



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2020 – 11:56 PM BST

PDB ID : 4YD9
Title : Crystal structure of squid hemocyanin
Authors : Matsuno, A.; Gai, Z.; Kato, K.; Tanaka, Y.; Yao, M.
Deposited on : 2015-02-21
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.14.6
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) : 2.14.6

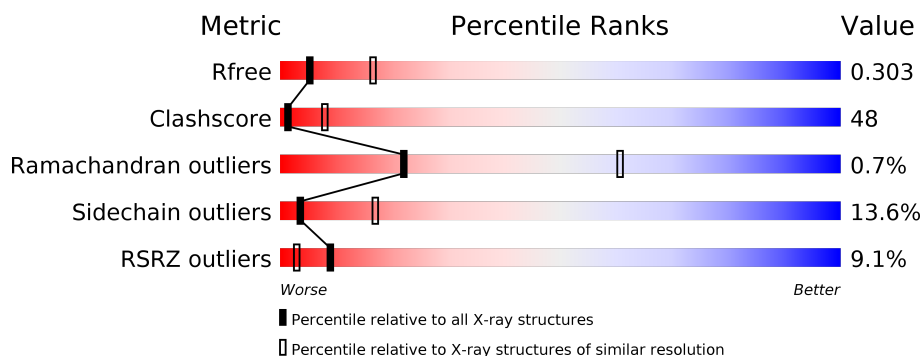
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 2092 (3.00-3.00) |
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 | 2000 | |
| 1 | D | 2000 | |
| 1 | G | 2000 | |
| 1 | J | 2000 | |
| 1 | M | 2000 | |
| 1 | P | 2000 | |


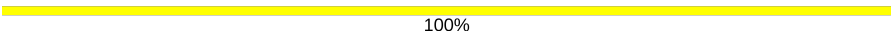


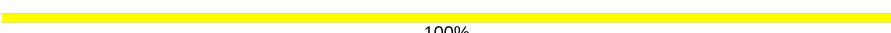
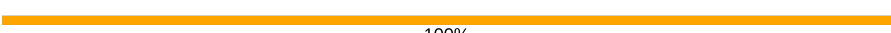








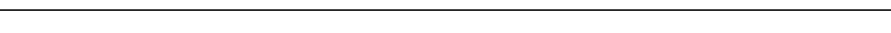

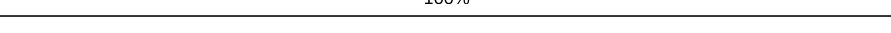

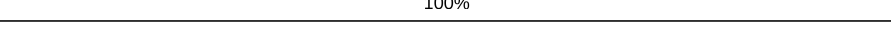
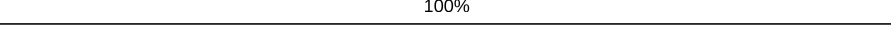
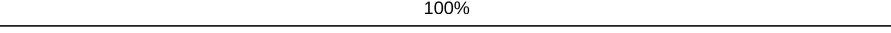
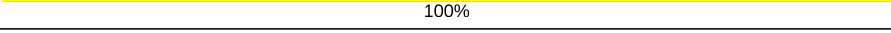

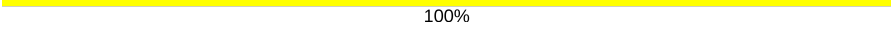

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | S | 2000 | |
| 1 | V | 2000 | |
| 1 | Y | 2000 | |
| 1 | b | 2000 | |
| 2 | B | 920 | |
| 2 | E | 920 | |
| 2 | H | 920 | |
| 2 | K | 920 | |
| 2 | N | 920 | |
| 2 | Q | 920 | |
| 2 | T | 920 | |
| 2 | W | 920 | |
| 2 | Z | 920 | |
| 2 | c | 920 | |
| 3 | C | 394 | |
| 3 | F | 394 | |
| 3 | I | 394 | |
| 3 | L | 394 | |
| 3 | O | 394 | |
| 3 | R | 394 | |
| 3 | U | 394 | |
| 3 | X | 394 | |
| 3 | a | 394 | |
| 3 | d | 394 | |
| 4 | 1 | 2 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 4 | 2 | 2 |  50% 50% |
| 4 | 4 | 2 |  100% |
| 4 | 6 | 2 |  50% 50% |
| 4 | 7 | 2 |  100% |
| 4 | 8 | 2 |  100% |
| 4 | 9 | 2 |  100% |
| 4 | BA | 2 |  100% |
| 4 | HA | 2 |  50% 50% |
| 4 | IA | 2 |  100% |
| 4 | JA | 2 |  50% 50% |
| 4 | MA | 2 |  100% |
| 4 | OA | 2 |  100% |
| 4 | QA | 2 |  50% 50% |
| 4 | RA | 2 |  50% 50% |
| 4 | e | 2 |  50% 50% |
| 4 | f | 2 |  100% |
| 4 | i | 2 |  50% 50% |
| 4 | j | 2 |  100% |
| 4 | m | 2 |  100% |
| 4 | n | 2 |  100% |
| 4 | o | 2 |  100% |
| 4 | p | 2 |  50% 50% |
| 4 | q | 2 |  100% |
| 4 | s | 2 |  50% 50% |
| 4 | t | 2 |  50% 50% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | u | 2 | 100% |
| 4 | v | 2 | 100% |
| 4 | x | 2 | 50% 50% |
| 5 | AA | 4 | 25% 50% 25% |
| 5 | FA | 4 | 100% |
| 5 | KA | 4 | 75% 25% |
| 5 | PA | 4 | 50% 50% |
| 5 | g | 4 | 50% 50% |
| 5 | l | 4 | 50% 50% |
| 6 | 3 | 3 | 33% 33% 33% |
| 6 | 5 | 3 | 100% |
| 6 | CA | 3 | 33% 67% |
| 6 | DA | 3 | 33% 67% |
| 6 | EA | 3 | 33% 33% 33% |
| 6 | GA | 3 | 100% |
| 6 | LA | 3 | 100% |
| 6 | NA | 3 | 67% 33% |
| 6 | h | 3 | 100% |
| 6 | k | 3 | 33% 67% |
| 6 | r | 3 | 67% 33% |
| 6 | w | 3 | 100% |
| 6 | y | 3 | 100% |
| 7 | z | 5 | 20% 80% |
| 8 | 0 | 4 | 25% 75% |

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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|---------|-----------|----------|---------|------------------|
| 6 | NAG | GA | 1 | - | - | X | - |
| 6 | NAG | GA | 2 | - | - | X | - |
| 6 | BMA | NA | 3 | - | - | - | X |
| 7 | MAN | z | 4 | - | - | - | X |
| 8 | NAG | 0 | 2 | - | - | X | - |
| 9 | CUO | A | 5001 | - | - | X | - |
| 9 | CUO | C | 3401[A] | - | - | X | - |
| 9 | CUO | C | 3401[B] | - | - | X | - |
| 9 | CUO | C | 3402[A] | - | - | X | - |
| 9 | CUO | C | 3402[B] | - | - | X | - |
| 9 | CUO | F | 3401[B] | - | - | X | - |
| 9 | CUO | F | 3402[A] | - | - | X | - |
| 9 | CUO | I | 3401[A] | - | - | X | - |
| 9 | CUO | I | 3402[A] | - | - | X | - |
| 9 | CUO | M | 2105 | - | - | X | - |
| 9 | CUO | O | 3401[A] | - | - | X | - |
| 9 | CUO | O | 3401[B] | - | - | X | - |
| 9 | CUO | P | 5015[C] | - | - | - | X |
| 9 | CUO | P | 5015[D] | - | - | - | X |
| 9 | CUO | S | 2104 | - | - | X | - |
| 9 | CUO | U | 3401[A] | - | - | X | - |
| 9 | CUO | U | 3401[B] | - | - | X | - |
| 9 | CUO | X | 3401[A] | - | - | X | X |
| 9 | CUO | X | 3401[B] | - | - | X | X |
| 9 | CUO | d | 3401[A] | - | - | - | X |
| 9 | CUO | d | 3401[B] | - | - | - | X |

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 261470 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 hemocyanin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | D | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | G | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | J | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | M | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | P | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | S | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | V | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | Y | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |
| 1 | b | 1656 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 13318 | 8513 | 2259 | 2478 | 68 | | | |

- Molecule 2 is a protein called hemocyanin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | B | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | E | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | H | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | K | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 2 | N | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | Q | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | T | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | W | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | Z | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |
| 2 | c | 825 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6704 | 4311 | 1128 | 1224 | 41 | | | |

- Molecule 3 is a protein called hemocyanin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 3 | C | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | F | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | I | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | L | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | O | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | R | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | U | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | X | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | a | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |
| 3 | d | 366 | Total | C | N | O | S | 0 | 366 | 0 |
| | | | 5912 | 3808 | 994 | 1076 | 34 | | | |

- Molecule 4 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 |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 4 | e | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | f | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | i | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | j | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | m | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | n | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | o | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | p | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | q | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | s | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | t | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | u | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | v | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | x | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 1 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 2 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 4 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 6 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 7 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 8 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | 9 | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | BA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 4 | HA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | IA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | JA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | MA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | OA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | QA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 4 | RA | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



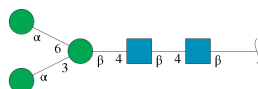
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 5 | g | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |
| 5 | l | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |
| 5 | AA | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |
| 5 | FA | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |
| 5 | KA | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |
| 5 | PA | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |

- Molecule 6 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.



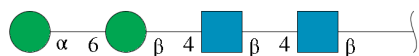
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 6 | h | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | k | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | r | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | w | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | y | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | 3 | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | 5 | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | CA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | DA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | EA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | GA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | LA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |
| 6 | NA | 3 | Total | C | N | O | 0 | 0 | 0 |
| | | | 39 | 22 | 2 | 15 | | | |

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



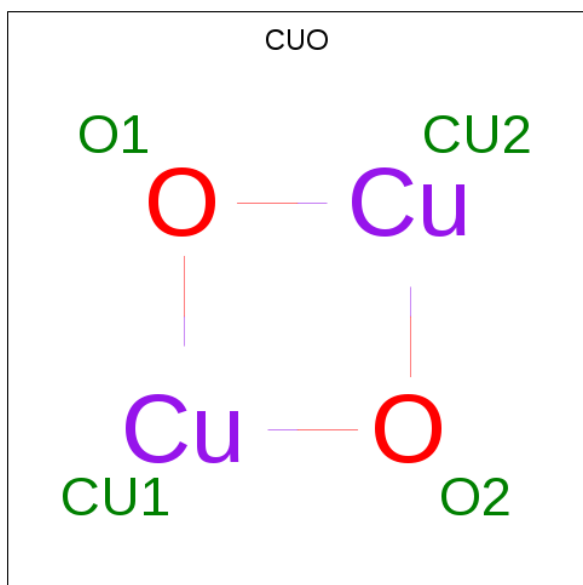
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 7 | z | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 61 | 34 | 2 | 25 | | | |

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



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

- Molecule 9 is CU2-O2 CLUSTER (three-letter code: CUO) (formula: Cu₂O₂).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 9 | A | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | A | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | A | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | A | 1 | Total | Cu | O | 0 | 1 |
| | | | 8 | 4 | 4 | | |
| 9 | B | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 9 | B | 1 | Total | Cu | O | 0 | 0 |
| | | | 4 | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 9 | C | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | C | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | D | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | D | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | D | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | D | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | D | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | E | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | E | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | F | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | F | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | G | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | G | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | G | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | G | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | G | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | H | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | H | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | I | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | I | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | J | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 9 | J | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | J | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | J | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | J | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | K | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | K | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | M | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | M | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | M | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | M | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | M | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | N | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | N | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | O | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | P | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | P | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | P | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | P | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | P | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | Q | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Q | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 9 | S | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | S | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | S | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | S | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | S | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | T | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | T | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | U | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | V | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | V | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | V | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | V | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | V | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | W | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | W | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | X | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | Y | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | Y | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Y | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Y | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Y | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |

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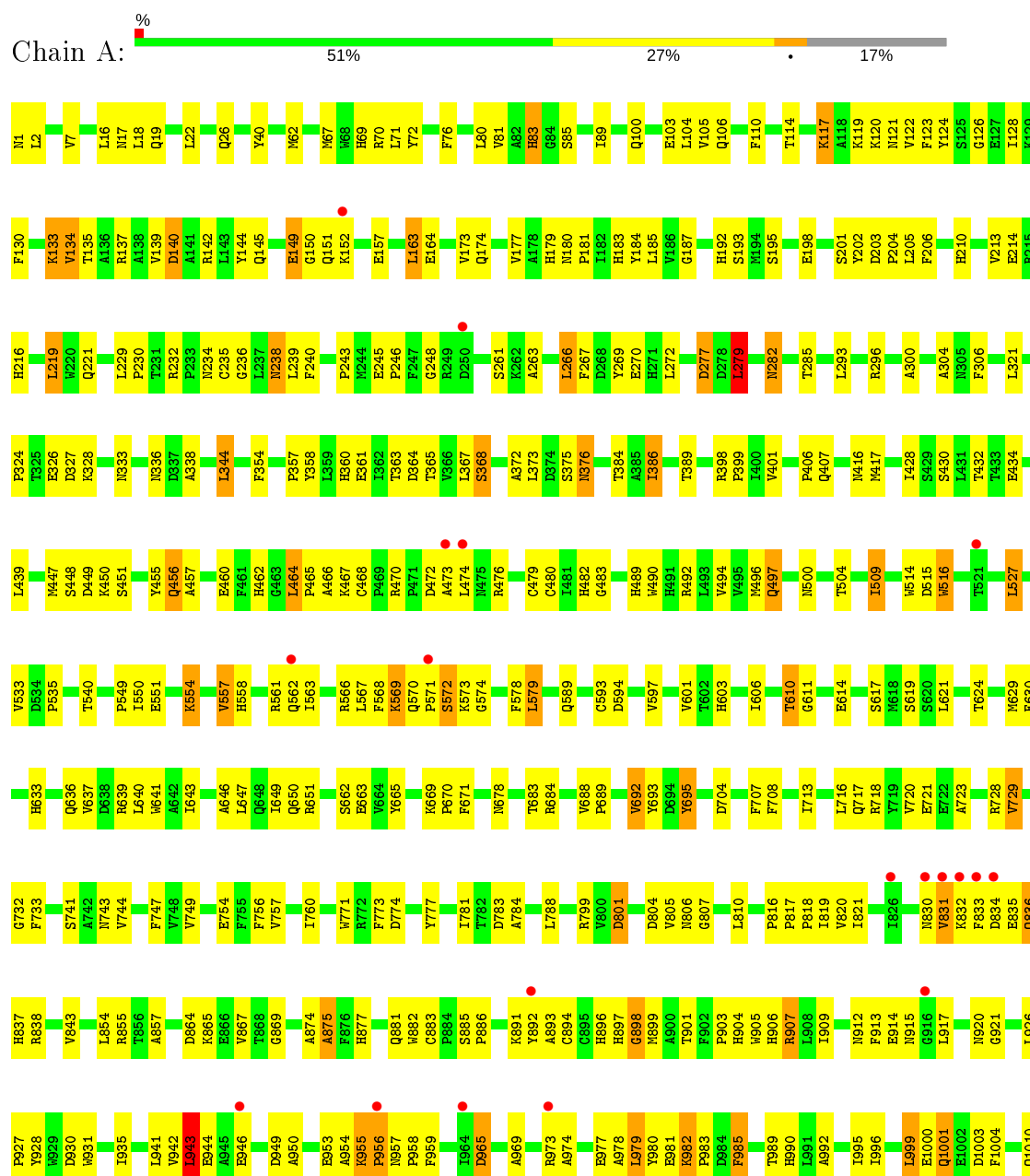
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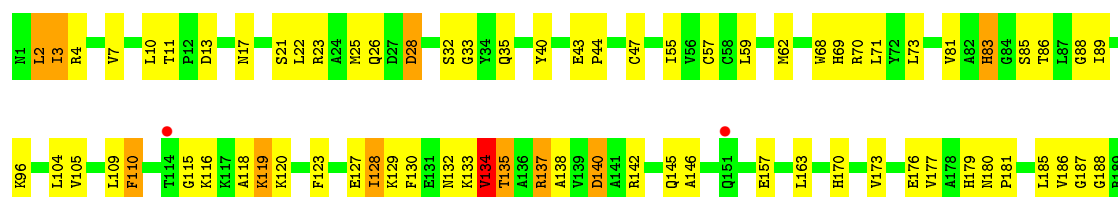
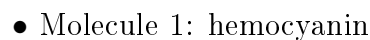
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|--------|---------|---------|
| 9 | Z | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | Z | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | b | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |
| 9 | b | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | b | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | b | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | b | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | c | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | c | 1 | Total 4 | Cu 2 | O 2 | 0 | 0 |
| 9 | d | 1 | Total 8 | Cu 4 | O 4 | 0 | 1 |

3 Residue-property plots [i](#)

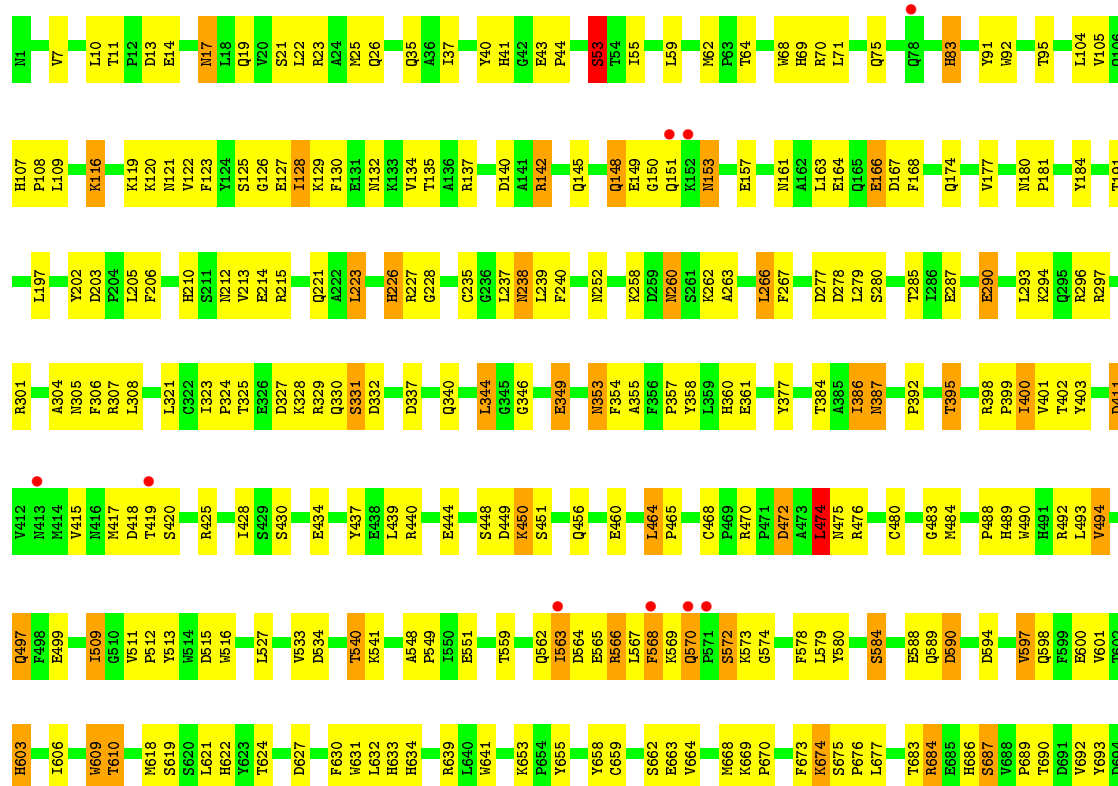
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: hemocyanin





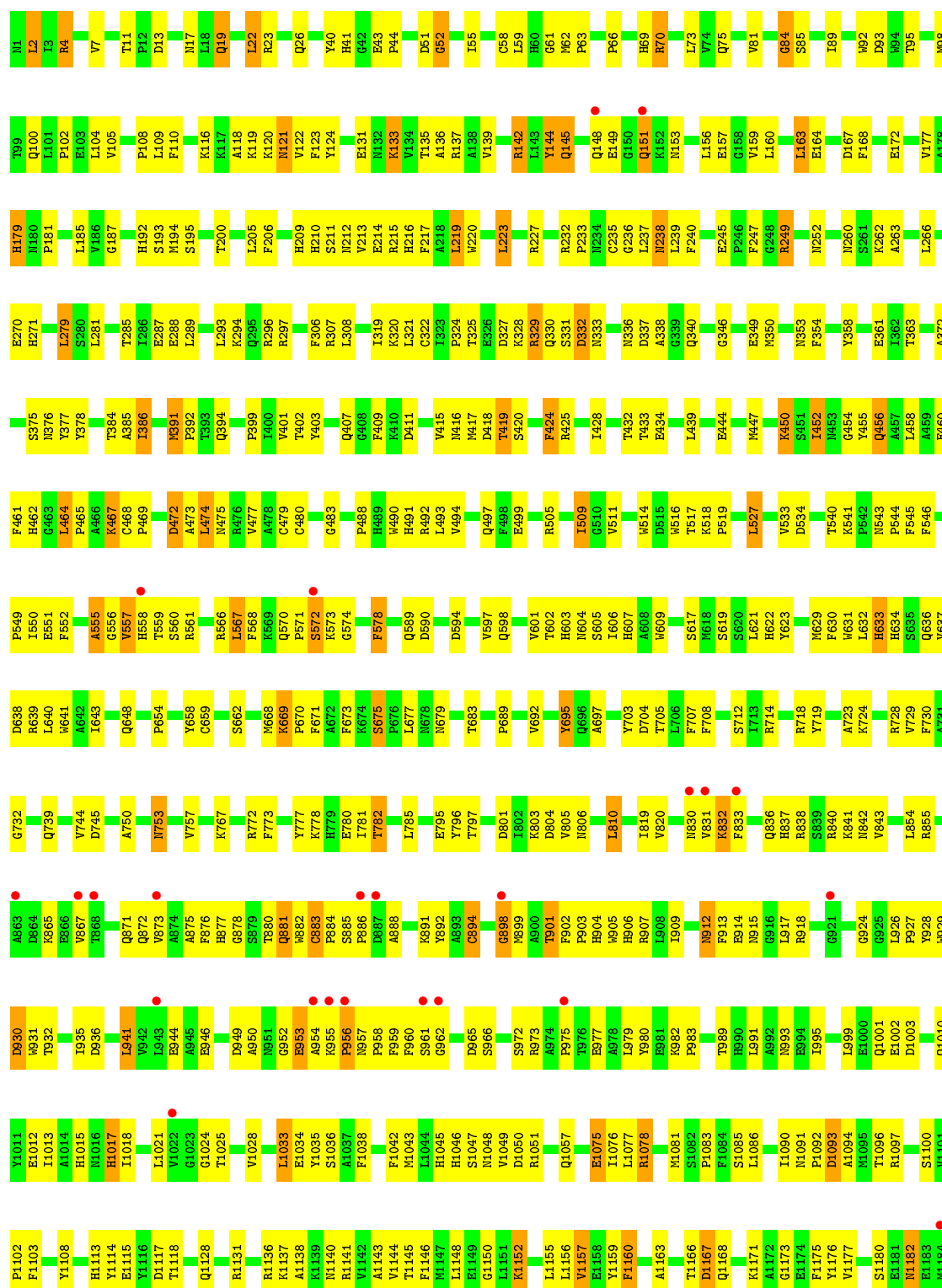
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|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| T1407 | L1408 | F1409 | V1410 | F1411 | E1412 | Q1413 | T1414 | V1308 | H1309 | T1310 | C1311 | G1312 | L1313 | H1314 | G1315 | H1316 | P1317 | V1318 | F1319 | P1320 | H1321 | W1322 | H1323 | R1324 | S1328 | L1329 | D1332 | E1333 | A1342 | V1343 | L1358 | E1361 | D1451 | H1457 | D1462 | E1470 | Q1472 | Y1473 | R1475 | L1476 | S1478 | Y1479 | C1484 | A1485 | P1492 | M1493 | R1494 | S1497 | N1498 | S1499 | T1500 | F1505 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| I1217 | T1221 | L1228 | K1229 | L1230 | T1232 | S1233 | V1234 | I1235 | Y1236 | G1239 | I1240 | G1241 | N1242 | F1243 | G1244 | R1247 | R1248 | W1249 | S1257 | R1258 | I1259 | R1260 | F1266 | M1271 | R1276 | A1277 | F1278 | K1279 | Q1280 | M1281 | A1282 | D1283 | R1286 | I1290 | V1296 | Q1299 | C1300 | P1301 | E1396 | L1397 | M1400 | R1406 | T1407 | L1408 | F1409 | V1410 | F1411 | E1412 | Q1413 | T1414 | V1415 | H1416 | G1417 | S1418 | L1419 | C1420 | D1421 | E1422 | F1423 | G1424 | H1425 | I1426 | J1427 | K1428 | L1429 | M1430 | N1431 | O1432 | P1433 | Q1434 | R1435 | S1436 | T1437 | U1438 | V1439 | W1440 | X1441 | Y1442 | Z1443 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| I1133 | N1140 | V1144 | L1148 | E1149 | K1152 | N1153 | S1154 | L1155 | L1156 | V1157 | F1160 | I1161 | G1165 | T1166 | Q1167 | Q1168 | K1169 | M1170 | K1171 | A1172 | G1173 | E1174 | F1175 | F1176 | V1177 | E1181 | N1182 | W1186 | K1187 | F1188 | R1189 | R1190 | P1191 | Y1192 | D1195 | I1196 | T1197 | Y1198 | V1199 | M1200 | M1203 | K1204 | L1205 | H1206 | D1209 | K1210 | Y1211 | T1212 | S1213 | P1214 | Q1215 | R1216 | U1217 | V1218 | W1219 | X1220 | Y1221 | Z1222 | A1223 | B1224 | C1225 | D1226 | E1227 | F1228 | G1229 | H1230 | I1231 | J1232 | K1233 | L1234 | M1235 | N1236 | O1237 | P1238 | Q1239 | R1240 | S1241 | T1242 | U1243 | V1244 | W1245 | X1246 | Y1247 | Z1248 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| T285 | L289 | R296 | R301 | A304 | N305 | F306 | N316 | V317 | R318 | I319 | K320 | L321 | C322 | T325 | E326 | R329 | N333 | N336 | D337 | R337 | R345 | F446 | H447 | S448 | D449 | K450 | S451 | L452 | Y455 | Q456 | E460 | F461 | H462 | G463 | L464 | P465 | S560 | R561 | L371 | V383 | T384 | A385 | T386 | Q394 | T395 | I396 | P397 | R398 | P399 | T400 | U401 | V402 | W403 | X404 | Y405 | Z406 | A407 | B408 | C409 | D410 | E411 | F412 | G413 | H414 | I415 | J416 | K417 | L418 | M419 | N420 | O421 | P422 | Q423 | R424 | S425 | T426 | U427 | V428 | W429 | X430 | Y431 | Z432 | A433 | B434 | C435 | D436 | E437 | F438 | G439 | H440 | I441 | J442 | K443 | L444 | M445 | N446 | O447 | P448 | Q449 | R450 | S451 | T452 | U453 | V454 | W455 | X456 | Y457 | Z458 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| F190 | T191 | H192 | S193 | M194 | S195 | T200 | D203 | P204 | L205 | F206 | F207 | L208 | H210 | V213 | E214 | R215 | K225 | H226 | R227 | T231 | C235 | D337 | N238 | L239 | F240 | H241 | P246 | R249 | D250 | T251 | T256 | T257 | K258 | L259 | R260 | T261 | K262 | N260 | S261 | K262 | A263 | L266 | E270 | F276 | D277 | D278 | L279 | N282 | T283 | U284 | V285 | W286 | X287 | Y288 | Z289 | A290 | B291 | C292 | D293 | E294 | F295 | G296 | H297 | I298 | J299 | K300 | L301 | M302 | N303 | O304 | P305 | Q306 | R307 | S308 | T309 | U310 | V311 | W312 | X313 | Y314 | Z315 | A316 | B317 | C318 | D319 | E320 | F321 | G322 | H323 | I324 | J325 | K326 | L327 | M328 | N329 | O330 | P331 | Q332 | R333 | S334 | T335 | U336 | V337 | W338 | X339 | Y340 | Z341 | A342 | B343 | C344 | D345 | E346 | F347 | G348 | H349 | I350 | J351 | K352 | L353 | M354 | N355 | O356 | P357 | Q358 | R359 | S360 | T361 | U362 | V363 | W364 | X365 | Y366 | Z367 | A368 | B369 | C370 | D371 | E372 | F373 | G374 | H375 | I376 | J377 | K378 | L379 | M380 | N381 | O382 | P383 | Q384 | R385 | S386 | T387 | U388 | V389 | W390 | X391 | Y392 | Z393 | A394 | B395 | C396 | D397 | E398 | F399 | G400 | H401 | I402 | J403 | K404 | L405 | M406 | N407 | O408 | P409 | Q410 | R411 | S412 | T413 | U414 | V415 | W416 | X417 | Y418 | Z419 | A420 | B421 | C422 | D423 | E424 | F425 | G426 | H427 | I428 | J429 | K430 | L431 | M432 | N433 | O434 | P435 | Q436 | R437 | S438 | T439 | U440 | V441 | W442 | X443 | Y444 | Z445 | A446 | B447 | C448 | D449 | E450 | F451 | G452 | H453 | I454 | J455 | K456 | L457 | M458 | N459 | O460 | P461 | Q462 | R463 | S464 | T465 | U466 | V467 | W468 | X469 | Y470 | Z471 | A472 | B473 | C474 | D475 | E476 | F477 | G478 | H479 | I480 | J481 | K482 | L483 | M484 | N485 | O486 | P487 | Q488 | R489 | S490 | T491 | U492 | V493 | W494 | X495 | Y496 | Z497 | A498 | B499 | C500 | D501 | E502 | F503 | G504 | H505 | I506 | J507 | K508 | L509 | M510 | N511 | O512 | P513 | Q514 | R515 | S516 | T517 | U518 | V519 | W520 | X521 | Y522 | Z523 | A524 | B525 | C526 | D527 | E528 | F529 | G530 | H531 | I532 | J533 | K534 | L535 | M536 | N537 | O538 | P539 | Q540 | R541 | S542 | T543 | U544 | V545 | W546 | X547 | Y548 | Z549 | A550 | B551 | C552 | D553 | E554 | F555 | G556 | H557 | I558 | J559 | K560 | L561 | M562 | N563 | O564 | P565 | Q566 | R567 | S568 | T569 | U570 | V571 | W572 | X573 | Y574 | Z575 | A576 | B577 | C578 | D579 | E580 | F581 | G582 | H583 | I584 | J585 | K586 | L587 | M588 | N589 | O590 | P591 | Q592 | R593 | S594 | T595 | U596 | V597 | W598 | X599 | Y600 | Z601 | A602 | B603 | C604 | D605 | E606 | F607 | G608 | H609 | I610 | J611 | K612 | L613 | M614 | N615 | O616 | P617 | Q618 | R619 | S620 | T621 | U622 | V623 | W624 | X625 | Y626 | Z627 | A628 | B629 | C630 | D631 | E632 | F633 | G634 | H635 | I636 | J637 | K638 | L639 | M640 | N641 | O642 | P643 | Q644 | R645 | S646 | T647 | U648 | V649 | W650 | X651 | Y652 | Z653 | A654 | B655 | C656 | D657 | E658 | F659 | G660 | H661 | I662 | J663 | K664 | L665 | M666 | N667 | O668 | P669 | Q670 | R671 | S672 | T673 | U674 | V675 | W676 | X677 | Y678 | Z679 | A680 | B681 | C682 | D683 | E684 | F685 | G686 | H687 | I688 | J689 | K690 | L691 | M692 | N693 | O694 | P695 | Q696 | R697 | S698 | T699 | U700 | V701 | W702 | X703 | Y704 | Z705 | A706 | B707 | C708 | D709 | E710 | F711 | G712 | H713 | I714 | J715 | K716 | L717 | M718 | N719 | O720 | P721 | Q722 | R723 | S724 | T725 | U726 | V727 | W728 | X729 | Y730 | Z731 | A732 | B733 | C734 | D735 | E736 | F737 | G738 | H739 | I740 | J741 | K742 | L743 | M744 | N745 | O746 | P747 | Q748 | R749 | S750 | T751 | U752 | V753 | W754 | X755 | Y756 | Z757 | A758 | B759 | C760 | D761 | E762 | F763 | G764 | H765 | I766 | J767 | K768 | L769 | M770 | N771 | O772 | P773 | Q774 | R775 | S776 | T777 | U778 | V779 | W780 | X781 | Y782 | Z783 | A784 | B785 | C786 | D787 | E788 | F789 | G790 | H791 | I792 | J793 | K794 | L795 | M796 | N797 | O798 | P799 | Q800 | R801 | S802 | T803 | U804 | V805 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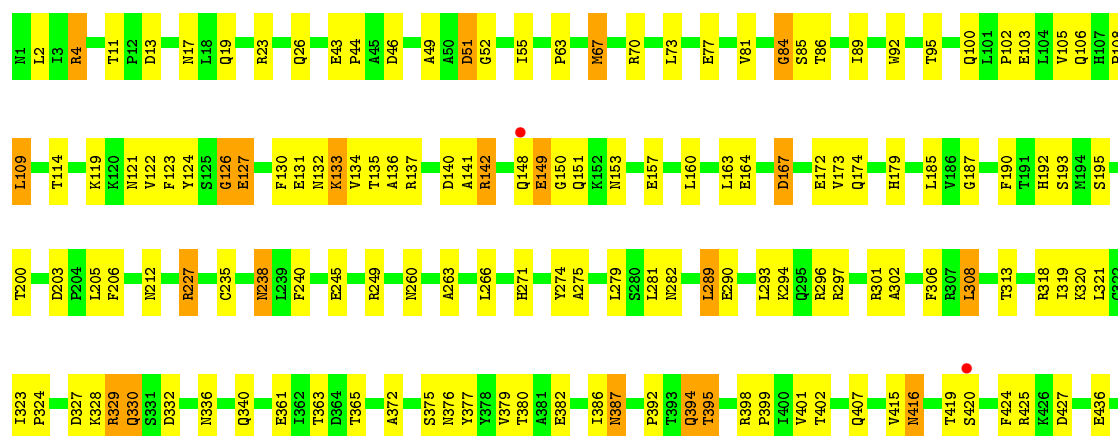




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| TRP | LEU | GLY | ILE | LVS | ALA | SER | ASP | VAL | ASN | THR | HIS | ILE | CYS | VAL | PRO | GLY | VAL | GLU | HIS | GLU | ASP | CYS | ASP | ASN |
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● Molecule 1: hemocyanin

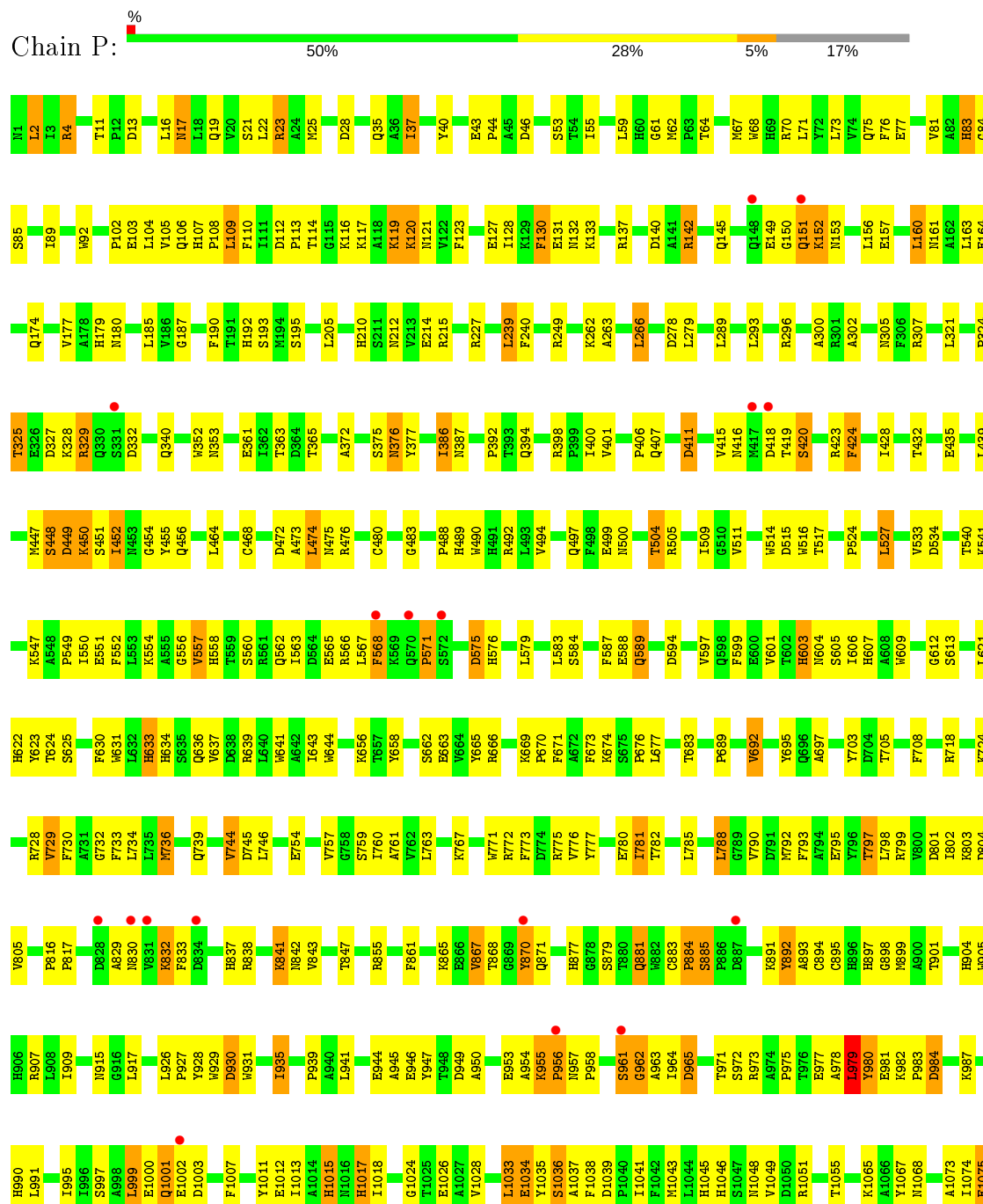


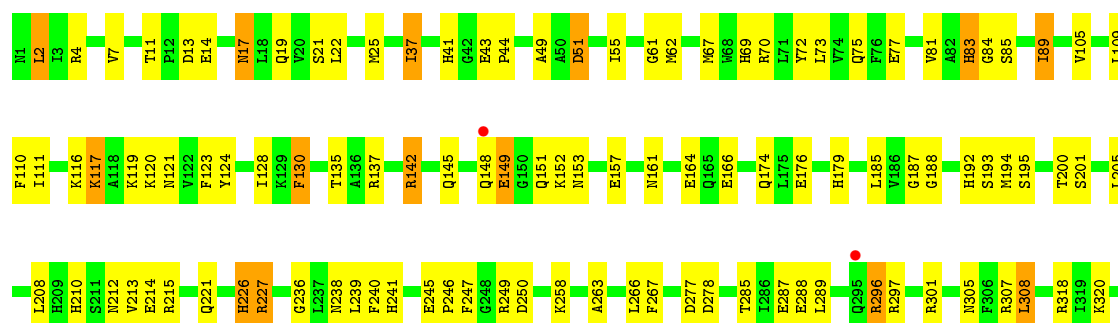
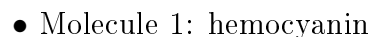


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- Molecule 1: hemocyanin

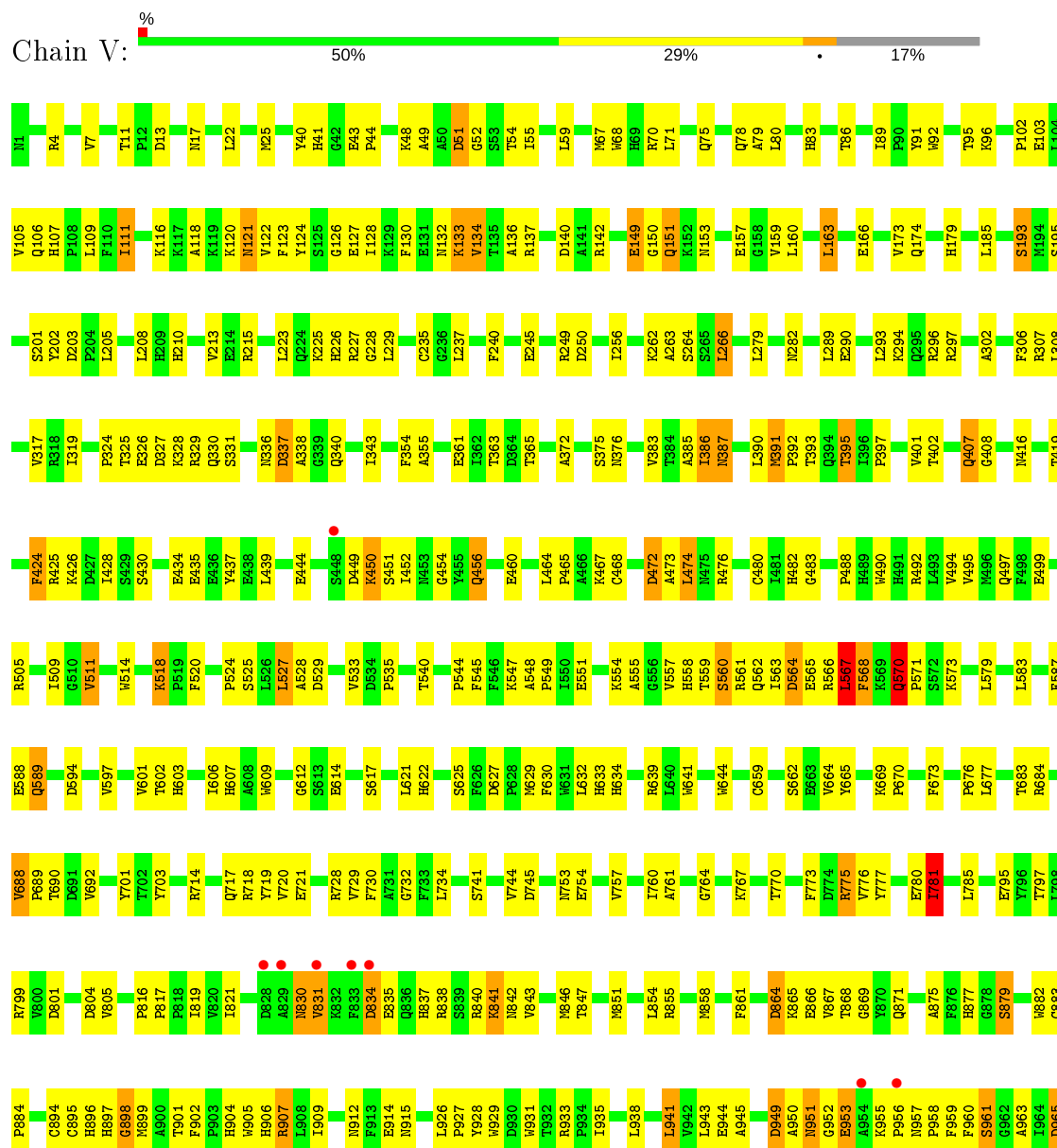


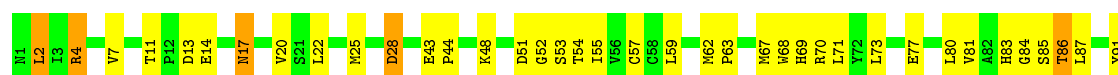


WORLDWIDE
PDB
PROTEIN DATA BANK

| | | | | | | |
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| LEU | GLU | ASN | PHE | THR | ALA | GLU |
| LEU | GLY | CYS | GLU | TYR | ASP | PHE |
| LEU | ALA | ALA | VAL | LYS | GLY | GLY |
| SER | LEU | LEU | LEU | HIS | SER | ASP |
| ARG | ASN | ASN | HIS | PRO | ASN | GLU |
| GLN | LEU | LEU | ASN | LYS | ILE | THR |
| SER | LEU | ASN | SER | THR | HIS | TRP |
| HIS | ASN | ILE | ILE | ASN | THR | ARG |
| ASP | ASP | HIS | HIS | GLU | ASP | ASP |
| ARG | ARG | PRO | SER | ASP | CYS | VAL |
| VAL | VAL | MET | TRP | ILE | LEU | VAL |
| PHE | PHE | ARG | ILE | GLU | HIS | THR |
| GLY | GLY | PRO | GLY | ASN | GLY | SER |
| PHE | PHE | PRO | PRO | PHE | MET | ALA |
| TRP | TRP | ASN | ASN | HIS | THR | ASN |
| LEU | LEU | LYS | PRO | HIS | PHE | ILE |
| SER | SER | THR | HIS | GLY | PRO | ARG |
| GLY | GLY | ALA | SER | LYS | HIS | ARG |
| ILE | ILE | ASN | MET | ILE | TRP | ASN |
| LYS | LYS | GLN | SER | SER | HIS | LEU |
| ALA | ALA | ASP | SER | PHE | ARG | LYS |
| SER | SER | HIS | LEU | ALA | LEU | ASP |
| ALA | ALA | LEU | ASP | ASP | TYR | LEU |
| ASP | ASP | THR | PHE | ALA | VAL | SER |
| VAL | VAL | PHE | ALA | VAL | SER | LYS |
| ILE | ILE | ASN | ALA | THR | LEU | GLU |
| ILE | ILE | ASN | TYR | VAL | VAL | ASP |
| HIS | HIS | SER | ASP | ARG | GLU | MET |
| ILE | ILE | ARG | PRO | LYS | ASN | PHE |
| CYS | CYS | PRO | ILE | PRO | GLU | SER |
| VAL | VAL | ASN | PHE | ARG | LEU | SER |
| PRO | PRO | ASP | PHE | ASP | LEU | ARG |
| ILE | ILE | VAL | LEU | GLN | ALA | ALA |
| GLY | GLY | PHE | HIS | LEU | ARG | ALA |
| VAL | VAL | ASP | HIS | PHE | GLY | PHE |
| GLU | GLU | TYR | SER | ASN | SER | LYS |
| GLU | GLU | ASN | THR | ASN | ASP | LYS |
| ASP | ASP | SER | VAL | ARG | VAL | MET |
| CYS | CYS | LEU | ARG | TYR | ALA | ASP |
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| | | PHE | ILE | HIS | TRP | ARG |
| | | ASN | TRP | ALA | ASP | GLY |
| | | SER | GLN | PHE | TRP | GLU |
| | | LEU | ASP | ALA | ILE | GLU |
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| | | SER | TYR | HIS | PHE | ALA |
| | | GLY | ARG | THR | ASP | PHE |
| | | LEU | LYS | ASP | LEU | GLY |
| | | SER | LEU | PHE | PRO | LEU |
| | | ILE | LEU | CYS | GLY | PRO |
| | | ARG | ASP | THR | ILE | ALA |
| | | LEU | TYR | PHE | GLN | ALA |
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- Molecule 1: hemocyanin

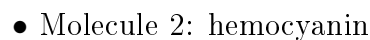


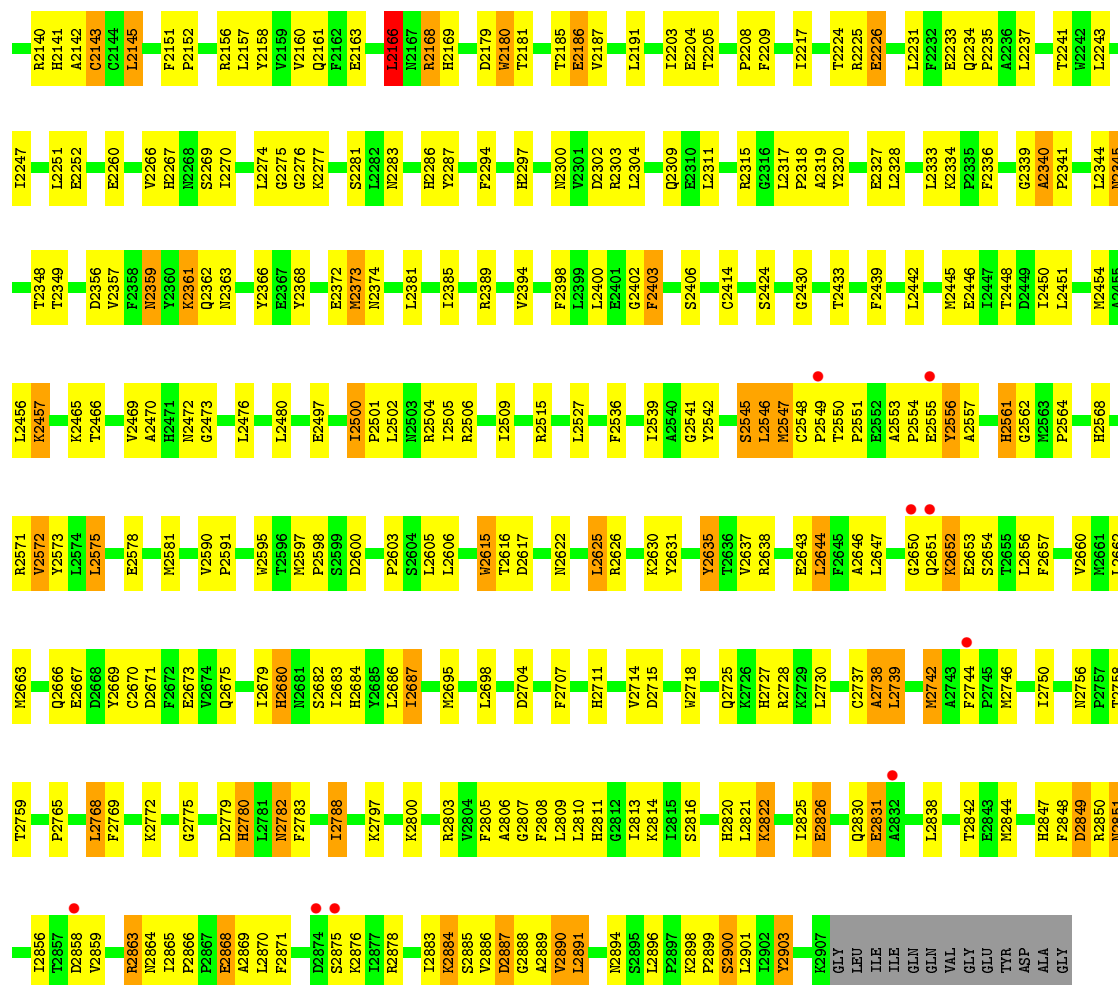


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| W92 | W93 | W94 | W95 | W96 | W97 | W98 | W99 | W100 | W101 | W102 | W103 | W104 | W105 | W106 | W107 | W108 | W109 | W110 | W111 | W112 | W113 | W114 | W115 | W116 | W117 | W118 | W119 | W120 | W121 | W122 | W123 | W124 | W125 | W126 | W127 | W128 | W129 | W130 | W131 | W132 | W133 | W134 | W135 | W136 | W137 | W138 | W139 | W140 | W141 | W142 | W143 | W144 | W145 | W146 | W147 | W148 | W149 | W150 | W151 | W152 | W153 | W154 | W155 | W156 | W157 | W158 | W159 | W160 | W161 | W162 | W163 | W164 | W165 | W166 | W167 | W168 | W169 | W170 | W171 | W172 | W173 | W174 | W175 | W176 | W177 | W178 | W179 | W180 | W181 | W182 | W183 | W184 | W185 | W186 | W187 | W188 | W189 | W190 | W191 | W192 | W193 | W194 | W195 | W196 | W197 | W198 | W199 | W200 | W201 | W202 | W203 | W204 | W205 | W206 | W207 | W208 | W209 | W210 | W211 | W212 | W213 | W214 | W215 | W216 | W217 | W218 | W219 | W220 | W221 | W222 | W223 | W224 | W225 | W226 | W227 | W228 | W229 | W230 | W231 | W232 | W233 | W234 | W235 | W236 | W237 | W238 | W239 | W240 | W241 | W242 | W243 | W244 | W245 | W246 | W247 | W248 | W249 | W250 | W251 | W252 | W253 | W254 | W255 | W256 | W257 | W258 | W259 | W260 | W261 | W262 | W263 | W264 | W265 | W266 | W267 | W268 | W269 | W270 | W271 | W272 | W273 | W274 | W275 | W276 | W277 | W278 | W279 | W280 | W281 | W282 | W283 | W284 | W285 | W286 | W287 | W288 | W289 | W290 | W291 | W292 | W293 | W294 | W295 | W296 | W297 | W298 | W299 | W300 | W301 | W302 | W303 | W304 | W305 | W306 | W307 | W308 | W309 | W310 | W311 | W312 | W313 | W314 | W315 | W316 | W317 | W318 | W319 | W320 | W321 | W322 | W323 | W324 | W325 | W326 | W327 | W328 | W329 | W330 | W331 | W332 | W333 | W334 | W335 | W336 | W337 | W338 | W339 | W340 | W341 | W342 | W343 | W344 | W345 | W346 | W347 | W348 | W349 | W350 | W351 | W352 | W353 | W354 | W355 | W356 | W357 | W358 | W359 | W360 | W361 | W362 | W363 | W364 | W365 | W366 | W367 | W368 | W369 | W370 | W371 | W372 | W373 | W374 | W375 | W376 | W377 | W378 | W379 | W380 | W381 | W382 | W383 | W384 | W385 | W386 | W387 | W388 | W389 | W390 | W391 | W392 | W393 | W394 | W395 | W396 | W397 | W398 | W399 | W400 | W401 | W402 | W403 | W404 | W405 | W406 | W407 | W408 | W409 | W410 | W411 | W412 | W413 | W414 | W415 | W416 | W417 | W418 | W419 | W420 | W421 | W422 | W423 | W424 | W425 | W426 | W427 | W428 | W429 | W430 | W431 | W432 | W433 | W434 | W435 | W436 | W437 | W438 | W439 | W440 | W441 | W442 | W443 | W444 | W445 | W446 | W447 | W448 | W449 | W450 | W451 | W452 | W453 | W454 | W455 | W456 | W457 | W458 | W459 | W460 | W461 | W462 | W463 | W464 | W465 | W466 | W467 | W468 | W469 | W470 | W471 | W472 | W473 | W474 | W475 | W476 | W477 | W478 | W479 | W480 | W481 | W482 | W483 | W484 | W485 | W486 | W487 | W488 | W489 | W490 | W491 | W492 | W493 | W494 | W495 | W496 | W497 | W498 | W499 | W500 | W501 | W502 | W503 | W504 | W505 | W506 | W507 | W508 | W509 | W510 | W511 | W512 | W513 | W514 | W515 | W516 | W517 | W518 | W519 | W520 | W521 | W522 | W523 | W524 | W525 | W526 | W527 | W528 | W529 | W530 | W531 | W532 | W533 | W534 | W535 | W536 | W537 | W538 | W539 | W540 | W541 | W542 | W543 | W544 | W545 | W546 | W547 | W548 | W549 | W550 | W551 | W552 | W553 | W554 | W555 | W556 | W557 | W558 | W559 | W560 | W561 | W562 | W563 | W564 | W565 | W566 | W567 | W568 | W569 | W570 | W571 | W572 | W573 | W574 | W575 | W576 | W577 | W578 | W579 | W580 | W581 | W582 | W583 | W584 | W585 | W586 | W587 | W588 | W589 | W590 | W591 | W592 | W593 | W594 | W595 | W596 | W597 | W598 | W599 | W600 | W601 | W602 | W603 | W604 | W605 | W606 | W607 | W608 | W609 | W610 | W611 | W612 | W613 | W614 | W615 | W616 | W617 | W618 | W619 | W620 | W621 | W622 | W623 | W624 | W625 | W626 | W627 | W628 | W629 | W630 | W631 | W632 | W633 | W634 | W635 | W636 | W637 | W638 | W639 | W640 | W641 | W642 | W643 | W644 | W645 | W646 | W647 | W648 | W649 | W650 | W651 | W652 | W653 | W654 | W655 | W656 | W657 | W658 | W659 | W660 | W661 | W662 | W663 | W664 | W665 | W666 | W667 | W668 | W669 | W670 | W671 | W672 | W673 | W674 | W675 | W676 | W677 | W678 | W679 | W680 | W681 | W682 | W683 | W684 | W685 | W686 | W687 | W688 | W689 | W690 | W691 | W692 | W693 | W694 | W695 | W696 | W697 | W698 | W699 | W700 | W701 | W702 | W703 | W704 | W705 | W706 | W707 | W708 | W709 | W710 | W711 | W712 | W713 | W714 | W715 | W716 | W717 | W718 | W719 | W720 | W721 | W722 | W723 | W724 | W725 | W726 | W727 | W728 | W729 | W730 | W731 | W732 | W733 | W734 | W735 | W736 | W737 | W738 | W739 | W740 | W741 | W742 | W743 | W744 | W745 | W746 | W747 | W748 | W749 | W750 | W751 | W752 | W753 | W754 | W755 | W756 | W757 | W758 | W759 | W760 | W761 | W762 | W763 | W764 | W765 | W766 | W767 | W768 | W769 | W770 | W771 | W772 | W773 | W774 | W775 | W776 | W777 | W778 | W779 | W780 | W781 | W782 | W783 | W784 | W785 | W786 | W787 | W788 | W789 | W790 | W791 | W792 | W793 | W794 | W795 | W796 | W797 | W798 | W799 | W800 | W801 | W802 | W803 | W804 | W805 | W806 | W807 | W808 | W809 | W810 | W811 | W812 | W813 | W814 | W815 | W816 | W817 | W818 | W819 | W820 | W821 | W822 | W823 | W824 | W825 | W826 | W827 | W828 | W829 | W830 | W831 | W832 | W833 | W834 | W835 | W836 | W837 | W838 | W839 | W840 | W841 | W842 | W843 | W844 | W845 | W846 | W847 | W848 | W849 | W850 | W851 | W852 | W853 | W854 | W855 | W856 | W857 | W858 | W859 | W860 | W861 | W862 | W863 | W864 | W865 | W866 | W867 | W868 | W869 | W870 | W871 | W872 | W873 | W874 | W875 | W876 | W877 | W878 | W879 | W880 | W881 | W882 | W883 | W884 | W885 | W886 | W887 | W888 | W889 | W890 | W891 | W892 | W893 | W894 | W895 | W896 | W897 | W898 | W899 | W900 | W901 | W902 | W903 | W904 | W905 | W906 | W907 | W908 | W909 | W910 | W911 | W912 | W913 | W914 | W915 | W916 | W917 | W918 | W919 | W920 | W921 | W922 | W923 | W924 | W925 | W926 | W927 | W928 | W929 | W930 | W931 | W932 | W933 | W934 | W935 | W936 | W937 | W938 | W939 | W940 | W941 | W942 | W943 | W944 | W945 | W946 | W947 | W948 | W949 | W950 | W951 | W952 | W953 | W954 | W955 | W956 | W957 | W958 | W959 | W960 | W961 | W962 | W963 | W964 | W965 | W966 | W967 | W968 | W969 | W970 | W971 | W972 | W973 | W974 | W975 | W976 | W977 | W978 | W979 | W980 | W981 | W982 | W983 | W984 | W985 | W986 | W987 | W988 | W989 | W990 | W991 | W992 | W993 | W994 | W995 | W996 | W997 | W998 | W999 | W1000 | W1001 | W1002 | W1003 | W1004 | W1005 | W1006 | W1007 | W1008 | W1009 | W1010 | W1011 | W1012 | W1013 | W1014 | W1015 | W1016 | W1017 | W1018 | W1019 | W1020 | W1021 | W1022 | W1023 | W1024 | W1025 | W1026 | W1027 | W1028 | W1029 | W1030 | W1031 | W1032 | W1033 | W1034 | W1035 | W1036 | W1037 | W1038 | W1039 | W1040 | W1041 | W1042 | W1043 | W1044 | W1045 | W1046 | W1047 | W1048 | W1049 | W1050 | W1051 | W1052 | W1053 | W1054 | W1055 | W1056 | W1057 | W1058 | W1059 | W1060 | W1061 | W1062 | W1063 | W1064 | W1065 | W1066 | W1067 | W1068 | W1069 | W1070 | W1071 | W1072 | W1073 | W1074 | W1075 | W1076 | W1077 | W1078 | W1079 | W1080 | W1081 | W1082 | W1083 | W1084 | W1085 | W1086 | W1087 | W1088 | W1089 | W1090 | W1091 | W1092 | W1093 | W1094 | W1095 | W1096 | W1097 | W1098 | W1099 | W1100 | W1101 | W1102 | W1103 | W1104 | W1105 | W1106 | W1107 | W1108 | W1109 | W1110 | W1111 | W1112 | W1113 | W1114 | W1115 | W1116 | W1117 | W1118 | W1119 | W1120 | W1121 | W1122 | W1123 | W1124 | W1125 | W1126 | W1127 | W1128 | W1129 | W1130 | W1131 | W1132 | W1133 | W1134 | W1135 | W1136 | W1137 | W1138 | W1139 | W1140 | W1141 | W1142 | W1143 | W1144 | W1145 | W1146 | W1147 | W1148 | W1149 | W1150 | W1151 | W1152 | W1153 | W1154 | W1155 | W1156 | W1157 | W1158 | W1159 | W1160 | W1161 | W1162 | W1163 | W1164 | W1165 | W1166 | W1167 | W1168 | W1169 | W1170 | W1171 | W1172 | W1173 | W1174 | W1175 | W1176 | W1177 | W1178 | W1179 | W1180 | W1181 | W1182 | W1183 | W1184 | W1185 | W1186 | W1187 | W1188 | W1189 | W1190 | W1191 | W1192 | W1193 | W1194 | W1195 | W1196 | W1197 | W1198 | W1199 | W1200 | W1201 | W1202 | W1203 | W1204 | W1205 | W1206 | W1207 | W1208 | W1209 | W1210 | W1211 | W1212 | W1213 | W1214 | W1215 | W1216 | W1217 | W1218 | W1219 | W1220 | W1221 | W1222 | W1223 | W1224 | W1225 | W1226 | W1227 | W1228 | W1229 | W1230 | W1231 | W1232 | W1233 | W1234 | W1235 | W1236 | W1237 | W1238 | W1239 | W1240 | W1241 | W1242 | W1243 | W1244 | W1245 | W1246 | W1247 | W1248 | W1249 | W1250 | W1251 | W1252 | W1253 | W1254 | W1255 | W1256 | W1257 | W1258 | W1259 | W1260 | W1261 | W1262 | W1263 | W1264 | W1265 | W1266 | W1267 | W1268 | W1269 | W1270 | W1271 | W1272 | W1273 | W1274 | W1275 | W1276 | W1277 | W1278 | W1279 | W1280 | W1281 | W1282 | W1283 | W1284 | W1285 | W1286 | W1287 | W1288 | W1289 | W1290 | W1291 | W1292 | W1293 | W1294 | W1295 | W1296 | W1297 | W1298 | W1299 | W1300 | W1301 | W1302 | W1303 | W1304 | W1305 | W1306 | W1307 | W1308 | W1309 | W1310 | W1311 | W1312 | W1313 | W1314 | W1315 | W1316 | W1317 | W1318 | W1319 | W1320 | W1321 | W1322 | W1323 | W1324 | W1325 | W1326 | W1327 | W1328 | W1329 | W1330 | W1331 | W1332 | W1333 | W1334 | W1335 | W1336 | W1337 | W1338 | W1339 | W1340 | W1341 | W1342 | W1343 | W1344 | W1345 | W1346 | W1347 | W1348 | W1349 | W1350 | W1351 | W1352 | W1353 | W1354 | W1355 | W1356 | W1357 | W1358 | W1359 | W1360 | W1361 | W1362 | W1363 | W1364 | W1365 | W1366 | W1367 | W1368 | W1369 | W1370 | W1371 | W1372 | W1373 | W1374 | W1375 | W1376 | W1377 | W1378 | W1379 | W1380 | W1381 | W1382 | W1383 | W1384 | W1385 | W1386 | W1387 | W1388 | W1389 | W1390 | W1391 | W1392 | W1393 | W1394 | W1395 | W1396 | W1397 | W1398 | W1399 | W1400 | W1401 | W1402 | W1403 | W1404 | W1405 | W1406 | W1407 | W1 |
|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|--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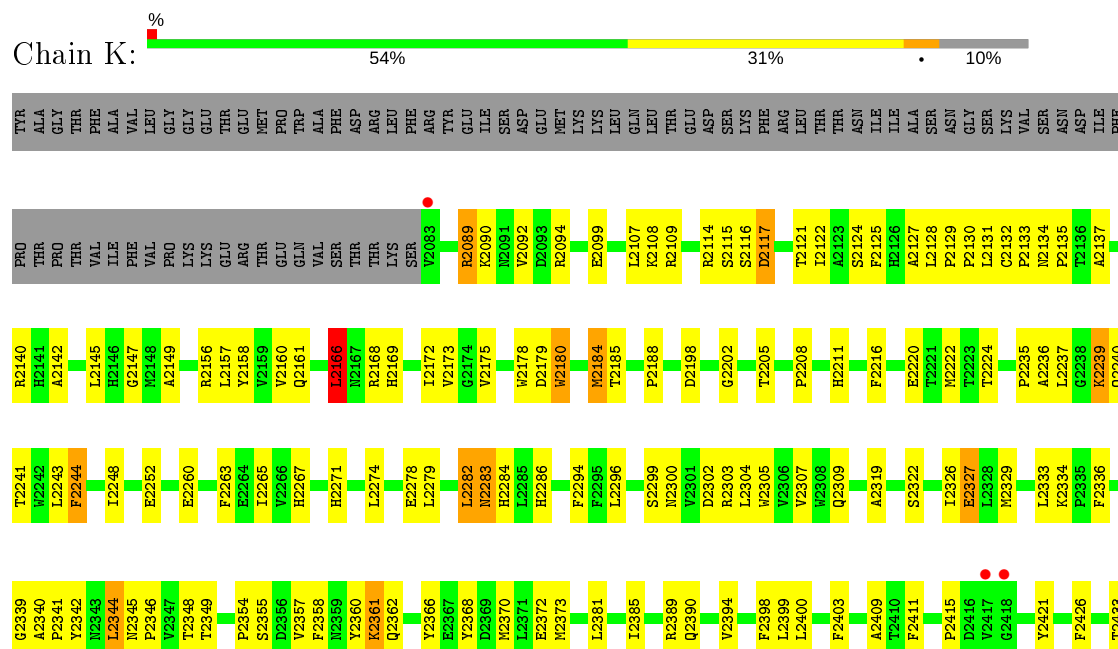


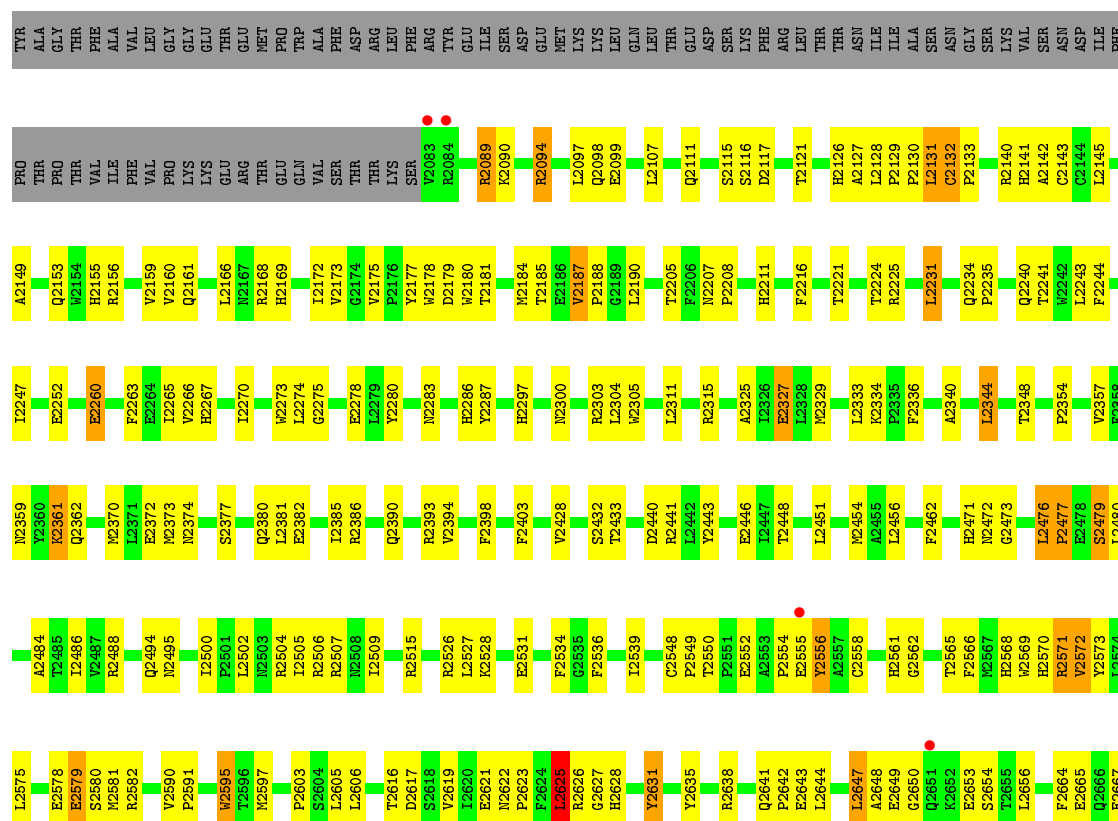
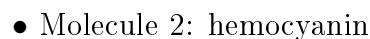
- Molecule 2: hemocyanin

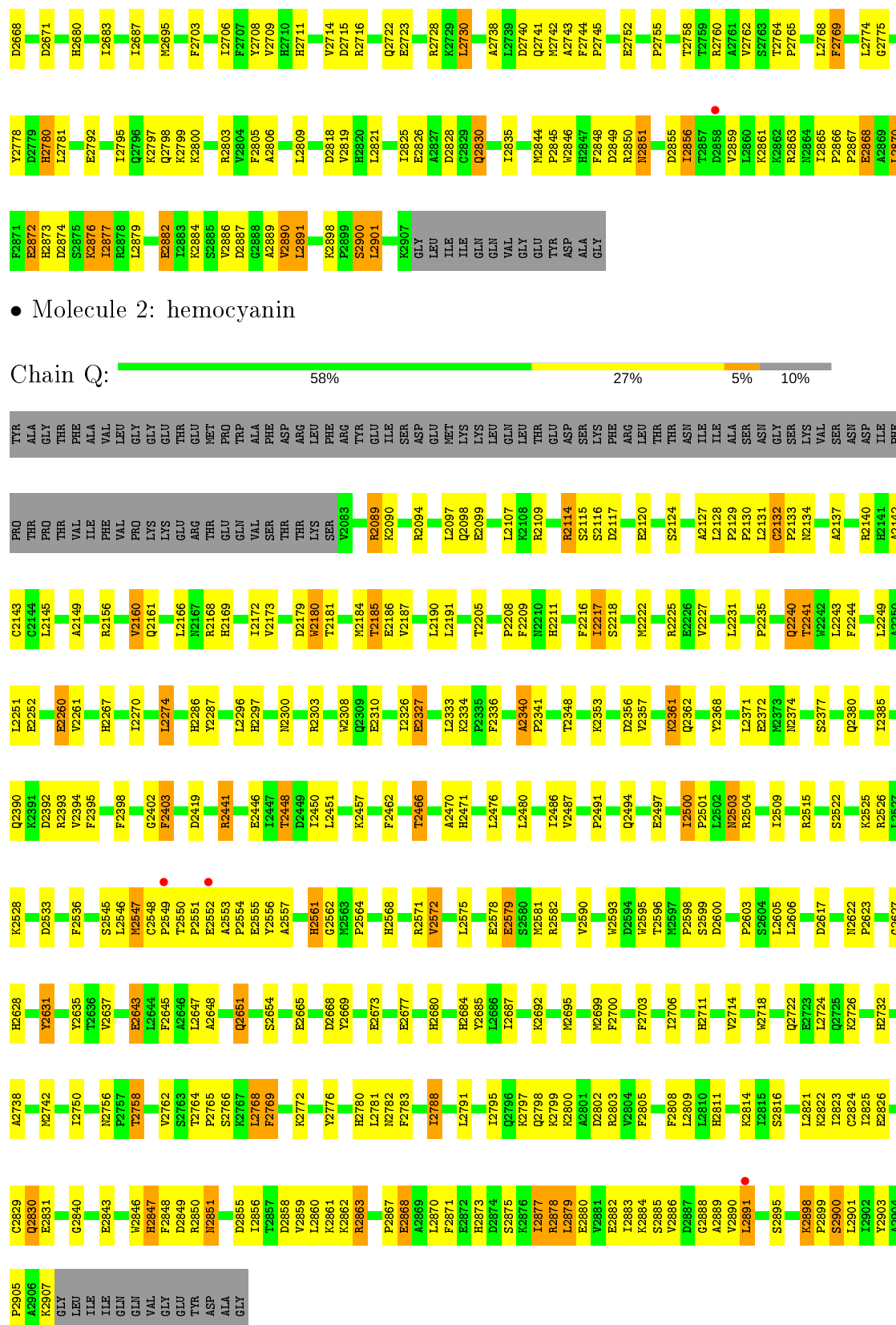




• Molecule 2: hemocyanin







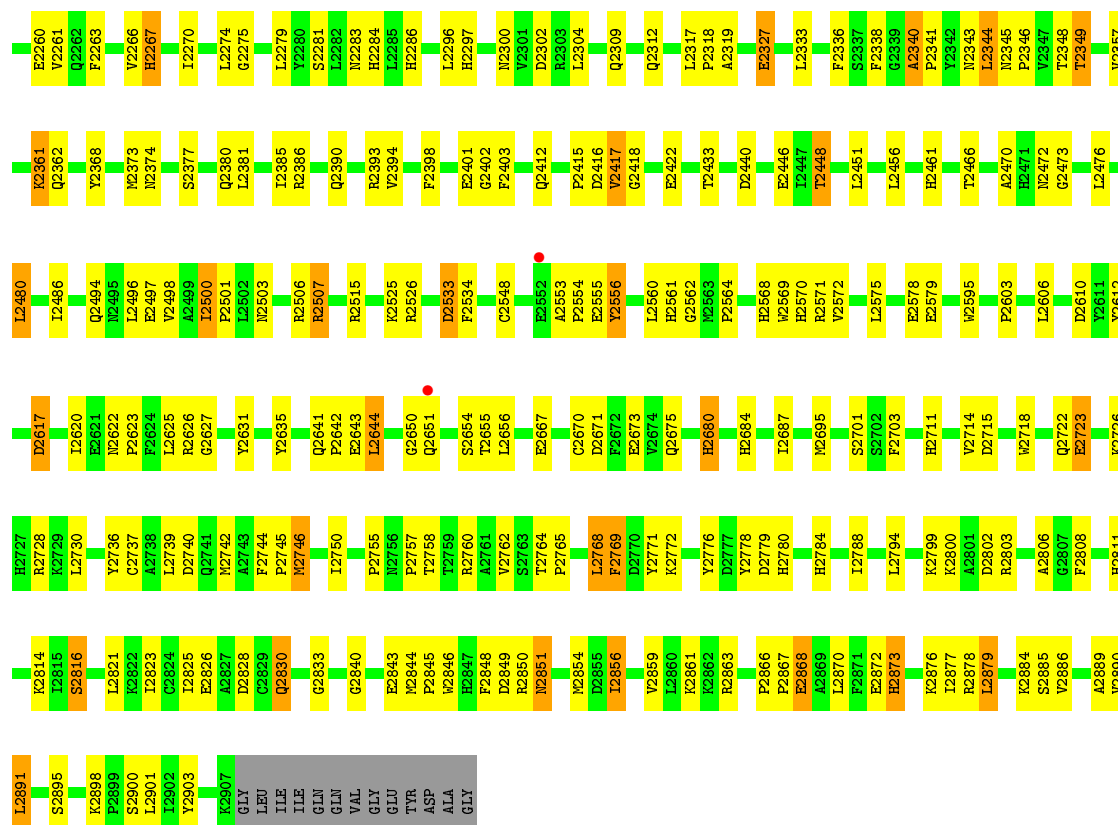
Chain T:  56% 29% 10%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| THR | ALA | GLY | THR | THR | ALA | VAL | LEU | GLY | GLY | THR | GLU | THR | MET | PRO | TRP | ALA | PHE | ASP | ARG | LEU | PHE | ARG | THR | GLU | THR | THR | ASN | ILE | ILE | ALA | SER | ASN | GLY | SER | LYS | VAL | SER | ASN | ASP | ILE | PHE | | | | | | | | | | | | | |
| PRO | THR | PRO | THR | VAL | ILE | PHE | VAL | PHE | PRO | LYS | LYS | GLU | ARG | THR | GLN | VAL | SER | THR | THR | LYS | SER | V2083 | R2089 | R2090 | R2091 | R2092 | R2093 | R2094 | L2097 | Q2098 | E2099 | I2104 | L2107 | R2108 | R2109 | M2110 | Q2111 | R2112 | R2113 | R2114 | S2115 | S2116 | D2117 | A2127 | L2128 | P2129 | L2130 | P2131 | Q2132 | P2133 | R2140 | Q2239 | R2141 | A2142 |
| C2143 | C2144 | L2145 | R2156 | V2160 | Q2161 | F2162 | E2163 | L2166 | N2167 | R2168 | H2169 | I2172 | V2173 | G2174 | V2175 | P2176 | Y2177 | W2178 | D2179 | K2180 | T2181 | M2184 | T2185 | E2186 | L2191 | T2201 | G2202 | I2203 | N2207 | P2208 | S2215 | F2216 | I2217 | S2218 | T2221 | M2222 | R2225 | F2232 | E2233 | Q2234 | P2235 | A2236 | L2237 | G2238 | R2239 | Q2240 | T2241 | | | | | | | |
| L2242 | L2243 | F2244 | E2252 | E2260 | V2261 | I2265 | V2266 | H2267 | H2271 | S2272 | W2273 | L2274 | G2275 | G2276 | L2279 | N2283 | H2284 | L2285 | H2286 | N2300 | R2303 | L2317 | F2318 | N2323 | E2327 | L2333 | K2334 | P2335 | F2336 | G2339 | A2340 | P2341 | Y2342 | R2343 | N2344 | N2345 | P2346 | T2347 | T2348 | T2349 | V2357 | F2358 | H2359 | Q2360 | T2361 | | | | | | | | | |
| Q2362 | E2370 | M2371 | E2372 | M2373 | L2381 | I2385 | R2386 | R2389 | Q2390 | V2394 | G2402 | F2403 | G2404 | S2405 | P2415 | D2416 | V2417 | G2418 | D2419 | S2424 | H2425 | N2435 | P2436 | R2441 | L2442 | Y2443 | K2444 | M2445 | E2446 | I2447 | T2448 | L2451 | M2454 | H2461 | L2476 | F2477 | E2478 | G2479 | L2480 | L2481 | R2488 | P2491 | | | | | | | | | | | | |
| L2496 | E2497 | V2498 | N2502 | L2503 | R2504 | L2505 | R2506 | S2507 | N2508 | L2509 | K2525 | R2526 | L2527 | K2528 | D2533 | F2536 | S2545 | L2546 | N2547 | C2548 | T2549 | P2551 | E2552 | A2553 | P2554 | E2555 | Y2556 | A2557 | C2558 | C2559 | L2560 | H2561 | H2568 | W2569 | R2570 | R2571 | V2572 | L2575 | H2576 | F2577 | E2578 | E2579 | M2580 | M2581 | F2703 | D2704 | H2584 | W2585 | T2586 | P2587 | P2588 | | | |
| N2601 | L2605 | L2606 | D2617 | N2622 | L2623 | R2626 | R2627 | H2628 | I2629 | L2630 | V2631 | E2632 | T2633 | T2634 | V2635 | R2638 | E2643 | L2644 | L2647 | A2648 | E2649 | T2652 | G2653 | Q2651 | R2652 | L2656 | L2662 | E2665 | E2677 | V2678 | L2679 | H2680 | R2681 | S2682 | I2683 | H2684 | I2687 | M2695 | F2705 | D2706 | V2709 | H2710 | | | | | | | | | | | | |
| H2711 | V2714 | W2718 | Q2722 | E2723 | K2726 | L2730 | P2731 | K2734 | A2738 | L2739 | D2740 | P2745 | F2749 | I2750 | N2754 | P2755 | P2756 | T2757 | T2758 | E2759 | R2760 | T2764 | S2765 | S2766 | K2767 | L2768 | F2769 | Y2771 | K2772 | S2773 | L2774 | G2775 | Y2776 | I2788 | L2795 | Q2798 | K2799 | K2800 | R2803 | V2804 | F2805 | A2806 | G2807 | | | | | | | | | | | |
| F2808 | L2809 | S2816 | V2819 | H2820 | L2821 | K2822 | C2824 | L2825 | I2826 | A2827 | D2828 | C2829 | Q2830 | E2831 | L2832 | Q2833 | F2836 | G2840 | E2843 | K2844 | P2845 | W2846 | H2847 | F2848 | D2849 | R2850 | N2851 | M2854 | D2855 | L2856 | T2857 | D2858 | V2859 | K2862 | R2863 | H2864 | I2865 | P2866 | P2867 | F2871 | E2872 | D2873 | S2874 | L2875 | K2876 | L2877 | R2878 | L2879 | E2882 | | | | | |
| I2883 | K2884 | V2886 | D2887 | G2888 | A2889 | V2890 | L2891 | D2892 | S2900 | L2901 | R2907 | GLY | LEU | ILE | ILE | GLN | VAL | GLY | GLY | THR | ASP | ALA | GLY | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

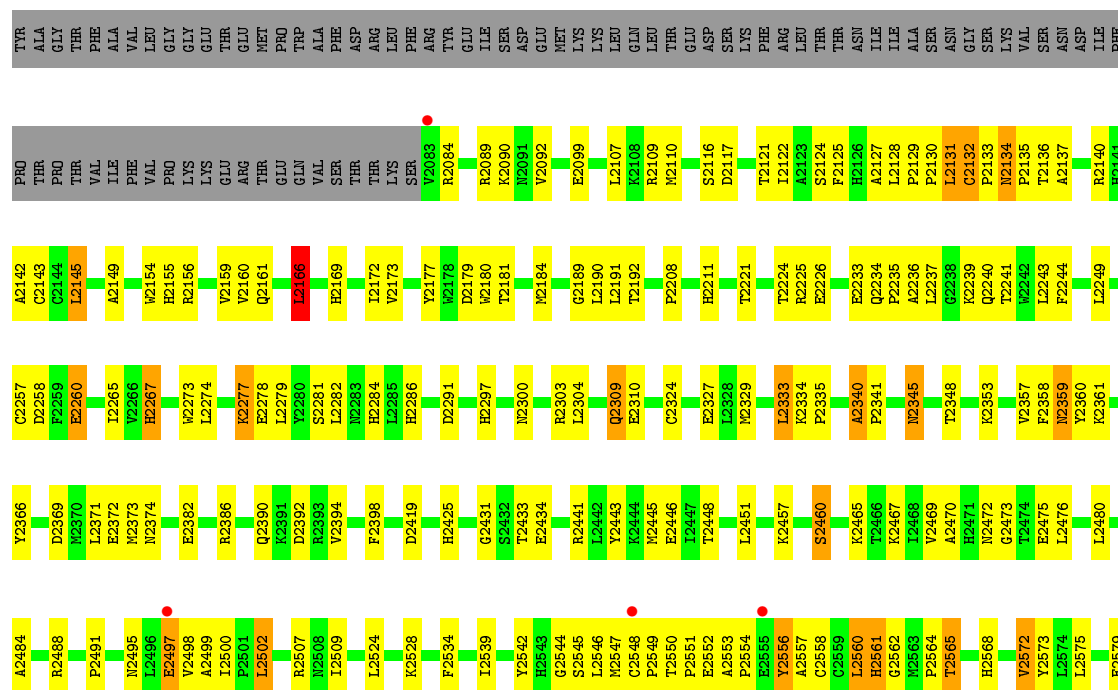
• Molecule 2: hemocyanin

Chain W:  59% 27% 10%

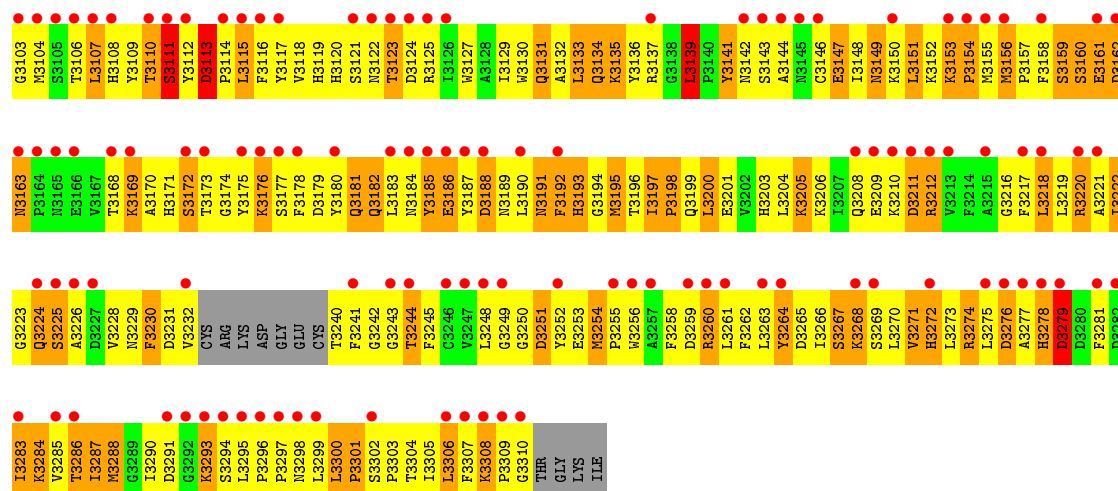
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|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| TYR | ALA | GLY | THR | PHE | ALA | VAL | LEU | GLY | GLY | GLU | THR | THR | PRO | MET | TRP | PHE | ASP | ARG | LEU | PHE | ARG | TYR | GLU | ILE | SER | ASP | GLU | MET | LYS | LYS | LEU | GLN | LEU | THR | GLU | ASP | ASP | LYS | PHE | ARG | LEU | THR | THR | ASN | ASN | ILE | ILE | ALA | SER | ASN | GLY | SER | LYS | VAL | SER | ASN | ASP | ILE | PHE |
| PRO | THR | PRO | THR | VAL | ILE | PHE | VAL | PRO | LYS | LYS | GLU | ARG | THR | THR | GLN | VAL | SER | THR | THR | LYS | SER | V2083 | R2089 | R2090 | R2091 | V2092 | R2093 | R2094 | E2099 | L2107 | K2108 | Q2111 | R2114 | S2115 | S2116 | T2121 | S2124 | A2127 | L2128 | P2129 | V2138 | A2142 | C2143 | C2144 | L2145 | R2156 | V2160 | | | | | | | | | | | | |
| Q2161 | F2162 | E2163 | L2166 | H2169 | V2175 | P2176 | G2177 | W2178 | L2179 | W2180 | T2181 | M2184 | T2185 | F2186 | V2187 | L2190 | L2191 | T2205 | P2208 | S2215 | F2216 | I2217 | S2218 | T2221 | R2225 | L2231 | F2232 | E2233 | Q2234 | P2235 | A2236 | L2237 | Q2240 | T2241 | W2242 | L2243 | F2244 | R2245 | N2246 | I2247 | I2248 | E2252 | Q2253 | T2254 | C2257 | | | | | | | | | | | | | | |



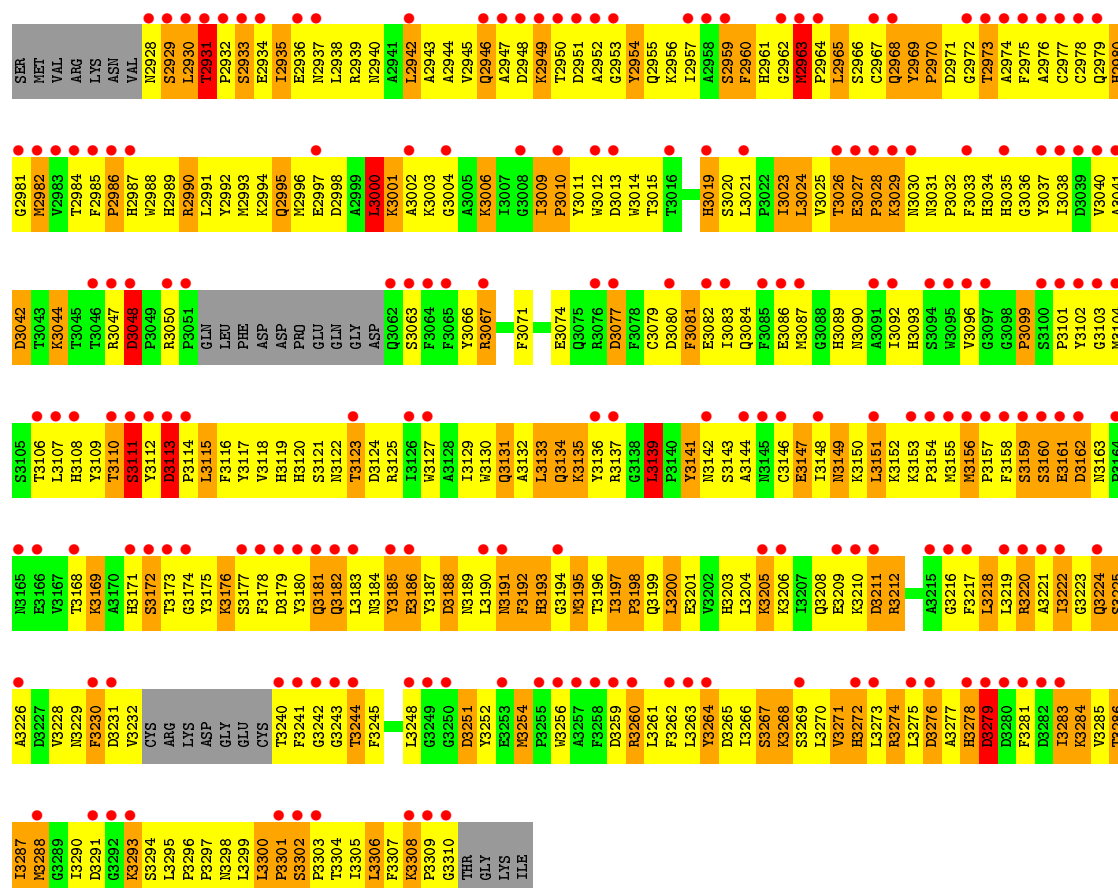
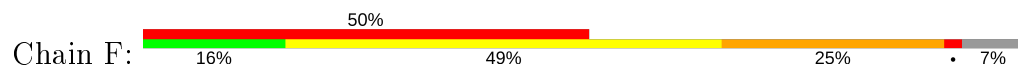
• Molecule 2: hemocyanin



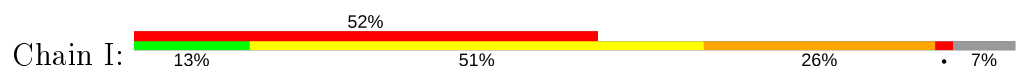




• Molecule 3: hemocyanin

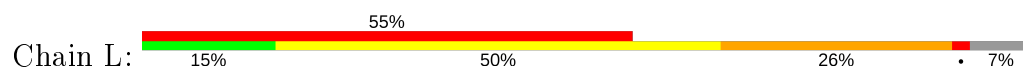


• Molecule 3: hemocyanin

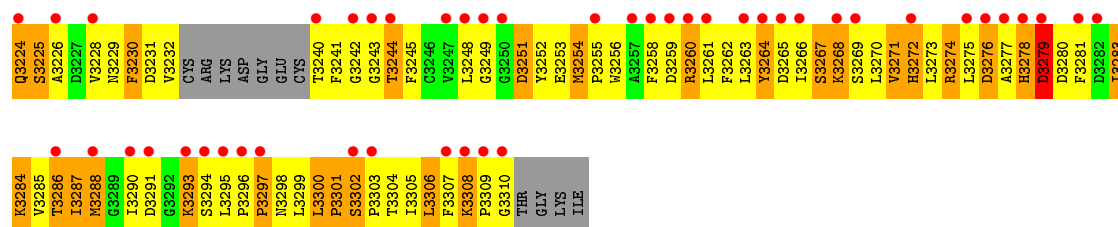


| | | | | | | | | | | | | |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| SER | G2981 | D3042 | T3106 | E3166 | D3227 | I3287 | D3227 | E3166 | T3106 | D3042 | G2981 | SER |
| MEI | M2982 | T3043 | L3107 | V3167 | V3228 | M3288 | V3228 | V3167 | L3107 | T3043 | M2982 | MEI |
| VAL | V2983 | K3044 | H3108 | K3168 | M3229 | G3289 | M3229 | K3168 | H3108 | K3044 | V2983 | VAL |
| ARG | T2984 | T3045 | Y3109 | K3169 | G3290 | I3290 | G3290 | K3169 | Y3109 | T3045 | T2984 | ARG |
| LVS | P2985 | T3046 | T3110 | A3170 | D3231 | D3291 | D3231 | A3170 | T3110 | T3046 | P2985 | LVS |
| ASN | P2986 | R3047 | S3111 | H3171 | D3232 | G3292 | D3232 | H3171 | S3111 | R3047 | P2986 | ASN |
| VAL | H2987 | D3048 | Y3112 | S3172 | CYS | K3293 | CYS | S3172 | Y3112 | D3048 | H2987 | VAL |
| N2928 | H2988 | P3049 | D3113 | T3173 | ARG | S3294 | ARG | T3173 | D3113 | P3049 | H2988 | N2928 |
| S2929 | H2989 | R3050 | P3114 | G3174 | LVS | L3295 | LVS | G3174 | P3114 | R3050 | H2989 | S2929 |
| L2930 | R2990 | P3051 | L3115 | V3175 | ASP | P3296 | ASP | V3175 | L3115 | P3051 | R2990 | L2930 |
| T2931 | R2991 | GLN | F3116 | K3176 | GLY | P3297 | GLY | K3176 | F3116 | GLN | R2991 | T2931 |
| P2932 | Y2992 | LEU | S3177 | S3177 | GLU | N3298 | GLU | S3177 | S3177 | LEU | Y2992 | P2932 |
| S2933 | M2993 | PHE | V3118 | P3178 | CYS | L3299 | CYS | P3178 | V3118 | PHE | M2993 | S2933 |
| E2934 | K2994 | ASP | H3119 | D3179 | T3240 | L3300 | T3240 | D3179 | H3119 | ASP | K2994 | E2934 |
| I2935 | Q2995 | ASP | H3120 | F3241 | F3241 | P3301 | F3241 | F3241 | H3120 | ASP | Q2995 | I2935 |
| E2936 | M2996 | PRO | Q3181 | Q3181 | G3242 | S3302 | G3242 | Q3181 | Q3181 | PRO | M2996 | E2936 |
| N2937 | E2997 | GLU | Q3182 | Q3182 | G3243 | P3303 | G3243 | Q3182 | Q3182 | GLU | E2997 | N2937 |
| L2938 | D2998 | GLN | L3183 | L3183 | T3244 | T3304 | T3244 | L3183 | L3183 | GLN | D2998 | L2938 |
| R2939 | L2999 | GLY | N3184 | N3184 | F3245 | I3305 | F3245 | N3184 | N3184 | GLY | L2999 | R2939 |
| N2940 | L3000 | ASP | R3125 | R3185 | G3246 | L3306 | G3246 | R3185 | R3125 | ASP | L3000 | N2940 |
| A2941 | K3001 | Q3062 | I3126 | E3186 | V3247 | F3307 | V3247 | E3186 | I3126 | Q3062 | K3001 | A2941 |
| L2942 | A3002 | S3063 | A3127 | Y3187 | L3248 | K3308 | L3248 | Y3187 | A3127 | S3063 | A3002 | L2942 |
| A2943 | K3003 | + | A3128 | D3188 | G3249 | P3309 | G3249 | D3188 | A3128 | + | K3003 | A2943 |
| V2944 | G3004 | Y3066 | I3129 | N3189 | G3250 | G3310 | G3250 | N3189 | I3129 | Y3066 | G3004 | V2944 |
| A2945 | A3005 | R3067 | H3130 | L3190 | D3251 | THR | D3251 | L3190 | H3130 | R3067 | A3005 | A2945 |
| Q2946 | K3006 | + | Q3131 | N3191 | Y3252 | GLY | Y3252 | N3191 | Q3131 | + | K3006 | Q2946 |
| A2947 | L3007 | F3071 | A3132 | F3192 | M3253 | LVS | M3253 | F3192 | A3132 | F3071 | L3007 | A2947 |
| D2948 | G3008 | + | L3133 | K3193 | N3254 | LVS | N3254 | K3193 | L3133 | + | G3008 | D2948 |
| K2949 | I3009 | Q3074 | G3134 | K3194 | P3255 | K3308 | P3255 | K3194 | G3134 | Q3074 | I3009 | K2949 |
| T2950 | P3010 | Q3075 | K3135 | N3195 | W3256 | T2950 | W3256 | N3195 | K3135 | Q3075 | P3010 | T2950 |
| D2951 | Y3011 | R3076 | Y3136 | T3196 | A3257 | D2951 | A3257 | T3196 | Y3136 | R3076 | Y3011 | D2951 |
| A2952 | H3012 | D3077 | R3137 | I3197 | P3258 | K3308 | P3258 | I3197 | R3137 | D3077 | H3012 | A2952 |
| G2953 | D3013 | F3078 | G3138 | F3198 | D3259 | G2953 | D3259 | F3198 | G3138 | F3078 | D3013 | G2953 |
| Y2954 | P3014 | D3079 | L3139 | Q3199 | R3260 | T2954 | R3260 | Q3199 | L3139 | D3079 | P3014 | Y2954 |
| Q2955 | T3015 | D3080 | P3140 | L3200 | F3261 | K3309 | F3261 | L3200 | P3140 | D3080 | T3015 | Q2955 |
| K2956 | T3016 | + | Y3141 | E3201 | F3262 | LVS | F3262 | Y3141 | Y3141 | + | T3016 | K2956 |
| L2957 | + | E3082 | N3142 | H3203 | L3263 | LVS | L3263 | H3203 | N3142 | E3082 | + | L2957 |
| A2958 | H3019 | L3083 | S3143 | L3204 | Y3264 | LVS | Y3264 | L3204 | S3143 | L3083 | H3019 | A2958 |
| S2959 | S3020 | Q3084 | A3144 | D3265 | D3265 | K3309 | D3265 | D3265 | A3144 | Q3084 | S3020 | S2959 |
| F2960 | L3021 | F3085 | N3145 | K3205 | I3266 | LVS | I3266 | K3205 | N3145 | F3085 | L3021 | F2960 |
| H2961 | P3022 | H3086 | C3146 | S3267 | S3267 | T2961 | S3267 | S3267 | C3146 | H3086 | P3022 | H2961 |
| G2962 | I3023 | M3087 | E3147 | K3268 | K3268 | G2962 | K3268 | K3268 | E3147 | M3087 | I3023 | G2962 |
| M2963 | L3024 | G3088 | I3148 | Q3208 | S3269 | M2963 | S3269 | Q3208 | I3148 | G3088 | L3024 | M2963 |
| P2964 | V3025 | H3089 | N3149 | E3209 | L3270 | P2964 | L3270 | E3209 | N3149 | H3089 | V3025 | P2964 |
| L2965 | T3026 | M3090 | K3150 | K3210 | M3271 | LVS | M3271 | K3210 | K3150 | M3090 | T3026 | L2965 |
| S2966 | E3027 | A3091 | L3151 | R3211 | H3272 | G2966 | H3272 | R3211 | L3151 | A3091 | E3027 | S2966 |
| C2967 | P3028 | H3092 | K3152 | R3212 | R3273 | T2967 | R3273 | R3212 | K3152 | H3092 | P3028 | C2967 |
| Q2968 | K3029 | H3093 | K3153 | K3274 | K3274 | Q2968 | K3274 | K3274 | K3153 | H3093 | K3029 | Q2968 |
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| T2972 | F3033 | G3097 | P3157 | L3218 | H3278 | T2972 | H3278 | L3218 | P3157 | G3097 | F3033 | T2972 |
| T2973 | H3034 | P3098 | F3158 | L3219 | D3279 | LVS | D3279 | L3219 | F3158 | P3098 | H3034 | T2973 |
| A2974 | H3035 | P3099 | S3159 | R3220 | R3280 | T2974 | R3280 | R3220 | S3159 | P3099 | H3035 | A2974 |
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| A2976 | Y3037 | P3101 | E3161 | I3222 | D3282 | A2976 | D3282 | I3222 | E3161 | P3101 | Y3037 | A2976 |
| C2977 | I3038 | Y3102 | D3162 | G3223 | I3283 | C2977 | I3283 | G3223 | D3162 | Y3102 | I3038 | C2977 |
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| P2979 | V3040 | M3104 | P3164 | S3225 | V3285 | P2979 | V3285 | P3164 | P3164 | M3104 | V3040 | P2979 |
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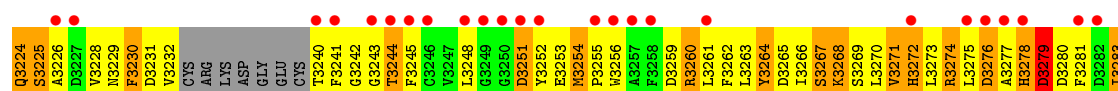
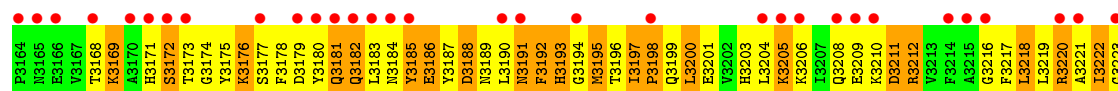
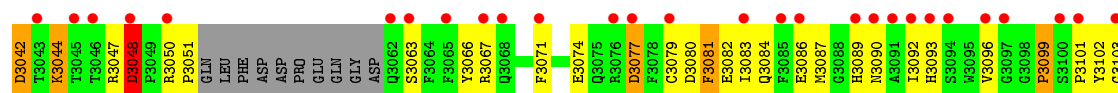
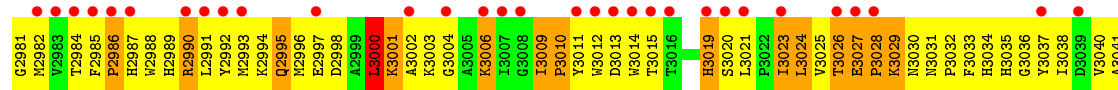
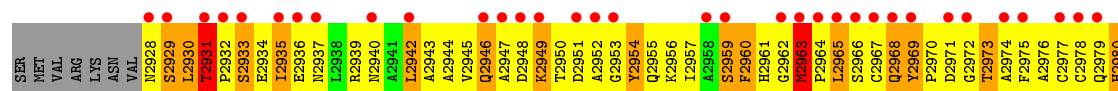
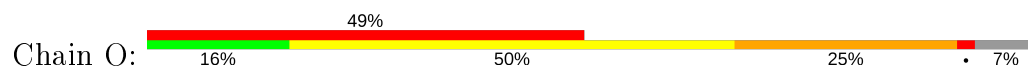
• Molecule 3: hemocyanin



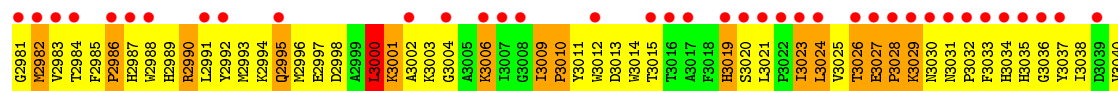
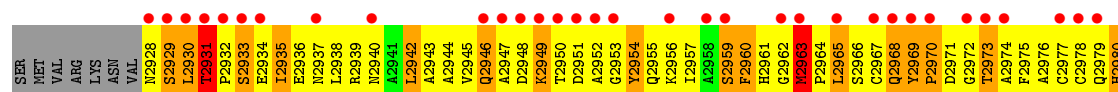
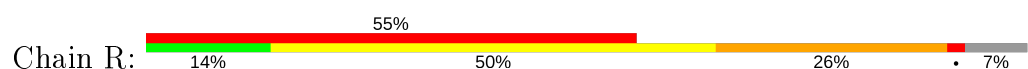
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| MET | M2982 | T3043 | S3105 | N3165 |
| VAL | V2983 | K3044 | L3106 | E3166 |
| ARG | T2984 | T3045 | L3107 | V3167 |
| LVS | P2985 | T3046 | H3108 | T3168 |
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| S2929 | H2989 | R3050 | S3112 | S3172 |
| L2930 | R2990 | P3051 | D3113 | T3173 |
| T2931 | R2991 | GLN | P3114 | G3174 |
| P2932 | Y2992 | LEU | L3115 | V3175 |
| S2933 | M2993 | PHE | F3116 | K3176 |
| E2934 | K2994 | ASP | Y3117 | S3177 |
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| E2936 | M2996 | PRO | H3119 | D3179 |
| N2937 | E2997 | GLU | R3120 | K3180 |
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| R2939 | L2999 | GLY | N3122 | Q3182 |
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| T2950 | P3010 | K3073 | L3133 | R3193 |
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| Y2954 | P3014 | D3077 | R3137 | L3197 |
| Q2955 | T3015 | F3078 | G3138 | K3198 |
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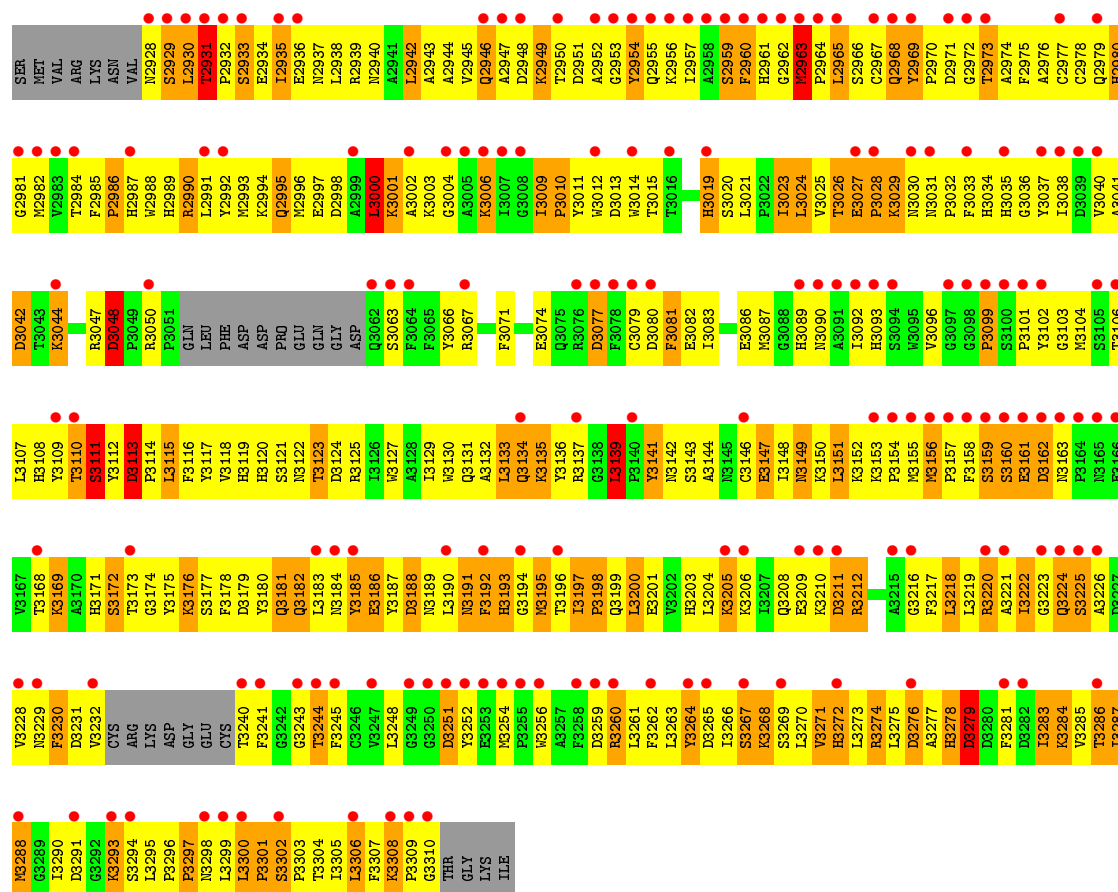


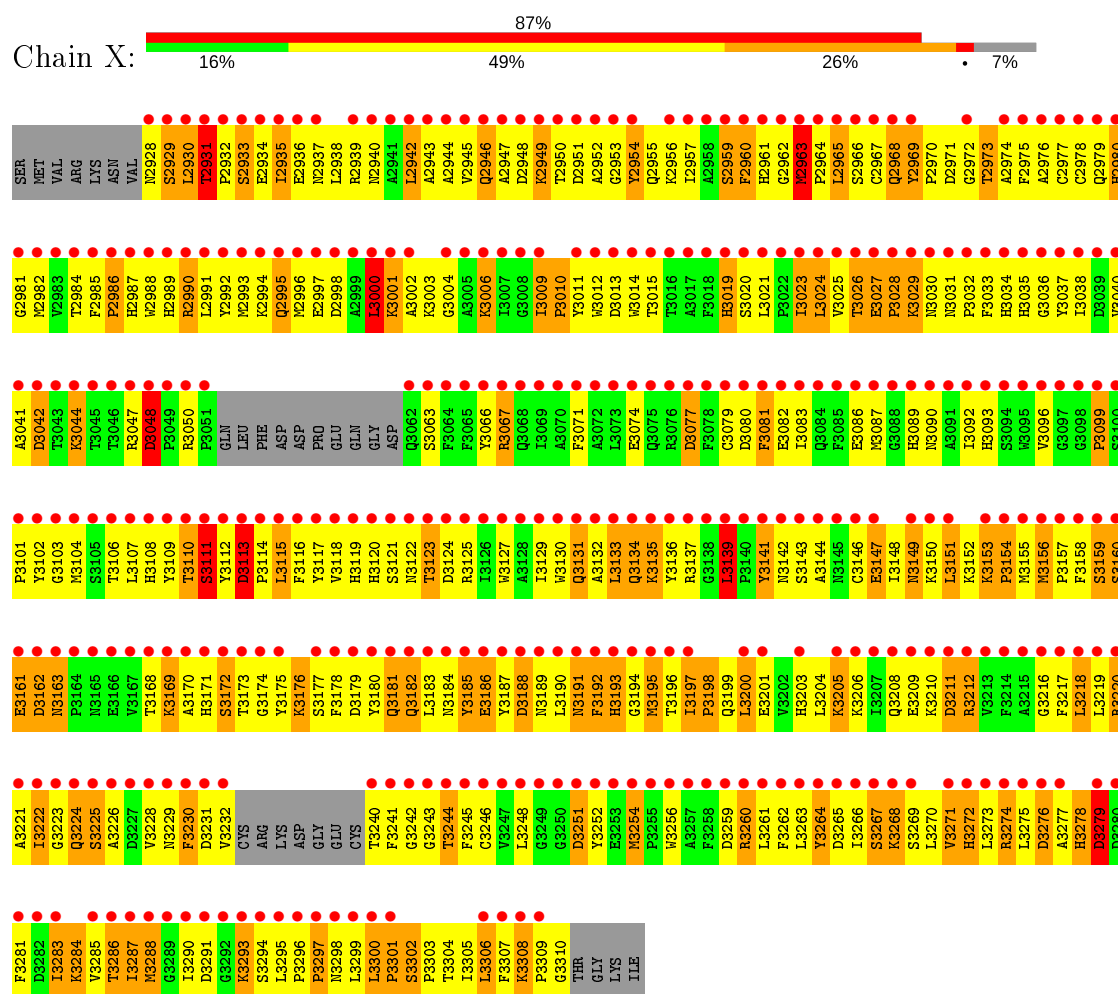
• Molecule 3: hemocyanin



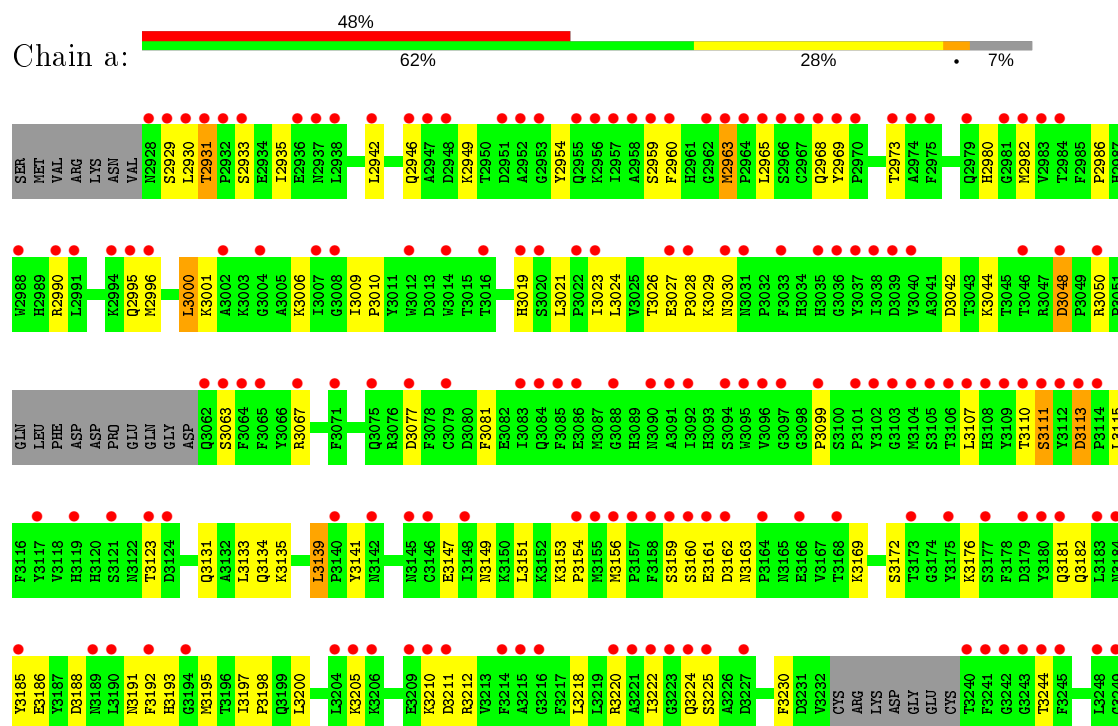
• Molecule 3: hemocyanin

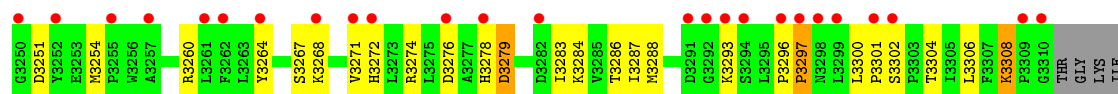




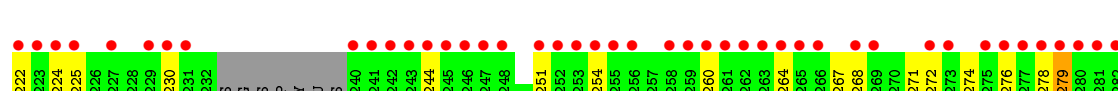
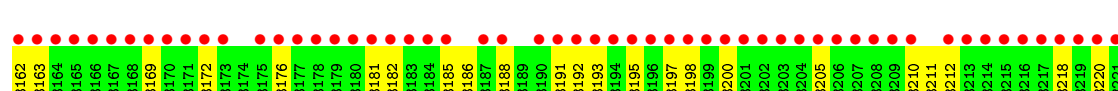
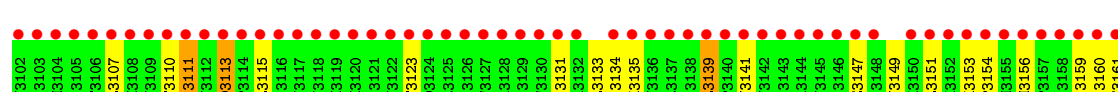
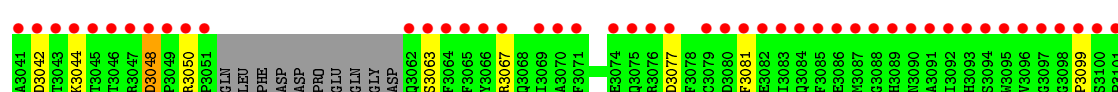
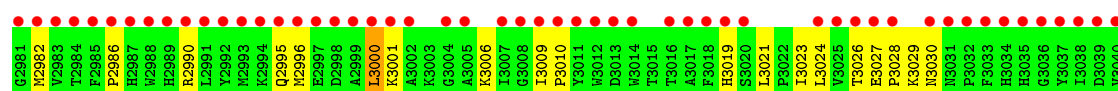
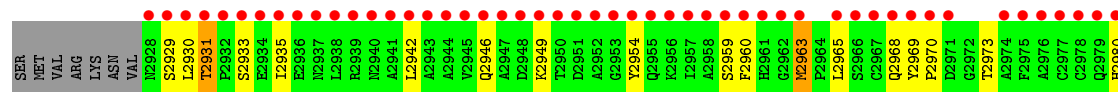
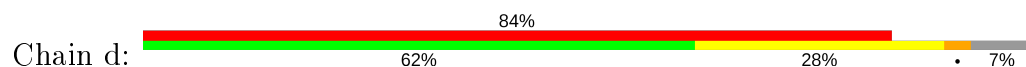


• Molecule 3: hemocyanin





• Molecule 3: hemocyanin



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



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

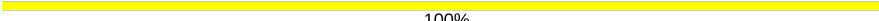


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:  50% 50%

MAG1
MAG2

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

Chain j:  100%

MAG1
MAG2

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

Chain m:  100%

MAG1
MAG2

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

Chain n:  100%

MAG1
MAG2

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

Chain o:  100%

MAG1
MAG2

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

Chain p:  50% 50%

MAG1
MAG2

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

Chain q:  100%

NAG1
NAG2

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

Chain s:  50% 50%

NAG1
NAG2

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

Chain t:  50% 50%


NAG1
NAG2

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

Chain u:  100%

NAG1
NAG2

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

Chain v:  100%

NAG1
NAG2

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

Chain x:  50% 50%

NAG1
NAG2

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

Chain 1:  50% 50%

NAG1
NAG2

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

Chain 2:  50% 50%



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

Chain 4:  100%



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

Chain 6:  50% 50%



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

Chain 7:  100%



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

Chain 8:  100%



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

Chain 9:  100%



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

Chain BA:  100%

MAG1
MAG2

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

Chain HA:  50% 50%MAG1
MAG2

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

Chain IA:  100%MAG1
MAG2

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

Chain JA:  50% 50%MAG1
MAG2

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

Chain MA:  100%MAG1
MAG2

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

Chain OA:  100%MAG1
MAG2

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

Chain QA:  50% 50%MAG1
MAG2

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

Chain RA: 


MAG1
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 

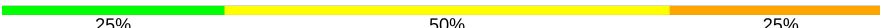

MAG1
MAG2
BMA3
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l: 


MAG1
MAG2
BMA3
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA: 



MAG1
MAG2
BMA3
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain FA: 


MAG1
MAG2
BMA3
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain KA: 

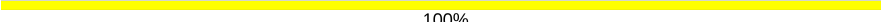

MAG1
MAG2
BMA3
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain PA:  50% 50%




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

Chain h:  100%



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

Chain k:  33% 67%

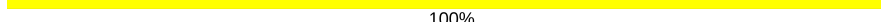


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  67% 33%

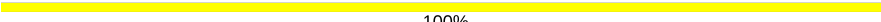


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:  100%



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

Chain y:  100%



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

Chain 3:  33% 33% 33%



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

Chain 5:  100%

UAG1
UAG2
BMA3

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

Chain CA:  33% 67%

UAG1
UAG2
BMA3

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

Chain DA:  33% 67%

UAG1
UAG2
BMA3

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

Chain EA:  33% 33% 33%

UAG1
UAG2
BMA3

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

Chain GA:  100%

UAG1
UAG2
BMA3

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

Chain LA:  100%

UAG1
UAG2
BMA3

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

Chain NA:  67% 33%



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

Chain z:  20% 80%



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

Chain 0:  25% 75%



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 171.37Å 538.66Å 310.92Å 90.00° 104.09° 90.00° | Depositor |
| Resolution (Å) | 49.10 – 3.00 49.10 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 98.9 (49.10-3.00) 89.6 (49.10-3.00) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.11 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.74 (at 3.01Å) | Xtriage |
| Refinement program | PHENIX 1.9_1692 | Depositor |
| R, R_{free} | 0.274 , 0.303 0.275 , 0.303 | Depositor DCC |
| R_{free} test set | 53588 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 64.8 | Xtriage |
| Anisotropy | 0.538 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.24 , 11.9 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$ | Xtriage |
| Estimated twinning fraction | 0.055 for h,-k,-h-l | Xtriage |
| F_o, F_c correlation | 0.86 | EDS |
| Total number of atoms | 261470 | wwPDB-VP |
| Average B, all atoms (Å ²) | 68.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: CUO, 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 | 0.29 | 0/13698 | 0.54 | 4/18607 (0.0%) |
| 1 | D | 0.29 | 0/13698 | 0.54 | 4/18607 (0.0%) |
| 1 | G | 0.28 | 0/13698 | 0.53 | 3/18607 (0.0%) |
| 1 | J | 0.29 | 0/13698 | 0.53 | 2/18607 (0.0%) |
| 1 | M | 0.28 | 0/13698 | 0.52 | 2/18607 (0.0%) |
| 1 | P | 0.28 | 0/13698 | 0.53 | 3/18607 (0.0%) |
| 1 | S | 0.27 | 0/13698 | 0.52 | 4/18607 (0.0%) |
| 1 | V | 0.28 | 0/13698 | 0.52 | 4/18607 (0.0%) |
| 1 | Y | 0.27 | 0/13698 | 0.51 | 3/18607 (0.0%) |
| 1 | b | 0.27 | 0/13698 | 0.52 | 3/18607 (0.0%) |
| 2 | B | 0.27 | 0/6909 | 0.51 | 2/9383 (0.0%) |
| 2 | E | 0.28 | 0/6909 | 0.52 | 1/9383 (0.0%) |
| 2 | H | 0.28 | 0/6909 | 0.51 | 2/9383 (0.0%) |
| 2 | K | 0.28 | 0/6909 | 0.52 | 2/9383 (0.0%) |
| 2 | N | 0.28 | 0/6909 | 0.50 | 1/9383 (0.0%) |
| 2 | Q | 0.27 | 0/6909 | 0.50 | 0/9383 |
| 2 | T | 0.27 | 0/6909 | 0.50 | 2/9383 (0.0%) |
| 2 | W | 0.26 | 0/6909 | 0.49 | 1/9383 (0.0%) |
| 2 | Z | 0.27 | 0/6909 | 0.49 | 1/9383 (0.0%) |
| 2 | c | 0.27 | 0/6909 | 0.49 | 0/9383 |
| 3 | C | 0.80 | 12/6100 (0.2%) | 0.90 | 34/8282 (0.4%) |
| 3 | F | 0.80 | 12/6100 (0.2%) | 0.90 | 34/8282 (0.4%) |
| 3 | I | 0.80 | 12/6100 (0.2%) | 0.90 | 34/8282 (0.4%) |
| 3 | L | 0.80 | 12/6100 (0.2%) | 0.91 | 34/8282 (0.4%) |
| 3 | O | 0.80 | 12/6100 (0.2%) | 0.90 | 34/8282 (0.4%) |
| 3 | R | 0.80 | 14/6100 (0.2%) | 0.90 | 34/8282 (0.4%) |
| 3 | U | 0.80 | 12/6100 (0.2%) | 0.91 | 34/8282 (0.4%) |
| 3 | X | 0.80 | 12/6100 (0.2%) | 0.90 | 34/8282 (0.4%) |
| 3 | a | 0.80 | 12/6100 (0.2%) | 0.90 | 34/8282 (0.4%) |
| 3 | d | 0.80 | 14/6100 (0.2%) | 0.90 | 34/8282 (0.4%) |
| All | All | 0.45 | 124/267070 (0.0%) | 0.63 | 384/362720 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 2 |
| 1 | D | 0 | 3 |
| 1 | G | 0 | 1 |
| 1 | J | 0 | 2 |
| 1 | M | 0 | 1 |
| 1 | S | 0 | 3 |
| 1 | Y | 0 | 1 |
| 1 | b | 0 | 2 |
| 2 | B | 0 | 1 |
| 2 | K | 0 | 3 |
| 2 | N | 0 | 1 |
| 2 | Q | 0 | 1 |
| 2 | T | 0 | 2 |
| 2 | W | 0 | 1 |
| 2 | Z | 0 | 2 |
| 2 | c | 0 | 1 |
| 3 | C | 0 | 4 |
| 3 | F | 0 | 4 |
| 3 | I | 0 | 4 |
| 3 | L | 0 | 4 |
| 3 | O | 0 | 4 |
| 3 | R | 0 | 4 |
| 3 | U | 0 | 4 |
| 3 | X | 0 | 4 |
| 3 | a | 0 | 4 |
| 3 | d | 0 | 4 |
| All | All | 0 | 67 |

The worst 5 of 124 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|---------|------|-------|------|-------------|----------|
| 3 | C | 3154[A] | PRO | N-CD | 5.36 | 1.55 | 1.47 |
| 3 | C | 3154[B] | PRO | N-CD | 5.36 | 1.55 | 1.47 |
| 3 | X | 3154[A] | PRO | N-CD | 5.25 | 1.55 | 1.47 |
| 3 | X | 3154[B] | PRO | N-CD | 5.25 | 1.55 | 1.47 |
| 3 | O | 3154[A] | PRO | N-CD | 5.24 | 1.55 | 1.47 |

The worst 5 of 384 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|------|------|----------|------|------------------------|---------------------|
| 1 | P | 979 | LEU | CA-CB-CG | 7.97 | 133.62 | 115.30 |
| 1 | V | 567 | LEU | CA-CB-CG | 7.90 | 133.47 | 115.30 |
| 1 | A | 279 | LEU | CA-CB-CG | 7.27 | 132.02 | 115.30 |
| 2 | K | 2546 | LEU | CA-CB-CG | 6.93 | 131.25 | 115.30 |
| 1 | M | 1230 | LEU | CA-CB-CG | 6.68 | 130.67 | 115.30 |

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|---------|------|-----------|
| 1 | A | 464 | LEU | Peptide |
| 1 | A | 982 | LYS | Peptide |
| 2 | B | 2127 | ALA | Peptide |
| 3 | C | 3113[A] | ASP | Mainchain |
| 3 | C | 3113[B] | ASP | Mainchain |

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 | 13318 | 0 | 12755 | 440 | 1 |
| 1 | D | 13318 | 0 | 12755 | 458 | 0 |
| 1 | G | 13318 | 0 | 12754 | 478 | 0 |
| 1 | J | 13318 | 0 | 12755 | 484 | 0 |
| 1 | M | 13318 | 0 | 12755 | 427 | 0 |
| 1 | P | 13318 | 0 | 12755 | 438 | 0 |
| 1 | S | 13318 | 0 | 12755 | 437 | 0 |
| 1 | V | 13318 | 0 | 12755 | 434 | 0 |
| 1 | Y | 13318 | 0 | 12744 | 397 | 0 |
| 1 | b | 13318 | 0 | 12754 | 0 | 1 |
| 2 | B | 6704 | 0 | 6445 | 197 | 0 |
| 2 | E | 6704 | 0 | 6445 | 232 | 0 |
| 2 | H | 6704 | 0 | 6445 | 230 | 0 |
| 2 | K | 6704 | 0 | 6445 | 209 | 0 |
| 2 | N | 6704 | 0 | 6445 | 192 | 0 |
| 2 | Q | 6704 | 0 | 6445 | 207 | 0 |
| 2 | T | 6704 | 0 | 6445 | 214 | 0 |
| 2 | W | 6704 | 0 | 6445 | 214 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | Z | 6704 | 0 | 6444 | 181 | 0 |
| 2 | c | 6704 | 0 | 6445 | 0 | 0 |
| 3 | C | 5912 | 0 | 5607 | 2272 | 0 |
| 3 | F | 5912 | 0 | 5599 | 1400 | 0 |
| 3 | I | 5912 | 0 | 5601 | 2391 | 0 |
| 3 | L | 5912 | 0 | 5604 | 2283 | 0 |
| 3 | O | 5912 | 0 | 5604 | 1994 | 0 |
| 3 | R | 5912 | 0 | 5597 | 2373 | 0 |
| 3 | U | 5912 | 0 | 5612 | 1410 | 0 |
| 3 | X | 5912 | 0 | 5598 | 1993 | 0 |
| 3 | a | 5912 | 0 | 5594 | 0 | 0 |
| 3 | d | 5912 | 0 | 5607 | 0 | 0 |
| 4 | 1 | 28 | 0 | 25 | 1 | 0 |
| 4 | 2 | 28 | 0 | 25 | 1 | 0 |
| 4 | 4 | 28 | 0 | 25 | 0 | 0 |
| 4 | 6 | 28 | 0 | 25 | 1 | 0 |
| 4 | 7 | 28 | 0 | 25 | 6 | 0 |
| 4 | 8 | 28 | 0 | 25 | 0 | 0 |
| 4 | 9 | 28 | 0 | 25 | 2 | 0 |
| 4 | BA | 28 | 0 | 25 | 5 | 0 |
| 4 | HA | 28 | 0 | 25 | 6 | 0 |
| 4 | IA | 28 | 0 | 25 | 0 | 0 |
| 4 | JA | 28 | 0 | 25 | 2 | 0 |
| 4 | MA | 28 | 0 | 25 | 8 | 0 |
| 4 | OA | 28 | 0 | 25 | 1 | 0 |
| 4 | QA | 28 | 0 | 25 | 0 | 0 |
| 4 | RA | 28 | 0 | 25 | 1 | 0 |
| 4 | e | 28 | 0 | 25 | 0 | 0 |
| 4 | f | 28 | 0 | 25 | 0 | 0 |
| 4 | i | 28 | 0 | 25 | 0 | 0 |
| 4 | j | 28 | 0 | 25 | 0 | 0 |
| 4 | m | 28 | 0 | 25 | 0 | 0 |
| 4 | n | 28 | 0 | 25 | 0 | 0 |
| 4 | o | 28 | 0 | 25 | 0 | 0 |
| 4 | p | 28 | 0 | 25 | 0 | 0 |
| 4 | q | 28 | 0 | 25 | 0 | 0 |
| 4 | s | 28 | 0 | 25 | 0 | 0 |
| 4 | t | 28 | 0 | 25 | 0 | 0 |
| 4 | u | 28 | 0 | 25 | 0 | 0 |
| 4 | v | 28 | 0 | 25 | 0 | 0 |
| 4 | x | 28 | 0 | 25 | 0 | 0 |
| 5 | AA | 50 | 0 | 43 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | FA | 50 | 0 | 43 | 2 | 0 |
| 5 | KA | 50 | 0 | 43 | 1 | 0 |
| 5 | PA | 50 | 0 | 43 | 1 | 0 |
| 5 | g | 50 | 0 | 43 | 0 | 0 |
| 5 | l | 50 | 0 | 43 | 0 | 0 |
| 6 | 3 | 39 | 0 | 34 | 3 | 0 |
| 6 | 5 | 39 | 0 | 34 | 2 | 0 |
| 6 | CA | 39 | 0 | 34 | 3 | 0 |
| 6 | DA | 39 | 0 | 34 | 2 | 0 |
| 6 | EA | 39 | 0 | 34 | 1 | 0 |
| 6 | GA | 39 | 0 | 34 | 9 | 0 |
| 6 | LA | 39 | 0 | 34 | 5 | 0 |
| 6 | NA | 39 | 0 | 34 | 2 | 0 |
| 6 | h | 39 | 0 | 34 | 0 | 0 |
| 6 | k | 39 | 0 | 34 | 0 | 0 |
| 6 | r | 39 | 0 | 34 | 0 | 0 |
| 6 | w | 39 | 0 | 34 | 0 | 0 |
| 6 | y | 39 | 0 | 34 | 0 | 0 |
| 7 | z | 61 | 0 | 52 | 0 | 0 |
| 8 | 0 | 50 | 0 | 43 | 8 | 0 |
| 9 | A | 24 | 0 | 0 | 2 | 0 |
| 9 | B | 8 | 0 | 0 | 0 | 0 |
| 9 | C | 16 | 0 | 0 | 14 | 0 |
| 9 | D | 24 | 0 | 0 | 2 | 0 |
| 9 | E | 8 | 0 | 0 | 0 | 0 |
| 9 | F | 16 | 0 | 0 | 7 | 0 |
| 9 | G | 24 | 0 | 0 | 1 | 0 |
| 9 | H | 8 | 0 | 0 | 0 | 0 |
| 9 | I | 16 | 0 | 0 | 12 | 0 |
| 9 | J | 24 | 0 | 0 | 2 | 0 |
| 9 | K | 8 | 0 | 0 | 0 | 0 |
| 9 | M | 24 | 0 | 0 | 3 | 0 |
| 9 | N | 8 | 0 | 0 | 0 | 0 |
| 9 | O | 8 | 0 | 0 | 10 | 0 |
| 9 | P | 24 | 0 | 0 | 0 | 0 |
| 9 | Q | 8 | 0 | 0 | 0 | 0 |
| 9 | S | 24 | 0 | 0 | 3 | 0 |
| 9 | T | 8 | 0 | 0 | 1 | 0 |
| 9 | U | 8 | 0 | 0 | 10 | 0 |
| 9 | V | 24 | 0 | 0 | 2 | 0 |
| 9 | W | 8 | 0 | 0 | 1 | 0 |
| 9 | X | 8 | 0 | 0 | 10 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 9 | Y | 24 | 0 | 0 | 3 | 0 |
| 9 | Z | 8 | 0 | 0 | 0 | 0 |
| 9 | b | 24 | 0 | 0 | 0 | 0 |
| 9 | c | 8 | 0 | 0 | 0 | 0 |
| 9 | d | 8 | 0 | 0 | 0 | 0 |
| All | All | 261470 | 0 | 249529 | 19298 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

The worst 5 of 19298 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) |
|---------------------|----------------------|--------------------------|-------------------|
| 3:C:3079[B]:CYS:CB | 3:L:3161[B]:GLU:HG2 | 1.22 | 1.65 |
| 3:C:2982[B]:MET:SD | 3:L:3156[B]:MET:HB2 | 1.37 | 1.64 |
| 3:C:2975[B]:PHE:CD1 | 3:L:3107[B]:LEU:HD11 | 1.28 | 1.63 |
| 3:I:3174[B]:GLY:CA | 3:R:3154[B]:PRO:HB3 | 1.17 | 1.62 |
| 3:O:3153[B]:LYS:CD | 3:X:3176[B]:LYS:HD3 | 1.31 | 1.60 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------|------------------------|--------------------------|-------------------|
| 1:A:1:ASN:N | 1:b:887:ASP:OD1[1_455] | 2.19 | 0.01 |

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 | 1654/2000 (83%) | 1552 (94%) | 89 (5%) | 13 (1%) | 19 57 |
| 1 | D | 1654/2000 (83%) | 1541 (93%) | 100 (6%) | 13 (1%) | 19 57 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|----|
| 1 | G | 1654/2000 (83%) | 1560 (94%) | 78 (5%) | 16 (1%) | 15 | 53 |
| 1 | J | 1654/2000 (83%) | 1537 (93%) | 103 (6%) | 14 (1%) | 19 | 57 |
| 1 | M | 1654/2000 (83%) | 1569 (95%) | 73 (4%) | 12 (1%) | 22 | 60 |
| 1 | P | 1654/2000 (83%) | 1562 (94%) | 78 (5%) | 14 (1%) | 19 | 57 |
| 1 | S | 1654/2000 (83%) | 1581 (96%) | 64 (4%) | 9 (0%) | 29 | 68 |
| 1 | V | 1654/2000 (83%) | 1570 (95%) | 68 (4%) | 16 (1%) | 15 | 53 |
| 1 | Y | 1654/2000 (83%) | 1580 (96%) | 66 (4%) | 8 (0%) | 29 | 68 |
| 1 | b | 1654/2000 (83%) | 1564 (95%) | 80 (5%) | 10 (1%) | 25 | 64 |
| 2 | B | 823/920 (90%) | 778 (94%) | 40 (5%) | 5 (1%) | 25 | 64 |
| 2 | E | 823/920 (90%) | 781 (95%) | 34 (4%) | 8 (1%) | 15 | 53 |
| 2 | H | 823/920 (90%) | 787 (96%) | 33 (4%) | 3 (0%) | 34 | 72 |
| 2 | K | 823/920 (90%) | 778 (94%) | 37 (4%) | 8 (1%) | 15 | 53 |
| 2 | N | 823/920 (90%) | 789 (96%) | 32 (4%) | 2 (0%) | 47 | 82 |
| 2 | Q | 823/920 (90%) | 787 (96%) | 32 (4%) | 4 (0%) | 29 | 68 |
| 2 | T | 823/920 (90%) | 794 (96%) | 22 (3%) | 7 (1%) | 17 | 55 |
| 2 | W | 823/920 (90%) | 791 (96%) | 28 (3%) | 4 (0%) | 29 | 68 |
| 2 | Z | 823/920 (90%) | 797 (97%) | 23 (3%) | 3 (0%) | 34 | 72 |
| 2 | c | 823/920 (90%) | 791 (96%) | 29 (4%) | 3 (0%) | 34 | 72 |
| 3 | C | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | F | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | I | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | L | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | O | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | R | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | U | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | X | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | a | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| 3 | d | 720/394 (183%) | 666 (92%) | 48 (7%) | 6 (1%) | 19 | 57 |
| All | All | 31970/33140 (96%) | 30149 (94%) | 1589 (5%) | 232 (1%) | 22 | 60 |

5 of 232 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1196 | ILE |
| 1 | D | 695 | TYR |
| 1 | D | 1196 | ILE |
| 1 | G | 331 | SER |
| 1 | G | 1086 | LEU |

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 | 1429/1738 (82%) | 1278 (89%) | 151 (11%) | 6 | 26 |
| 1 | D | 1429/1738 (82%) | 1267 (89%) | 162 (11%) | 6 | 24 |
| 1 | G | 1429/1738 (82%) | 1264 (88%) | 165 (12%) | 5 | 24 |
| 1 | J | 1429/1738 (82%) | 1266 (89%) | 163 (11%) | 5 | 24 |
| 1 | M | 1429/1738 (82%) | 1284 (90%) | 145 (10%) | 7 | 29 |
| 1 | P | 1429/1738 (82%) | 1264 (88%) | 165 (12%) | 5 | 24 |
| 1 | S | 1429/1738 (82%) | 1269 (89%) | 160 (11%) | 6 | 24 |
| 1 | V | 1429/1738 (82%) | 1270 (89%) | 159 (11%) | 6 | 25 |
| 1 | Y | 1429/1738 (82%) | 1261 (88%) | 168 (12%) | 5 | 22 |
| 1 | b | 1429/1738 (82%) | 1277 (89%) | 152 (11%) | 6 | 26 |
| 2 | B | 731/814 (90%) | 666 (91%) | 65 (9%) | 9 | 35 |
| 2 | E | 731/814 (90%) | 655 (90%) | 76 (10%) | 7 | 27 |
| 2 | H | 731/814 (90%) | 634 (87%) | 97 (13%) | 4 | 17 |
| 2 | K | 731/814 (90%) | 656 (90%) | 75 (10%) | 7 | 28 |
| 2 | N | 731/814 (90%) | 652 (89%) | 79 (11%) | 6 | 26 |
| 2 | Q | 731/814 (90%) | 654 (90%) | 77 (10%) | 7 | 27 |
| 2 | T | 731/814 (90%) | 660 (90%) | 71 (10%) | 8 | 31 |
| 2 | W | 731/814 (90%) | 659 (90%) | 72 (10%) | 8 | 30 |
| 2 | Z | 731/814 (90%) | 655 (90%) | 76 (10%) | 7 | 27 |
| 2 | c | 731/814 (90%) | 652 (89%) | 79 (11%) | 6 | 26 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|------------|-------------|----|
| 3 | C | 636/343 (185%) | 432 (68%) | 204 (32%) | 0 | 1 |
| 3 | F | 636/343 (185%) | 432 (68%) | 204 (32%) | 0 | 1 |
| 3 | I | 636/343 (185%) | 432 (68%) | 204 (32%) | 0 | 1 |
| 3 | L | 636/343 (185%) | 430 (68%) | 206 (32%) | 0 | 1 |
| 3 | O | 636/343 (185%) | 430 (68%) | 206 (32%) | 0 | 1 |
| 3 | R | 636/343 (185%) | 432 (68%) | 204 (32%) | 0 | 1 |
| 3 | U | 636/343 (185%) | 432 (68%) | 204 (32%) | 0 | 1 |
| 3 | X | 636/343 (185%) | 432 (68%) | 204 (32%) | 0 | 1 |
| 3 | a | 636/343 (185%) | 432 (68%) | 204 (32%) | 0 | 1 |
| 3 | d | 636/343 (185%) | 432 (68%) | 204 (32%) | 0 | 1 |
| All | All | 27960/28950 (97%) | 23559 (84%) | 4401 (16%) | 3 | 13 |

5 of 4401 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|---------|------|
| 2 | N | 2887 | ASP |
| 3 | R | 2959[B] | SER |
| 1 | b | 1053 | TRP |
| 3 | O | 3024[B] | LEU |
| 1 | P | 376 | ASN |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 300 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | M | 192 | HIS |
| 1 | P | 679 | ASN |
| 1 | b | 779 | HIS |
| 1 | M | 881 | GLN |
| 2 | N | 2230 | HIS |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

130 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$ |
| 8 | NAG | 0 | 1 | 1,8 | 14,14,15 | 0.72 | 1 (7%) | 17,19,21 | 1.49 | 2 (11%) |
| 8 | NAG | 0 | 2 | 8 | 14,14,15 | 0.52 | 0 | 17,19,21 | 1.50 | 4 (23%) |
| 8 | BMA | 0 | 3 | 8 | 11,11,12 | 0.22 | 0 | 15,15,17 | 1.90 | 4 (26%) |
| 8 | MAN | 0 | 4 | 8 | 11,11,12 | 0.32 | 0 | 15,15,17 | 0.89 | 1 (6%) |
| 4 | NAG | 1 | 1 | 1,4 | 14,14,15 | 0.44 | 0 | 17,19,21 | 1.03 | 1 (5%) |
| 4 | NAG | 1 | 2 | 4 | 14,14,15 | 0.42 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 4 | NAG | 2 | 1 | 2,4 | 14,14,15 | 1.05 | 1 (7%) | 17,19,21 | 1.42 | 2 (11%) |
| 4 | NAG | 2 | 2 | 4 | 14,14,15 | 0.31 | 0 | 17,19,21 | 0.73 | 0 |
| 6 | NAG | 3 | 1 | 1,6 | 14,14,15 | 0.96 | 1 (7%) | 17,19,21 | 1.45 | 2 (11%) |
| 6 | NAG | 3 | 2 | 6 | 14,14,15 | 0.40 | 0 | 17,19,21 | 0.77 | 0 |
| 6 | BMA | 3 | 3 | 6 | 11,11,12 | 0.26 | 0 | 15,15,17 | 0.62 | 0 |
| 4 | NAG | 4 | 1 | 1,4 | 14,14,15 | 0.72 | 1 (7%) | 17,19,21 | 1.24 | 2 (11%) |
| 4 | NAG | 4 | 2 | 4 | 14,14,15 | 0.41 | 0 | 17,19,21 | 1.19 | 2 (11%) |
| 6 | NAG | 5 | 1 | 1,6 | 14,14,15 | 0.71 | 0 | 17,19,21 | 1.26 | 1 (5%) |
| 6 | NAG | 5 | 2 | 6 | 14,14,15 | 0.31 | 0 | 17,19,21 | 1.00 | 1 (5%) |
| 6 | BMA | 5 | 3 | 6 | 11,11,12 | 0.28 | 0 | 15,15,17 | 1.31 | 2 (13%) |
| 4 | NAG | 6 | 1 | 1,4 | 14,14,15 | 0.90 | 1 (7%) | 17,19,21 | 1.93 | 2 (11%) |
| 4 | NAG | 6 | 2 | 4 | 14,14,15 | 0.41 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 4 | NAG | 7 | 1 | 2,4 | 14,14,15 | 0.81 | 1 (7%) | 17,19,21 | 1.49 | 2 (11%) |
| 4 | NAG | 7 | 2 | 4 | 14,14,15 | 0.43 | 0 | 17,19,21 | 1.07 | 2 (11%) |
| 4 | NAG | 8 | 1 | 1,4 | 14,14,15 | 0.94 | 1 (7%) | 17,19,21 | 1.85 | 2 (11%) |
| 4 | NAG | 8 | 2 | 4 | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.69 | 1 (5%) |
| 4 | NAG | 9 | 1 | 1,4 | 14,14,15 | 0.89 | 1 (7%) | 17,19,21 | 1.51 | 3 (17%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAG | 9 | 2 | 4 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.78 | 1 (5%) |
| 5 | NAG | AA | 1 | 1,5 | 14,14,15 | 0.66 | 0 | 17,19,21 | 1.16 | 3 (17%) |
| 5 | NAG | AA | 2 | 5 | 14,14,15 | 0.42 | 0 | 17,19,21 | 0.88 | 1 (5%) |
| 5 | BMA | AA | 3 | 5 | 11,11,12 | 0.29 | 0 | 15,15,17 | 1.93 | 3 (20%) |
| 5 | MAN | AA | 4 | 5 | 11,11,12 | 0.24 | 0 | 15,15,17 | 0.53 | 0 |
| 4 | NAG | BA | 1 | 1,4 | 14,14,15 | 0.71 | 0 | 17,19,21 | 1.37 | 3 (17%) |
| 4 | NAG | BA | 2 | 4 | 14,14,15 | 0.57 | 0 | 17,19,21 | 1.10 | 1 (5%) |
| 6 | NAG | CA | 1 | 2,6 | 14,14,15 | 1.04 | 1 (7%) | 17,19,21 | 1.54 | 1 (5%) |
| 6 | NAG | CA | 2 | 6 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.94 | 1 (5%) |
| 6 | BMA | CA | 3 | 6 | 11,11,12 | 0.22 | 0 | 15,15,17 | 0.68 | 0 |
| 6 | NAG | DA | 1 | 1,6 | 14,14,15 | 0.76 | 1 (7%) | 17,19,21 | 1.17 | 1 (5%) |
| 6 | NAG | DA | 2 | 6 | 14,14,15 | 0.31 | 0 | 17,19,21 | 1.22 | 2 (11%) |
| 6 | BMA | DA | 3 | 6 | 11,11,12 | 0.25 | 0 | 15,15,17 | 1.01 | 1 (6%) |
| 6 | NAG | EA | 1 | 1,6 | 14,14,15 | 0.79 | 1 (7%) | 17,19,21 | 1.35 | 2 (11%) |
| 6 | NAG | EA | 2 | 6 | 14,14,15 | 0.37 | 0 | 17,19,21 | 2.26 | 4 (23%) |
| 6 | BMA | EA | 3 | 6 | 11,11,12 | 0.23 | 0 | 15,15,17 | 0.78 | 0 |
| 5 | NAG | FA | 1 | 1,5 | 14,14,15 | 0.78 | 1 (7%) | 17,19,21 | 1.36 | 2 (11%) |
| 5 | NAG | FA | 2 | 5 | 14,14,15 | 0.48 | 0 | 17,19,21 | 0.90 | 1 (5%) |
| 5 | BMA | FA | 3 | 5 | 11,11,12 | 0.61 | 0 | 15,15,17 | 1.41 | 2 (13%) |
| 5 | MAN | FA | 4 | 5 | 11,11,12 | 0.21 | 0 | 15,15,17 | 1.29 | 2 (13%) |
| 6 | NAG | GA | 1 | 1,6 | 14,14,15 | 0.71 | 0 | 17,19,21 | 1.32 | 1 (5%) |
| 6 | NAG | GA | 2 | 6 | 14,14,15 | 0.42 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 6 | BMA | GA | 3 | 6 | 11,11,12 | 0.31 | 0 | 15,15,17 | 1.09 | 2 (13%) |
| 4 | NAG | HA | 1 | 2,4 | 14,14,15 | 0.68 | 0 | 17,19,21 | 1.23 | 2 (11%) |
| 4 | NAG | HA | 2 | 4 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.61 | 0 |
| 4 | NAG | IA | 1 | 1,4 | 14,14,15 | 0.80 | 1 (7%) | 17,19,21 | 1.50 | 2 (11%) |
| 4 | NAG | IA | 2 | 4 | 14,14,15 | 0.54 | 0 | 17,19,21 | 0.92 | 1 (5%) |
| 4 | NAG | JA | 1 | 1,4 | 14,14,15 | 0.82 | 1 (7%) | 17,19,21 | 1.23 | 1 (5%) |
| 4 | NAG | JA | 2 | 4 | 14,14,15 | 0.35 | 0 | 17,19,21 | 0.75 | 0 |
| 5 | NAG | KA | 1 | 1,5 | 14,14,15 | 0.72 | 0 | 17,19,21 | 1.86 | 5 (29%) |
| 5 | NAG | KA | 2 | 5 | 14,14,15 | 0.37 | 0 | 17,19,21 | 1.30 | 2 (11%) |
| 5 | BMA | KA | 3 | 5 | 11,11,12 | 0.29 | 0 | 15,15,17 | 1.45 | 1 (6%) |
| 5 | MAN | KA | 4 | 5 | 11,11,12 | 0.42 | 0 | 15,15,17 | 1.92 | 3 (20%) |
| 6 | NAG | LA | 1 | 1,6 | 14,14,15 | 0.98 | 1 (7%) | 17,19,21 | 2.35 | 4 (23%) |
| 6 | NAG | LA | 2 | 6 | 14,14,15 | 0.46 | 0 | 17,19,21 | 1.16 | 2 (11%) |
| 6 | BMA | LA | 3 | 6 | 11,11,12 | 0.22 | 0 | 15,15,17 | 0.79 | 1 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAG | MA | 1 | 2,4 | 14,14,15 | 0.99 | 1 (7%) | 17,19,21 | 2.38 | 3 (17%) |
| 4 | NAG | MA | 2 | 4 | 14,14,15 | 0.32 | 0 | 17,19,21 | 1.69 | 3 (17%) |
| 6 | NAG | NA | 1 | 1,6 | 14,14,15 | 0.72 | 1 (7%) | 17,19,21 | 1.02 | 1 (5%) |
| 6 | NAG | NA | 2 | 6 | 14,14,15 | 0.37 | 0 | 17,19,21 | 0.84 | 0 |
| 6 | BMA | NA | 3 | 6 | 11,11,12 | 0.25 | 0 | 15,15,17 | 0.95 | 1 (6%) |
| 4 | NAG | OA | 1 | 1,4 | 14,14,15 | 1.17 | 1 (7%) | 17,19,21 | 1.59 | 2 (11%) |
| 4 | NAG | OA | 2 | 4 | 14,14,15 | 0.55 | 0 | 17,19,21 | 0.98 | 1 (5%) |
| 5 | NAG | PA | 1 | 1,5 | 14,14,15 | 0.66 | 0 | 17,19,21 | 1.13 | 1 (5%) |
| 5 | NAG | PA | 2 | 5 | 14,14,15 | 0.37 | 0 | 17,19,21 | 0.98 | 1 (5%) |
| 5 | BMA | PA | 3 | 5 | 11,11,12 | 0.61 | 0 | 15,15,17 | 2.27 | 4 (26%) |
| 5 | MAN | PA | 4 | 5 | 11,11,12 | 0.27 | 0 | 15,15,17 | 0.90 | 1 (6%) |
| 4 | NAG | QA | 1 | 1,4 | 14,14,15 | 0.57 | 0 | 17,19,21 | 2.49 | 5 (29%) |
| 4 | NAG | QA | 2 | 4 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.69 | 0 |
| 4 | NAG | RA | 1 | 2,4 | 14,14,15 | 1.13 | 1 (7%) | 17,19,21 | 2.16 | 4 (23%) |
| 4 | NAG | RA | 2 | 4 | 14,14,15 | 0.45 | 0 | 17,19,21 | 0.72 | 0 |
| 4 | NAG | e | 1 | 1,4 | 14,14,15 | 0.60 | 0 | 17,19,21 | 1.67 | 4 (23%) |
| 4 | NAG | e | 2 | 4 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.52 | 0 |
| 4 | NAG | f | 1 | 1,4 | 14,14,15 | 0.90 | 1 (7%) | 17,19,21 | 1.42 | 2 (11%) |
| 4 | NAG | f | 2 | 4 | 14,14,15 | 0.24 | 0 | 17,19,21 | 1.01 | 1 (5%) |
| 5 | NAG | g | 1 | 1,5 | 14,14,15 | 0.60 | 0 | 17,19,21 | 1.51 | 2 (11%) |
| 5 | NAG | g | 2 | 5 | 14,14,15 | 0.50 | 0 | 17,19,21 | 1.05 | 0 |
| 5 | BMA | g | 3 | 5 | 11,11,12 | 0.49 | 0 | 15,15,17 | 2.19 | 4 (26%) |
| 5 | MAN | g | 4 | 5 | 11,11,12 | 0.24 | 0 | 15,15,17 | 0.73 | 0 |
| 6 | NAG | h | 1 | 1,6 | 14,14,15 | 0.62 | 0 | 17,19,21 | 1.14 | 2 (11%) |
| 6 | NAG | h | 2 | 6 | 14,14,15 | 0.57 | 0 | 17,19,21 | 1.09 | 1 (5%) |
| 6 | BMA | h | 3 | 6 | 11,11,12 | 0.26 | 0 | 15,15,17 | 1.15 | 2 (13%) |
| 4 | NAG | i | 1 | 2,4 | 14,14,15 | 1.06 | 1 (7%) | 17,19,21 | 1.23 | 2 (11%) |
| 4 | NAG | i | 2 | 4 | 14,14,15 | 0.42 | 0 | 17,19,21 | 0.86 | 0 |
| 4 | NAG | j | 1 | 1,4 | 14,14,15 | 1.00 | 1 (7%) | 17,19,21 | 1.65 | 2 (11%) |
| 4 | NAG | j | 2 | 4 | 14,14,15 | 0.49 | 0 | 17,19,21 | 1.36 | 3 (17%) |
| 6 | NAG | k | 1 | 1,6 | 14,14,15 | 0.78 | 1 (7%) | 17,19,21 | 1.10 | 1 (5%) |
| 6 | NAG | k | 2 | 6 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.66 | 1 (5%) |
| 6 | BMA | k | 3 | 6 | 11,11,12 | 0.25 | 0 | 15,15,17 | 0.53 | 0 |
| 5 | NAG | l | 1 | 1,5 | 14,14,15 | 0.69 | 0 | 17,19,21 | 1.21 | 1 (5%) |
| 5 | NAG | l | 2 | 5 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.61 | 0 |
| 5 | BMA | l | 3 | 5 | 11,11,12 | 0.27 | 0 | 15,15,17 | 0.83 | 0 |
| 5 | MAN | l | 4 | 5 | 11,11,12 | 0.27 | 0 | 15,15,17 | 0.99 | 1 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAG | m | 1 | 1,4 | 14,14,15 | 0.40 | 0 | 17,19,21 | 0.97 | 1 (5%) |
| 4 | NAG | m | 2 | 4 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.91 | 1 (5%) |
| 4 | NAG | n | 1 | 2,4 | 14,14,15 | 0.53 | 0 | 17,19,21 | 1.57 | 3 (17%) |
| 4 | NAG | n | 2 | 4 | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.99 | 1 (5%) |
| 4 | NAG | o | 1 | 1,4 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.00 | 1 (5%) |
| 4 | NAG | o | 2 | 4 | 14,14,15 | 0.43 | 0 | 17,19,21 | 1.13 | 2 (11%) |
| 4 | NAG | p | 1 | 4 | 14,14,15 | 0.89 | 1 (7%) | 17,19,21 | 1.94 | 4 (23%) |
| 4 | NAG | p | 2 | 4 | 14,14,15 | 0.30 | 0 | 17,19,21 | 0.67 | 0 |
| 4 | NAG | q | 1 | 1,4 | 14,14,15 | 0.56 | 0 | 17,19,21 | 1.18 | 2 (11%) |
| 4 | NAG | q | 2 | 4 | 14,14,15 | 0.51 | 0 | 17,19,21 | 0.87 | 1 (5%) |
| 6 | NAG | r | 1 | 1,6 | 14,14,15 | 0.69 | 0 | 17,19,21 | 1.73 | 4 (23%) |
| 6 | NAG | r | 2 | 6 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.02 | 0 |
| 6 | BMA | r | 3 | 6 | 11,11,12 | 0.23 | 0 | 15,15,17 | 0.63 | 0 |
| 4 | NAG | s | 1 | 2,4 | 14,14,15 | 0.80 | 1 (7%) | 17,19,21 | 1.22 | 2 (11%) |
| 4 | NAG | s | 2 | 4 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.77 | 0 |
| 4 | NAG | t | 1 | 1,4 | 14,14,15 | 0.64 | 0 | 17,19,21 | 1.50 | 3 (17%) |
| 4 | NAG | t | 2 | 4 | 14,14,15 | 0.31 | 0 | 17,19,21 | 0.54 | 0 |
| 4 | NAG | u | 1 | 1,4 | 14,14,15 | 0.83 | 1 (7%) | 17,19,21 | 1.64 | 3 (17%) |
| 4 | NAG | u | 2 | 4 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.85 | 1 (5%) |
| 4 | NAG | v | 1 | 1,4 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.11 | 1 (5%) |
| 4 | NAG | v | 2 | 4 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.93 | 1 (5%) |
| 6 | NAG | w | 1 | 1,6 | 14,14,15 | 0.71 | 1 (7%) | 17,19,21 | 1.90 | 4 (23%) |
| 6 | NAG | w | 2 | 6 | 14,14,15 | 0.42 | 0 | 17,19,21 | 1.17 | 1 (5%) |
| 6 | BMA | w | 3 | 6 | 11,11,12 | 0.30 | 0 | 15,15,17 | 0.84 | 1 (6%) |
| 4 | NAG | x | 1 | 2,4 | 14,14,15 | 0.50 | 0 | 17,19,21 | 0.91 | 0 |
| 4 | NAG | x | 2 | 4 | 14,14,15 | 0.48 | 0 | 17,19,21 | 1.03 | 1 (5%) |
| 6 | NAG | y | 1 | 1,6 | 14,14,15 | 0.86 | 1 (7%) | 17,19,21 | 1.18 | 1 (5%) |
| 6 | NAG | y | 2 | 6 | 14,14,15 | 0.35 | 0 | 17,19,21 | 1.92 | 4 (23%) |
| 6 | BMA | y | 3 | 6 | 11,11,12 | 0.22 | 0 | 15,15,17 | 1.24 | 2 (13%) |
| 7 | NAG | z | 1 | 1,7 | 14,14,15 | 1.07 | 1 (7%) | 17,19,21 | 2.10 | 3 (17%) |
| 7 | NAG | z | 2 | 7 | 14,14,15 | 0.58 | 0 | 17,19,21 | 1.58 | 3 (17%) |
| 7 | BMA | z | 3 | 7 | 11,11,12 | 0.45 | 0 | 15,15,17 | 2.58 | 5 (33%) |
| 7 | MAN | z | 4 | 7 | 11,11,12 | 0.42 | 0 | 15,15,17 | 1.98 | 4 (26%) |
| 7 | MAN | z | 5 | 7 | 11,11,12 | 0.22 | 0 | 15,15,17 | 0.63 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 8 | NAG | 0 | 1 | 1,8 | - | 2/6/23/26 | 0/1/1/1 |
| 8 | NAG | 0 | 2 | 8 | - | 2/6/23/26 | 0/1/1/1 |
| 8 | BMA | 0 | 3 | 8 | - | 0/2/19/22 | 0/1/1/1 |
| 8 | MAN | 0 | 4 | 8 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | 1 | 1 | 1,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | 1 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | 2 | 1 | 2,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | 2 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | 3 | 1 | 1,6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | 3 | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | 3 | 3 | 6 | - | 2/2/19/22 | 0/1/1/1 |
| 4 | NAG | 4 | 1 | 1,4 | - | 5/6/23/26 | 0/1/1/1 |
| 4 | NAG | 4 | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | 5 | 1 | 1,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | 5 | 2 | 6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | BMA | 5 | 3 | 6 | - | 2/2/19/22 | 0/1/1/1 |
| 4 | NAG | 6 | 1 | 1,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | 6 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | 7 | 1 | 2,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | 7 | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | 8 | 1 | 1,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | 8 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | 9 | 1 | 1,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | 9 | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | AA | 1 | 1,5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | AA | 2 | 5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | BMA | AA | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | AA | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | BA | 1 | 1,4 | - | 5/6/23/26 | 0/1/1/1 |
| 4 | NAG | BA | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | CA | 1 | 2,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | CA | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | CA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | DA | 1 | 1,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | DA | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | DA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 6 | NAG | EA | 1 | 1,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | EA | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | EA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | FA | 1 | 1,5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | FA | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | FA | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | FA | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | GA | 1 | 1,6 | - | 5/6/23/26 | 0/1/1/1 |
| 6 | NAG | GA | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | GA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | HA | 1 | 2,4 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | NAG | HA | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | IA | 1 | 1,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | IA | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | JA | 1 | 1,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | JA | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | KA | 1 | 1,5 | - | 4/6/23/26 | 0/1/1/1 |
| 5 | NAG | KA | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | KA | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | KA | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | LA | 1 | 1,6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | LA | 2 | 6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | BMA | LA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | MA | 1 | 2,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | MA | 2 | 4 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | NAG | NA | 1 | 1,6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | NA | 2 | 6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | BMA | NA | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | OA | 1 | 1,4 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | NAG | OA | 2 | 4 | - | 3/6/23/26 | 0/1/1/1 |
| 5 | NAG | PA | 1 | 1,5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | PA | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | PA | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | PA | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | QA | 1 | 1,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | QA | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | RA | 1 | 2,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | RA | 2 | 4 | - | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4 | NAG | e | 1 | 1,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | e | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | f | 1 | 1,4 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | f | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | g | 1 | 1,5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | g | 2 | 5 | - | 3/6/23/26 | 0/1/1/1 |
| 5 | BMA | g | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 5 | MAN | g | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | h | 1 | 1,6 | - | 3/6/23/26 | 0/1/1/1 |
| 6 | NAG | h | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | h | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | i | 1 | 2,4 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | NAG | i | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | j | 1 | 1,4 | - | 5/6/23/26 | 0/1/1/1 |
| 4 | NAG | j | 2 | 4 | - | 6/6/23/26 | 0/1/1/1 |
| 6 | NAG | k | 1 | 1,6 | - | 6/6/23/26 | 0/1/1/1 |
| 6 | NAG | k | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | k | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | l | 1 | 1,5 | - | 2/6/23/26 | 0/1/1/1 |
| 5 | NAG | l | 2 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | BMA | l | 3 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 5 | MAN | l | 4 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | m | 1 | 1,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | m | 2 | 4 | - | 6/6/23/26 | 0/1/1/1 |
| 4 | NAG | n | 1 | 2,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | n | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | o | 1 | 1,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | o | 2 | 4 | - | 1/6/23/26 | 0/1/1/1 |
| 4 | NAG | p | 1 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | p | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | q | 1 | 1,4 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | q | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | r | 1 | 1,6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | r | 2 | 6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | BMA | r | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | s | 1 | 2,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | s | 2 | 4 | - | 4/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4 | NAG | t | 1 | 1,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | t | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | u | 1 | 1,4 | - | 4/6/23/26 | 0/1/1/1 |
| 4 | NAG | u | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | v | 1 | 1,4 | - | 2/6/23/26 | 0/1/1/1 |
| 4 | NAG | v | 2 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | w | 1 | 1,6 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | w | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | w | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | x | 1 | 2,4 | - | 3/6/23/26 | 0/1/1/1 |
| 4 | NAG | x | 2 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | y | 1 | 1,6 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | y | 2 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | y | 3 | 6 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | NAG | z | 1 | 1,7 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | NAG | z | 2 | 7 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | BMA | z | 3 | 7 | - | 2/2/19/22 | 0/1/1/1 |
| 7 | MAN | z | 4 | 7 | - | 1/2/19/22 | 0/1/1/1 |
| 7 | MAN | z | 5 | 7 | - | 1/2/19/22 | 0/1/1/1 |

The worst 5 of 29 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4 | OA | 1 | NAG | C1-C2 | 4.08 | 1.58 | 1.52 |
| 4 | 2 | 1 | NAG | C1-C2 | 3.75 | 1.57 | 1.52 |
| 4 | i | 1 | NAG | C1-C2 | 3.72 | 1.57 | 1.52 |
| 4 | RA | 1 | NAG | C1-C2 | 3.70 | 1.57 | 1.52 |
| 7 | z | 1 | NAG | C1-C2 | 3.65 | 1.57 | 1.52 |

The worst 5 of 216 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6 | LA | 1 | NAG | C1-O5-C5 | 8.01 | 123.04 | 112.19 |
| 4 | MA | 1 | NAG | C1-O5-C5 | 7.93 | 122.94 | 112.19 |
| 4 | RA | 1 | NAG | C1-O5-C5 | 7.38 | 122.19 | 112.19 |
| 4 | QA | 1 | NAG | C2-N2-C7 | -7.33 | 112.46 | 122.90 |
| 7 | z | 1 | NAG | C1-O5-C5 | 7.09 | 121.79 | 112.19 |

There are no chirality outliers.

5 of 240 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 4 | IA | 1 | NAG | C8-C7-N2-C2 |
| 4 | IA | 1 | NAG | O7-C7-N2-C2 |
| 4 | e | 1 | NAG | C8-C7-N2-C2 |
| 4 | e | 1 | NAG | O7-C7-N2-C2 |
| 6 | NA | 2 | NAG | C8-C7-N2-C2 |

There are no ring outliers.

48 monomers are involved in 74 short contacts:

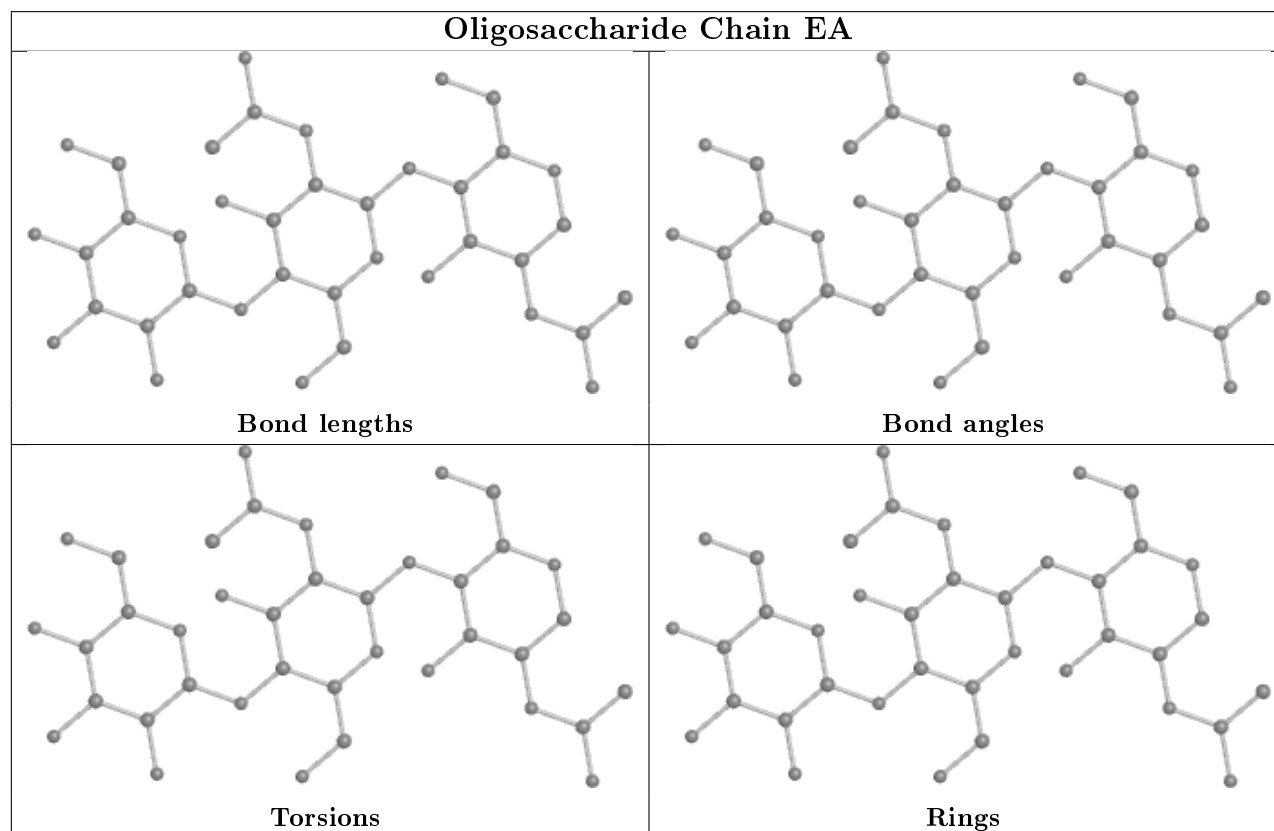
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | 7 | 2 | NAG | 6 | 0 |
| 6 | NA | 2 | NAG | 2 | 0 |
| 6 | 3 | 2 | NAG | 1 | 0 |
| 6 | CA | 2 | NAG | 3 | 0 |
| 4 | OA | 1 | NAG | 1 | 0 |
| 6 | GA | 1 | NAG | 7 | 0 |
| 4 | 6 | 1 | NAG | 1 | 0 |
| 6 | CA | 1 | NAG | 2 | 0 |
| 4 | 2 | 1 | NAG | 1 | 0 |
| 4 | 1 | 1 | NAG | 1 | 0 |
| 8 | 0 | 2 | NAG | 8 | 0 |
| 4 | 9 | 1 | NAG | 2 | 0 |
| 6 | 5 | 2 | NAG | 2 | 0 |
| 5 | KA | 1 | NAG | 1 | 0 |
| 6 | EA | 1 | NAG | 1 | 0 |
| 5 | FA | 2 | NAG | 1 | 0 |
| 6 | 5 | 1 | NAG | 1 | 0 |
| 6 | LA | 1 | NAG | 3 | 0 |
| 6 | 5 | 3 | BMA | 1 | 0 |
| 4 | JA | 1 | NAG | 2 | 0 |
| 4 | 7 | 1 | NAG | 6 | 0 |
| 5 | PA | 1 | NAG | 1 | 0 |
| 6 | DA | 1 | NAG | 2 | 0 |
| 6 | DA | 2 | NAG | 2 | 0 |
| 8 | 0 | 1 | NAG | 6 | 0 |
| 6 | LA | 2 | NAG | 5 | 0 |
| 4 | MA | 1 | NAG | 6 | 0 |
| 5 | PA | 2 | NAG | 1 | 0 |
| 6 | GA | 3 | BMA | 2 | 0 |
| 4 | OA | 2 | NAG | 1 | 0 |
| 6 | LA | 3 | BMA | 1 | 0 |
| 4 | JA | 2 | NAG | 1 | 0 |
| 4 | HA | 2 | NAG | 2 | 0 |

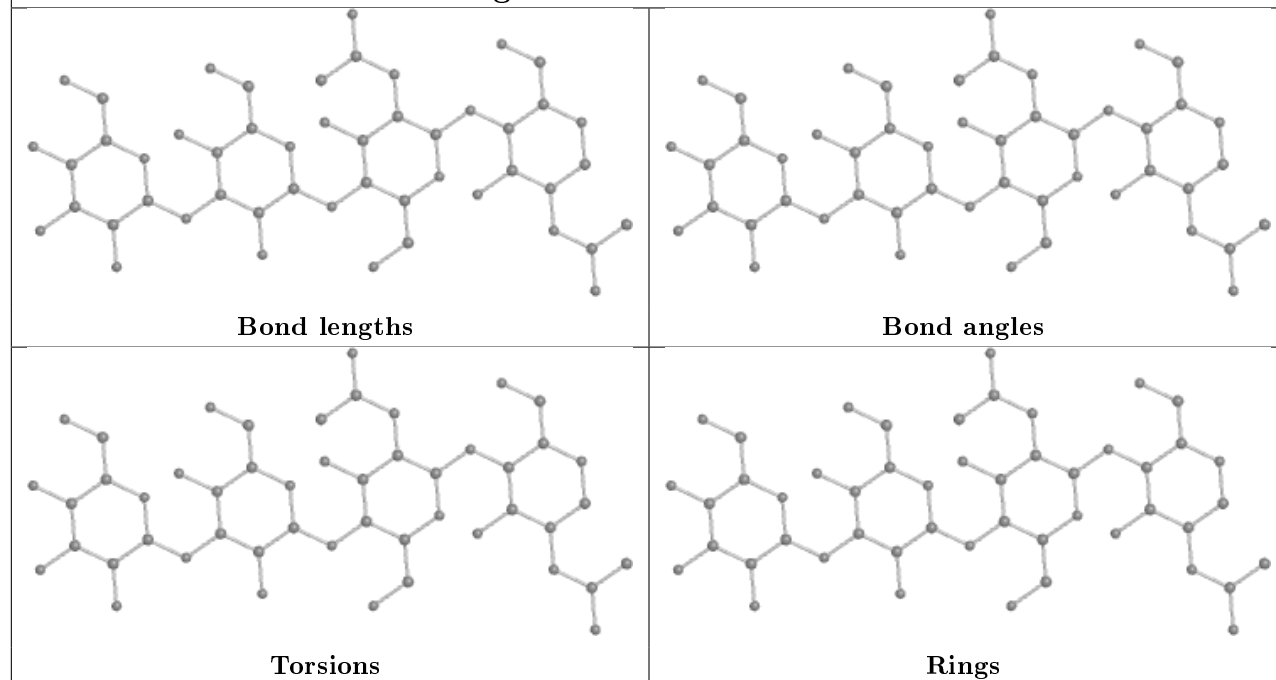
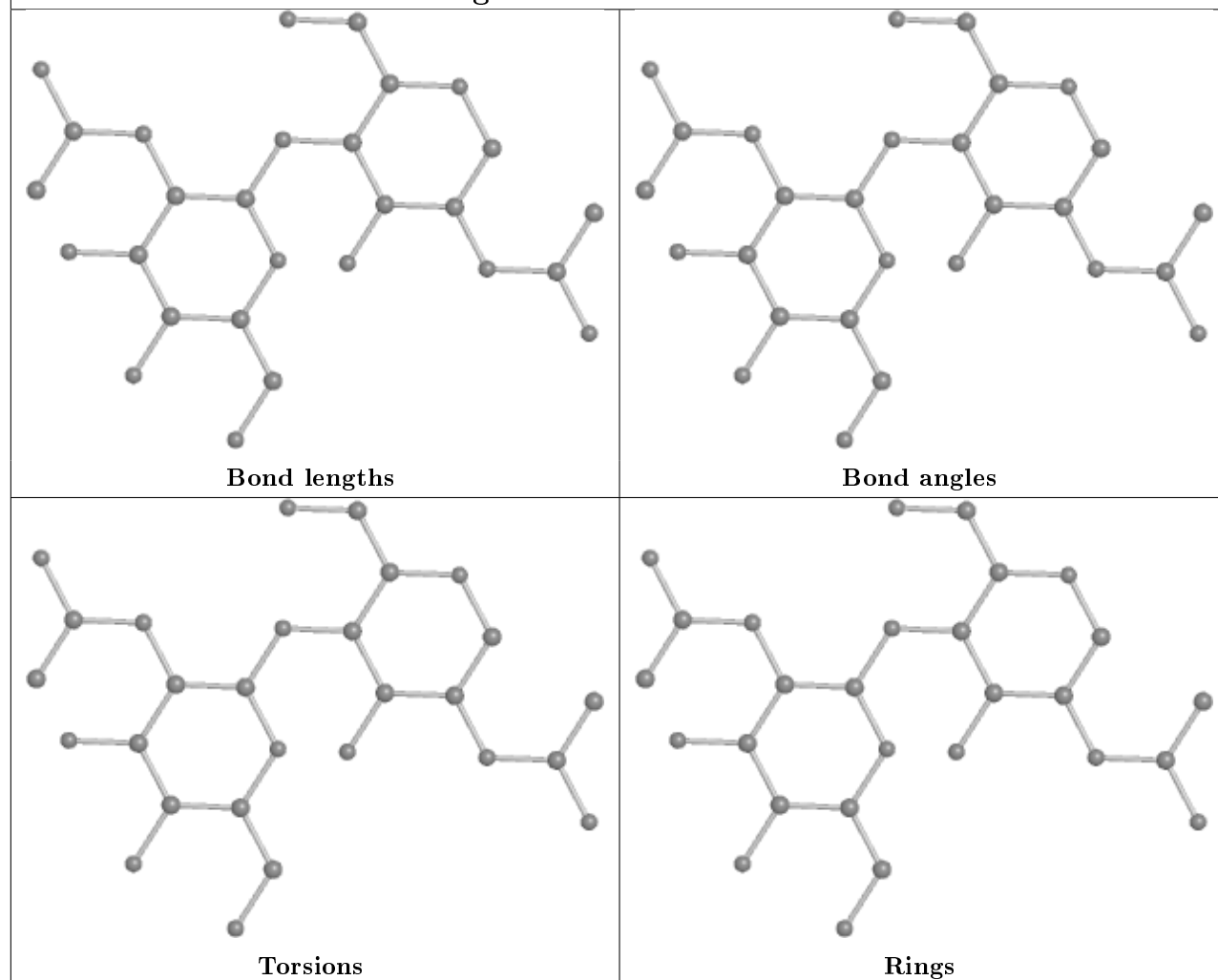
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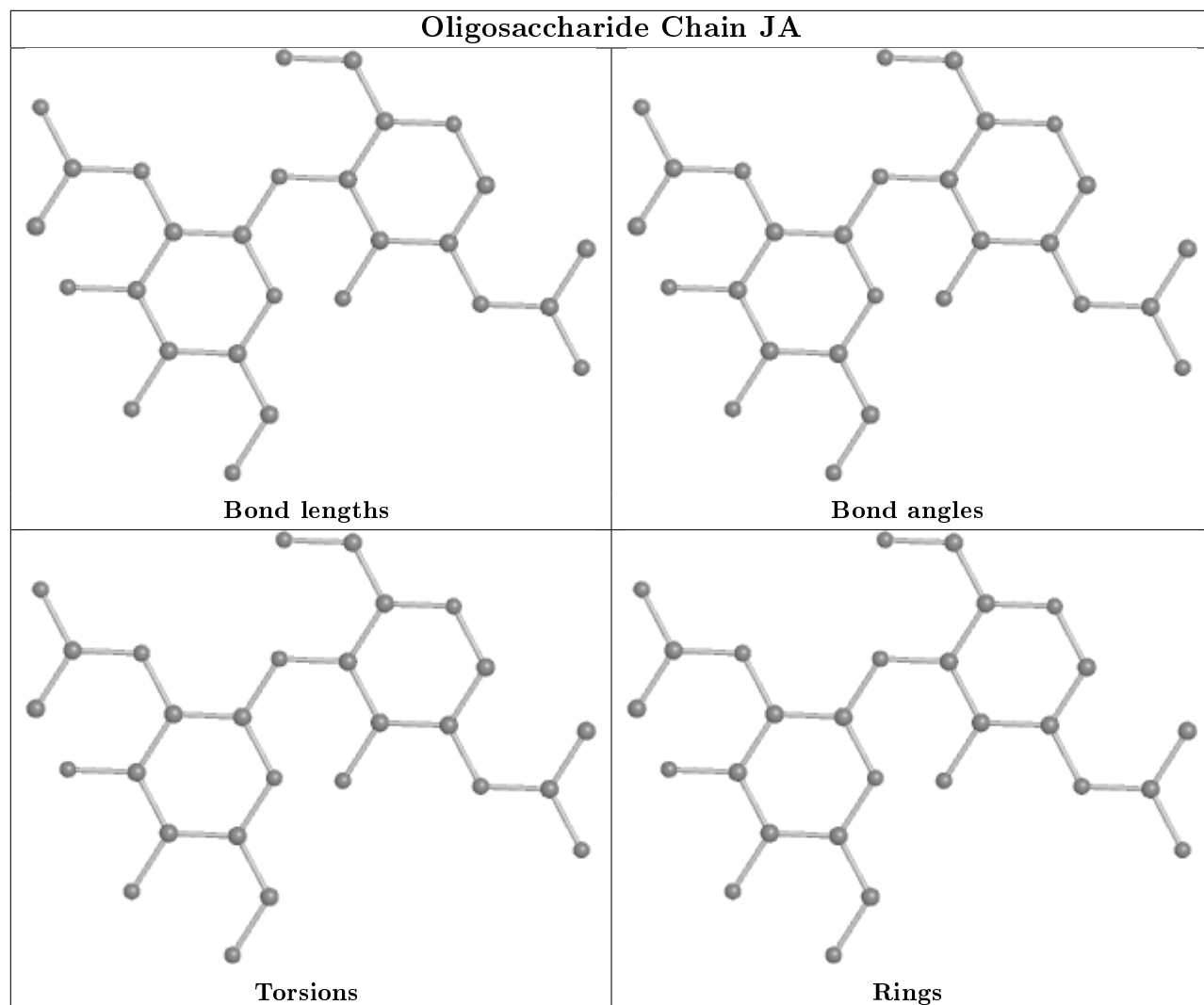
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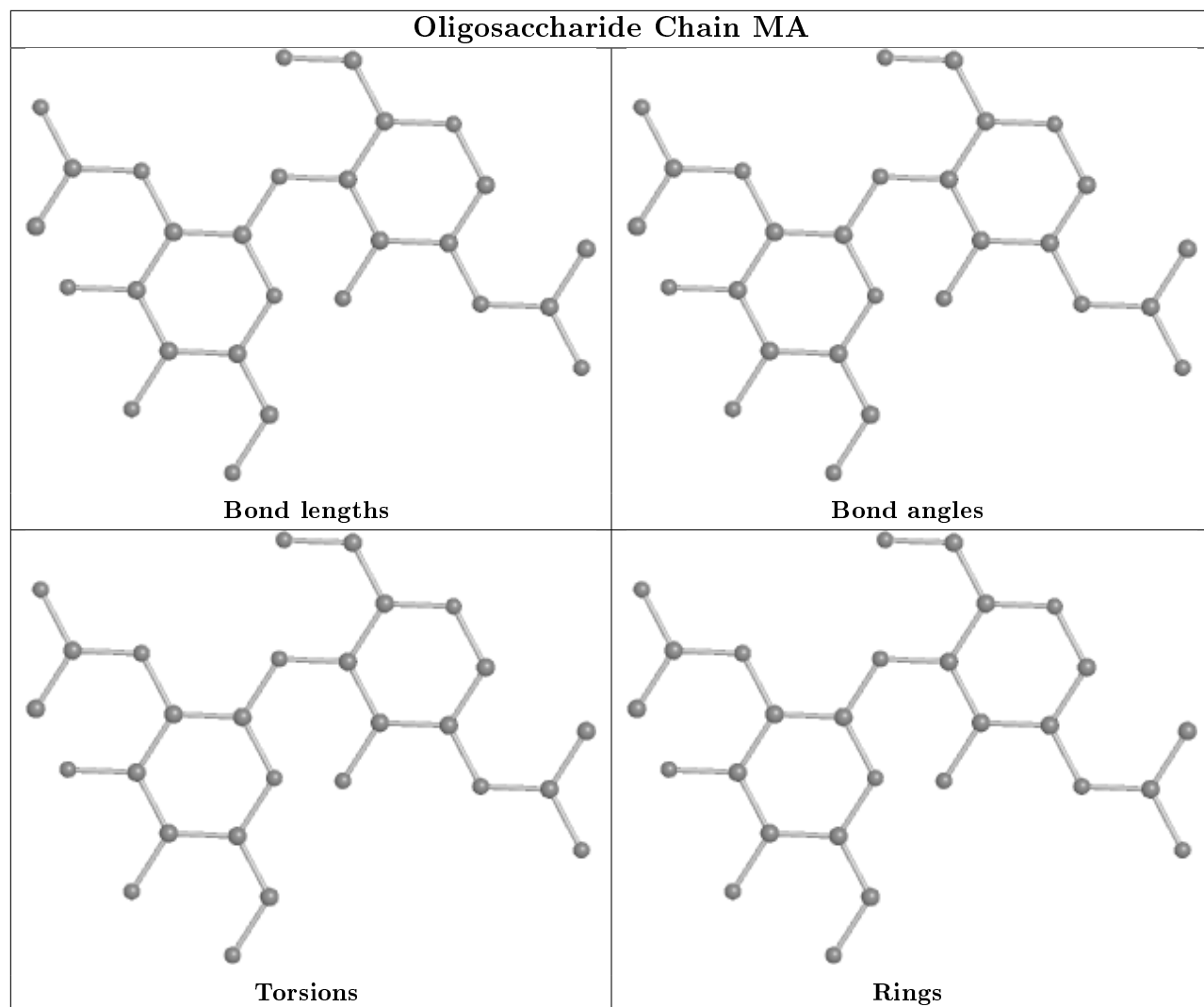
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 5 | FA | 3 | BMA | 1 | 0 |
| 4 | RA | 1 | NAG | 1 | 0 |
| 5 | AA | 1 | NAG | 1 | 0 |
| 4 | BA | 1 | NAG | 3 | 0 |
| 4 | BA | 2 | NAG | 3 | 0 |
| 6 | NA | 1 | NAG | 2 | 0 |
| 5 | FA | 1 | NAG | 1 | 0 |
| 6 | 3 | 1 | NAG | 3 | 0 |
| 4 | MA | 2 | NAG | 5 | 0 |
| 4 | RA | 2 | NAG | 1 | 0 |
| 8 | 0 | 3 | BMA | 1 | 0 |
| 6 | GA | 2 | NAG | 9 | 0 |
| 4 | 9 | 2 | NAG | 1 | 0 |
| 4 | HA | 1 | NAG | 4 | 0 |
| 5 | FA | 4 | MAN | 1 | 0 |

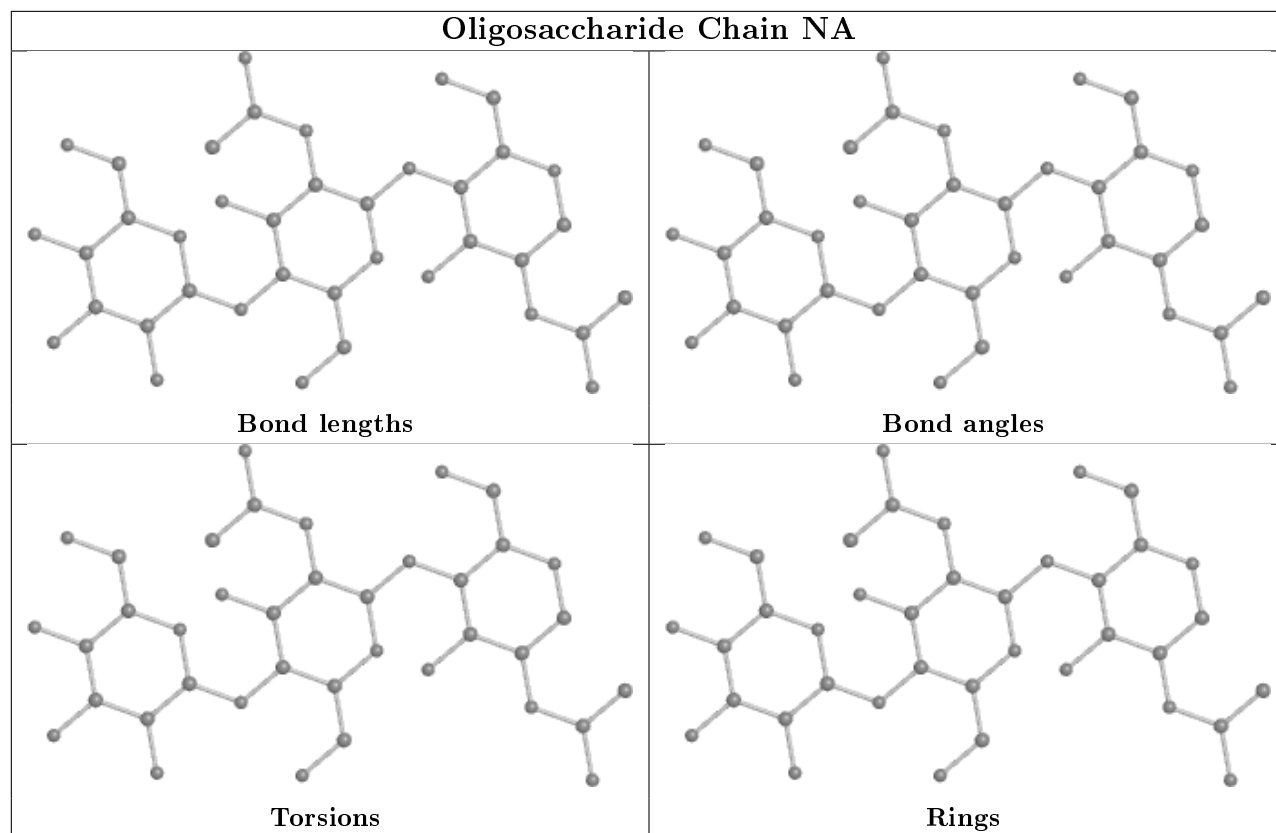
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

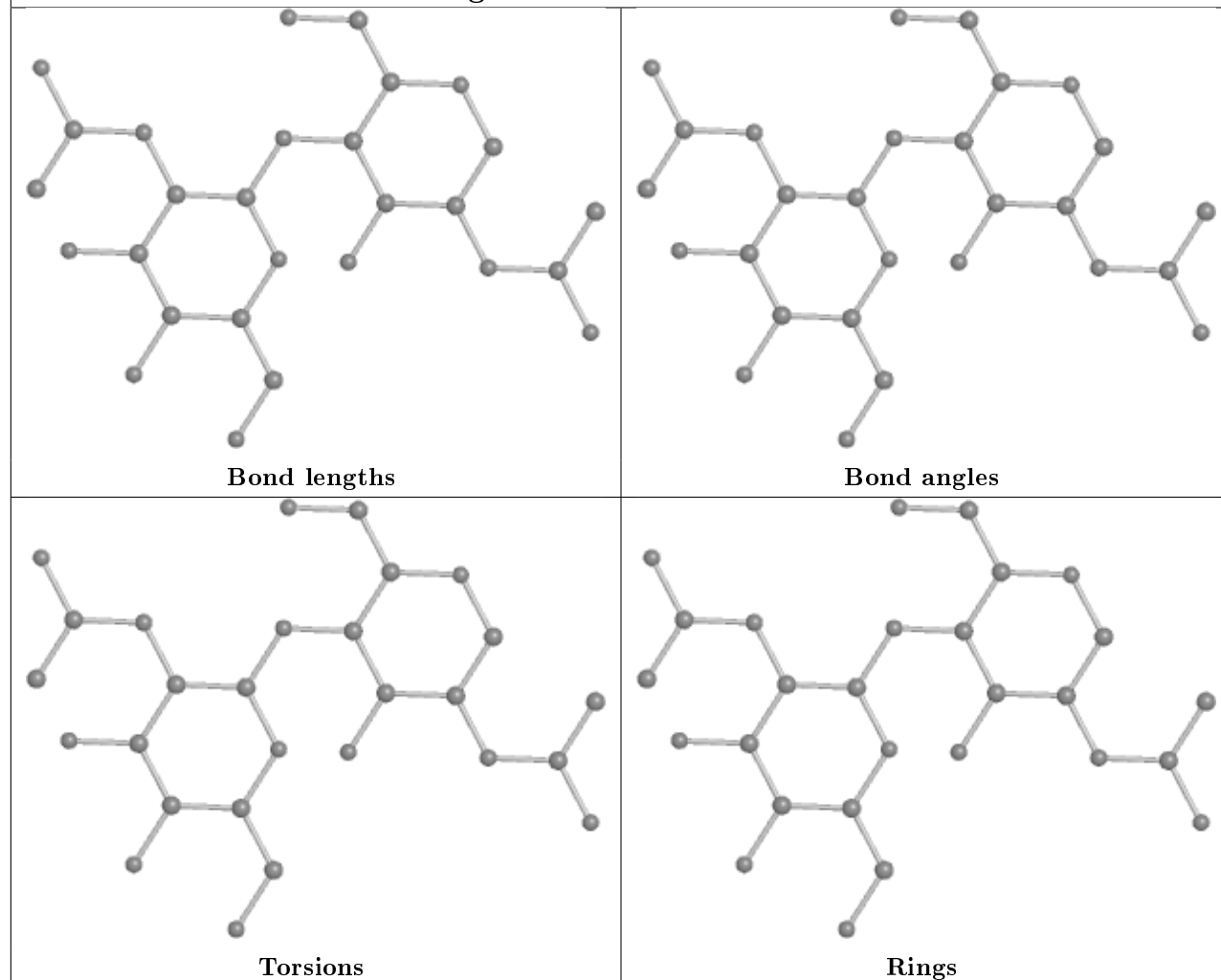
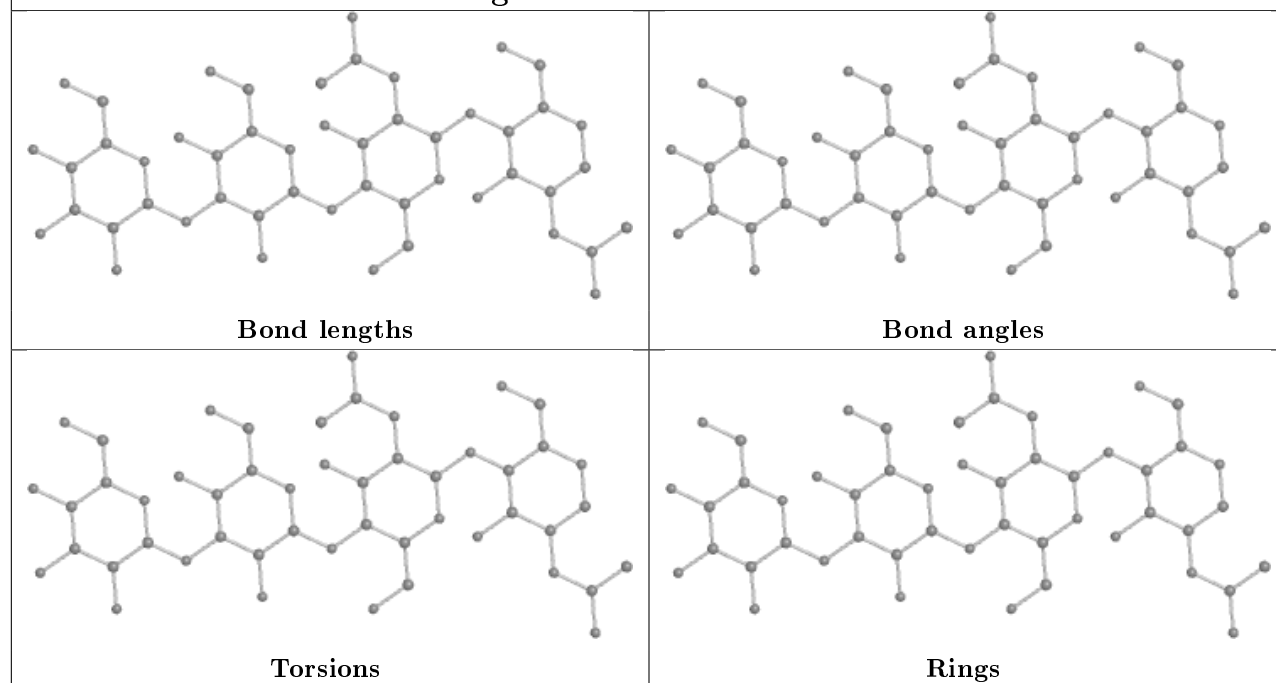


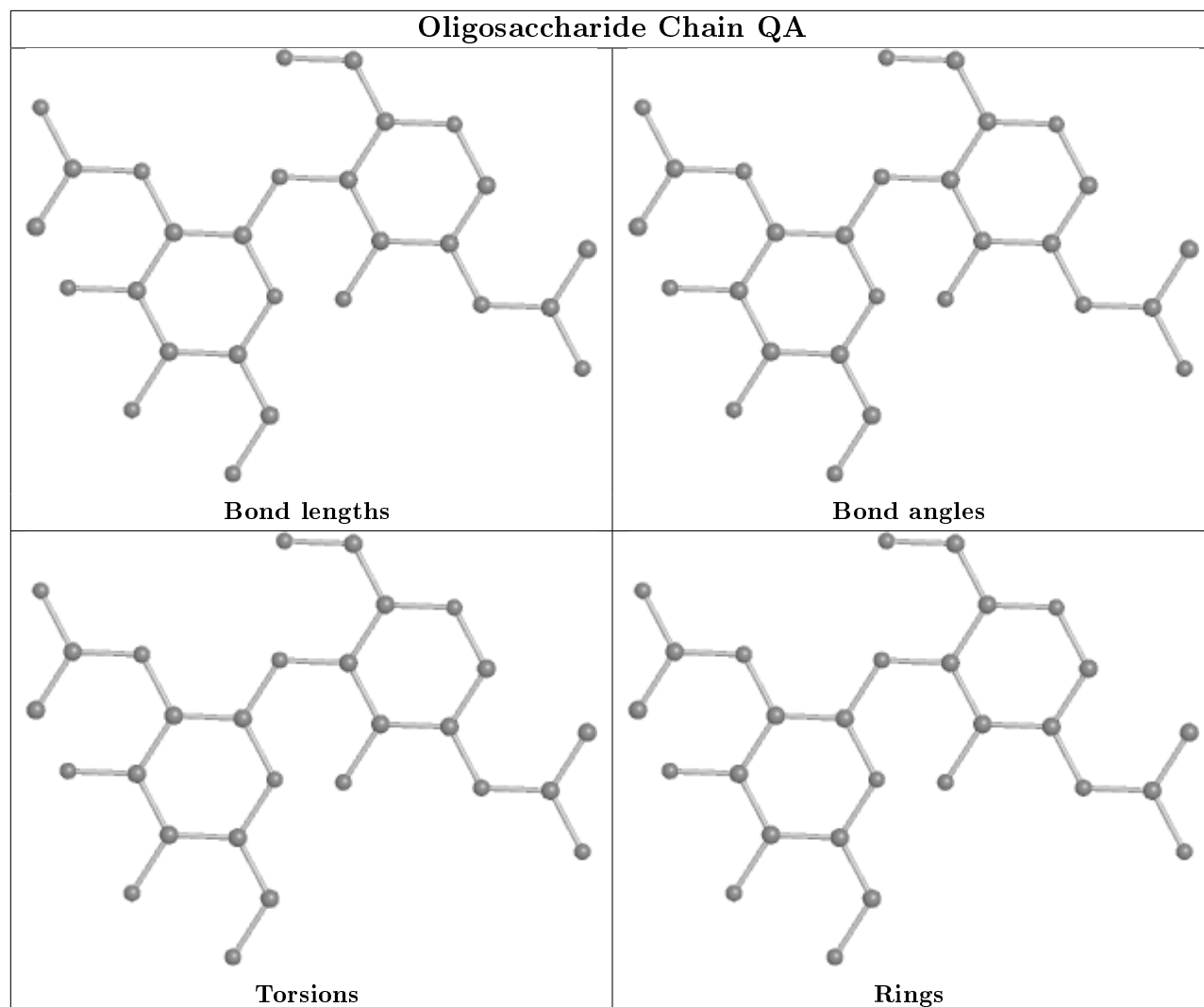
Oligosaccharide Chain FA**Oligosaccharide Chain IA**

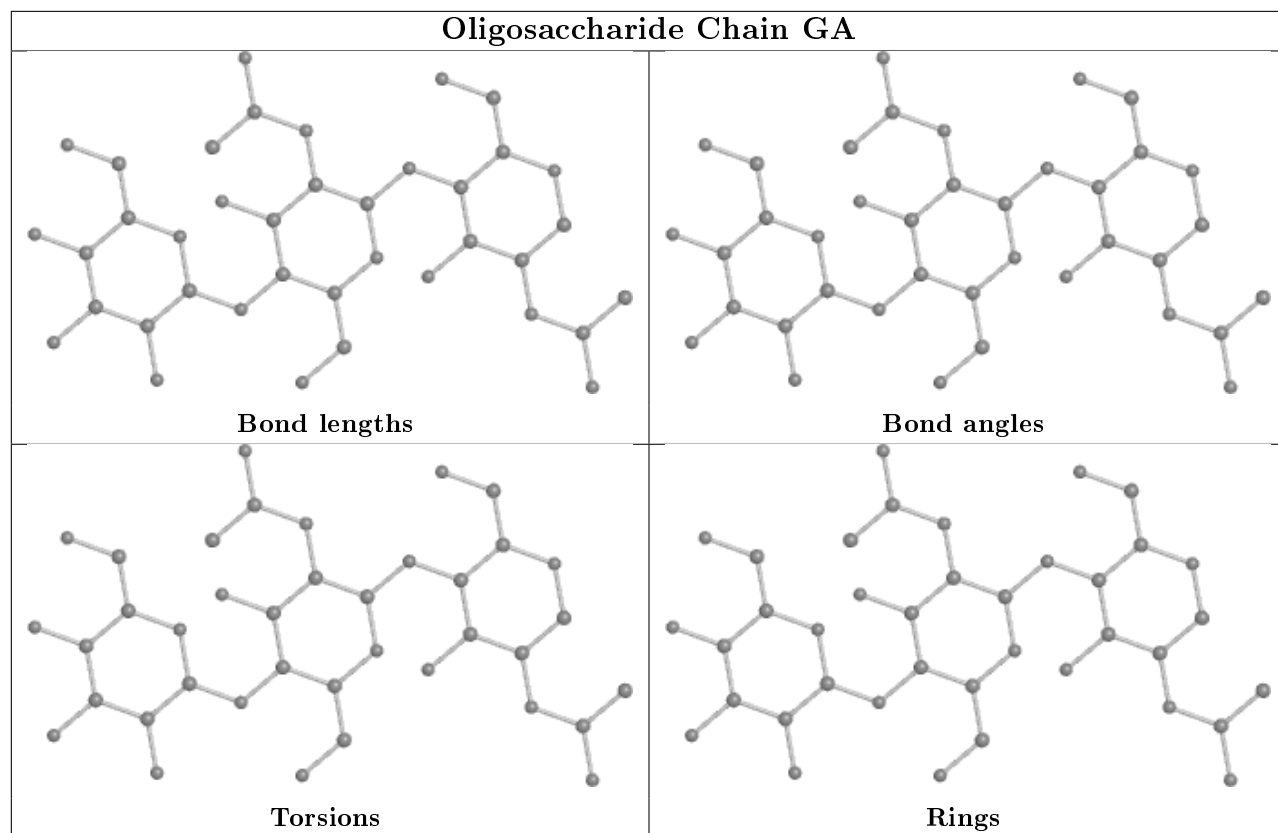
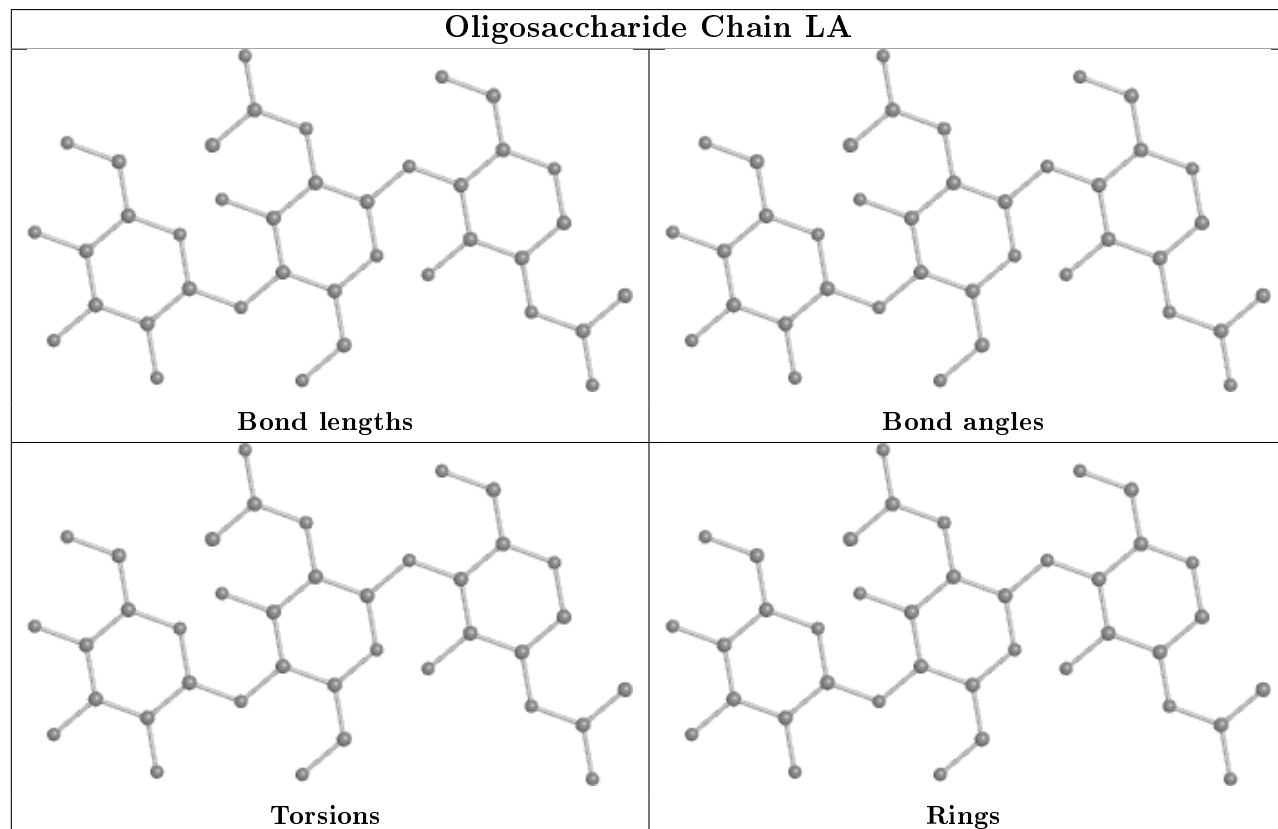
Oligosaccharide Chain JA

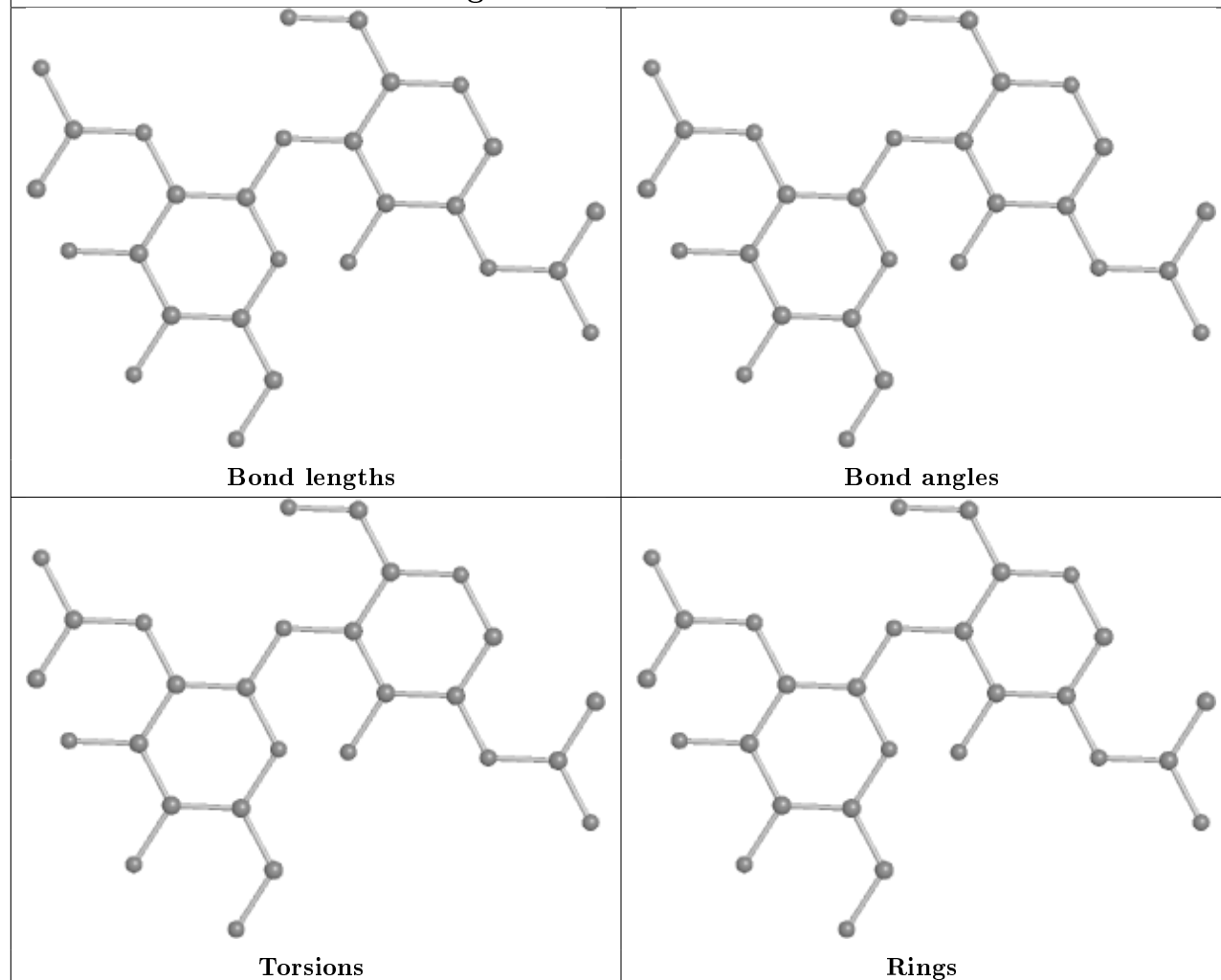
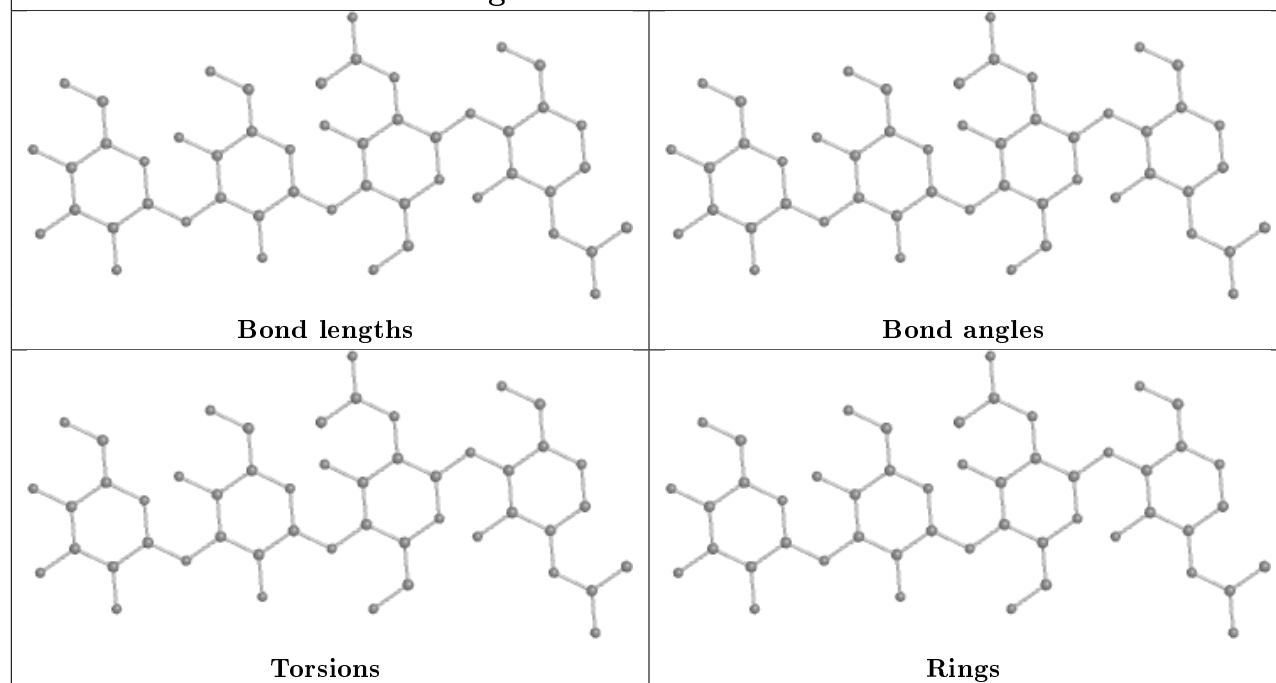


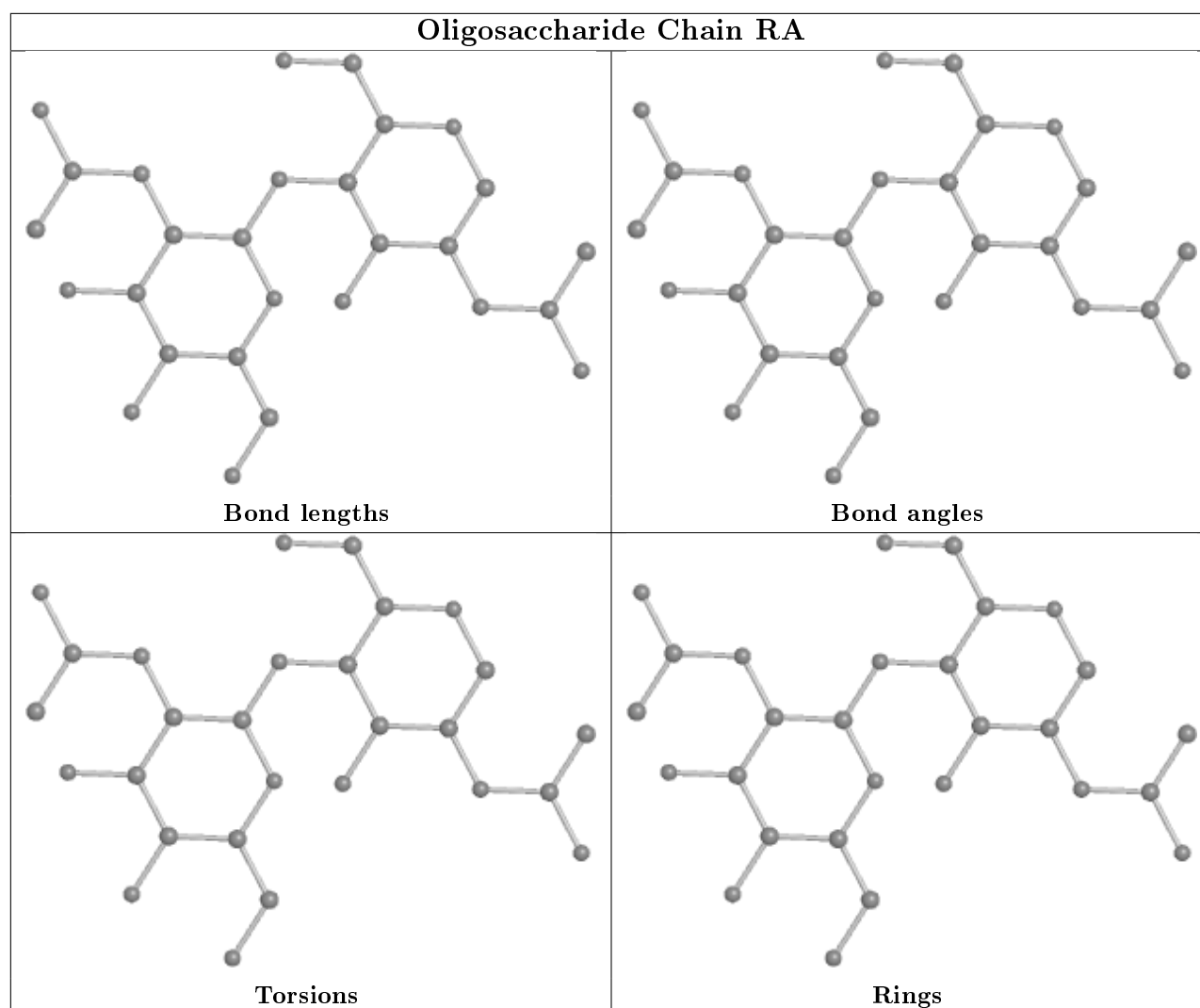


Oligosaccharide Chain OA**Oligosaccharide Chain PA**



Oligosaccharide Chain GA**Oligosaccharide Chain LA**

Oligosaccharide Chain HA**Oligosaccharide Chain KA**



5.6 Ligand geometry [i](#)

100 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|---------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 9 | CUO | U | 3401[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | T | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | S | 2105 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | I | 3401[B] | 3 | 0,4,4 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|---------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 9 | CUO | C | 3402[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | A | 5004 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | D | 5016[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Q | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | S | 2102 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | b | 2102 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | b | 2105 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | D | 5001 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | c | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | D | 5016[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | N | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | P | 5015[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | G | 2105 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | K | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | M | 2104 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | S | 2104 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | V | 5003 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | O | 3401[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | O | 3401[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | J | 5014[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | b | 2103 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Z | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | d | 3401[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | J | 5001 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | d | 3401[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | D | 5004 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | G | 2101[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | F | 3402[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | F | 3402[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | J | 5002 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | c | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Y | 2102 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | G | 2102 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | E | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | V | 5018[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | M | 2101[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | P | 5001 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | b | 2104 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Y | 2105 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | M | 2105 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | U | 3401[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | T | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | V | 5002 | 1 | 0,4,4 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|---------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 9 | CUO | I | 3401[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | C | 3402[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | J | 5003 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | D | 5003 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | C | 3401[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | E | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | S | 2103 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | C | 3401[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | M | 2102 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | J | 5004 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Y | 2103 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | P | 5004 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | b | 2101[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | D | 5002 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Q | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | b | 2101[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | G | 2104 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | G | 2103 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | P | 5015[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | W | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Y | 2101[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | J | 5014[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | S | 2101[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Z | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | A | 5016[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Y | 2101[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | F | 3401[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | F | 3401[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | K | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | N | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | I | 3402[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | A | 5016[D] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | B | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | S | 2101[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | I | 3402[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | G | 2101[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | A | 5002 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | M | 2103 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | P | 5003 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | B | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | Y | 2104 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | W | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | V | 5004 | 1 | 0,4,4 | 0.00 | - | - | | |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|---------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 9 | CUO | X | 3401[A] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | V | 5001 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | X | 3401[B] | 3 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | P | 5002 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | M | 2101[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | H | 3002 | 2 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | V | 5018[C] | - | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | A | 5003 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | A | 5001 | 1 | 0,4,4 | 0.00 | - | - | | |
| 9 | CUO | H | 3001 | 2 | 0,4,4 | 0.00 | - | - | | |

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 |
|-----|------|-------|---------|------|---------|----------|---------|
| 9 | CUO | U | 3401[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | T | 3001 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | S | 2105 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | I | 3401[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | C | 3402[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | A | 5004 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | D | 5016[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | Q | 3001 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | S | 2102 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | b | 2102 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | b | 2105 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | D | 5001 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | c | 3001 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | D | 5016[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | N | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | P | 5015[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | G | 2105 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | K | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | M | 2104 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | S | 2104 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | V | 5003 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | O | 3401[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | O | 3401[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | J | 5014[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | b | 2103 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | Z | 3001 | 2 | - | - | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|---------|------|---------|----------|---------|
| 9 | CUO | d | 3401[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | J | 5001 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | d | 3401[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | D | 5004 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | G | 2101[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | F | 3402[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | F | 3402[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | J | 5002 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | c | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | Y | 2102 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | G | 2102 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | E | 3001 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | V | 5018[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | M | 2101[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | P | 5001 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | b | 2104 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | Y | 2105 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | M | 2105 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | U | 3401[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | T | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | V | 5002 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | I | 3401[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | C | 3402[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | J | 5003 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | D | 5003 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | C | 3401[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | E | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | S | 2103 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | C | 3401[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | M | 2102 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | J | 5004 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | Y | 2103 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | P | 5004 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | b | 2101[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | D | 5002 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | Q | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | b | 2101[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | G | 2104 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | G | 2103 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | P | 5015[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | W | 3001 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | Y | 2101[C] | - | - | - | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|---------|------|---------|----------|---------|
| 9 | CUO | J | 5014[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | S | 2101[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | Z | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | A | 5016[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | Y | 2101[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | F | 3401[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | F | 3401[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | K | 3001 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | N | 3001 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | I | 3402[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | A | 5016[D] | - | - | - | 0/1/1/1 |
| 9 | CUO | B | 3001 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | S | 2101[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | I | 3402[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | G | 2101[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | A | 5002 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | M | 2103 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | P | 5003 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | B | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | Y | 2104 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | W | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | V | 5004 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | X | 3401[A] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | V | 5001 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | X | 3401[B] | 3 | - | - | 0/1/1/1 |
| 9 | CUO | P | 5002 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | M | 2101[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | H | 3002 | 2 | - | - | 0/1/1/1 |
| 9 | CUO | V | 5018[C] | - | - | - | 0/1/1/1 |
| 9 | CUO | A | 5003 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | A | 5001 | 1 | - | - | 0/1/1/1 |
| 9 | CUO | H | 3001 | 2 | - | - | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 83 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|---------|------|---------|--------------|
| 9 | U | 3401[B] | CUO | 5 | 0 |
| 9 | I | 3401[B] | CUO | 1 | 0 |
| 9 | C | 3402[B] | CUO | 2 | 0 |
| 9 | S | 2102 | CUO | 1 | 0 |
| 9 | D | 5001 | CUO | 1 | 0 |
| 9 | M | 2104 | CUO | 1 | 0 |
| 9 | S | 2104 | CUO | 2 | 0 |
| 9 | V | 5003 | CUO | 1 | 0 |
| 9 | O | 3401[B] | CUO | 5 | 0 |
| 9 | O | 3401[A] | CUO | 5 | 0 |
| 9 | J | 5001 | CUO | 1 | 0 |
| 9 | D | 5004 | CUO | 1 | 0 |
| 9 | F | 3402[A] | CUO | 5 | 0 |
| 9 | J | 5002 | CUO | 1 | 0 |
| 9 | Y | 2102 | CUO | 1 | 0 |
| 9 | Y | 2105 | CUO | 1 | 0 |
| 9 | M | 2105 | CUO | 2 | 0 |
| 9 | U | 3401[A] | CUO | 5 | 0 |
| 9 | T | 3002 | CUO | 1 | 0 |
| 9 | I | 3401[A] | CUO | 5 | 0 |
| 9 | C | 3402[A] | CUO | 5 | 0 |
| 9 | C | 3401[B] | CUO | 2 | 0 |
| 9 | C | 3401[A] | CUO | 5 | 0 |
| 9 | G | 2104 | CUO | 1 | 0 |
| 9 | F | 3401[B] | CUO | 2 | 0 |
| 9 | I | 3402[B] | CUO | 1 | 0 |
| 9 | I | 3402[A] | CUO | 5 | 0 |
| 9 | Y | 2104 | CUO | 1 | 0 |
| 9 | W | 3002 | CUO | 1 | 0 |
| 9 | V | 5004 | CUO | 1 | 0 |
| 9 | X | 3401[A] | CUO | 5 | 0 |
| 9 | X | 3401[B] | CUO | 5 | 0 |
| 9 | A | 5001 | CUO | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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 | 1656/2000 (82%) | -0.30 | 28 (1%) 70 41 | 36, 70, 118, 164 | 0 |
| 1 | D | 1656/2000 (82%) | -0.30 | 34 (2%) 63 34 | 37, 67, 114, 176 | 0 |
| 1 | G | 1656/2000 (82%) | -0.33 | 24 (1%) 75 49 | 31, 68, 109, 152 | 0 |
| 1 | J | 1656/2000 (82%) | -0.30 | 31 (1%) 66 37 | 30, 64, 119, 162 | 0 |
| 1 | M | 1656/2000 (82%) | -0.40 | 21 (1%) 77 51 | 29, 56, 109, 157 | 0 |
| 1 | P | 1656/2000 (82%) | -0.44 | 19 (1%) 80 56 | 27, 53, 97, 176 | 0 |
| 1 | S | 1656/2000 (82%) | -0.40 | 32 (1%) 66 37 | 31, 60, 108, 164 | 0 |
| 1 | V | 1656/2000 (82%) | -0.46 | 15 (0%) 84 63 | 26, 55, 105, 154 | 0 |
| 1 | Y | 1656/2000 (82%) | -0.36 | 17 (1%) 82 59 | 31, 66, 112, 160 | 0 |
| 1 | b | 1656/2000 (82%) | -0.41 | 17 (1%) 82 59 | 30, 60, 105, 161 | 0 |
| 2 | B | 825/920 (89%) | -0.52 | 4 (0%) 91 75 | 32, 57, 101, 140 | 0 |
| 2 | E | 825/920 (89%) | -0.48 | 8 (0%) 82 59 | 30, 59, 106, 137 | 0 |
| 2 | H | 825/920 (89%) | -0.42 | 10 (1%) 79 54 | 31, 63, 112, 147 | 0 |
| 2 | K | 825/920 (89%) | -0.43 | 6 (0%) 87 69 | 34, 60, 101, 158 | 0 |
| 2 | N | 825/920 (89%) | -0.54 | 5 (0%) 89 72 | 21, 46, 92, 135 | 0 |
| 2 | Q | 825/920 (89%) | -0.54 | 3 (0%) 92 79 | 26, 49, 100, 134 | 0 |
| 2 | T | 825/920 (89%) | -0.51 | 3 (0%) 92 79 | 30, 53, 93, 137 | 0 |
| 2 | W | 825/920 (89%) | -0.54 | 2 (0%) 95 87 | 25, 53, 99, 129 | 0 |
| 2 | Z | 825/920 (89%) | -0.51 | 5 (0%) 89 72 | 25, 52, 95, 130 | 0 |
| 2 | c | 825/920 (89%) | -0.52 | 6 (0%) 87 69 | 26, 55, 103, 135 | 0 |
| 3 | C | 366/394 (92%) | 2.76 | 232 (63%) 0 0 | 68, 90, 99, 110 | 0 |
| 3 | F | 366/394 (92%) | 2.44 | 196 (53%) 0 0 | 56, 78, 88, 107 | 0 |
| 3 | I | 366/394 (92%) | 2.52 | 204 (55%) 0 0 | 57, 79, 91, 111 | 0 |
| 3 | L | 366/394 (92%) | 2.61 | 215 (58%) 0 0 | 64, 89, 99, 106 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å ²) | Q<0.9 |
|-----|-------|-------------------|--------|-----------|---|---|-----------------------|-------|
| 3 | O | 366/394 (92%) | 2.37 | 192 (52%) | 0 | 0 | 52, 75, 95, 107 | 0 |
| 3 | R | 366/394 (92%) | 2.52 | 215 (58%) | 0 | 0 | 59, 79, 90, 109 | 0 |
| 3 | U | 366/394 (92%) | 2.28 | 171 (46%) | 0 | 0 | 52, 74, 93, 103 | 0 |
| 3 | X | 366/394 (92%) | 4.89 | 344 (93%) | 0 | 0 | 79, 102, 111, 116 | 0 |
| 3 | a | 366/394 (92%) | 2.40 | 190 (51%) | 0 | 0 | 54, 76, 88, 96 | 0 |
| 3 | d | 366/394 (92%) | 4.59 | 331 (90%) | 0 | 0 | 81, 99, 107, 111 | 0 |
| All | All | 28470/33140 (85%) | 0.02 | 2580 (9%) | 9 | 3 | 21, 63, 107, 176 | 0 |

The worst 5 of 2580 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|---------|------|------|
| 3 | d | 2977[A] | CYS | 16.0 |
| 3 | d | 3101[A] | PRO | 15.1 |
| 3 | X | 2979[A] | GLN | 14.3 |
| 3 | a | 3062[A] | GLN | 13.4 |
| 3 | O | 3062[A] | GLN | 12.9 |

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

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

6.3 Carbohydrates ⓘ

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 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 6 | BMA | CA | 3 | 11/12 | 0.39 | 0.29 | 96,123,130,130 | 0 |
| 5 | BMA | FA | 3 | 11/12 | 0.58 | 0.23 | 85,101,110,113 | 0 |
| 7 | BMA | z | 3 | 11/12 | 0.59 | 0.40 | 124,134,140,150 | 0 |
| 7 | MAN | z | 4 | 11/12 | 0.60 | 0.44 | 135,140,150,154 | 0 |
| 4 | NAG | x | 2 | 14/15 | 0.62 | 0.23 | 104,115,125,125 | 0 |
| 7 | MAN | z | 5 | 11/12 | 0.63 | 0.36 | 121,135,151,154 | 0 |
| 6 | BMA | GA | 3 | 11/12 | 0.64 | 0.29 | 130,136,142,143 | 0 |
| 4 | NAG | 4 | 2 | 14/15 | 0.66 | 0.32 | 78,96,107,116 | 0 |
| 6 | BMA | 5 | 3 | 11/12 | 0.68 | 0.19 | 98,114,124,127 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 5 | MAN | g | 4 | 11/12 | 0.70 | 0.20 | 103,117,133,133 | 0 |
| 5 | MAN | KA | 4 | 11/12 | 0.70 | 0.32 | 87,103,122,135 | 0 |
| 6 | BMA | LA | 3 | 11/12 | 0.70 | 0.25 | 101,110,119,119 | 0 |
| 8 | BMA | 0 | 3 | 11/12 | 0.71 | 0.25 | 97,112,128,130 | 0 |
| 6 | BMA | h | 3 | 11/12 | 0.72 | 0.31 | 108,114,120,126 | 0 |
| 5 | MAN | l | 4 | 11/12 | 0.72 | 0.21 | 114,118,122,128 | 0 |
| 5 | MAN | FA | 4 | 11/12 | 0.72 | 0.31 | 94,107,126,132 | 0 |
| 4 | NAG | s | 2 | 14/15 | 0.73 | 0.36 | 89,102,108,116 | 0 |
| 4 | NAG | 7 | 2 | 14/15 | 0.74 | 0.32 | 69,83,101,104 | 0 |
| 6 | BMA | EA | 3 | 11/12 | 0.74 | 0.35 | 104,115,132,134 | 0 |
| 6 | BMA | NA | 3 | 11/12 | 0.74 | 0.49 | 102,117,134,138 | 0 |
| 5 | BMA | l | 3 | 11/12 | 0.75 | 0.26 | 98,113,119,128 | 0 |
| 6 | BMA | y | 3 | 11/12 | 0.76 | 0.30 | 102,116,123,123 | 0 |
| 4 | NAG | t | 2 | 14/15 | 0.76 | 0.25 | 50,90,102,103 | 0 |
| 6 | BMA | 3 | 3 | 11/12 | 0.76 | 0.18 | 114,119,149,149 | 0 |
| 4 | NAG | 1 | 2 | 14/15 | 0.76 | 0.26 | 91,104,121,126 | 0 |
| 6 | BMA | r | 3 | 11/12 | 0.77 | 0.28 | 111,120,128,129 | 0 |
| 8 | MAN | 0 | 4 | 11/12 | 0.78 | 0.20 | 94,114,123,126 | 0 |
| 4 | NAG | BA | 2 | 14/15 | 0.79 | 0.19 | 62,82,95,101 | 0 |
| 5 | NAG | g | 2 | 14/15 | 0.80 | 0.29 | 99,105,109,109 | 0 |
| 6 | NAG | w | 2 | 14/15 | 0.80 | 0.19 | 88,104,108,111 | 0 |
| 6 | BMA | k | 3 | 11/12 | 0.81 | 0.23 | 110,119,126,133 | 0 |
| 7 | NAG | z | 2 | 14/15 | 0.81 | 0.29 | 92,105,121,128 | 0 |
| 4 | NAG | QA | 2 | 14/15 | 0.81 | 0.16 | 97,115,121,125 | 0 |
| 6 | NAG | LA | 1 | 14/15 | 0.81 | 0.21 | 78,87,93,98 | 0 |
| 4 | NAG | f | 2 | 14/15 | 0.81 | 0.27 | 106,116,123,129 | 0 |
| 6 | NAG | DA | 2 | 14/15 | 0.81 | 0.26 | 78,91,95,98 | 0 |
| 4 | NAG | m | 1 | 14/15 | 0.81 | 0.19 | 77,91,99,104 | 0 |
| 4 | NAG | n | 2 | 14/15 | 0.82 | 0.28 | 72,91,105,110 | 0 |
| 5 | NAG | FA | 2 | 14/15 | 0.82 | 0.20 | 74,88,101,105 | 0 |
| 6 | NAG | CA | 2 | 14/15 | 0.82 | 0.30 | 88,97,115,124 | 0 |
| 5 | NAG | l | 2 | 14/15 | 0.82 | 0.21 | 69,84,96,97 | 0 |
| 5 | MAN | PA | 4 | 11/12 | 0.82 | 0.15 | 107,112,125,133 | 0 |
| 5 | MAN | AA | 4 | 11/12 | 0.83 | 0.18 | 114,125,132,145 | 0 |
| 4 | NAG | e | 2 | 14/15 | 0.83 | 0.23 | 69,83,96,102 | 0 |
| 4 | NAG | QA | 1 | 14/15 | 0.83 | 0.22 | 97,107,114,118 | 0 |
| 6 | BMA | w | 3 | 11/12 | 0.83 | 0.30 | 107,110,117,128 | 0 |
| 4 | NAG | 9 | 2 | 14/15 | 0.83 | 0.25 | 73,97,113,113 | 0 |
| 4 | NAG | u | 2 | 14/15 | 0.84 | 0.22 | 86,100,114,132 | 0 |
| 6 | NAG | w | 1 | 14/15 | 0.84 | 0.21 | 78,100,106,118 | 0 |
| 6 | NAG | GA | 2 | 14/15 | 0.84 | 0.17 | 88,108,127,131 | 0 |
| 6 | NAG | h | 2 | 14/15 | 0.84 | 0.15 | 84,94,107,114 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 6 | NAG | 5 | 2 | 14/15 | 0.84 | 0.17 | 61,77,95,103 | 0 |
| 6 | NAG | EA | 2 | 14/15 | 0.84 | 0.20 | 70,82,98,108 | 0 |
| 4 | NAG | x | 1 | 14/15 | 0.84 | 0.15 | 80,94,105,105 | 0 |
| 4 | NAG | i | 2 | 14/15 | 0.84 | 0.26 | 84,92,107,111 | 0 |
| 4 | NAG | MA | 2 | 14/15 | 0.84 | 0.19 | 84,93,116,127 | 0 |
| 4 | NAG | v | 2 | 14/15 | 0.85 | 0.19 | 82,97,104,106 | 0 |
| 4 | NAG | 1 | 1 | 14/15 | 0.85 | 0.19 | 88,96,102,103 | 0 |
| 5 | NAG | KA | 2 | 14/15 | 0.85 | 0.19 | 67,81,92,93 | 0 |
| 4 | NAG | 8 | 2 | 14/15 | 0.85 | 0.19 | 64,84,98,101 | 0 |
| 5 | BMA | KA | 3 | 11/12 | 0.85 | 0.26 | 79,99,114,127 | 0 |
| 6 | BMA | DA | 3 | 11/12 | 0.85 | 0.24 | 82,103,108,108 | 0 |
| 7 | NAG | z | 1 | 14/15 | 0.86 | 0.16 | 79,85,93,96 | 0 |
| 5 | BMA | PA | 3 | 11/12 | 0.86 | 0.17 | 96,97,104,125 | 0 |
| 8 | NAG | 0 | 2 | 14/15 | 0.86 | 0.16 | 58,78,82,90 | 0 |
| 6 | NAG | 3 | 1 | 14/15 | 0.86 | 0.19 | 46,67,81,90 | 0 |
| 4 | NAG | o | 1 | 14/15 | 0.86 | 0.22 | 61,73,85,88 | 0 |
| 5 | NAG | PA | 2 | 14/15 | 0.86 | 0.15 | 72,80,89,91 | 0 |
| 4 | NAG | JA | 2 | 14/15 | 0.86 | 0.21 | 82,92,100,100 | 0 |
| 4 | NAG | m | 2 | 14/15 | 0.86 | 0.23 | 80,95,108,108 | 0 |
| 5 | BMA | AA | 3 | 11/12 | 0.87 | 0.14 | 112,120,124,127 | 0 |
| 4 | NAG | p | 2 | 14/15 | 0.87 | 0.14 | 54,72,84,88 | 0 |
| 6 | NAG | r | 1 | 14/15 | 0.87 | 0.25 | 79,88,107,112 | 0 |
| 5 | BMA | g | 3 | 11/12 | 0.88 | 0.17 | 110,124,133,139 | 0 |
| 6 | NAG | CA | 1 | 14/15 | 0.88 | 0.17 | 59,71,83,91 | 0 |
| 6 | NAG | k | 1 | 14/15 | 0.88 | 0.15 | 71,83,92,99 | 0 |
| 4 | NAG | IA | 2 | 14/15 | 0.88 | 0.15 | 75,89,96,100 | 0 |
| 4 | NAG | 6 | 2 | 14/15 | 0.88 | 0.21 | 49,73,85,91 | 0 |
| 4 | NAG | HA | 2 | 14/15 | 0.88 | 0.20 | 71,82,95,107 | 0 |
| 4 | NAG | JA | 1 | 14/15 | 0.88 | 0.19 | 70,80,88,90 | 0 |
| 5 | NAG | g | 1 | 14/15 | 0.88 | 0.18 | 57,79,95,97 | 0 |
| 4 | NAG | 6 | 1 | 14/15 | 0.89 | 0.19 | 74,81,89,91 | 0 |
| 4 | NAG | i | 1 | 14/15 | 0.89 | 0.19 | 59,68,91,95 | 0 |
| 6 | NAG | 3 | 2 | 14/15 | 0.89 | 0.17 | 61,82,96,102 | 0 |
| 4 | NAG | t | 1 | 14/15 | 0.89 | 0.15 | 53,69,82,85 | 0 |
| 6 | NAG | GA | 1 | 14/15 | 0.89 | 0.28 | 79,97,106,109 | 0 |
| 6 | NAG | h | 1 | 14/15 | 0.89 | 0.14 | 85,93,112,115 | 0 |
| 6 | NAG | LA | 2 | 14/15 | 0.90 | 0.14 | 76,89,100,104 | 0 |
| 4 | NAG | p | 1 | 14/15 | 0.90 | 0.14 | 47,61,75,75 | 0 |
| 4 | NAG | e | 1 | 14/15 | 0.90 | 0.11 | 62,79,86,94 | 0 |
| 4 | NAG | 9 | 1 | 14/15 | 0.90 | 0.15 | 87,95,100,108 | 0 |
| 4 | NAG | RA | 1 | 14/15 | 0.90 | 0.21 | 75,83,99,108 | 0 |
| 5 | NAG | AA | 2 | 14/15 | 0.90 | 0.17 | 87,92,98,104 | 0 |

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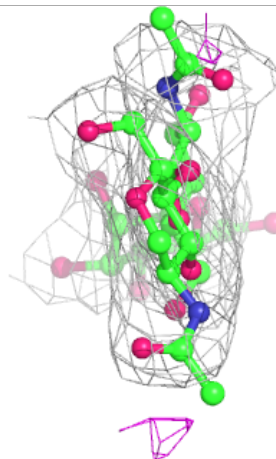
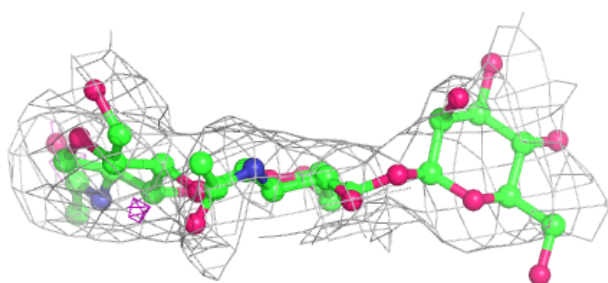
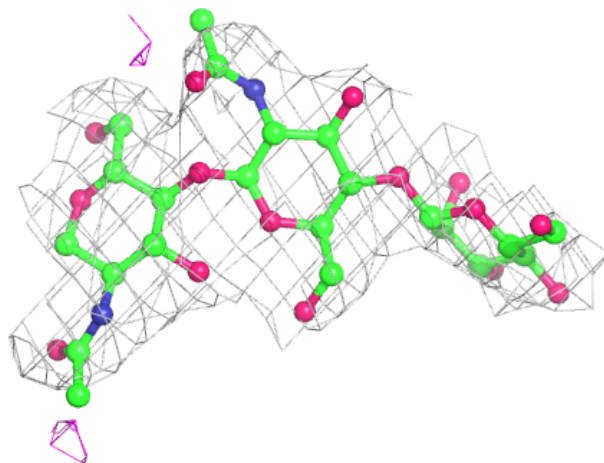
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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 4 | NAG | o | 2 | 14/15 | 0.90 | 0.20 | 43,67,86,87 | 0 |
| 4 | NAG | u | 1 | 14/15 | 0.90 | 0.22 | 73,78,87,92 | 0 |
| 4 | NAG | 2 | 1 | 14/15 | 0.90 | 0.14 | 41,56,75,80 | 0 |
| 4 | NAG | HA | 1 | 14/15 | 0.90 | 0.15 | 56,63,83,93 | 0 |
| 4 | NAG | 8 | 1 | 14/15 | 0.90 | 0.16 | 57,62,72,81 | 0 |
| 4 | NAG | v | 1 | 14/15 | 0.91 | 0.19 | 64,80,91,91 | 0 |
| 6 | NAG | NA | 2 | 14/15 | 0.91 | 0.23 | 61,80,101,112 | 0 |
| 4 | NAG | f | 1 | 14/15 | 0.91 | 0.13 | 88,95,105,109 | 0 |
| 5 | NAG | PA | 1 | 14/15 | 0.91 | 0.19 | 62,72,77,78 | 0 |
| 6 | NAG | r | 2 | 14/15 | 0.91 | 0.13 | 84,91,98,102 | 0 |
| 4 | NAG | IA | 1 | 14/15 | 0.91 | 0.15 | 51,66,83,92 | 0 |
| 8 | NAG | 0 | 1 | 14/15 | 0.91 | 0.19 | 60,67,72,81 | 0 |
| 6 | NAG | k | 2 | 14/15 | 0.91 | 0.14 | 88,104,119,123 | 0 |
| 4 | NAG | BA | 1 | 14/15 | 0.91 | 0.16 | 80,84,96,97 | 0 |
| 4 | NAG | OA | 2 | 14/15 | 0.91 | 0.16 | 55,73,85,91 | 0 |
| 4 | NAG | n | 1 | 14/15 | 0.92 | 0.17 | 67,77,90,98 | 0 |
| 6 | NAG | DA | 1 | 14/15 | 0.92 | 0.17 | 50,66,77,82 | 0 |
| 5 | NAG | l | 1 | 14/15 | 0.92 | 0.15 | 52,57,72,76 | 0 |
| 4 | NAG | RA | 2 | 14/15 | 0.92 | 0.24 | 83,92,102,114 | 0 |
| 4 | NAG | 2 | 2 | 14/15 | 0.92 | 0.20 | 53,71,87,100 | 0 |
| 4 | NAG | q | 2 | 14/15 | 0.92 | 0.16 | 80,88,92,93 | 0 |
| 4 | NAG | s | 1 | 14/15 | 0.93 | 0.18 | 71,77,85,90 | 0 |
| 6 | NAG | EA | 1 | 14/15 | 0.93 | 0.15 | 46,58,71,75 | 0 |
| 6 | NAG | y | 1 | 14/15 | 0.93 | 0.13 | 52,67,74,75 | 0 |
| 4 | NAG | q | 1 | 14/15 | 0.93 | 0.15 | 56,67,78,80 | 0 |
| 4 | NAG | j | 1 | 14/15 | 0.93 | 0.16 | 59,67,76,76 | 0 |
| 5 | NAG | FA | 1 | 14/15 | 0.93 | 0.16 | 49,68,77,78 | 0 |
| 4 | NAG | j | 2 | 14/15 | 0.94 | 0.19 | 49,57,73,79 | 0 |
| 6 | NAG | y | 2 | 14/15 | 0.94 | 0.22 | 65,83,94,109 | 0 |
| 6 | NAG | NA | 1 | 14/15 | 0.94 | 0.13 | 56,62,71,72 | 0 |
| 4 | NAG | OA | 1 | 14/15 | 0.94 | 0.11 | 57,70,80,85 | 0 |
| 4 | NAG | 7 | 1 | 14/15 | 0.94 | 0.14 | 57,70,83,84 | 0 |
| 5 | NAG | AA | 1 | 14/15 | 0.95 | 0.14 | 61,71,75,75 | 0 |
| 4 | NAG | 4 | 1 | 14/15 | 0.95 | 0.08 | 57,70,74,80 | 0 |
| 6 | NAG | 5 | 1 | 14/15 | 0.95 | 0.16 | 52,60,70,76 | 0 |
| 4 | NAG | MA | 1 | 14/15 | 0.95 | 0.10 | 69,77,85,86 | 0 |
| 5 | NAG | KA | 1 | 14/15 | 0.96 | 0.13 | 60,66,76,78 | 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.

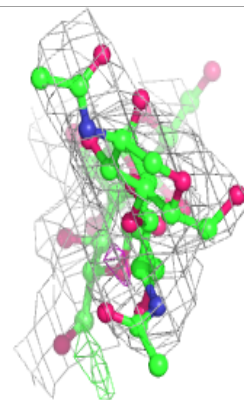
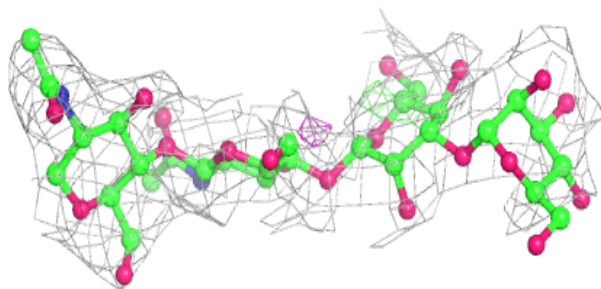
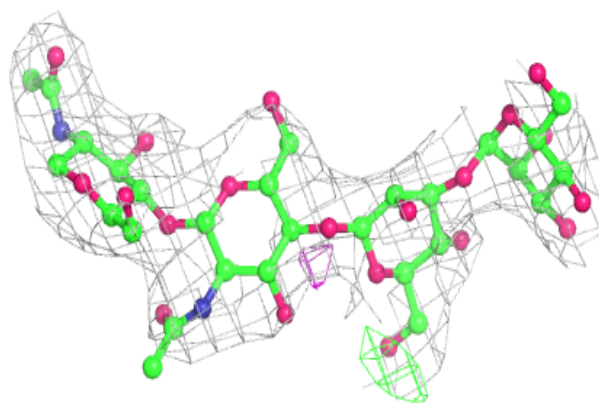
Electron density around Chain EA:

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

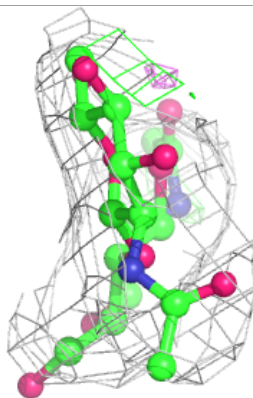
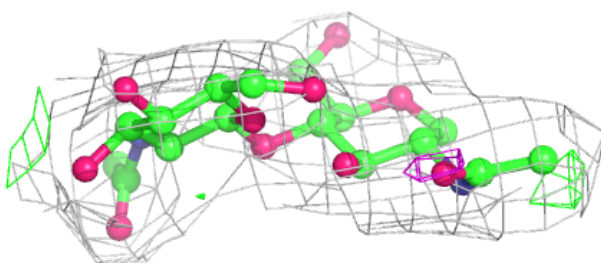
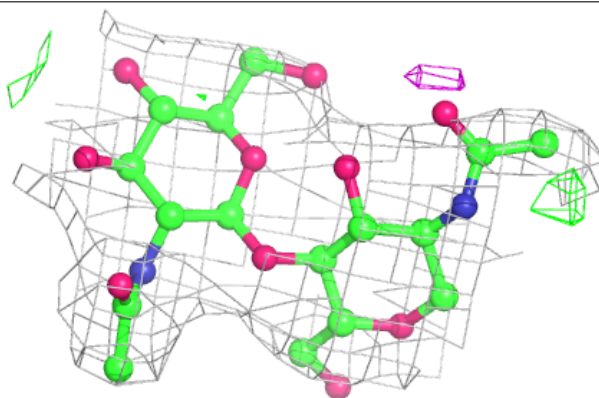


Electron density around Chain FA:

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

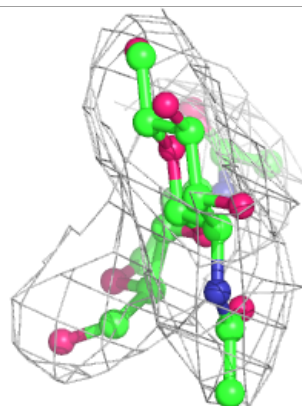
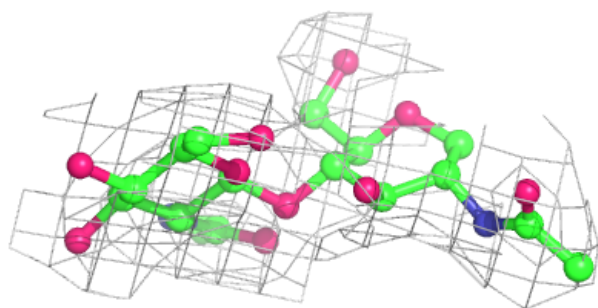
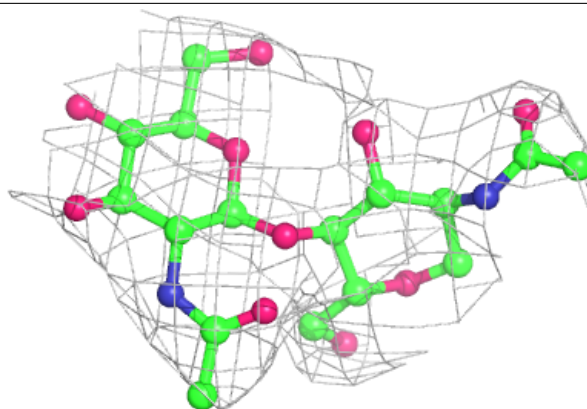
**Electron density around Chain IA:**

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

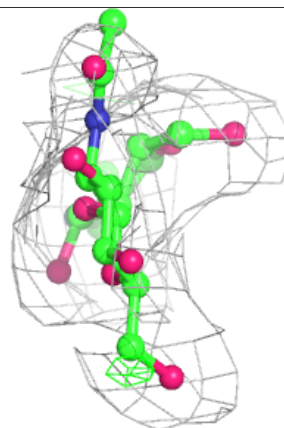
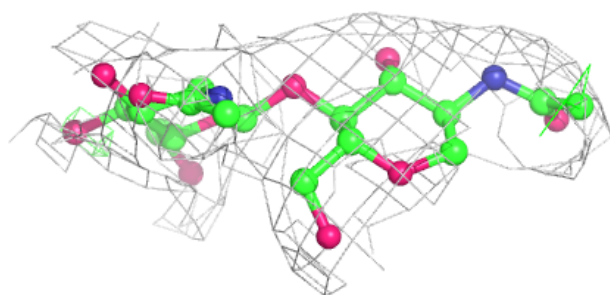
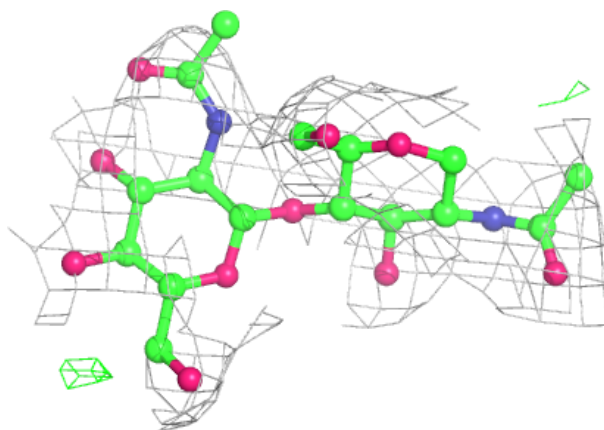


Electron density around Chain JA:

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

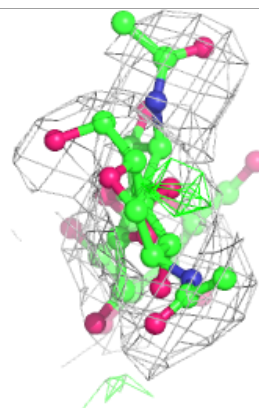
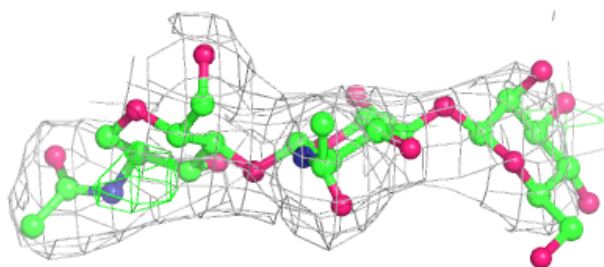
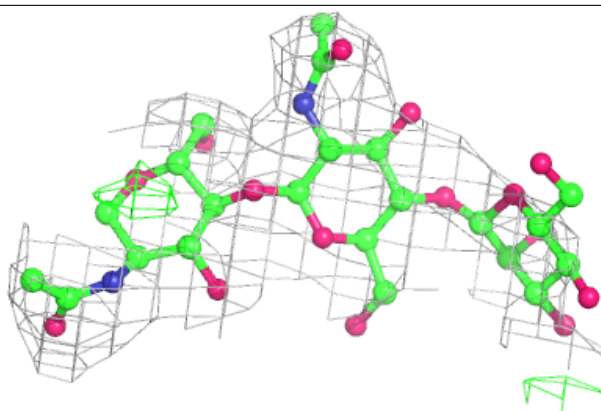
**Electron density around Chain MA:**

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

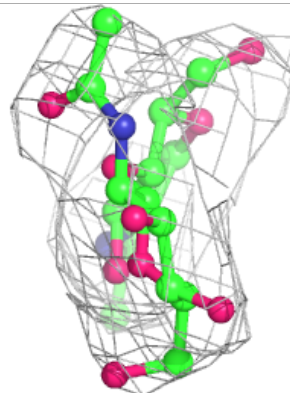
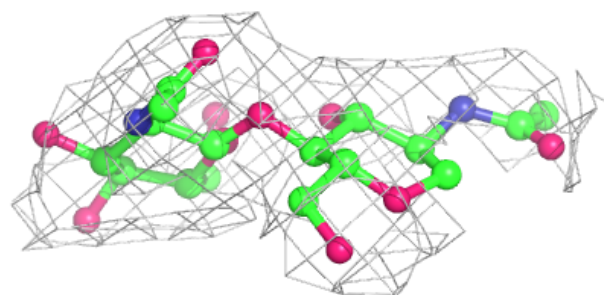
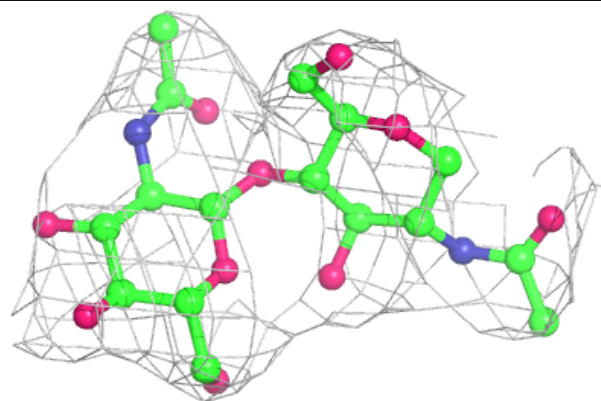


Electron density around Chain NA:

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

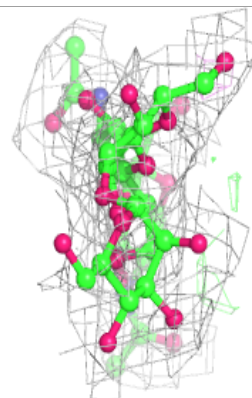
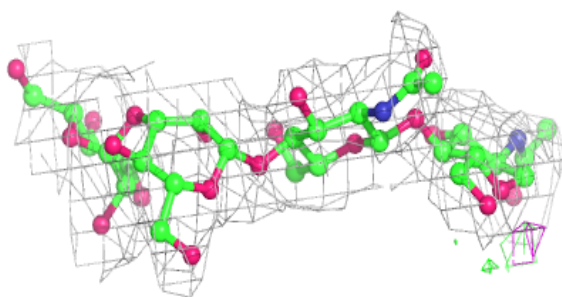
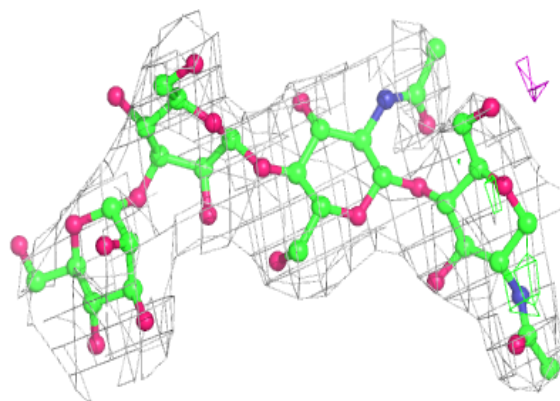
**Electron density around Chain OA:**

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

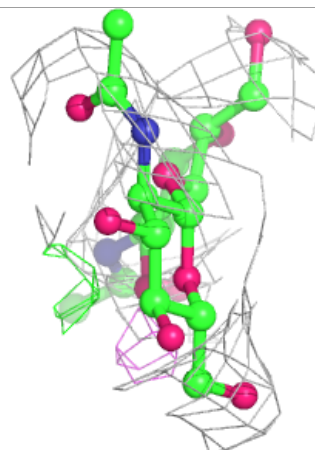
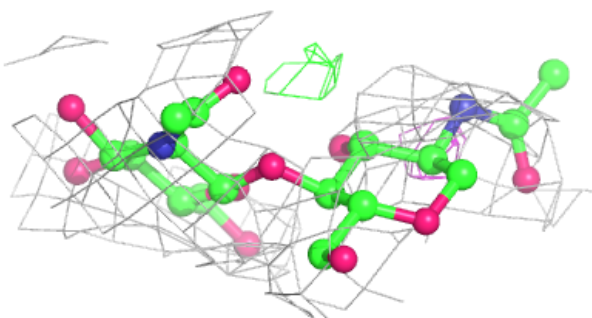
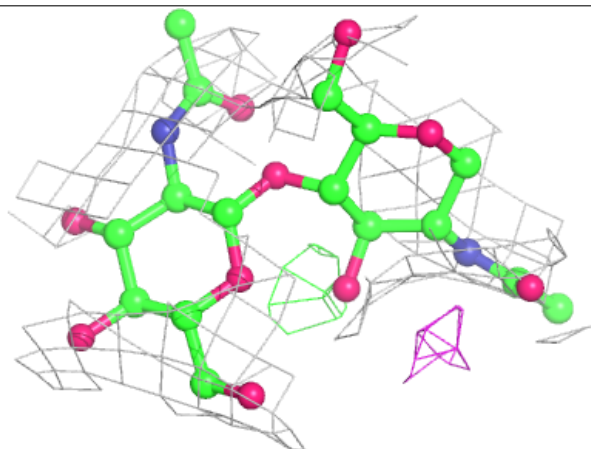


Electron density around Chain PA:

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

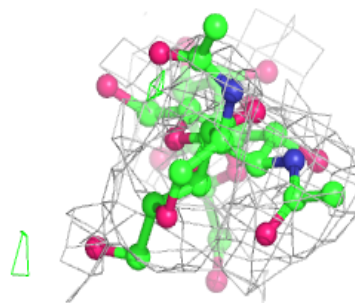
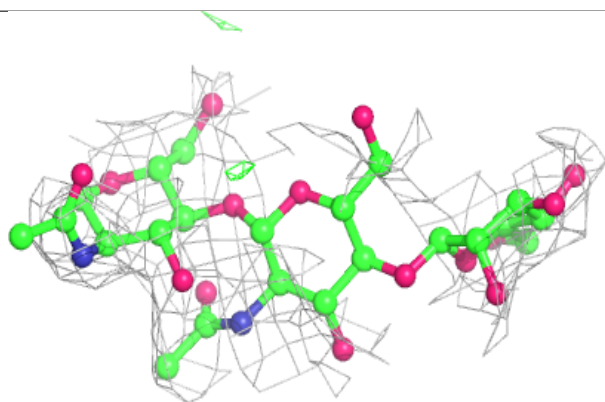
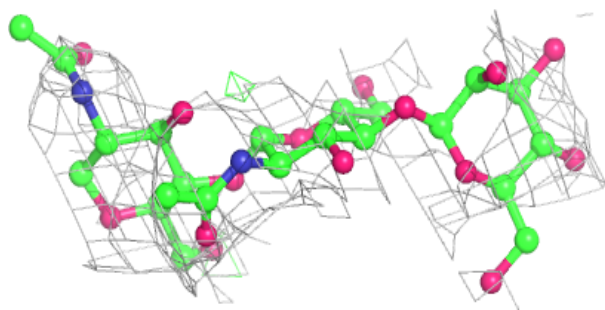
**Electron density around Chain QA:**

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

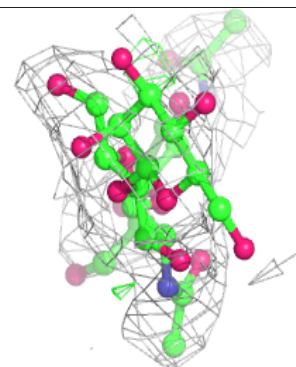
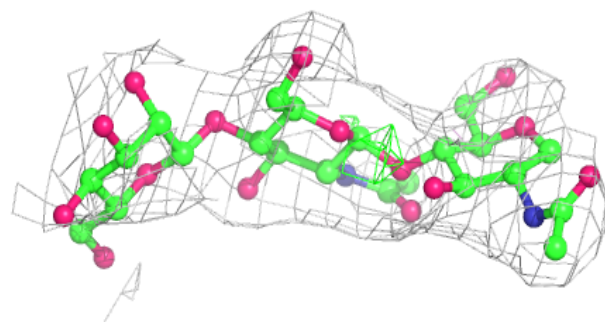
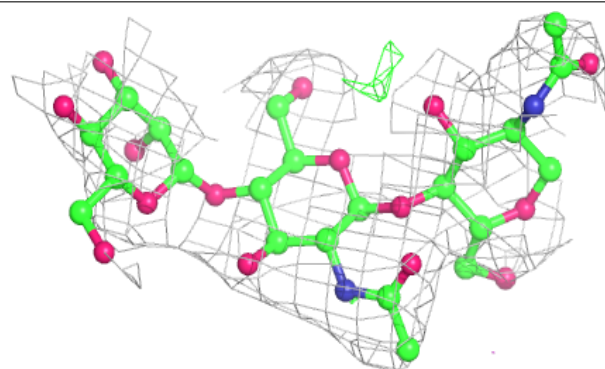


Electron density around Chain GA:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

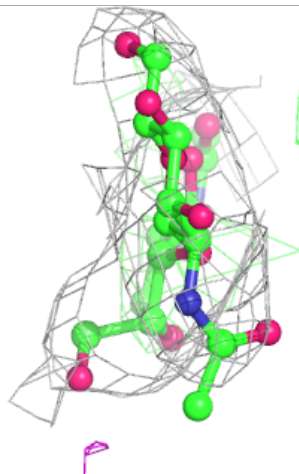
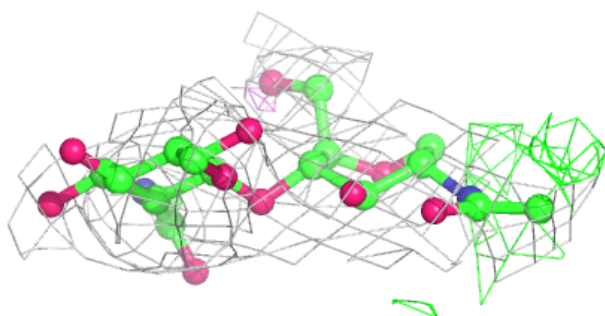
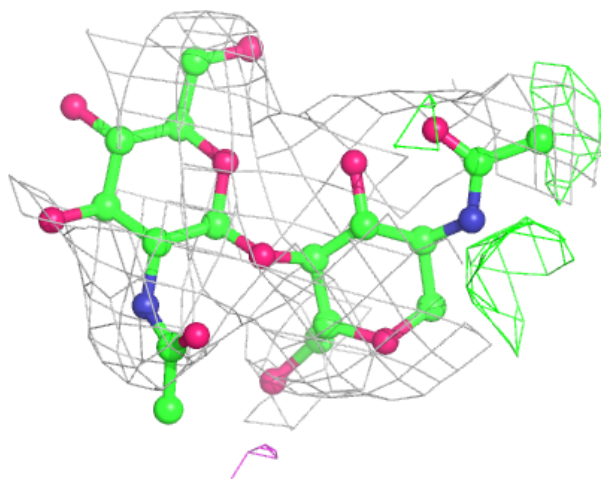
**Electron density around Chain LA:**

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



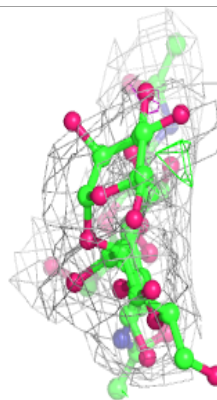
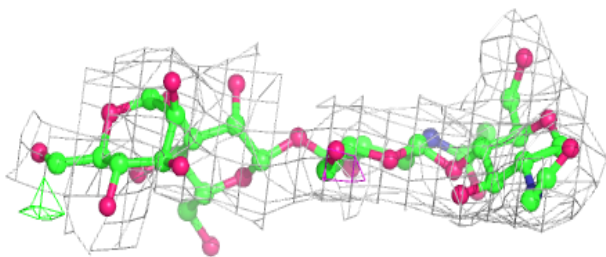
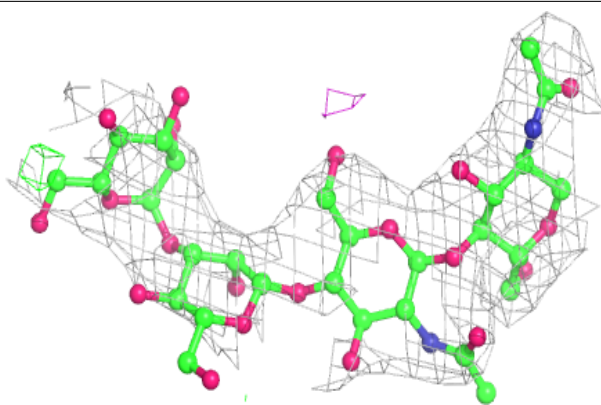
Electron density around Chain HA:

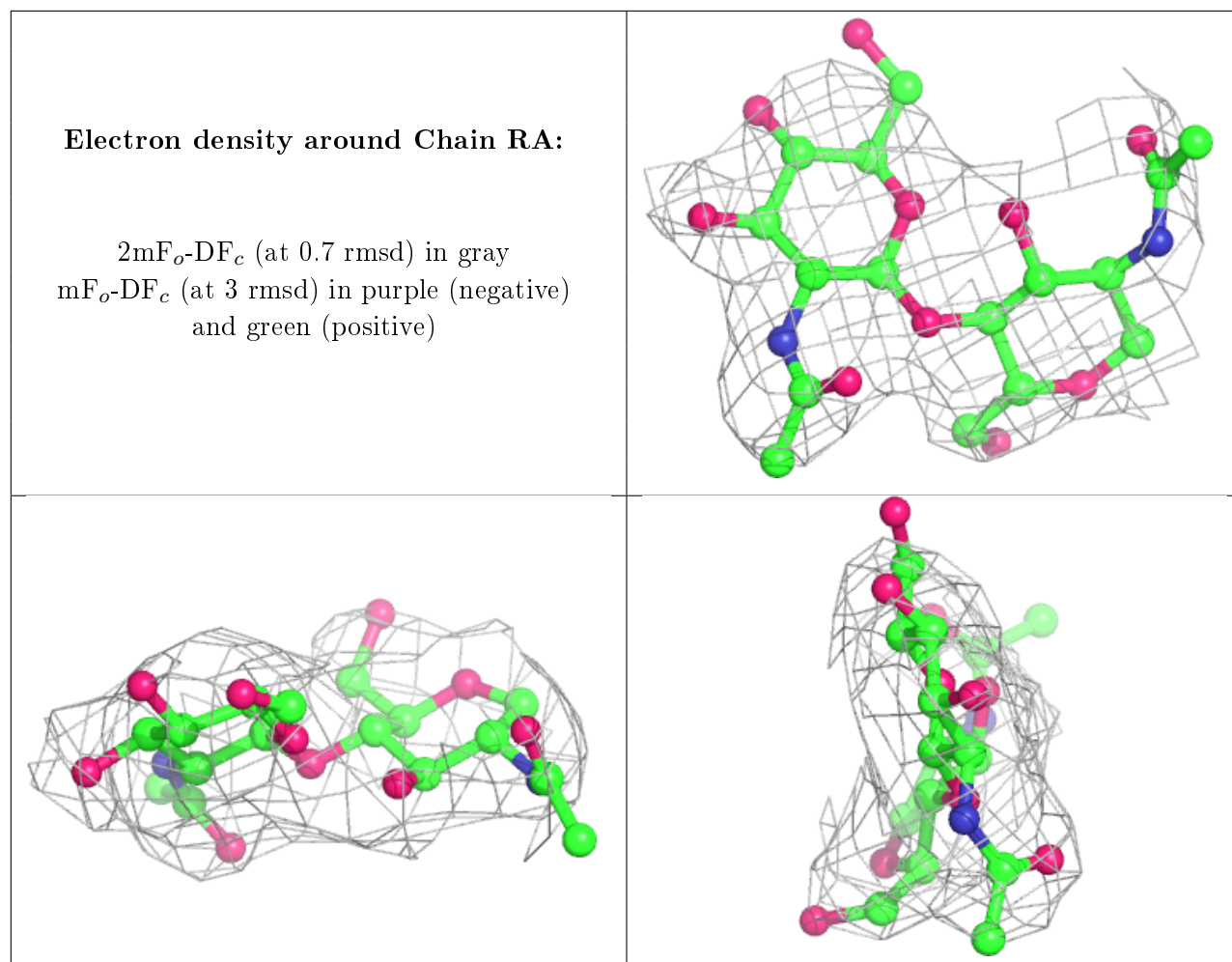
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain KA:

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





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 9 | CUO | X | 3401[A] | 4/4 | 0.39 | 0.56 | 121,121,121,121 | 4 |
| 9 | CUO | X | 3401[B] | 4/4 | 0.39 | 0.56 | 121,121,121,121 | 4 |
| 9 | CUO | I | 3402[B] | 4/4 | 0.49 | 0.23 | 84,84,84,84 | 4 |
| 9 | CUO | I | 3402[A] | 4/4 | 0.49 | 0.23 | 84,84,84,84 | 4 |
| 9 | CUO | V | 5018[D] | 4/4 | 0.52 | 0.36 | 113,113,113,113 | 4 |
| 9 | CUO | P | 5015[C] | 4/4 | 0.52 | 0.42 | 114,114,114,114 | 4 |
| 9 | CUO | P | 5015[D] | 4/4 | 0.52 | 0.42 | 114,114,114,114 | 4 |
| 9 | CUO | V | 5018[C] | 4/4 | 0.52 | 0.36 | 113,113,113,113 | 4 |
| 9 | CUO | D | 5016[D] | 4/4 | 0.59 | 0.30 | 109,109,109,109 | 4 |
| 9 | CUO | D | 5016[C] | 4/4 | 0.59 | 0.30 | 109,109,109,109 | 4 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|---------|-------|------|------|----------------------------|-------|
| 9 | CUO | J | 5014[C] | 4/4 | 0.59 | 0.31 | 98,98,98,98 | 4 |
| 9 | CUO | J | 5014[D] | 4/4 | 0.59 | 0.31 | 98,98,98,98 | 4 |
| 9 | CUO | d | 3401[A] | 4/4 | 0.60 | 0.43 | 111,111,111,111 | 4 |
| 9 | CUO | d | 3401[B] | 4/4 | 0.60 | 0.43 | 111,111,111,111 | 4 |
| 9 | CUO | A | 5016[D] | 4/4 | 0.62 | 0.20 | 95,95,95,95 | 4 |
| 9 | CUO | A | 5016[C] | 4/4 | 0.62 | 0.20 | 95,95,95,95 | 4 |
| 9 | CUO | S | 2101[D] | 4/4 | 0.65 | 0.27 | 94,94,94,94 | 4 |
| 9 | CUO | S | 2101[C] | 4/4 | 0.65 | 0.27 | 94,94,94,94 | 4 |
| 9 | CUO | O | 3401[A] | 4/4 | 0.67 | 0.32 | 85,85,85,85 | 4 |
| 9 | CUO | O | 3401[B] | 4/4 | 0.67 | 0.32 | 85,85,85,85 | 4 |
| 9 | CUO | b | 2101[D] | 4/4 | 0.68 | 0.31 | 106,106,106,106 | 4 |
| 9 | CUO | b | 2101[C] | 4/4 | 0.68 | 0.31 | 106,106,106,106 | 4 |
| 9 | CUO | G | 2101[C] | 4/4 | 0.69 | 0.28 | 104,104,104,104 | 4 |
| 9 | CUO | U | 3401[B] | 4/4 | 0.69 | 0.36 | 81,81,81,81 | 4 |
| 9 | CUO | U | 3401[A] | 4/4 | 0.69 | 0.36 | 81,81,81,81 | 4 |
| 9 | CUO | G | 2101[D] | 4/4 | 0.69 | 0.28 | 104,104,104,104 | 4 |
| 9 | CUO | F | 3401[B] | 4/4 | 0.70 | 0.23 | 86,86,86,86 | 4 |
| 9 | CUO | F | 3401[A] | 4/4 | 0.70 | 0.23 | 86,86,86,86 | 4 |
| 9 | CUO | C | 3401[B] | 4/4 | 0.71 | 0.28 | 99,99,99,99 | 4 |
| 9 | CUO | C | 3401[A] | 4/4 | 0.71 | 0.28 | 99,99,99,99 | 4 |
| 9 | CUO | M | 2101[C] | 4/4 | 0.71 | 0.27 | 103,103,103,103 | 4 |
| 9 | CUO | M | 2101[D] | 4/4 | 0.71 | 0.27 | 103,103,103,103 | 4 |
| 9 | CUO | Y | 2101[D] | 4/4 | 0.72 | 0.28 | 99,99,99,99 | 4 |
| 9 | CUO | Y | 2101[C] | 4/4 | 0.72 | 0.28 | 99,99,99,99 | 4 |
| 9 | CUO | C | 3402[A] | 4/4 | 0.73 | 0.31 | 100,100,100,100 | 4 |
| 9 | CUO | C | 3402[B] | 4/4 | 0.73 | 0.31 | 100,100,100,100 | 4 |
| 9 | CUO | F | 3402[B] | 4/4 | 0.74 | 0.28 | 85,85,85,85 | 4 |
| 9 | CUO | F | 3402[A] | 4/4 | 0.74 | 0.28 | 85,85,85,85 | 4 |
| 9 | CUO | I | 3401[B] | 4/4 | 0.76 | 0.21 | 84,84,84,84 | 4 |
| 9 | CUO | I | 3401[A] | 4/4 | 0.76 | 0.21 | 84,84,84,84 | 4 |
| 9 | CUO | E | 3001 | 4/4 | 0.89 | 0.13 | 55,55,80,85 | 0 |
| 9 | CUO | Y | 2104 | 4/4 | 0.90 | 0.13 | 69,75,80,100 | 0 |
| 9 | CUO | M | 2104 | 4/4 | 0.90 | 0.10 | 58,70,74,76 | 0 |
| 9 | CUO | V | 5003 | 4/4 | 0.90 | 0.11 | 66,79,89,90 | 0 |
| 9 | CUO | G | 2104 | 4/4 | 0.90 | 0.17 | 58,85,92,97 | 0 |
| 9 | CUO | c | 3001 | 4/4 | 0.90 | 0.16 | 48,56,77,80 | 0 |
| 9 | CUO | A | 5001 | 4/4 | 0.90 | 0.12 | 70,73,87,92 | 0 |
| 9 | CUO | B | 3001 | 4/4 | 0.91 | 0.15 | 49,55,75,88 | 0 |
| 9 | CUO | b | 2104 | 4/4 | 0.91 | 0.13 | 60,75,83,94 | 0 |
| 9 | CUO | A | 5002 | 4/4 | 0.91 | 0.17 | 55,75,89,91 | 0 |
| 9 | CUO | D | 5001 | 4/4 | 0.92 | 0.14 | 64,68,95,98 | 0 |
| 9 | CUO | V | 5002 | 4/4 | 0.92 | 0.14 | 50,61,67,72 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 9 | CUO | b | 2105 | 4/4 | 0.92 | 0.11 | 54,57,68,74 | 0 |
| 9 | CUO | P | 5003 | 4/4 | 0.93 | 0.14 | 45,54,76,83 | 0 |
| 9 | CUO | T | 3002 | 4/4 | 0.93 | 0.13 | 52,69,74,84 | 0 |
| 9 | CUO | J | 5001 | 4/4 | 0.93 | 0.12 | 49,52,60,69 | 0 |
| 9 | CUO | S | 2104 | 4/4 | 0.93 | 0.11 | 74,79,82,87 | 0 |
| 9 | CUO | G | 2103 | 4/4 | 0.93 | 0.14 | 49,58,62,73 | 0 |
| 9 | CUO | N | 3001 | 4/4 | 0.93 | 0.14 | 36,39,74,80 | 0 |
| 9 | CUO | Y | 2103 | 4/4 | 0.93 | 0.18 | 58,65,82,85 | 0 |
| 9 | CUO | J | 5003 | 4/4 | 0.94 | 0.09 | 89,96,96,103 | 0 |
| 9 | CUO | D | 5003 | 4/4 | 0.94 | 0.08 | 60,62,67,79 | 0 |
| 9 | CUO | S | 2105 | 4/4 | 0.94 | 0.13 | 45,45,62,71 | 0 |
| 9 | CUO | B | 3002 | 4/4 | 0.94 | 0.14 | 57,58,80,91 | 0 |
| 9 | CUO | b | 2103 | 4/4 | 0.94 | 0.13 | 55,59,71,73 | 0 |
| 9 | CUO | W | 3002 | 4/4 | 0.94 | 0.12 | 58,62,70,77 | 0 |
| 9 | CUO | J | 5002 | 4/4 | 0.94 | 0.13 | 53,56,80,83 | 0 |
| 9 | CUO | S | 2102 | 4/4 | 0.94 | 0.13 | 54,65,85,90 | 0 |
| 9 | CUO | P | 5002 | 4/4 | 0.94 | 0.12 | 56,59,75,82 | 0 |
| 9 | CUO | Z | 3002 | 4/4 | 0.94 | 0.11 | 48,68,69,72 | 0 |
| 9 | CUO | D | 5002 | 4/4 | 0.94 | 0.14 | 51,60,82,85 | 0 |
| 9 | CUO | A | 5003 | 4/4 | 0.94 | 0.07 | 79,87,89,89 | 0 |
| 9 | CUO | Q | 3002 | 4/4 | 0.94 | 0.10 | 53,62,64,73 | 0 |
| 9 | CUO | b | 2102 | 4/4 | 0.95 | 0.10 | 60,63,73,78 | 0 |
| 9 | CUO | P | 5001 | 4/4 | 0.95 | 0.13 | 36,38,56,71 | 0 |
| 9 | CUO | N | 3002 | 4/4 | 0.95 | 0.12 | 48,51,70,74 | 0 |
| 9 | CUO | M | 2105 | 4/4 | 0.95 | 0.12 | 48,60,61,62 | 0 |
| 9 | CUO | W | 3001 | 4/4 | 0.95 | 0.13 | 37,41,72,78 | 0 |
| 9 | CUO | c | 3002 | 4/4 | 0.95 | 0.08 | 70,71,79,80 | 0 |
| 9 | CUO | J | 5004 | 4/4 | 0.95 | 0.11 | 49,58,62,63 | 0 |
| 9 | CUO | Y | 2102 | 4/4 | 0.95 | 0.10 | 59,67,69,83 | 0 |
| 9 | CUO | P | 5004 | 4/4 | 0.95 | 0.13 | 40,48,67,68 | 0 |
| 9 | CUO | Q | 3001 | 4/4 | 0.95 | 0.12 | 37,43,64,70 | 0 |
| 9 | CUO | K | 3002 | 4/4 | 0.95 | 0.11 | 52,69,75,79 | 0 |
| 9 | CUO | H | 3001 | 4/4 | 0.95 | 0.11 | 58,60,72,78 | 0 |
| 9 | CUO | S | 2103 | 4/4 | 0.96 | 0.13 | 49,52,72,80 | 0 |
| 9 | CUO | V | 5001 | 4/4 | 0.96 | 0.15 | 39,39,64,66 | 0 |
| 9 | CUO | Y | 2105 | 4/4 | 0.96 | 0.10 | 47,59,61,62 | 0 |
| 9 | CUO | A | 5004 | 4/4 | 0.96 | 0.11 | 51,60,67,70 | 0 |
| 9 | CUO | Z | 3001 | 4/4 | 0.96 | 0.12 | 46,54,67,69 | 0 |
| 9 | CUO | K | 3001 | 4/4 | 0.96 | 0.08 | 57,73,73,80 | 0 |
| 9 | CUO | G | 2105 | 4/4 | 0.96 | 0.08 | 58,60,66,69 | 0 |
| 9 | CUO | T | 3001 | 4/4 | 0.96 | 0.13 | 44,59,84,85 | 0 |
| 9 | CUO | V | 5004 | 4/4 | 0.96 | 0.12 | 44,50,62,65 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 9 | CUO | M | 2102 | 4/4 | 0.97 | 0.11 | 41,52,59,63 | 0 |
| 9 | CUO | M | 2103 | 4/4 | 0.97 | 0.11 | 50,59,66,68 | 0 |
| 9 | CUO | G | 2102 | 4/4 | 0.97 | 0.10 | 57,62,65,70 | 0 |
| 9 | CUO | H | 3002 | 4/4 | 0.97 | 0.08 | 67,79,83,84 | 0 |
| 9 | CUO | E | 3002 | 4/4 | 0.98 | 0.06 | 57,61,67,68 | 0 |
| 9 | CUO | D | 5004 | 4/4 | 0.98 | 0.07 | 52,54,59,62 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.