



wwPDB Geometry-Only Validation Summary Report ⓘ

Mar 8, 2026 – 11:42 AM UTC

PDB ID : 3IRK / pdb_00003irk
Title : Solution Structure of Heparin dp30
Authors : Khan, S.; Gor, J.; Mulloy, B.; Perkins, S.J.
Deposited on : 2009-08-24
Resolution : Not provided

This is a wwPDB Geometry-Only 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

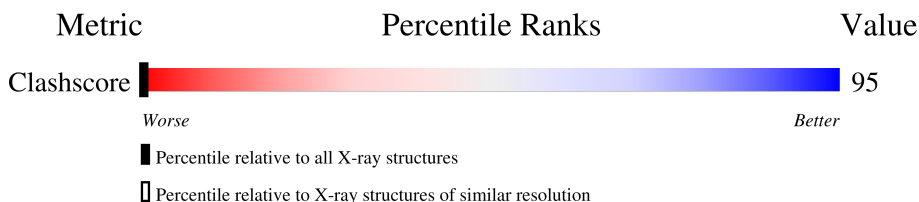
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

SOLUTION SCATTERING

The reported resolution of this entry is unknown.


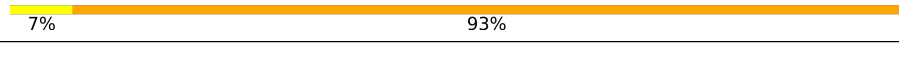

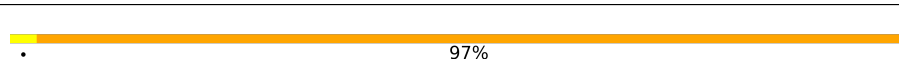

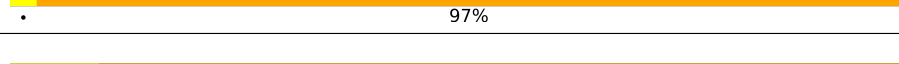
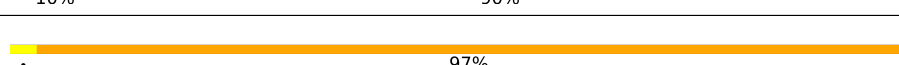



Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|------------|-----------------------------|---|
| Clashscore | 190562 | - |

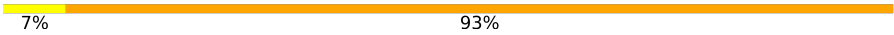
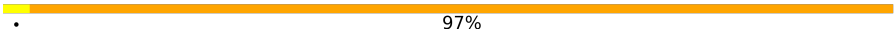


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 1-A | 30 |  10% 90% |
| 1 | 10-A | 30 |  7% 93% |
| 1 | 11-A | 30 |  13% 87% |
| 1 | 12-A | 30 |  20% 80% |
| 1 | 13-A | 30 |  . 97% |
| 1 | 14-A | 30 |  17% 83% |
| 1 | 2-A | 30 |  . 97% |
| 1 | 3-A | 30 |  10% 90% |
| 1 | 4-A | 30 |  . 97% |
| 1 | 5-A | 30 |  17% 83% |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain | |
|-----|-------|--------|--|-----|
| 1 | 6-A | 30 |  | 93% |
| 1 | 7-A | 30 |  | 97% |
| 1 | 8-A | 30 |  | 87% |
| 1 | 9-A | 30 |  | 90% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | IDS | 1-A | 10 | - | - | X | - |
| 1 | SGN | 1-A | 11 | - | - | X | - |
| 1 | SGN | 1-A | 23 | - | - | X | - |
| 1 | IDS | 1-A | 24 | - | - | X | - |
| 1 | SGN | 1-A | 25 | - | - | X | - |
| 1 | IDS | 10-A | 28 | - | - | X | - |
| 1 | IDS | 11-A | 12 | - | - | X | - |
| 1 | SGN | 11-A | 13 | - | - | X | - |
| 1 | IDS | 11-A | 16 | - | - | X | - |
| 1 | SGN | 11-A | 17 | - | - | X | - |
| 1 | IDS | 11-A | 18 | - | - | X | - |
| 1 | IDS | 11-A | 20 | - | - | X | - |
| 1 | SGN | 11-A | 23 | - | - | X | - |
| 1 | IDS | 11-A | 24 | - | - | X | - |
| 1 | SGN | 11-A | 5 | - | - | X | - |
| 1 | IDS | 11-A | 6 | - | - | X | - |
| 1 | IDS | 12-A | 24 | - | - | X | - |
| 1 | SGN | 12-A | 27 | - | - | X | - |
| 1 | IDS | 12-A | 28 | - | - | X | - |
| 1 | IDS | 12-A | 6 | - | - | X | - |
| 1 | SGN | 12-A | 7 | - | - | X | - |
| 1 | IDS | 13-A | 12 | - | - | X | - |
| 1 | SGN | 13-A | 13 | - | - | X | - |
| 1 | SGN | 13-A | 15 | - | - | X | - |
| 1 | IDS | 13-A | 16 | - | - | X | - |
| 1 | IDS | 13-A | 18 | - | - | X | - |
| 1 | IDS | 13-A | 28 | - | - | X | - |
| 1 | SGN | 13-A | 29 | - | - | X | - |
| 1 | IDS | 13-A | 4 | - | - | X | - |
| 1 | SGN | 13-A | 5 | - | - | X | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | IDS | 14-A | 12 | - | - | X | - |
| 1 | IDS | 14-A | 20 | - | - | X | - |
| 1 | SGN | 14-A | 23 | - | - | X | - |
| 1 | IDS | 14-A | 24 | - | - | X | - |
| 1 | IDS | 14-A | 6 | - | - | X | - |
| 1 | SGN | 14-A | 7 | - | - | X | - |
| 1 | SGN | 2-A | 23 | - | - | X | - |
| 1 | IDS | 2-A | 24 | - | - | X | - |
| 1 | IDS | 2-A | 26 | - | - | X | - |
| 1 | SGN | 2-A | 27 | - | - | X | - |
| 1 | SGN | 3-A | 13 | - | - | X | - |
| 1 | IDS | 3-A | 14 | - | - | X | - |
| 1 | IDS | 3-A | 16 | - | - | X | - |
| 1 | IDS | 3-A | 20 | - | - | X | - |
| 1 | SGN | 3-A | 21 | - | - | X | - |
| 1 | IDS | 3-A | 22 | - | - | X | - |
| 1 | SGN | 3-A | 29 | - | - | X | - |
| 1 | SGN | 3-A | 3 | - | - | X | - |
| 1 | IDS | 3-A | 30 | - | - | X | - |
| 1 | IDS | 3-A | 4 | - | - | X | - |
| 1 | SGN | 3-A | 5 | - | - | X | - |
| 1 | IDS | 4-A | 10 | - | - | X | - |
| 1 | SGN | 4-A | 11 | - | - | X | - |
| 1 | IDS | 4-A | 12 | - | - | X | - |
| 1 | SGN | 4-A | 13 | - | - | X | - |
| 1 | IDS | 4-A | 16 | - | - | X | - |
| 1 | IDS | 4-A | 18 | - | - | X | - |
| 1 | SGN | 4-A | 19 | - | - | X | - |
| 1 | IDS | 4-A | 20 | - | - | X | - |
| 1 | SGN | 4-A | 23 | - | - | X | - |
| 1 | IDS | 4-A | 24 | - | - | X | - |
| 1 | SGN | 4-A | 25 | - | - | X | - |
| 1 | IDS | 4-A | 6 | - | - | X | - |
| 1 | SGN | 4-A | 7 | - | - | X | - |
| 1 | SGN | 4-A | 9 | - | - | X | - |
| 1 | IDS | 5-A | 14 | - | - | X | - |
| 1 | SGN | 5-A | 15 | - | - | X | - |
| 1 | IDS | 5-A | 22 | - | - | X | - |
| 1 | SGN | 5-A | 25 | - | - | X | - |
| 1 | IDS | 5-A | 26 | - | - | X | - |
| 1 | IDS | 5-A | 28 | - | - | X | - |
| 1 | IDS | 6-A | 12 | - | - | X | - |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 1 | SGN | 6-A | 13 | - | - | X | - |
| 1 | SGN | 6-A | 15 | - | - | X | - |
| 1 | IDS | 6-A | 16 | - | - | X | - |
| 1 | IDS | 6-A | 18 | - | - | X | - |
| 1 | IDS | 6-A | 24 | - | - | X | - |
| 1 | IDS | 6-A | 30 | - | - | X | - |
| 1 | IDS | 7-A | 10 | - | - | X | - |
| 1 | IDS | 7-A | 16 | - | - | X | - |
| 1 | SGN | 7-A | 17 | - | - | X | - |
| 1 | IDS | 7-A | 2 | - | - | X | - |
| 1 | IDS | 7-A | 22 | - | - | X | - |
| 1 | IDS | 7-A | 24 | - | - | X | - |
| 1 | IDS | 7-A | 26 | - | - | X | - |
| 1 | SGN | 7-A | 3 | - | - | X | - |
| 1 | IDS | 7-A | 4 | - | - | X | - |
| 1 | SGN | 7-A | 9 | - | - | X | - |
| 1 | IDS | 8-A | 10 | - | - | X | - |
| 1 | IDS | 8-A | 18 | - | - | X | - |
| 1 | SGN | 8-A | 23 | - | - | X | - |
| 1 | IDS | 8-A | 24 | - | - | X | - |
| 1 | SGN | 8-A | 9 | - | - | X | - |
| 1 | IDS | 9-A | 12 | - | - | X | - |
| 1 | SGN | 9-A | 13 | - | - | X | - |
| 1 | IDS | 9-A | 14 | - | - | X | - |
| 1 | SGN | 9-A | 15 | - | - | X | - |
| 1 | IDS | 9-A | 16 | - | - | X | - |
| 1 | SGN | 9-A | 17 | - | - | X | - |
| 1 | IDS | 9-A | 18 | - | - | X | - |
| 1 | SGN | 9-A | 19 | - | - | X | - |
| 1 | IDS | 9-A | 20 | - | - | X | - |
| 1 | SGN | 9-A | 21 | - | - | X | - |
| 1 | IDS | 9-A | 22 | - | - | X | - |
| 1 | SGN | 9-A | 23 | - | - | X | - |
| 1 | IDS | 9-A | 24 | - | - | X | - |
| 1 | SGN | 9-A | 25 | - | - | X | - |
| 1 | IDS | 9-A | 26 | - | - | X | - |
| 1 | IDS | 9-A | 6 | - | - | X | - |

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|----|---------|---------|-------|
| 1 | 7-A | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 180 | 15 | 285 | 45 | | | |
| 1 | 8-A | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 180 | 15 | 285 | 45 | | | |
| 1 | 9-A | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 180 | 15 | 285 | 45 | | | |
| 1 | 10-A | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 180 | 15 | 285 | 45 | | | |
| 1 | 11-A | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 180 | 15 | 285 | 45 | | | |
| 1 | 12-A | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 180 | 15 | 285 | 45 | | | |
| 1 | 13-A | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 180 | 15 | 285 | 45 | | | |
| 1 | 14-A | 30 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 525 | 180 | 15 | 285 | 45 | | | |

Chain 6-A:  7% 93%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| SGN1 | IDS2 | SGN3 | IDS4 | SGN5 | IDS6 | SGN7 | IDS8 | SGN9 | IDS10 | SGN11 | IDS12 | SGN13 | IDS14 | SGN15 | IDS16 | SGN17 | IDS18 | SGN19 | IDS20 | SGN21 | IDS22 | SGN23 | IDS24 | SGN25 | IDS26 | SGN27 | IDS28 | SGN29 | IDS30 |
|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

● Molecule 1: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain 7-A:  97%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| SGN1 | IDS2 | SGN3 | IDS4 | SGN5 | IDS6 | SGN7 | IDS8 | SGN9 | IDS10 | SGN11 | IDS12 | SGN13 | IDS14 | SGN15 | IDS16 | SGN17 | IDS18 | SGN19 | IDS20 | SGN21 | IDS22 | SGN23 | IDS24 | SGN25 | IDS26 | SGN27 | IDS28 | SGN29 | IDS30 |
|------|------|------|------|------|------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|

● Molecule 1: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain 8-A:  13% 87%

| |
|-------|
| SGN1 |
| IDS2 |
| SGN3 |
| IDS4 |
| SGN5 |
| IDS6 |
| SGN7 |
| IDS8 |
| SGN9 |
| IDS10 |
| SGN11 |
| IDS12 |
| SGN13 |
| IDS14 |
| SGN15 |
| IDS16 |
| SGN17 |
| IDS18 |
| SGN19 |
| IDS20 |
| SGN21 |
| IDS22 |
| SGN23 |
| IDS24 |
| SGN25 |
| IDS26 |
| SGN27 |
| IDS28 |
| SGN29 |
| IDS30 |

- Molecule 1: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain 13-A: .

97%

| |
|-------|
| SGN1 |
| IDS2 |
| SGN3 |
| IDS4 |
| SGN5 |
| IDS6 |
| SGN7 |
| IDS8 |
| SGN9 |
| IDS10 |
| SGN11 |
| IDS12 |
| SGN13 |
| IDS14 |
| SGN15 |
| IDS16 |
| SGN17 |
| IDS18 |
| SGN19 |
| IDS20 |
| SGN21 |
| IDS22 |
| SGN23 |
| IDS24 |
| SGN25 |
| IDS26 |
| SGN27 |
| IDS28 |
| SGN29 |
| IDS30 |

- Molecule 1: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain 14-A:

17%

83%

| |
|-------|
| SGN1 |
| IDS2 |
| SGN3 |
| IDS4 |
| SGN5 |
| IDS6 |
| SGN7 |
| IDS8 |
| SGN9 |
| IDS10 |
| SGN11 |
| IDS12 |
| SGN13 |
| IDS14 |
| SGN15 |
| IDS16 |
| SGN17 |
| IDS18 |
| SGN19 |
| IDS20 |
| SGN21 |
| IDS22 |
| SGN23 |
| IDS24 |
| SGN25 |
| IDS26 |
| SGN27 |
| IDS28 |
| SGN29 |
| IDS30 |

4 Model quality

4.1 Standard geometry

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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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 | 1-A | 525 | 0 | 162 | 51 | 0 |
| 1 | 2-A | 525 | 0 | 164 | 50 | 0 |
| 1 | 3-A | 525 | 0 | 164 | 79 | 0 |
| 1 | 4-A | 525 | 0 | 164 | 104 | 0 |
| 1 | 5-A | 525 | 0 | 163 | 45 | 0 |
| 1 | 6-A | 525 | 0 | 162 | 64 | 0 |
| 1 | 7-A | 525 | 0 | 161 | 73 | 0 |
| 1 | 8-A | 525 | 0 | 165 | 53 | 0 |
| 1 | 9-A | 525 | 0 | 165 | 111 | 0 |
| 1 | 10-A | 525 | 0 | 163 | 43 | 0 |
| 1 | 11-A | 525 | 0 | 162 | 59 | 0 |
| 1 | 12-A | 525 | 0 | 163 | 55 | 0 |
| 1 | 13-A | 525 | 0 | 163 | 73 | 0 |
| 1 | 14-A | 525 | 0 | 164 | 57 | 0 |
| All | All | 7350 | 0 | 2285 | 917 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 95.

The worst 5 of 917 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|----------------|--------------------------|-------------------|
| 1:A:27:SGN:H61 | 1:A:28:IDS:S | 1.48 | 1.51 |
| 1:A:17:SGN:C6 | 1:A:18:IDS:O2S | 1.65 | 1.45 |
| 1:A:28:IDS:H3 | 1:A:29:SGN:N2 | 1.21 | 1.44 |
| 1:A:18:IDS:H3 | 1:A:19:SGN:N2 | 1.29 | 1.43 |
| 1:A:6:IDS:H3 | 1:A:7:SGN:N2 | 1.13 | 1.42 |

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

4.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

420 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$ |
| 1 | SGN | 1-A | 1 | 1 | 20,20,20 | 1.13 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 1-A | 10 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 1-A | 11 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 1-A | 12 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 1-A | 13 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 1-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 1-A | 15 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 1-A | 16 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 1-A | 17 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 1-A | 18 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 1-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 1-A | 2 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | IDS | 1-A | 20 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 1-A | 21 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 1-A | 22 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 1-A | 23 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 1-A | 24 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 1-A | 25 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 1-A | 26 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 1-A | 27 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 1-A | 28 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 1-A | 29 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 1-A | 3 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 1-A | 30 | 1 | 15,15,17 | 1.54 | 2 (13%) | 14,22,26 | 1.45 | 2 (14%) |
| 1 | IDS | 1-A | 4 | 1 | 16,16,17 | 1.45 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 1-A | 5 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 1-A | 6 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 1-A | 7 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 1-A | 8 | 1 | 16,16,17 | 1.44 | 3 (18%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 1-A | 9 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 10-A | 1 | 1 | 20,20,20 | 1.12 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 10-A | 10 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 10-A | 11 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | IDS | 10-A | 12 | 1 | 16,16,17 | 1.39 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 10-A | 13 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 10-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 10-A | 15 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 10-A | 16 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 10-A | 17 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 10-A | 18 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 10-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 10-A | 2 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | IDS | 10-A | 20 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 10-A | 21 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 10-A | 22 | 1 | 16,16,17 | 1.42 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 10-A | 23 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 10-A | 24 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 10-A | 25 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 10-A | 26 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 10-A | 27 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 10-A | 28 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 10-A | 29 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 10-A | 3 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 10-A | 30 | 1 | 15,15,17 | 1.57 | 3 (20%) | 14,22,26 | 1.45 | 2 (14%) |
| 1 | IDS | 10-A | 4 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 10-A | 5 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 10-A | 6 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 10-A | 7 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 10-A | 8 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 10-A | 9 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 11-A | 1 | 1 | 20,20,20 | 1.15 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 11-A | 10 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 11-A | 11 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 11-A | 12 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.21 | 2 (12%) |
| 1 | SGN | 11-A | 13 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 11-A | 14 | 1 | 16,16,17 | 1.46 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 11-A | 15 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 11-A | 16 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | SGN | 11-A | 17 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 11-A | 18 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 11-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 11-A | 2 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | IDS | 11-A | 20 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 11-A | 21 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 11-A | 22 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 11-A | 23 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 11-A | 24 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 11-A | 25 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 11-A | 26 | 1 | 16,16,17 | 1.42 | 3 (18%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 11-A | 27 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 11-A | 28 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 11-A | 29 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | SGN | 11-A | 3 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 11-A | 30 | 1 | 15,15,17 | 1.53 | 2 (13%) | 14,22,26 | 1.45 | 2 (14%) |
| 1 | IDS | 11-A | 4 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 11-A | 5 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 11-A | 6 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 11-A | 7 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 11-A | 8 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 11-A | 9 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.11 | 1 (4%) |
| 1 | SGN | 12-A | 1 | 1 | 20,20,20 | 1.14 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 12-A | 10 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 12-A | 11 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 12-A | 12 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 12-A | 13 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 12-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 12-A | 15 | 1 | 19,19,20 | 1.26 | 1 (5%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 12-A | 16 | 1 | 16,16,17 | 1.42 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 12-A | 17 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 12-A | 18 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 12-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 12-A | 2 | 1 | 16,16,17 | 1.42 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | IDS | 12-A | 20 | 1 | 16,16,17 | 1.45 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | SGN | 12-A | 21 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 12-A | 22 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 12-A | 23 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 12-A | 24 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 12-A | 25 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 12-A | 26 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 12-A | 27 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 12-A | 28 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 12-A | 29 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 12-A | 3 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 12-A | 30 | 1 | 15,15,17 | 1.53 | 2 (13%) | 14,22,26 | 1.45 | 2 (14%) |
| 1 | IDS | 12-A | 4 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 12-A | 5 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 12-A | 6 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 12-A | 7 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 12-A | 8 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 12-A | 9 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 13-A | 1 | 1 | 20,20,20 | 1.13 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 13-A | 10 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 13-A | 11 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 13-A | 12 | 1 | 16,16,17 | 1.39 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 13-A | 13 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 13-A | 14 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 13-A | 15 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 13-A | 16 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 13-A | 17 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 13-A | 18 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 13-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 13-A | 2 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | IDS | 13-A | 20 | 1 | 16,16,17 | 1.44 | 3 (18%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 13-A | 21 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 13-A | 22 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 13-A | 23 | 1 | 19,19,20 | 1.29 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 13-A | 24 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 13-A | 25 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | IDS | 13-A | 26 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 13-A | 27 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 13-A | 28 | 1 | 16,16,17 | 1.45 | 3 (18%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 13-A | 29 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 13-A | 3 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 13-A | 30 | 1 | 15,15,17 | 1.54 | 2 (13%) | 14,22,26 | 1.45 | 2 (14%) |
| 1 | IDS | 13-A | 4 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 13-A | 5 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 13-A | 6 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 13-A | 7 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 13-A | 8 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 13-A | 9 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 14-A | 1 | 1 | 20,20,20 | 1.14 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 14-A | 10 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 14-A | 11 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 14-A | 12 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 14-A | 13 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 14-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 14-A | 15 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 14-A | 16 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 14-A | 17 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 14-A | 18 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 14-A | 19 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 14-A | 2 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | IDS | 14-A | 20 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.21 | 2 (12%) |
| 1 | SGN | 14-A | 21 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 14-A | 22 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 14-A | 23 | 1 | 19,19,20 | 1.25 | 1 (5%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 14-A | 24 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 14-A | 25 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 14-A | 26 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 14-A | 27 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 14-A | 28 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 14-A | 29 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 14-A | 3 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | IDS | 14-A | 30 | 1 | 15,15,17 | 1.56 | 2 (13%) | 14,22,26 | 1.44 | 2 (14%) |
| 1 | IDS | 14-A | 4 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 14-A | 5 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 14-A | 6 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 14-A | 7 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 14-A | 8 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 14-A | 9 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 2-A | 1 | 1 | 20,20,20 | 1.14 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 2-A | 10 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 2-A | 11 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 2-A | 12 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 2-A | 13 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 2-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 2-A | 15 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 2-A | 16 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 2-A | 17 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 2-A | 18 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 2-A | 19 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 2-A | 2 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | IDS | 2-A | 20 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 2-A | 21 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 2-A | 22 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 2-A | 23 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 2-A | 24 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 2-A | 25 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 2-A | 26 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 2-A | 27 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 2-A | 28 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 2-A | 29 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 2-A | 3 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 2-A | 30 | 1 | 15,15,17 | 1.54 | 2 (13%) | 14,22,26 | 1.44 | 2 (14%) |
| 1 | IDS | 2-A | 4 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 2-A | 5 | 1 | 19,19,20 | 1.25 | 1 (5%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 2-A | 6 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 2-A | 7 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | IDS | 2-A | 8 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 2-A | 9 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 3-A | 1 | 1 | 20,20,20 | 1.15 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 3-A | 10 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 3-A | 11 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 3-A | 12 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 3-A | 13 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 3-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 3-A | 15 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 3-A | 16 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 3-A | 17 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 3-A | 18 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 3-A | 19 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 3-A | 2 | 1 | 16,16,17 | 1.40 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | IDS | 3-A | 20 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 3-A | 21 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 3-A | 22 | 1 | 16,16,17 | 1.42 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 3-A | 23 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 3-A | 24 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 3-A | 25 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 3-A | 26 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 3-A | 27 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 3-A | 28 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 3-A | 29 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 3-A | 3 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 3-A | 30 | 1 | 15,15,17 | 1.54 | 2 (13%) | 14,22,26 | 1.44 | 2 (14%) |
| 1 | IDS | 3-A | 4 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 3-A | 5 | 1 | 19,19,20 | 1.25 | 1 (5%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 3-A | 6 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 3-A | 7 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 3-A | 8 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 3-A | 9 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.11 | 1 (4%) |
| 1 | SGN | 4-A | 1 | 1 | 20,20,20 | 1.14 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 4-A | 10 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 4-A | 11 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | IDS | 4-A | 12 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 4-A | 13 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 4-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 4-A | 15 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 4-A | 16 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 4-A | 17 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 4-A | 18 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 4-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 4-A | 2 | 1 | 16,16,17 | 1.40 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | IDS | 4-A | 20 | 1 | 16,16,17 | 1.44 | 3 (18%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 4-A | 21 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 4-A | 22 | 1 | 16,16,17 | 1.40 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 4-A | 23 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 4-A | 24 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 4-A | 25 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 4-A | 26 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 4-A | 27 | 1 | 19,19,20 | 1.29 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 4-A | 28 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 4-A | 29 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 4-A | 3 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 4-A | 30 | 1 | 15,15,17 | 1.56 | 3 (20%) | 14,22,26 | 1.44 | 2 (14%) |
| 1 | IDS | 4-A | 4 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 4-A | 5 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 4-A | 6 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 4-A | 7 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 4-A | 8 | 1 | 16,16,17 | 1.42 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 4-A | 9 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 5-A | 1 | 1 | 20,20,20 | 1.14 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 5-A | 10 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 11 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 5-A | 12 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 5-A | 13 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 5-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 15 | 1 | 19,19,20 | 1.24 | 1 (5%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 5-A | 16 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | SGN | 5-A | 17 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 5-A | 18 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 5-A | 19 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 5-A | 2 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | IDS | 5-A | 20 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 21 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 5-A | 22 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 23 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 5-A | 24 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 5-A | 25 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 5-A | 26 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 27 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 5-A | 28 | 1 | 16,16,17 | 1.44 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 29 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.11 | 1 (4%) |
| 1 | SGN | 5-A | 3 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 5-A | 30 | 1 | 15,15,17 | 1.55 | 2 (13%) | 14,22,26 | 1.45 | 2 (14%) |
| 1 | IDS | 5-A | 4 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 5 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 5-A | 6 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 7 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 5-A | 8 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 5-A | 9 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 6-A | 1 | 1 | 20,20,20 | 1.13 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 6-A | 10 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 6-A | 11 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 6-A | 12 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 6-A | 13 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 6-A | 15 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 16 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 6-A | 17 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 18 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 6-A | 19 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 2 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | IDS | 6-A | 20 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | SGN | 6-A | 21 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 22 | 1 | 16,16,17 | 1.40 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 6-A | 23 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 24 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 6-A | 25 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 26 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 6-A | 27 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.11 | 1 (4%) |
| 1 | IDS | 6-A | 28 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 6-A | 29 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 6-A | 3 | 1 | 19,19,20 | 1.23 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 30 | 1 | 15,15,17 | 1.54 | 2 (13%) | 14,22,26 | 1.44 | 2 (14%) |
| 1 | IDS | 6-A | 4 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 6-A | 5 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 6 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 6-A | 7 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 6-A | 8 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 6-A | 9 | 1 | 19,19,20 | 1.23 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 7-A | 1 | 1 | 20,20,20 | 1.15 | 1 (5%) | 25,31,31 | 0.99 | 1 (4%) |
| 1 | IDS | 7-A | 10 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 7-A | 11 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 7-A | 12 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 7-A | 13 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.11 | 1 (4%) |
| 1 | IDS | 7-A | 14 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 7-A | 15 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 7-A | 16 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 7-A | 17 | 1 | 19,19,20 | 1.29 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 7-A | 18 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 7-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 7-A | 2 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | IDS | 7-A | 20 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 7-A | 21 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 7-A | 22 | 1 | 16,16,17 | 1.40 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 7-A | 23 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 7-A | 24 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 7-A | 25 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | IDS | 7-A | 26 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 7-A | 27 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 7-A | 28 | 1 | 16,16,17 | 1.45 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 7-A | 29 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 7-A | 3 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 7-A | 30 | 1 | 15,15,17 | 1.55 | 2 (13%) | 14,22,26 | 1.44 | 2 (14%) |
| 1 | IDS | 7-A | 4 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 7-A | 5 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 7-A | 6 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 7-A | 7 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 7-A | 8 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 7-A | 9 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 8-A | 1 | 1 | 20,20,20 | 1.13 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 8-A | 10 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 11 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 8-A | 12 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 13 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 8-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 8-A | 15 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 8-A | 16 | 1 | 16,16,17 | 1.40 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 17 | 1 | 19,19,20 | 1.29 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 8-A | 18 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 8-A | 2 | 1 | 16,16,17 | 1.42 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | IDS | 8-A | 20 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 21 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 8-A | 22 | 1 | 16,16,17 | 1.40 | 3 (18%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 8-A | 23 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 8-A | 24 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 25 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 8-A | 26 | 1 | 16,16,17 | 1.44 | 3 (18%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 8-A | 27 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 8-A | 28 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 29 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 8-A | 3 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | IDS | 8-A | 30 | 1 | 15,15,17 | 1.53 | 2 (13%) | 14,22,26 | 1.45 | 2 (14%) |
| 1 | IDS | 8-A | 4 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 8-A | 5 | 1 | 19,19,20 | 1.24 | 1 (5%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 8-A | 6 | 1 | 16,16,17 | 1.44 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 7 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 8-A | 8 | 1 | 16,16,17 | 1.45 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 8-A | 9 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 9-A | 1 | 1 | 20,20,20 | 1.12 | 1 (5%) | 25,31,31 | 1.00 | 1 (4%) |
| 1 | IDS | 9-A | 10 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 9-A | 11 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 9-A | 12 | 1 | 16,16,17 | 1.41 | 3 (18%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 9-A | 13 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 9-A | 14 | 1 | 16,16,17 | 1.44 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 9-A | 15 | 1 | 19,19,20 | 1.25 | 1 (5%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 9-A | 16 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 9-A | 17 | 1 | 19,19,20 | 1.28 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 9-A | 18 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.18 | 2 (12%) |
| 1 | SGN | 9-A | 19 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.09 | 1 (4%) |
| 1 | IDS | 9-A | 2 | 1 | 16,16,17 | 1.42 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | IDS | 9-A | 20 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 9-A | 21 | 1 | 19,19,20 | 1.27 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 9-A | 22 | 1 | 16,16,17 | 1.43 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 9-A | 23 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 9-A | 24 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 9-A | 25 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 9-A | 26 | 1 | 16,16,17 | 1.43 | 2 (12%) | 16,24,26 | 1.20 | 2 (12%) |
| 1 | SGN | 9-A | 27 | 1 | 19,19,20 | 1.26 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 9-A | 28 | 1 | 16,16,17 | 1.42 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 9-A | 29 | 1 | 19,19,20 | 1.24 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | SGN | 9-A | 3 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 9-A | 30 | 1 | 15,15,17 | 1.53 | 2 (13%) | 14,22,26 | 1.44 | 2 (14%) |
| 1 | IDS | 9-A | 4 | 1 | 16,16,17 | 1.45 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 9-A | 5 | 1 | 19,19,20 | 1.26 | 1 (5%) | 23,29,31 | 1.10 | 1 (4%) |
| 1 | IDS | 9-A | 6 | 1 | 16,16,17 | 1.41 | 2 (12%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 9-A | 7 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 1 | IDS | 9-A | 8 | 1 | 16,16,17 | 1.44 | 3 (18%) | 16,24,26 | 1.19 | 2 (12%) |
| 1 | SGN | 9-A | 9 | 1 | 19,19,20 | 1.25 | 2 (10%) | 23,29,31 | 1.10 | 1 (4%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | SGN | 1-A | 1 | 1 | - | 8/11/31/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 10 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 11 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 12 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 13 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 14 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 15 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 16 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 17 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 18 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 19 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 2 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | IDS | 1-A | 20 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 21 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 22 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 23 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 24 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 25 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 26 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 27 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 28 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 29 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | SGN | 1-A | 3 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 30 | 1 | - | 3/9/22/29 | 0/1/1/1 |
| 1 | IDS | 1-A | 4 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 5 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 1-A | 6 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 7 | 1 | - | 3/11/28/31 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | IDS | 1-A | 8 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 1-A | 9 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | SGN | 10-A | 1 | 1 | - | 4/11/31/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 10 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 11 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 12 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 13 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 14 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 15 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 16 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 17 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 18 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 19 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 2 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | IDS | 10-A | 20 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 21 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 22 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 23 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 24 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 25 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 26 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 27 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 28 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 29 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | SGN | 10-A | 3 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 30 | 1 | - | 1/9/22/29 | 0/1/1/1 |
| 1 | IDS | 10-A | 4 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 5 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 6 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 7 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 10-A | 8 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 10-A | 9 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | SGN | 11-A | 1 | 1 | - | 4/11/31/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 10 | 1 | - | 7/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 11 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 12 | 1 | - | 3/9/26/29 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | SGN | 11-A | 13 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 14 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 15 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 16 | 1 | - | 6/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 17 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 18 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 19 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 2 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | IDS | 11-A | 20 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 21 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 22 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 23 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 24 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 25 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 26 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 27 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 28 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 29 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | SGN | 11-A | 3 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 30 | 1 | - | 0/9/22/29 | 0/1/1/1 |
| 1 | IDS | 11-A | 4 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 5 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 6 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 7 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 11-A | 8 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 11-A | 9 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | SGN | 12-A | 1 | 1 | - | 0/11/31/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 10 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 11 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 12 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 13 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 14 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 15 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 16 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 17 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 18 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 19 | 1 | - | 3/11/28/31 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | IDS | 12-A | 2 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | IDS | 12-A | 20 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 21 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 22 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 23 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 24 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 25 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 26 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 27 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 28 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 29 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | SGN | 12-A | 3 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 30 | 1 | - | 2/9/22/29 | 0/1/1/1 |
| 1 | IDS | 12-A | 4 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 5 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 6 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 7 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 12-A | 8 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 12-A | 9 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | SGN | 13-A | 1 | 1 | - | 8/11/31/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 10 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 11 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 12 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 13 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 14 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 15 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 16 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 17 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 18 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 19 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 2 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | IDS | 13-A | 20 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 21 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 22 | 1 | - | 7/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 23 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 24 | 1 | - | 4/9/26/29 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | SGN | 13-A | 25 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 26 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 27 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 28 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 29 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | SGN | 13-A | 3 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 30 | 1 | - | 0/9/22/29 | 0/1/1/1 |
| 1 | IDS | 13-A | 4 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 5 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 6 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 7 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 13-A | 8 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 13-A | 9 | 1 | - | 9/11/28/31 | 0/1/1/1 |
| 1 | SGN | 14-A | 1 | 1 | - | 3/11/31/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 10 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 11 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 12 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 13 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 14 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 15 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 16 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 17 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 18 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 19 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 2 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | IDS | 14-A | 20 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 21 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 22 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 23 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 24 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 25 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 26 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 27 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 28 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 29 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | SGN | 14-A | 3 | 1 | - | 5/11/28/31 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | IDS | 14-A | 30 | 1 | - | 0/9/22/29 | 0/1/1/1 |
| 1 | IDS | 14-A | 4 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 5 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 6 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 7 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 14-A | 8 | 1 | - | 7/9/26/29 | 0/1/1/1 |
| 1 | SGN | 14-A | 9 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | SGN | 2-A | 1 | 1 | - | 3/11/31/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 10 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 11 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 12 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 13 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 14 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 15 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 16 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 17 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 18 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 19 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 2 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | IDS | 2-A | 20 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 21 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 22 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 23 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 24 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 25 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 26 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 27 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 28 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 29 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | SGN | 2-A | 3 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 30 | 1 | - | 2/9/22/29 | 0/1/1/1 |
| 1 | IDS | 2-A | 4 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 5 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 6 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 2-A | 7 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 2-A | 8 | 1 | - | 3/9/26/29 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | SGN | 2-A | 9 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | SGN | 3-A | 1 | 1 | - | 7/11/31/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 10 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 11 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 12 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 13 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 14 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 15 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 16 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 17 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 18 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 19 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 2 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | IDS | 3-A | 20 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 21 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 22 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 23 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 24 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 25 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 26 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 27 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 28 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 29 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | SGN | 3-A | 3 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 30 | 1 | - | 3/9/22/29 | 0/1/1/1 |
| 1 | IDS | 3-A | 4 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 5 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 6 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 7 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 3-A | 8 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 3-A | 9 | 1 | - | 9/11/28/31 | 0/1/1/1 |
| 1 | SGN | 4-A | 1 | 1 | - | 4/11/31/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 10 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 11 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 12 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 13 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 14 | 1 | - | 0/9/26/29 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | SGN | 4-A | 15 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 16 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 17 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 18 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 19 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 2 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | IDS | 4-A | 20 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 21 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 22 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 23 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 24 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 25 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 26 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 27 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 28 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 29 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | SGN | 4-A | 3 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 30 | 1 | - | 4/9/22/29 | 0/1/1/1 |
| 1 | IDS | 4-A | 4 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 5 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 6 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 7 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 4-A | 8 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 4-A | 9 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | SGN | 5-A | 1 | 1 | - | 7/11/31/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 10 | 1 | - | 7/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 11 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 12 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 13 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 14 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 15 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 16 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 17 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 18 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 19 | 1 | - | 3/11/28/31 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | IDS | 5-A | 2 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | IDS | 5-A | 20 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 21 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 22 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 23 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 24 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 25 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 26 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 27 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 28 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 29 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | SGN | 5-A | 3 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 30 | 1 | - | 1/9/22/29 | 0/1/1/1 |
| 1 | IDS | 5-A | 4 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 5 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 6 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 7 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 5-A | 8 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 5-A | 9 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | SGN | 6-A | 1 | 1 | - | 5/11/31/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 10 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 11 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 12 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 13 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 14 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 15 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 16 | 1 | - | 6/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 17 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 18 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 19 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 2 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | IDS | 6-A | 20 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 21 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 22 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 23 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 24 | 1 | - | 2/9/26/29 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 1 | SGN | 6-A | 25 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 26 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 27 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 28 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 29 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | SGN | 6-A | 3 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 30 | 1 | - | 1/9/22/29 | 0/1/1/1 |
| 1 | IDS | 6-A | 4 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 5 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 6 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 7 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 6-A | 8 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 6-A | 9 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | SGN | 7-A | 1 | 1 | - | 10/11/31/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 10 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 11 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 12 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 13 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 14 | 1 | - | 6/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 15 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 16 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 17 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 18 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 19 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 2 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | IDS | 7-A | 20 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 21 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 22 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 23 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 24 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 25 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 26 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 27 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 28 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 29 | 1 | - | 6/11/28/31 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | SGN | 7-A | 3 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 30 | 1 | - | 1/9/22/29 | 0/1/1/1 |
| 1 | IDS | 7-A | 4 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 5 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 6 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 7 | 1 | - | 8/11/28/31 | 0/1/1/1 |
| 1 | IDS | 7-A | 8 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 7-A | 9 | 1 | - | 0/11/28/31 | 0/1/1/1 |
| 1 | SGN | 8-A | 1 | 1 | - | 5/11/31/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 10 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 11 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 12 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 13 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 14 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 15 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 16 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 17 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 18 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 19 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 2 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | IDS | 8-A | 20 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 21 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 22 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 23 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 24 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 25 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 26 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 27 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 28 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 29 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | SGN | 8-A | 3 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 30 | 1 | - | 2/9/22/29 | 0/1/1/1 |
| 1 | IDS | 8-A | 4 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 5 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 8-A | 6 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 7 | 1 | - | 1/11/28/31 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 1 | IDS | 8-A | 8 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 8-A | 9 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | SGN | 9-A | 1 | 1 | - | 5/11/31/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 10 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 11 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 12 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 13 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 14 | 1 | - | 3/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 15 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 16 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 17 | 1 | - | 1/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 18 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 19 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 2 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | IDS | 9-A | 20 | 1 | - | 1/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 21 | 1 | - | 7/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 22 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 23 | 1 | - | 5/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 24 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 25 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 26 | 1 | - | 5/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 27 | 1 | - | 6/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 28 | 1 | - | 2/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 29 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | SGN | 9-A | 3 | 1 | - | 4/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 30 | 1 | - | 2/9/22/29 | 0/1/1/1 |
| 1 | IDS | 9-A | 4 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 5 | 1 | - | 3/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 6 | 1 | - | 4/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 7 | 1 | - | 2/11/28/31 | 0/1/1/1 |
| 1 | IDS | 9-A | 8 | 1 | - | 0/9/26/29 | 0/1/1/1 |
| 1 | SGN | 9-A | 9 | 1 | - | 6/11/28/31 | 0/1/1/1 |

The worst 5 of 868 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | 4-A | 27 | SGN | S1-N2 | 3.83 | 1.64 | 1.59 |
| 1 | 7-A | 17 | SGN | S1-N2 | 3.82 | 1.64 | 1.59 |
| 1 | 8-A | 17 | SGN | S1-N2 | 3.82 | 1.64 | 1.59 |
| 1 | 2-A | 4 | IDS | O2-C2 | -3.82 | 1.41 | 1.47 |
| 1 | 9-A | 4 | IDS | O2-C2 | -3.82 | 1.41 | 1.47 |

The worst 5 of 630 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 1 | 5-A | 30 | IDS | O6B-C6-C5 | 3.46 | 121.70 | 112.71 |
| 1 | 11-A | 30 | IDS | O6B-C6-C5 | 3.45 | 121.69 | 112.71 |
| 1 | 13-A | 30 | IDS | O6B-C6-C5 | 3.44 | 121.66 | 112.71 |
| 1 | 6-A | 30 | IDS | O6B-C6-C5 | 3.44 | 121.65 | 112.71 |
| 1 | 10-A | 30 | IDS | O6B-C6-C5 | 3.44 | 121.65 | 112.71 |

There are no chirality outliers.

5 of 1369 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 1 | 1-A | 1 | SGN | C4-C5-C6-O6 |
| 1 | 1-A | 1 | SGN | O5-C5-C6-O6 |
| 1 | 1-A | 1 | SGN | C2-N2-S1-O2S |
| 1 | 1-A | 1 | SGN | C2-N2-S1-O3S |
| 1 | 2-A | 1 | SGN | C2-N2-S1-O1S |

There are no ring outliers.

379 monomers are involved in 917 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 3-A | 8 | IDS | 1 | 0 |
| 1 | 4-A | 14 | IDS | 2 | 0 |
| 1 | 9-A | 17 | SGN | 12 | 0 |
| 1 | 2-A | 17 | SGN | 2 | 0 |
| 1 | 12-A | 19 | SGN | 3 | 0 |
| 1 | 2-A | 30 | IDS | 4 | 0 |
| 1 | 9-A | 9 | SGN | 5 | 0 |
| 1 | 14-A | 12 | IDS | 7 | 0 |
| 1 | 1-A | 6 | IDS | 3 | 0 |
| 1 | 8-A | 9 | SGN | 9 | 0 |
| 1 | 1-A | 9 | SGN | 4 | 0 |
| 1 | 3-A | 29 | SGN | 11 | 0 |
| 1 | 7-A | 17 | SGN | 8 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 4-A | 22 | IDS | 4 | 0 |
| 1 | 8-A | 28 | IDS | 5 | 0 |
| 1 | 10-A | 2 | IDS | 3 | 0 |
| 1 | 11-A | 11 | SGN | 1 | 0 |
| 1 | 13-A | 14 | IDS | 3 | 0 |
| 1 | 5-A | 18 | IDS | 2 | 0 |
| 1 | 8-A | 20 | IDS | 1 | 0 |
| 1 | 7-A | 4 | IDS | 8 | 0 |
| 1 | 6-A | 22 | IDS | 4 | 0 |
| 1 | 13-A | 22 | IDS | 2 | 0 |
| 1 | 13-A | 19 | SGN | 6 | 0 |
| 1 | 5-A | 25 | SGN | 9 | 0 |
| 1 | 6-A | 28 | IDS | 1 | 0 |
| 1 | 8-A | 6 | IDS | 3 | 0 |
| 1 | 3-A | 12 | IDS | 2 | 0 |
| 1 | 10-A | 19 | SGN | 4 | 0 |
| 1 | 3-A | 20 | IDS | 12 | 0 |
| 1 | 10-A | 16 | IDS | 2 | 0 |
| 1 | 9-A | 5 | SGN | 2 | 0 |
| 1 | 2-A | 19 | SGN | 1 | 0 |
| 1 | 6-A | 10 | IDS | 3 | 0 |
| 1 | 13-A | 10 | IDS | 5 | 0 |
| 1 | 7-A | 27 | SGN | 6 | 0 |
| 1 | 3-A | 18 | IDS | 1 | 0 |
| 1 | 7-A | 8 | IDS | 3 | 0 |
| 1 | 12-A | 15 | SGN | 5 | 0 |
| 1 | 5-A | 3 | SGN | 2 | 0 |
| 1 | 13-A | 12 | IDS | 11 | 0 |
| 1 | 10-A | 3 | SGN | 5 | 0 |
| 1 | 1-A | 28 | IDS | 3 | 0 |
| 1 | 3-A | 25 | SGN | 5 | 0 |
| 1 | 7-A | 15 | SGN | 2 | 0 |
| 1 | 11-A | 8 | IDS | 2 | 0 |
| 1 | 4-A | 5 | SGN | 1 | 0 |
| 1 | 3-A | 14 | IDS | 6 | 0 |
| 1 | 7-A | 14 | IDS | 2 | 0 |
| 1 | 10-A | 14 | IDS | 4 | 0 |
| 1 | 8-A | 14 | IDS | 3 | 0 |
| 1 | 4-A | 16 | IDS | 8 | 0 |
| 1 | 9-A | 18 | IDS | 13 | 0 |
| 1 | 13-A | 5 | SGN | 10 | 0 |
| 1 | 14-A | 15 | SGN | 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 1-A | 14 | IDS | 2 | 0 |
| 1 | 6-A | 21 | SGN | 3 | 0 |
| 1 | 9-A | 25 | SGN | 19 | 0 |
| 1 | 3-A | 22 | IDS | 10 | 0 |
| 1 | 13-A | 15 | SGN | 7 | 0 |
| 1 | 13-A | 28 | IDS | 14 | 0 |
| 1 | 9-A | 19 | SGN | 18 | 0 |
| 1 | 2-A | 11 | SGN | 3 | 0 |
| 1 | 4-A | 24 | IDS | 10 | 0 |
| 1 | 12-A | 17 | SGN | 1 | 0 |
| 1 | 8-A | 18 | IDS | 7 | 0 |
| 1 | 9-A | 1 | SGN | 2 | 0 |
| 1 | 2-A | 21 | SGN | 5 | 0 |
| 1 | 3-A | 10 | IDS | 5 | 0 |
| 1 | 9-A | 3 | SGN | 3 | 0 |
| 1 | 4-A | 8 | IDS | 5 | 0 |
| 1 | 13-A | 2 | IDS | 3 | 0 |
| 1 | 12-A | 21 | SGN | 2 | 0 |
| 1 | 8-A | 16 | IDS | 2 | 0 |
| 1 | 4-A | 17 | SGN | 4 | 0 |
| 1 | 11-A | 24 | IDS | 7 | 0 |
| 1 | 11-A | 27 | SGN | 2 | 0 |
| 1 | 10-A | 12 | IDS | 1 | 0 |
| 1 | 5-A | 24 | IDS | 1 | 0 |
| 1 | 7-A | 21 | SGN | 6 | 0 |
| 1 | 9-A | 8 | IDS | 5 | 0 |
| 1 | 7-A | 13 | SGN | 2 | 0 |
| 1 | 13-A | 26 | IDS | 2 | 0 |
| 1 | 2-A | 13 | SGN | 1 | 0 |
| 1 | 6-A | 30 | IDS | 6 | 0 |
| 1 | 12-A | 16 | IDS | 5 | 0 |
| 1 | 4-A | 4 | IDS | 2 | 0 |
| 1 | 1-A | 11 | SGN | 8 | 0 |
| 1 | 6-A | 5 | SGN | 2 | 0 |
| 1 | 12-A | 30 | IDS | 1 | 0 |
| 1 | 5-A | 17 | SGN | 2 | 0 |
| 1 | 12-A | 23 | SGN | 1 | 0 |
| 1 | 13-A | 4 | IDS | 7 | 0 |
| 1 | 11-A | 21 | SGN | 6 | 0 |
| 1 | 7-A | 5 | SGN | 2 | 0 |
| 1 | 10-A | 21 | SGN | 1 | 0 |
| 1 | 7-A | 26 | IDS | 8 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 7-A | 23 | SGN | 6 | 0 |
| 1 | 11-A | 13 | SGN | 7 | 0 |
| 1 | 5-A | 13 | SGN | 3 | 0 |
| 1 | 4-A | 20 | IDS | 15 | 0 |
| 1 | 2-A | 23 | SGN | 9 | 0 |
| 1 | 8-A | 15 | SGN | 3 | 0 |
| 1 | 9-A | 27 | SGN | 2 | 0 |
| 1 | 14-A | 23 | SGN | 8 | 0 |
| 1 | 1-A | 29 | SGN | 1 | 0 |
| 1 | 6-A | 2 | IDS | 2 | 0 |
| 1 | 7-A | 10 | IDS | 14 | 0 |
| 1 | 11-A | 26 | IDS | 1 | 0 |
| 1 | 11-A | 20 | IDS | 8 | 0 |
| 1 | 14-A | 11 | SGN | 4 | 0 |
| 1 | 13-A | 30 | IDS | 1 | 0 |
| 1 | 11-A | 16 | IDS | 6 | 0 |
| 1 | 13-A | 23 | SGN | 1 | 0 |
| 1 | 1-A | 3 | SGN | 2 | 0 |
| 1 | 6-A | 17 | SGN | 6 | 0 |
| 1 | 7-A | 2 | IDS | 6 | 0 |
| 1 | 7-A | 22 | IDS | 9 | 0 |
| 1 | 11-A | 10 | IDS | 2 | 0 |
| 1 | 14-A | 2 | IDS | 3 | 0 |
| 1 | 10-A | 10 | IDS | 4 | 0 |
| 1 | 4-A | 27 | SGN | 4 | 0 |
| 1 | 8-A | 12 | IDS | 2 | 0 |
| 1 | 3-A | 17 | SGN | 5 | 0 |
| 1 | 10-A | 17 | SGN | 2 | 0 |
| 1 | 6-A | 3 | SGN | 4 | 0 |
| 1 | 2-A | 10 | IDS | 3 | 0 |
| 1 | 4-A | 1 | SGN | 2 | 0 |
| 1 | 14-A | 25 | SGN | 6 | 0 |
| 1 | 3-A | 4 | IDS | 12 | 0 |
| 1 | 5-A | 4 | IDS | 2 | 0 |
| 1 | 8-A | 24 | IDS | 12 | 0 |
| 1 | 10-A | 4 | IDS | 4 | 0 |
| 1 | 14-A | 5 | SGN | 2 | 0 |
| 1 | 3-A | 6 | IDS | 5 | 0 |
| 1 | 2-A | 2 | IDS | 1 | 0 |
| 1 | 9-A | 21 | SGN | 8 | 0 |
| 1 | 5-A | 2 | IDS | 5 | 0 |
| 1 | 5-A | 22 | IDS | 6 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 10-A | 22 | IDS | 2 | 0 |
| 1 | 14-A | 3 | SGN | 3 | 0 |
| 1 | 14-A | 6 | IDS | 6 | 0 |
| 1 | 9-A | 13 | SGN | 10 | 0 |
| 1 | 3-A | 3 | SGN | 7 | 0 |
| 1 | 5-A | 9 | SGN | 1 | 0 |
| 1 | 10-A | 26 | IDS | 2 | 0 |
| 1 | 3-A | 30 | IDS | 11 | 0 |
| 1 | 10-A | 30 | IDS | 2 | 0 |
| 1 | 14-A | 24 | IDS | 10 | 0 |
| 1 | 14-A | 18 | IDS | 1 | 0 |
| 1 | 4-A | 21 | SGN | 5 | 0 |
| 1 | 6-A | 15 | SGN | 12 | 0 |
| 1 | 14-A | 7 | SGN | 9 | 0 |
| 1 | 1-A | 13 | SGN | 2 | 0 |
| 1 | 8-A | 5 | SGN | 3 | 0 |
| 1 | 13-A | 11 | SGN | 2 | 0 |
| 1 | 13-A | 1 | SGN | 3 | 0 |
| 1 | 5-A | 14 | IDS | 9 | 0 |
| 1 | 6-A | 27 | SGN | 1 | 0 |
| 1 | 9-A | 2 | IDS | 5 | 0 |
| 1 | 8-A | 10 | IDS | 11 | 0 |
| 1 | 1-A | 16 | IDS | 2 | 0 |
| 1 | 6-A | 8 | IDS | 5 | 0 |
| 1 | 8-A | 2 | IDS | 1 | 0 |
| 1 | 6-A | 19 | SGN | 2 | 0 |
| 1 | 4-A | 6 | IDS | 12 | 0 |
| 1 | 7-A | 20 | IDS | 1 | 0 |
| 1 | 12-A | 28 | IDS | 13 | 0 |
| 1 | 14-A | 8 | IDS | 4 | 0 |
| 1 | 2-A | 29 | SGN | 5 | 0 |
| 1 | 1-A | 12 | IDS | 1 | 0 |
| 1 | 7-A | 28 | IDS | 3 | 0 |
| 1 | 8-A | 25 | SGN | 6 | 0 |
| 1 | 12-A | 29 | SGN | 1 | 0 |
| 1 | 14-A | 19 | SGN | 5 | 0 |
| 1 | 6-A | 13 | SGN | 7 | 0 |
| 1 | 2-A | 15 | SGN | 2 | 0 |
| 1 | 5-A | 27 | SGN | 4 | 0 |
| 1 | 12-A | 11 | SGN | 6 | 0 |
| 1 | 11-A | 5 | SGN | 7 | 0 |
| 1 | 8-A | 11 | SGN | 2 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 11-A | 28 | IDS | 2 | 0 |
| 1 | 5-A | 15 | SGN | 7 | 0 |
| 1 | 13-A | 29 | SGN | 10 | 0 |
| 1 | 6-A | 23 | SGN | 3 | 0 |
| 1 | 12-A | 13 | SGN | 5 | 0 |
| 1 | 7-A | 16 | IDS | 7 | 0 |
| 1 | 3-A | 19 | SGN | 4 | 0 |
| 1 | 10-A | 29 | SGN | 5 | 0 |
| 1 | 4-A | 13 | SGN | 12 | 0 |
| 1 | 11-A | 6 | IDS | 7 | 0 |
| 1 | 1-A | 27 | SGN | 2 | 0 |
| 1 | 3-A | 15 | SGN | 2 | 0 |
| 1 | 4-A | 2 | IDS | 4 | 0 |
| 1 | 10-A | 15 | SGN | 4 | 0 |
| 1 | 6-A | 4 | IDS | 2 | 0 |
| 1 | 13-A | 21 | SGN | 4 | 0 |
| 1 | 9-A | 14 | IDS | 11 | 0 |
| 1 | 13-A | 13 | SGN | 12 | 0 |
| 1 | 5-A | 16 | IDS | 1 | 0 |
| 1 | 14-A | 14 | IDS | 5 | 0 |
| 1 | 11-A | 17 | SGN | 7 | 0 |
| 1 | 4-A | 19 | SGN | 16 | 0 |
| 1 | 3-A | 27 | SGN | 1 | 0 |
| 1 | 7-A | 11 | SGN | 6 | 0 |
| 1 | 2-A | 9 | SGN | 1 | 0 |
| 1 | 14-A | 22 | IDS | 5 | 0 |
| 1 | 5-A | 23 | SGN | 5 | 0 |
| 1 | 12-A | 20 | IDS | 4 | 0 |
| 1 | 5-A | 21 | SGN | 3 | 0 |
| 1 | 8-A | 22 | IDS | 2 | 0 |
| 1 | 14-A | 13 | SGN | 6 | 0 |
| 1 | 12-A | 5 | SGN | 1 | 0 |
| 1 | 9-A | 23 | SGN | 9 | 0 |
| 1 | 8-A | 19 | SGN | 5 | 0 |
| 1 | 13-A | 9 | SGN | 6 | 0 |
| 1 | 14-A | 26 | IDS | 1 | 0 |
| 1 | 4-A | 28 | IDS | 4 | 0 |
| 1 | 6-A | 24 | IDS | 6 | 0 |
| 1 | 6-A | 18 | IDS | 6 | 0 |
| 1 | 7-A | 29 | SGN | 2 | 0 |
| 1 | 6-A | 7 | SGN | 2 | 0 |
| 1 | 1-A | 5 | SGN | 2 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 13-A | 20 | IDS | 3 | 0 |
| 1 | 5-A | 26 | IDS | 9 | 0 |
| 1 | 1-A | 23 | SGN | 7 | 0 |
| 1 | 6-A | 25 | SGN | 5 | 0 |
| 1 | 13-A | 25 | SGN | 3 | 0 |
| 1 | 7-A | 12 | IDS | 2 | 0 |
| 1 | 14-A | 21 | SGN | 2 | 0 |
| 1 | 4-A | 15 | SGN | 6 | 0 |
| 1 | 3-A | 13 | SGN | 7 | 0 |
| 1 | 5-A | 30 | IDS | 1 | 0 |
| 1 | 10-A | 13 | SGN | 1 | 0 |
| 1 | 2-A | 26 | IDS | 10 | 0 |
| 1 | 12-A | 25 | SGN | 6 | 0 |
| 1 | 5-A | 10 | IDS | 1 | 0 |
| 1 | 2-A | 16 | IDS | 1 | 0 |
| 1 | 11-A | 4 | IDS | 4 | 0 |
| 1 | 14-A | 4 | IDS | 5 | 0 |
| 1 | 1-A | 4 | IDS | 3 | 0 |
| 1 | 1-A | 24 | IDS | 6 | 0 |
| 1 | 1-A | 22 | IDS | 5 | 0 |
| 1 | 1-A | 2 | IDS | 5 | 0 |
| 1 | 12-A | 12 | IDS | 3 | 0 |
| 1 | 1-A | 25 | SGN | 7 | 0 |
| 1 | 11-A | 9 | SGN | 2 | 0 |
| 1 | 7-A | 6 | IDS | 1 | 0 |
| 1 | 4-A | 12 | IDS | 12 | 0 |
| 1 | 3-A | 21 | SGN | 13 | 0 |
| 1 | 2-A | 24 | IDS | 10 | 0 |
| 1 | 2-A | 18 | IDS | 3 | 0 |
| 1 | 2-A | 12 | IDS | 1 | 0 |
| 1 | 8-A | 17 | SGN | 2 | 0 |
| 1 | 2-A | 7 | SGN | 4 | 0 |
| 1 | 4-A | 11 | SGN | 7 | 0 |
| 1 | 12-A | 18 | IDS | 1 | 0 |
| 1 | 12-A | 7 | SGN | 10 | 0 |
| 1 | 11-A | 25 | SGN | 2 | 0 |
| 1 | 1-A | 21 | SGN | 2 | 0 |
| 1 | 2-A | 25 | SGN | 3 | 0 |
| 1 | 7-A | 24 | IDS | 8 | 0 |
| 1 | 7-A | 18 | IDS | 2 | 0 |
| 1 | 9-A | 26 | IDS | 13 | 0 |
| 1 | 13-A | 3 | SGN | 2 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 7-A | 7 | SGN | 3 | 0 |
| 1 | 8-A | 7 | SGN | 1 | 0 |
| 1 | 9-A | 16 | IDS | 11 | 0 |
| 1 | 9-A | 20 | IDS | 15 | 0 |
| 1 | 1-A | 18 | IDS | 1 | 0 |
| 1 | 11-A | 14 | IDS | 2 | 0 |
| 1 | 11-A | 12 | IDS | 8 | 0 |
| 1 | 10-A | 6 | IDS | 3 | 0 |
| 1 | 3-A | 23 | SGN | 6 | 0 |
| 1 | 2-A | 3 | SGN | 2 | 0 |
| 1 | 1-A | 7 | SGN | 6 | 0 |
| 1 | 10-A | 23 | SGN | 3 | 0 |
| 1 | 7-A | 25 | SGN | 4 | 0 |
| 1 | 3-A | 26 | IDS | 4 | 0 |
| 1 | 14-A | 17 | SGN | 4 | 0 |
| 1 | 2-A | 4 | IDS | 2 | 0 |
| 1 | 13-A | 18 | IDS | 6 | 0 |
| 1 | 8-A | 30 | IDS | 1 | 0 |
| 1 | 8-A | 23 | SGN | 7 | 0 |
| 1 | 12-A | 27 | SGN | 13 | 0 |
| 1 | 2-A | 8 | IDS | 1 | 0 |
| 1 | 11-A | 18 | IDS | 6 | 0 |
| 1 | 8-A | 21 | SGN | 3 | 0 |
| 1 | 4-A | 29 | SGN | 1 | 0 |
| 1 | 10-A | 18 | IDS | 4 | 0 |
| 1 | 9-A | 12 | IDS | 7 | 0 |
| 1 | 11-A | 7 | SGN | 5 | 0 |
| 1 | 10-A | 7 | SGN | 2 | 0 |
| 1 | 12-A | 8 | IDS | 4 | 0 |
| 1 | 5-A | 28 | IDS | 6 | 0 |
| 1 | 2-A | 20 | IDS | 4 | 0 |
| 1 | 10-A | 25 | SGN | 2 | 0 |
| 1 | 8-A | 4 | IDS | 1 | 0 |
| 1 | 4-A | 10 | IDS | 15 | 0 |
| 1 | 5-A | 29 | SGN | 3 | 0 |
| 1 | 7-A | 9 | SGN | 9 | 0 |
| 1 | 6-A | 14 | IDS | 4 | 0 |
| 1 | 1-A | 8 | IDS | 4 | 0 |
| 1 | 7-A | 19 | SGN | 1 | 0 |
| 1 | 4-A | 25 | SGN | 8 | 0 |
| 1 | 11-A | 22 | IDS | 3 | 0 |
| 1 | 3-A | 11 | SGN | 6 | 0 |

Continued on next page...

Continued from previous page...

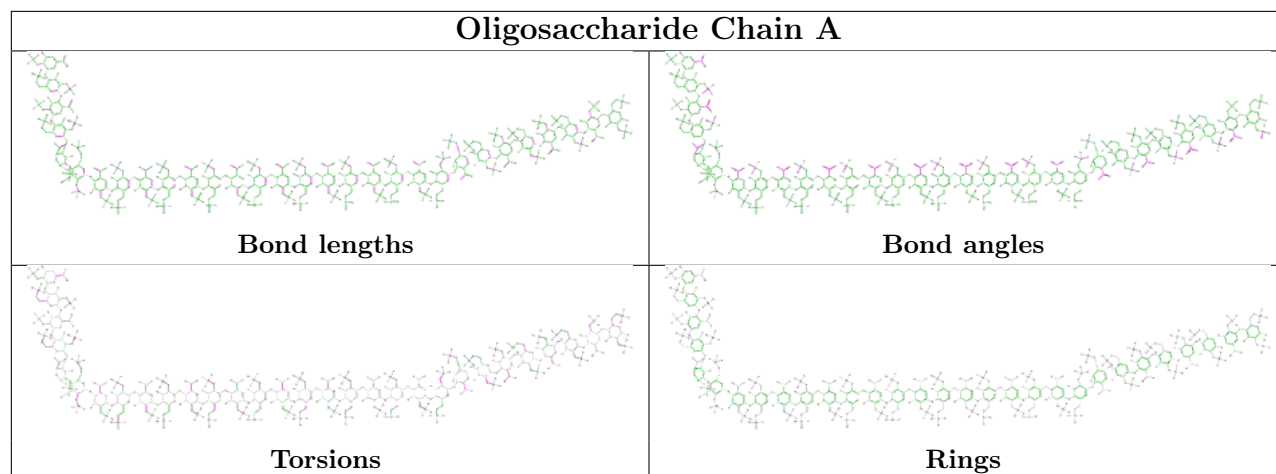
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 9-A | 6 | IDS | 6 | 0 |
| 1 | 12-A | 6 | IDS | 7 | 0 |
| 1 | 2-A | 14 | IDS | 2 | 0 |
| 1 | 2-A | 27 | SGN | 10 | 0 |
| 1 | 10-A | 8 | IDS | 3 | 0 |
| 1 | 4-A | 26 | IDS | 3 | 0 |
| 1 | 12-A | 24 | IDS | 7 | 0 |
| 1 | 9-A | 7 | SGN | 4 | 0 |
| 1 | 11-A | 15 | SGN | 6 | 0 |
| 1 | 2-A | 28 | IDS | 5 | 0 |
| 1 | 3-A | 5 | SGN | 11 | 0 |
| 1 | 13-A | 6 | IDS | 5 | 0 |
| 1 | 4-A | 7 | SGN | 11 | 0 |
| 1 | 6-A | 11 | SGN | 5 | 0 |
| 1 | 9-A | 22 | IDS | 7 | 0 |
| 1 | 2-A | 22 | IDS | 1 | 0 |
| 1 | 4-A | 18 | IDS | 7 | 0 |
| 1 | 2-A | 1 | SGN | 1 | 0 |
| 1 | 10-A | 27 | SGN | 4 | 0 |
| 1 | 6-A | 16 | IDS | 10 | 0 |
| 1 | 7-A | 3 | SGN | 9 | 0 |
| 1 | 6-A | 20 | IDS | 1 | 0 |
| 1 | 13-A | 24 | IDS | 1 | 0 |
| 1 | 10-A | 28 | IDS | 6 | 0 |
| 1 | 14-A | 1 | SGN | 3 | 0 |
| 1 | 13-A | 7 | SGN | 2 | 0 |
| 1 | 3-A | 2 | IDS | 1 | 0 |
| 1 | 6-A | 9 | SGN | 6 | 0 |
| 1 | 3-A | 24 | IDS | 3 | 0 |
| 1 | 10-A | 24 | IDS | 3 | 0 |
| 1 | 12-A | 22 | IDS | 2 | 0 |
| 1 | 11-A | 3 | SGN | 1 | 0 |
| 1 | 8-A | 1 | SGN | 1 | 0 |
| 1 | 14-A | 9 | SGN | 1 | 0 |
| 1 | 9-A | 29 | SGN | 1 | 0 |
| 1 | 12-A | 10 | IDS | 5 | 0 |
| 1 | 6-A | 6 | IDS | 2 | 0 |
| 1 | 6-A | 12 | IDS | 10 | 0 |
| 1 | 5-A | 11 | SGN | 1 | 0 |
| 1 | 14-A | 16 | IDS | 5 | 0 |
| 1 | 4-A | 9 | SGN | 14 | 0 |
| 1 | 10-A | 11 | SGN | 4 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 1 | 1-A | 1 | SGN | 5 | 0 |
| 1 | 5-A | 1 | SGN | 5 | 0 |
| 1 | 9-A | 15 | SGN | 11 | 0 |
| 1 | 1-A | 26 | IDS | 3 | 0 |
| 1 | 4-A | 23 | SGN | 9 | 0 |
| 1 | 1-A | 20 | IDS | 2 | 0 |
| 1 | 5-A | 20 | IDS | 1 | 0 |
| 1 | 13-A | 8 | IDS | 1 | 0 |
| 1 | 8-A | 29 | SGN | 6 | 0 |
| 1 | 1-A | 10 | IDS | 11 | 0 |
| 1 | 11-A | 23 | SGN | 9 | 0 |
| 1 | 11-A | 19 | SGN | 4 | 0 |
| 1 | 9-A | 28 | IDS | 2 | 0 |
| 1 | 13-A | 16 | IDS | 7 | 0 |
| 1 | 6-A | 29 | SGN | 6 | 0 |
| 1 | 3-A | 16 | IDS | 6 | 0 |
| 1 | 9-A | 24 | IDS | 18 | 0 |
| 1 | 5-A | 12 | IDS | 1 | 0 |
| 1 | 14-A | 20 | IDS | 6 | 0 |
| 1 | 2-A | 6 | IDS | 3 | 0 |
| 1 | 8-A | 13 | SGN | 5 | 0 |
| 1 | 9-A | 11 | SGN | 3 | 0 |
| 1 | 13-A | 27 | SGN | 5 | 0 |
| 1 | 4-A | 3 | SGN | 4 | 0 |
| 1 | 1-A | 17 | SGN | 3 | 0 |
| 1 | 12-A | 14 | IDS | 4 | 0 |
| 1 | 3-A | 9 | SGN | 1 | 0 |
| 1 | 10-A | 9 | SGN | 2 | 0 |
| 1 | 10-A | 5 | SGN | 4 | 0 |
| 1 | 7-A | 1 | SGN | 5 | 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.



4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.