



Full wwPDB Geometry-Only Validation Report ⓘ

Mar 8, 2026 – 05:27 AM UTC

PDB ID : 3IRI / pdb_00003iri
Title : Solution Structure of Heparin dp18
Authors : Khan, S.; Gor, J.; Mulloy, B.; Perkins, S.J.
Deposited on : 2009-08-24
Resolution : Not provided

This is a Full wwPDB Geometry-Only Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

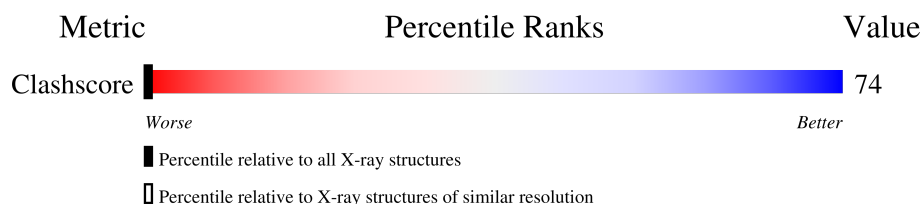
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION SCATTERING

The reported resolution of this entry is unknown.

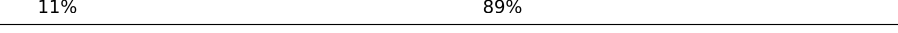
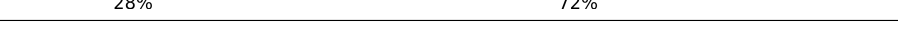
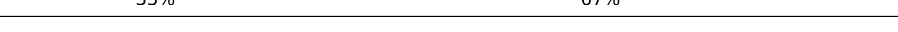
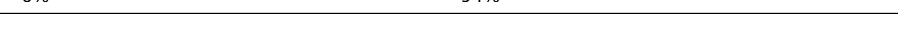
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	18	 11% 89%
1	2-A	18	 6% 94%
1	3-A	18	 6% 94%
1	4-A	18	 22% 78%
1	5-A	18	 11% 89%
1	6-A	18	 11% 89%
1	7-A	18	 28% 72%
1	8-A	18	 33% 67%
1	9-A	18	 6% 94%

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	SGN	1-A	13	-	-	X	-
1	IDS	1-A	16	-	-	X	-
1	SGN	1-A	17	-	-	X	-
1	SGN	1-A	5	-	-	X	-
1	IDS	1-A	6	-	-	X	-
1	IDS	2-A	10	-	-	X	-
1	SGN	2-A	11	-	-	X	-
1	IDS	2-A	2	-	-	X	-
1	SGN	2-A	3	-	-	X	-
1	IDS	2-A	6	-	-	X	-
1	SGN	2-A	9	-	-	X	-
1	SGN	3-A	17	-	-	X	-
1	IDS	3-A	18	-	-	X	-
1	IDS	3-A	6	-	-	X	-
1	SGN	3-A	7	-	-	X	-
1	SGN	3-A	9	-	-	X	-
1	SGN	4-A	7	-	-	X	-
1	IDS	4-A	8	-	-	X	-
1	IDS	5-A	12	-	-	X	-
1	IDS	6-A	10	-	-	X	-
1	SGN	6-A	11	-	-	X	-
1	IDS	6-A	12	-	-	X	-
1	SGN	6-A	13	-	-	X	-
1	IDS	6-A	14	-	-	X	-
1	IDS	6-A	4	-	-	X	-
1	IDS	7-A	16	-	-	X	-
1	SGN	8-A	11	X	-	-	-
1	SGN	8-A	15	-	-	X	-
1	SGN	8-A	7	-	-	X	-
1	IDS	9-A	2	-	-	X	-

o-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 3-A:  6% 94%

SGN1	IDS2	SGN3	IDS4	SGN5	IDS6	SGN7	IDS8	SGN9	IDS10	SGN11	IDS12	SGN13	IDS14	SGN15	IDS16	SGN17	IDS18
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• 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

Chain 4-A:  22% 78%

SGN1	IDS2	SGN3	IDS4	SGN5	IDS6	SGN7	IDS8	SGN9	IDS10	SGN11	IDS12	SGN13	IDS14	SGN15	IDS16	SGN17	IDS18
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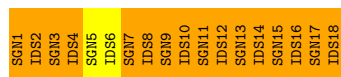
• Molecule 1: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic 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

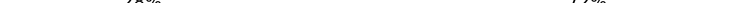
Chain 5-A:  11% 89%

SGN1	IDS2	SGN3	IDS4	SGN5	IDS6	SGN7	IDS8	SGN9	IDS10	SGN11	IDS12	SGN13	IDS14	SGN15	IDS16	SGN17	IDS18
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• Molecule 1: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha

Chain 6-A: 11% 89%



Chain 7-A:  28% 72%



Chain 8-A: 33% 67%

SGN1
IDS2
SGN3
IDS4
SGN5
IDS6
SGN7
IDS8
SGN9
IDS10
SGN11
IDS12
SGN13
IDS14
SGN15
IDS16
SGN17
IDS18

4 Model quality

4.1 Standard geometry

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

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	315	0	99	36	0
1	2-A	315	0	99	40	0
1	3-A	315	0	96	45	0
1	4-A	315	0	100	26	0
1	5-A	315	0	95	19	0
1	6-A	315	0	100	36	0
1	7-A	315	0	98	17	0
1	8-A	315	0	97	24	0
1	9-A	315	0	98	31	0
All	All	2835	0	882	274	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 74.

All (274) 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:15:SGN:C6	1:A:16:IDS:O2S	1.67	1.42
1:A:15:SGN:C6	1:A:16:IDS:S	2.10	1.40
1:A:8:IDS:H3	1:A:9:SGN:N2	1.28	1.40
1:A:15:SGN:C6	1:A:16:IDS:O2S	1.68	1.40
1:A:17:SGN:H61	1:A:18:IDS:S	1.65	1.35
1:A:12:IDS:O6A	1:A:13:SGN:C5	1.72	1.34
1:A:17:SGN:H61	1:A:18:IDS:O1S	1.28	1.33
1:A:7:SGN:C6	1:A:8:IDS:O2S	1.77	1.32
1:A:3:SGN:O3	1:A:4:IDS:H5	1.32	1.29
1:A:2:IDS:O3	1:A:3:SGN:O1S	1.53	1.26
1:A:16:IDS:H3	1:A:17:SGN:N2	1.24	1.25
1:A:8:IDS:O3	1:A:9:SGN:S1	1.94	1.24
1:A:3:SGN:O3	1:A:4:IDS:C5	1.87	1.21
1:A:17:SGN:C6	1:A:18:IDS:O2S	1.88	1.20
1:A:17:SGN:H61	1:A:18:IDS:O2S	1.04	1.19
1:A:10:IDS:H3	1:A:11:SGN:N2	1.45	1.17
1:A:16:IDS:C3	1:A:17:SGN:N2	2.05	1.16
1:A:10:IDS:O6A	1:A:11:SGN:H5	1.44	1.15
1:A:14:IDS:O3	1:A:15:SGN:O1S	1.64	1.15
1:A:13:SGN:O3	1:A:14:IDS:H5	1.48	1.14
1:A:12:IDS:O6A	1:A:13:SGN:H5	1.42	1.13
1:A:3:SGN:O6	1:A:4:IDS:O5	1.68	1.11
1:A:7:SGN:H61	1:A:8:IDS:O2S	1.38	1.11
1:A:7:SGN:O6	1:A:8:IDS:O2S	1.68	1.11
1:A:14:IDS:C3	1:A:15:SGN:O1S	1.99	1.10
1:A:16:IDS:O6A	1:A:17:SGN:H5	1.49	1.10
1:A:13:SGN:C6	1:A:14:IDS:O2S	2.00	1.09
1:A:8:IDS:O3	1:A:9:SGN:O1S	1.70	1.08
1:A:6:IDS:H3	1:A:7:SGN:N2	1.67	1.07
1:A:2:IDS:O3	1:A:3:SGN:S1	2.13	1.06
1:A:1:SGN:O3	1:A:2:IDS:H5	1.55	1.06
1:A:7:SGN:O4S	1:A:8:IDS:O1S	1.74	1.04
1:A:7:SGN:S2	1:A:8:IDS:O2S	2.15	1.04
1:A:17:SGN:C6	1:A:18:IDS:O1S	2.07	1.03
1:A:1:SGN:O4S	1:A:2:IDS:O1S	1.76	1.03
1:A:7:SGN:O3	1:A:8:IDS:H5	1.58	1.03
1:A:11:SGN:O3	1:A:12:IDS:O6B	1.73	1.03
1:A:8:IDS:C3	1:A:9:SGN:N2	2.23	1.02
1:A:6:IDS:C3	1:A:7:SGN:N2	2.22	1.02
1:A:11:SGN:O3	1:A:12:IDS:C5	2.08	1.01
1:A:3:SGN:O3	1:A:4:IDS:C5	2.08	1.01
1:A:8:IDS:O3	1:A:9:SGN:O3S	1.75	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:IDS:O3	1:A:7:SGN:O3S	1.79	1.00
1:A:1:SGN:H61	1:A:2:IDS:O2S	1.61	1.00
1:A:3:SGN:HO3	1:A:4:IDS:C6	1.75	1.00
1:A:6:IDS:O3	1:A:7:SGN:S1	2.18	0.99
1:A:12:IDS:O6A	1:A:13:SGN:C6	2.09	0.99
1:A:7:SGN:O4S	1:A:8:IDS:S	2.20	0.99
1:A:11:SGN:O3	1:A:12:IDS:C6	2.11	0.99
1:A:15:SGN:C5	1:A:16:IDS:O2S	2.09	0.99
1:A:12:IDS:O3	1:A:13:SGN:O1S	1.83	0.97
1:A:1:SGN:C6	1:A:2:IDS:O2S	2.14	0.96
1:A:14:IDS:H3	1:A:15:SGN:O1S	1.66	0.96
1:A:15:SGN:H61	1:A:16:IDS:O2S	1.64	0.96
1:A:7:SGN:H61	1:A:8:IDS:O2S	1.65	0.95
1:A:10:IDS:O6A	1:A:11:SGN:C5	2.14	0.95
1:A:13:SGN:H61	1:A:14:IDS:O2S	1.64	0.95
1:A:3:SGN:O3	1:A:4:IDS:C6	2.13	0.95
1:A:6:IDS:O3	1:A:7:SGN:S1	2.24	0.95
1:A:1:SGN:O4S	1:A:2:IDS:C1	2.15	0.94
1:A:14:IDS:H3	1:A:15:SGN:S1	2.07	0.94
1:A:3:SGN:O3	1:A:4:IDS:H5	1.67	0.94
1:A:6:IDS:O3	1:A:7:SGN:O3S	1.83	0.94
1:A:6:IDS:H3	1:A:7:SGN:N2	1.82	0.94
1:A:8:IDS:O6A	1:A:9:SGN:H5	1.68	0.93
1:A:4:IDS:O3	1:A:5:SGN:O1S	1.85	0.93
1:A:6:IDS:O3	1:A:7:SGN:O1S	1.85	0.93
1:A:6:IDS:O3	1:A:7:SGN:O1S	1.86	0.92
1:A:6:IDS:H3	1:A:7:SGN:S1	2.10	0.92
1:A:3:SGN:O3	1:A:4:IDS:C6	2.20	0.90
1:A:13:SGN:O4S	1:A:14:IDS:O5	1.91	0.89
1:A:15:SGN:O4S	1:A:16:IDS:O1S	1.91	0.88
1:A:15:SGN:C6	1:A:16:IDS:O2S	2.21	0.87
1:A:15:SGN:O5S	1:A:16:IDS:O5	1.92	0.87
1:A:1:SGN:O4S	1:A:2:IDS:S	2.32	0.87
1:A:13:SGN:O4S	1:A:15:SGN:N2	2.07	0.86
1:A:13:SGN:O3	1:A:14:IDS:C5	2.23	0.86
1:A:12:IDS:O6A	1:A:13:SGN:H62	1.75	0.85
1:A:12:IDS:O3	1:A:13:SGN:N2	2.11	0.83
1:A:3:SGN:S2	1:A:4:IDS:O5	2.36	0.83
1:A:7:SGN:O4S	1:A:8:IDS:O2S	1.96	0.83
1:A:5:SGN:C6	1:A:6:IDS:O1S	2.26	0.83
1:A:12:IDS:O3	1:A:13:SGN:N2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:SGN:H61	1:A:18:IDS:O2S	1.79	0.82
1:A:12:IDS:O6A	1:A:13:SGN:O5	1.96	0.81
1:A:9:SGN:O4S	1:A:10:IDS:C6	2.29	0.81
1:A:6:IDS:H3	1:A:7:SGN:N2	1.96	0.81
1:A:8:IDS:H3	1:A:9:SGN:S1	2.21	0.81
1:A:8:IDS:C3	1:A:9:SGN:O1S	2.29	0.81
1:A:4:IDS:O6A	1:A:5:SGN:H5	1.80	0.81
1:A:8:IDS:O3	1:A:9:SGN:O1S	1.98	0.80
1:A:6:IDS:H3	1:A:7:SGN:S1	2.21	0.80
1:A:1:SGN:O3	1:A:2:IDS:H5	1.82	0.80
1:A:7:SGN:O3	1:A:8:IDS:H5	1.82	0.80
1:A:1:SGN:O1S	1:A:1:SGN:H1	1.80	0.80
1:A:17:SGN:C6	1:A:18:IDS:S	2.61	0.80
1:A:11:SGN:H61	1:A:12:IDS:O2S	1.83	0.79
1:A:5:SGN:H62	1:A:6:IDS:O1S	1.83	0.79
1:A:6:IDS:O3	1:A:7:SGN:N2	2.17	0.78
1:A:15:SGN:H61	1:A:16:IDS:C1	2.13	0.77
1:A:11:SGN:O3	1:A:12:IDS:H5	1.83	0.77
1:A:11:SGN:H61	1:A:12:IDS:C1	2.15	0.77
1:A:6:IDS:O3	1:A:7:SGN:O1S	2.02	0.76
1:A:10:IDS:C3	1:A:11:SGN:N2	2.39	0.76
1:A:5:SGN:H61	1:A:6:IDS:S	2.25	0.76
1:A:1:SGN:O3	1:A:2:IDS:C5	2.35	0.75
1:A:8:IDS:O2	1:A:9:SGN:O3S	2.04	0.75
1:A:6:IDS:O3	1:A:7:SGN:N2	2.17	0.75
1:A:17:SGN:H61	1:A:18:IDS:S	2.26	0.75
1:A:3:SGN:O5S	1:A:4:IDS:O5	2.04	0.75
1:A:10:IDS:O2	1:A:11:SGN:O3S	2.03	0.74
1:A:8:IDS:H3	1:A:9:SGN:O1S	1.87	0.74
1:A:5:SGN:C6	1:A:6:IDS:S	2.75	0.74
1:A:13:SGN:C5	1:A:14:IDS:O2S	2.35	0.74
1:A:1:SGN:H61	1:A:2:IDS:C1	2.17	0.74
1:A:3:SGN:O6	1:A:4:IDS:C1	2.36	0.73
1:A:16:IDS:O3	1:A:17:SGN:N2	2.21	0.72
1:A:5:SGN:O6	1:A:6:IDS:C1	2.38	0.71
1:A:6:IDS:H3	1:A:7:SGN:O3S	1.91	0.71
1:A:17:SGN:H61	1:A:18:IDS:O2S	1.90	0.71
1:A:13:SGN:H61	1:A:14:IDS:S	2.30	0.71
1:A:9:SGN:O3	1:A:10:IDS:C6	2.39	0.70
1:A:7:SGN:S2	1:A:8:IDS:S	2.87	0.70
1:A:7:SGN:H61	1:A:8:IDS:C1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:SGN:H61	1:A:6:IDS:C1	2.21	0.69
1:A:6:IDS:C3	1:A:7:SGN:S1	2.80	0.69
1:A:15:SGN:S2	1:A:16:IDS:O5	2.50	0.69
1:A:6:IDS:O3	1:A:7:SGN:S1	2.48	0.69
1:A:14:IDS:C3	1:A:15:SGN:N2	2.55	0.69
1:A:6:IDS:H4	1:A:7:SGN:O1S	1.92	0.69
1:A:15:SGN:H5	1:A:16:IDS:O2S	1.92	0.69
1:A:10:IDS:O3	1:A:11:SGN:O3S	2.11	0.68
1:A:16:IDS:O6A	1:A:17:SGN:O5	2.12	0.68
1:A:4:IDS:H3	1:A:5:SGN:O1S	1.94	0.68
1:A:8:IDS:H3	1:A:9:SGN:S1	2.33	0.68
1:A:5:SGN:H61	1:A:6:IDS:O1S	1.95	0.67
1:A:9:SGN:H61	1:A:10:IDS:O2S	1.93	0.67
1:A:8:IDS:O3	1:A:9:SGN:N2	2.28	0.66
1:A:10:IDS:O3	1:A:11:SGN:O3S	2.13	0.66
1:A:11:SGN:O6	1:A:12:IDS:O5	2.12	0.66
1:A:11:SGN:O3	1:A:12:IDS:H5	1.95	0.66
1:A:9:SGN:O4S	1:A:10:IDS:O5	2.14	0.66
1:A:9:SGN:H61	1:A:10:IDS:C1	2.26	0.66
1:A:12:IDS:C6	1:A:13:SGN:H5	2.24	0.66
1:A:6:IDS:O3	1:A:7:SGN:N2	2.29	0.66
1:A:14:IDS:H3	1:A:15:SGN:N2	2.11	0.66
1:A:13:SGN:S2	1:A:14:IDS:O5	2.54	0.66
1:A:13:SGN:H61	1:A:14:IDS:C1	2.26	0.65
1:A:10:IDS:O3	1:A:11:SGN:S1	2.54	0.65
1:A:2:IDS:O6A	1:A:3:SGN:H62	1.97	0.65
1:A:9:SGN:O3	1:A:10:IDS:C5	2.44	0.65
1:A:7:SGN:O3	1:A:8:IDS:C5	2.41	0.65
1:A:2:IDS:O6B	1:A:3:SGN:H5	1.97	0.64
1:A:1:SGN:O3	1:A:2:IDS:C5	2.39	0.64
1:A:11:SGN:H61	1:A:12:IDS:C1	2.28	0.64
1:A:1:SGN:HO3	1:A:2:IDS:H5	1.63	0.64
1:A:17:SGN:O4S	1:A:18:IDS:O1S	2.16	0.64
1:A:9:SGN:O4S	1:A:10:IDS:O1S	2.15	0.64
1:A:3:SGN:O5S	1:A:4:IDS:O4	2.17	0.63
1:A:12:IDS:O3	1:A:13:SGN:S1	2.50	0.63
1:A:14:IDS:H3	1:A:15:SGN:N2	2.13	0.62
1:A:2:IDS:C6	1:A:3:SGN:H5	2.30	0.62
1:A:6:IDS:C3	1:A:7:SGN:O1S	2.47	0.61
1:A:16:IDS:O6A	1:A:17:SGN:H62	1.99	0.61
1:A:8:IDS:O6A	1:A:9:SGN:H5	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:SGN:S2	1:A:2:IDS:O5	2.58	0.61
1:A:3:SGN:O5S	1:A:4:IDS:C5	2.49	0.61
1:A:13:SGN:H5	1:A:14:IDS:O2S	1.99	0.61
1:A:1:SGN:H61	1:A:2:IDS:O2S	2.01	0.61
1:A:5:SGN:H61	1:A:6:IDS:C1	2.30	0.60
1:A:14:IDS:H3	1:A:15:SGN:N2	2.15	0.60
1:A:13:SGN:H62	1:A:14:IDS:O2S	1.98	0.60
1:A:6:IDS:C3	1:A:7:SGN:O3S	2.50	0.60
1:A:2:IDS:C6	1:A:3:SGN:C5	2.80	0.59
1:A:5:SGN:H61	1:A:6:IDS:C1	2.32	0.59
1:A:1:SGN:O3	1:A:2:IDS:C6	2.50	0.59
1:A:17:SGN:C5	1:A:18:IDS:O2S	2.50	0.59
1:A:16:IDS:O6A	1:A:17:SGN:C5	2.51	0.59
1:A:16:IDS:C3	1:A:17:SGN:N2	2.65	0.59
1:A:1:SGN:S2	1:A:2:IDS:C1	2.90	0.59
1:A:13:SGN:HO3	1:A:14:IDS:H5	1.61	0.58
1:A:9:SGN:O3	1:A:10:IDS:C5	2.51	0.58
1:A:7:SGN:O3	1:A:8:IDS:H5	2.02	0.58
1:A:2:IDS:O3	1:A:3:SGN:O3S	2.21	0.58
1:A:5:SGN:H62	1:A:6:IDS:S	2.41	0.58
1:A:13:SGN:O4S	1:A:14:IDS:C1	2.52	0.57
1:A:11:SGN:O3	1:A:12:IDS:C5	2.52	0.57
1:A:5:SGN:C6	1:A:6:IDS:O2S	2.52	0.57
1:A:9:SGN:H61	1:A:10:IDS:C1	2.35	0.57
1:A:16:IDS:O6A	1:A:17:SGN:C5	2.39	0.57
1:A:11:SGN:C6	1:A:12:IDS:C1	2.82	0.56
1:A:17:SGN:H61	1:A:18:IDS:O2S	2.05	0.56
1:A:1:SGN:O4	1:A:2:IDS:O2S	2.24	0.56
1:A:17:SGN:H5	1:A:18:IDS:O2S	2.06	0.56
1:A:9:SGN:O3	1:A:10:IDS:O5	2.21	0.56
1:A:10:IDS:O6A	1:A:11:SGN:C6	2.53	0.56
1:A:2:IDS:C3	1:A:3:SGN:O1S	2.49	0.56
1:A:9:SGN:O4S	1:A:10:IDS:C5	2.54	0.56
1:A:6:IDS:O2	1:A:7:SGN:O3S	2.24	0.55
1:A:11:SGN:H5	1:A:12:IDS:O2S	2.06	0.55
1:A:1:SGN:O1S	1:A:1:SGN:H1	2.07	0.55
1:A:13:SGN:H61	1:A:14:IDS:C1	2.37	0.54
1:A:9:SGN:O3	1:A:10:IDS:C6	2.55	0.54
1:A:17:SGN:H61	1:A:18:IDS:C1	2.38	0.54
1:A:16:IDS:H3	1:A:17:SGN:N2	2.23	0.53
1:A:15:SGN:H62	1:A:16:IDS:O2S	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:SGN:H5	1:A:16:IDS:O2S	2.08	0.53
1:A:10:IDS:O6A	1:A:11:SGN:C5	2.56	0.53
1:A:8:IDS:C3	1:A:9:SGN:S1	2.95	0.53
1:A:7:SGN:O3	1:A:8:IDS:C5	2.56	0.52
1:A:11:SGN:O3	1:A:12:IDS:O6B	2.26	0.52
1:A:9:SGN:O4S	1:A:10:IDS:O6B	2.27	0.52
1:A:13:SGN:C6	1:A:14:IDS:C1	2.88	0.52
1:A:6:IDS:C3	1:A:7:SGN:S1	2.95	0.52
1:A:1:SGN:O1S	1:A:1:SGN:H1	2.10	0.52
1:A:11:SGN:C6	1:A:12:IDS:C1	2.87	0.52
1:A:11:SGN:O3	1:A:12:IDS:O5	2.27	0.52
1:A:16:IDS:C3	1:A:17:SGN:N2	2.73	0.51
1:A:11:SGN:O5S	1:A:12:IDS:C6	2.58	0.51
1:A:2:IDS:C6	1:A:3:SGN:H5	2.40	0.51
1:A:10:IDS:C6	1:A:11:SGN:H5	2.33	0.51
1:A:8:IDS:O6A	1:A:9:SGN:C5	2.49	0.50
1:A:16:IDS:O3	1:A:17:SGN:S1	2.69	0.50
1:A:17:SGN:O3	1:A:18:IDS:O6B	2.29	0.49
1:A:16:IDS:O6A	1:A:17:SGN:C6	2.61	0.49
1:A:7:SGN:O3	1:A:8:IDS:H5	2.12	0.49
1:A:9:SGN:C6	1:A:10:IDS:C1	2.91	0.48
1:A:14:IDS:O3	1:A:15:SGN:O1S	2.31	0.48
1:A:1:SGN:O5S	1:A:2:IDS:O5	2.31	0.48
1:A:8:IDS:H3	1:A:9:SGN:O3S	2.13	0.48
1:A:1:SGN:C5	1:A:2:IDS:O2S	2.62	0.48
1:A:15:SGN:C5	1:A:16:IDS:O2S	2.55	0.48
1:A:13:SGN:O3	1:A:14:IDS:C6	2.60	0.48
1:A:15:SGN:S2	1:A:16:IDS:C1	3.02	0.47
1:A:10:IDS:O6A	1:A:11:SGN:H62	2.14	0.47
1:A:15:SGN:O3	1:A:16:IDS:O6B	2.32	0.47
1:A:1:SGN:O1S	1:A:1:SGN:C1	2.55	0.47
1:A:2:IDS:O6B	1:A:3:SGN:H5	2.14	0.47
1:A:9:SGN:O1S	1:A:9:SGN:C1	2.63	0.47
1:A:16:IDS:C2	1:A:17:SGN:O3S	2.29	0.47
1:A:9:SGN:O3	1:A:10:IDS:H5	2.15	0.47
1:A:17:SGN:C6	1:A:18:IDS:O2S	2.60	0.47
1:A:9:SGN:HO3	1:A:10:IDS:C5	2.24	0.47
1:A:13:SGN:H61	1:A:14:IDS:C1	2.45	0.46
1:A:12:IDS:H3	1:A:13:SGN:N2	2.30	0.46
1:A:15:SGN:H61	1:A:16:IDS:C1	2.45	0.46
1:A:2:IDS:C4	1:A:3:SGN:O1S	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:IDS:C4	1:A:7:SGN:O1S	2.61	0.46
1:A:15:SGN:O4	1:A:16:IDS:O2S	2.34	0.45
1:A:1:SGN:O4S	1:A:2:IDS:O2	2.34	0.45
1:A:6:IDS:C3	1:A:7:SGN:N2	2.79	0.45
1:A:11:SGN:H5	1:A:12:IDS:S	2.56	0.45
1:A:11:SGN:O6	1:A:12:IDS:C1	2.65	0.45
1:A:10:IDS:O6A	1:A:11:SGN:O5	2.35	0.44
1:A:3:SGN:HO3	1:A:4:IDS:C6	2.27	0.44
1:A:1:SGN:H61	1:A:2:IDS:S	2.55	0.44
1:A:12:IDS:C3	1:A:13:SGN:N2	2.80	0.44
1:A:1:SGN:HO3	1:A:2:IDS:C6	2.28	0.44
1:A:9:SGN:O3	1:A:10:IDS:O6B	2.35	0.44
1:A:2:IDS:C6	1:A:3:SGN:H62	2.48	0.43
1:A:12:IDS:C3	1:A:13:SGN:N2	2.82	0.43
1:A:2:IDS:C6	1:A:3:SGN:C5	2.97	0.43
1:A:17:SGN:C5	1:A:18:IDS:O2S	2.66	0.43
1:A:6:IDS:C3	1:A:7:SGN:N2	2.82	0.42
1:A:3:SGN:O4	1:A:4:IDS:O2S	2.36	0.42
1:A:15:SGN:H62	1:A:16:IDS:S	2.41	0.42
1:A:2:IDS:O6A	1:A:3:SGN:C6	2.66	0.42
1:A:4:IDS:H3	1:A:5:SGN:N2	2.35	0.42
1:A:6:IDS:H3	1:A:7:SGN:N2	2.35	0.42
1:A:17:SGN:C6	1:A:18:IDS:C1	2.98	0.41
1:A:12:IDS:H3	1:A:13:SGN:N2	2.34	0.41
1:A:15:SGN:C6	1:A:16:IDS:C1	2.98	0.41
1:A:5:SGN:H61	1:A:6:IDS:O2S	2.21	0.41
1:A:2:IDS:H4	1:A:3:SGN:O1S	2.21	0.40

There are no symmetry-related clashes.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

There are no protein molecules in this entry.

4.3.2 Protein sidechains ⓘ

There are no protein molecules in this entry.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates ⓘ

162 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	1.43	2 (12%)	16,24,26	1.19	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	1.39	2 (12%)	16,24,26	1.20	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	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	15	1	19,19,20	1.25	1 (5%)	23,29,31	1.11	1 (4%)
1	IDS	1-A	16	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	17	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	1-A	18	1	15,15,17	1.54	2 (13%)	14,22,26	1.43	2 (14%)
1	IDS	1-A	2	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	4	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	5	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	6	1	16,16,17	1.40	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	1-A	7	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	8	1	16,16,17	1.45	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	9	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	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	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	2-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	2-A	12	1	16,16,17	1.39	2 (12%)	16,24,26	1.19	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	1.19	2 (12%)
1	SGN	2-A	15	1	19,19,20	1.26	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	16	1	16,16,17	1.43	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	2-A	17	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	18	1	15,15,17	1.55	2 (13%)	14,22,26	1.43	2 (14%)
1	IDS	2-A	2	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	5	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	2-A	6	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	2-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	8	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	2-A	9	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	3-A	1	1	20,20,20	1.13	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	3-A	10	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	11	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	3-A	12	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	13	1	19,19,20	1.25	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	1.25	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	17	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	3-A	18	1	15,15,17	1.54	2 (13%)	14,22,26	1.44	2 (14%)
1	IDS	3-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	3-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
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	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	6	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	7	1	19,19,20	1.25	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	1.19	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	3-A	9	1	19,19,20	1.23	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	4-A	1	1	20,20,20	1.13	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	1.19	2 (12%)
1	SGN	4-A	11	1	19,19,20	1.28	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	4-A	12	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	14	1	16,16,17	1.44	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	4-A	15	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	4-A	17	1	19,19,20	1.29	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	18	1	15,15,17	1.56	2 (13%)	14,22,26	1.43	2 (14%)
1	IDS	4-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	3	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	4-A	5	1	19,19,20	1.26	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	1.19	2 (12%)
1	SGN	4-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	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	1.13	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	5-A	10	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	5-A	11	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	5-A	12	1	16,16,17	1.41	3 (18%)	16,24,26	1.20	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	1.45	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	5-A	15	1	19,19,20	1.27	1 (5%)	23,29,31	1.11	1 (4%)
1	IDS	5-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
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	15,15,17	1.55	2 (13%)	14,22,26	1.42	2 (14%)
1	IDS	5-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	5-A	3	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	5	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	5-A	6	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	5-A	7	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	5-A	8	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	5-A	9	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	6-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	6-A	10	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	11	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	12	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	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	1.45	2 (12%)	16,24,26	1.18	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	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	17	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	6-A	18	1	15,15,17	1.53	2 (13%)	14,22,26	1.43	2 (14%)
1	IDS	6-A	2	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	3	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	4	1	16,16,17	1.45	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	5	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	6	1	16,16,17	1.41	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	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	9	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	7-A	1	1	20,20,20	1.13	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	7-A	10	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	7-A	11	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	12	1	16,16,17	1.41	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	7-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	14	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	7-A	15	1	19,19,20	1.25	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	16	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	17	1	19,19,20	1.29	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	18	1	15,15,17	1.55	2 (13%)	14,22,26	1.43	2 (14%)
1	IDS	7-A	2	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	7-A	5	1	19,19,20	1.25	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	6	1	16,16,17	1.42	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	7-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	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	1.26	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	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	11	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	8-A	12	1	16,16,17	1.40	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	8-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	14	1	16,16,17	1.45	2 (12%)	16,24,26	1.18	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	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	17	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	18	1	15,15,17	1.54	2 (13%)	14,22,26	1.43	2 (14%)
1	IDS	8-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	8-A	5	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	6	1	16,16,17	1.41	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	8-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	8	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	9-A	1	1	20,20,20	1.15	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	9-A	10	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	11	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	12	1	16,16,17	1.40	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	14	1	16,16,17	1.47	3 (18%)	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	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	9-A	17	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	18	1	15,15,17	1.55	2 (13%)	14,22,26	1.43	2 (14%)
1	IDS	9-A	2	1	16,16,17	1.41	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	9-A	3	1	19,19,20	1.24	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	9-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	9-A	5	1	19,19,20	1.27	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	6	1	16,16,17	1.40	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	7	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	8	1	16,16,17	1.44	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	9-A	9	1	19,19,20	1.24	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	-	6/11/31/31	0/1/1/1
1	IDS	1-A	10	1	-	4/9/26/29	0/1/1/1
1	SGN	1-A	11	1	-	4/11/28/31	0/1/1/1
1	IDS	1-A	12	1	-	0/9/26/29	0/1/1/1
1	SGN	1-A	13	1	-	1/11/28/31	0/1/1/1
1	IDS	1-A	14	1	-	5/9/26/29	0/1/1/1
1	SGN	1-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	1-A	16	1	-	6/9/26/29	0/1/1/1
1	SGN	1-A	17	1	-	1/11/28/31	0/1/1/1
1	IDS	1-A	18	1	-	2/9/22/29	0/1/1/1
1	IDS	1-A	2	1	-	0/9/26/29	0/1/1/1
1	SGN	1-A	3	1	-	8/11/28/31	0/1/1/1
1	IDS	1-A	4	1	-	5/9/26/29	0/1/1/1
1	SGN	1-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	6	1	-	3/9/26/29	0/1/1/1
1	SGN	1-A	7	1	-	1/11/28/31	0/1/1/1
1	IDS	1-A	8	1	-	4/9/26/29	0/1/1/1
1	SGN	1-A	9	1	-	8/11/28/31	0/1/1/1
1	SGN	2-A	1	1	-	5/11/31/31	0/1/1/1
1	IDS	2-A	10	1	-	1/9/26/29	0/1/1/1
1	SGN	2-A	11	1	-	2/11/28/31	0/1/1/1
1	IDS	2-A	12	1	-	2/9/26/29	0/1/1/1
1	SGN	2-A	13	1	-	2/11/28/31	0/1/1/1
1	IDS	2-A	14	1	-	3/9/26/29	0/1/1/1
1	SGN	2-A	15	1	-	4/11/28/31	0/1/1/1
1	IDS	2-A	16	1	-	4/9/26/29	0/1/1/1

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

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

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

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

All (324) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	14	IDS	O2-C2	-3.81	1.41	1.47
1	6-A	4	IDS	O2-C2	-3.80	1.41	1.47
1	6-A	14	IDS	O2-C2	-3.79	1.41	1.47
1	4-A	15	SGN	S1-N2	3.79	1.64	1.59
1	5-A	14	IDS	O2-C2	-3.79	1.41	1.47
1	4-A	17	SGN	S1-N2	3.78	1.64	1.59
1	5-A	4	IDS	O2-C2	-3.78	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	14	IDS	O2-C2	-3.78	1.41	1.47
1	7-A	11	SGN	S1-N2	3.77	1.64	1.59
1	8-A	4	IDS	O2-C2	-3.77	1.41	1.47
1	3-A	14	IDS	O2-C2	-3.77	1.41	1.47
1	7-A	4	IDS	O2-C2	-3.76	1.41	1.47
1	3-A	4	IDS	O2-C2	-3.76	1.41	1.47
1	2-A	14	IDS	O2-C2	-3.75	1.41	1.47
1	9-A	4	IDS	O2-C2	-3.75	1.41	1.47
1	4-A	14	IDS	O2-C2	-3.75	1.41	1.47
1	8-A	5	SGN	S1-N2	3.75	1.64	1.59
1	2-A	15	SGN	S1-N2	3.75	1.64	1.59
1	2-A	5	SGN	S1-N2	3.75	1.64	1.59
1	6-A	17	SGN	S1-N2	3.75	1.64	1.59
1	4-A	4	IDS	O2-C2	-3.74	1.41	1.47
1	4-A	5	SGN	S1-N2	3.73	1.64	1.59
1	9-A	15	SGN	S1-N2	3.73	1.64	1.59
1	2-A	4	IDS	O2-C2	-3.73	1.41	1.47
1	4-A	18	IDS	O2-C2	-3.73	1.41	1.47
1	7-A	17	SGN	S1-N2	3.73	1.64	1.59
1	7-A	18	IDS	O2-C2	-3.73	1.41	1.47
1	1-A	4	IDS	O2-C2	-3.73	1.41	1.47
1	8-A	18	IDS	O2-C2	-3.73	1.41	1.47
1	8-A	17	SGN	S1-N2	3.72	1.64	1.59
1	2-A	17	SGN	S1-N2	3.72	1.64	1.59
1	1-A	14	IDS	O2-C2	-3.72	1.41	1.47
1	1-A	18	IDS	O2-C2	-3.71	1.41	1.47
1	1-A	11	SGN	S1-N2	3.71	1.64	1.59
1	5-A	5	SGN	S1-N2	3.71	1.64	1.59
1	4-A	3	SGN	S1-N2	3.71	1.64	1.59
1	1-A	5	SGN	S1-N2	3.71	1.64	1.59
1	3-A	12	IDS	O2-C2	-3.70	1.41	1.47
1	9-A	13	SGN	S1-N2	3.70	1.64	1.59
1	6-A	15	SGN	S1-N2	3.70	1.64	1.59
1	6-A	5	SGN	S1-N2	3.70	1.64	1.59
1	5-A	15	SGN	S1-N2	3.70	1.64	1.59
1	6-A	8	IDS	O2-C2	-3.70	1.41	1.47
1	8-A	15	SGN	S1-N2	3.70	1.64	1.59
1	6-A	3	SGN	S1-N2	3.70	1.64	1.59
1	5-A	17	SGN	S1-N2	3.69	1.64	1.59
1	7-A	15	SGN	S1-N2	3.69	1.64	1.59
1	4-A	12	IDS	O2-C2	-3.69	1.41	1.47
1	5-A	3	SGN	S1-N2	3.69	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	14	IDS	O2-C2	-3.69	1.41	1.47
1	3-A	15	SGN	S1-N2	3.69	1.64	1.59
1	7-A	10	IDS	O2-C2	-3.69	1.41	1.47
1	1-A	8	IDS	O2-C2	-3.68	1.41	1.47
1	6-A	10	IDS	O2-C2	-3.68	1.41	1.47
1	3-A	17	SGN	S1-N2	3.68	1.64	1.59
1	9-A	18	IDS	O2-C2	-3.68	1.41	1.47
1	8-A	10	IDS	O2-C2	-3.68	1.41	1.47
1	1-A	10	IDS	O2-C2	-3.68	1.41	1.47
1	4-A	11	SGN	S1-N2	3.68	1.64	1.59
1	9-A	11	SGN	S1-N2	3.68	1.64	1.59
1	9-A	8	IDS	O2-C2	-3.67	1.41	1.47
1	3-A	11	SGN	S1-N2	3.67	1.64	1.59
1	4-A	10	IDS	O2-C2	-3.67	1.41	1.47
1	9-A	5	SGN	S1-N2	3.67	1.64	1.59
1	2-A	11	SGN	S1-N2	3.67	1.64	1.59
1	1-A	16	IDS	O2-C2	-3.67	1.41	1.47
1	7-A	16	IDS	O2-C2	-3.67	1.41	1.47
1	1-A	15	SGN	S1-N2	3.67	1.64	1.59
1	9-A	17	SGN	S1-N2	3.67	1.64	1.59
1	3-A	10	IDS	O2-C2	-3.66	1.41	1.47
1	1-A	7	SGN	S1-N2	3.66	1.64	1.59
1	5-A	18	IDS	O2-C2	-3.66	1.41	1.47
1	3-A	18	IDS	O2-C2	-3.66	1.41	1.47
1	1-A	3	SGN	S1-N2	3.66	1.64	1.59
1	9-A	1	SGN	S1-N2	3.66	1.64	1.59
1	1-A	2	IDS	O2-C2	-3.65	1.41	1.47
1	6-A	12	IDS	O2-C2	-3.65	1.41	1.47
1	3-A	5	SGN	S1-N2	3.65	1.64	1.59
1	2-A	16	IDS	O2-C2	-3.65	1.41	1.47
1	2-A	18	IDS	O2-C2	-3.65	1.41	1.47
1	5-A	8	IDS	O2-C2	-3.65	1.41	1.47
1	1-A	17	SGN	S1-N2	3.65	1.64	1.59
1	2-A	10	IDS	O2-C2	-3.65	1.41	1.47
1	5-A	11	SGN	S1-N2	3.65	1.64	1.59
1	5-A	6	IDS	O2-C2	-3.65	1.41	1.47
1	6-A	2	IDS	O2-C2	-3.64	1.41	1.47
1	7-A	7	SGN	S1-N2	3.64	1.64	1.59
1	8-A	6	IDS	O2-C2	-3.64	1.41	1.47
1	5-A	12	IDS	O2-C2	-3.64	1.41	1.47
1	8-A	11	SGN	S1-N2	3.64	1.64	1.59
1	2-A	8	IDS	O2-C2	-3.64	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	13	SGN	S1-N2	3.64	1.64	1.59
1	6-A	18	IDS	O2-C2	-3.64	1.41	1.47
1	4-A	6	IDS	O2-C2	-3.64	1.41	1.47
1	6-A	6	IDS	O2-C2	-3.64	1.41	1.47
1	9-A	10	IDS	O2-C2	-3.64	1.41	1.47
1	7-A	12	IDS	O2-C2	-3.64	1.41	1.47
1	4-A	16	IDS	O2-C2	-3.64	1.41	1.47
1	2-A	6	IDS	O2-C2	-3.64	1.41	1.47
1	8-A	12	IDS	O2-C2	-3.64	1.41	1.47
1	2-A	7	SGN	S1-N2	3.63	1.64	1.59
1	7-A	5	SGN	S1-N2	3.63	1.64	1.59
1	2-A	2	IDS	O2-C2	-3.63	1.41	1.47
1	2-A	13	SGN	S1-N2	3.63	1.64	1.59
1	5-A	2	IDS	O2-C2	-3.63	1.41	1.47
1	5-A	10	IDS	O2-C2	-3.63	1.41	1.47
1	4-A	13	SGN	S1-N2	3.62	1.64	1.59
1	2-A	12	IDS	O2-C2	-3.62	1.41	1.47
1	5-A	16	IDS	O2-C2	-3.62	1.41	1.47
1	8-A	3	SGN	S1-N2	3.62	1.64	1.59
1	4-A	8	IDS	O2-C2	-3.62	1.41	1.47
1	3-A	3	SGN	S1-N2	3.61	1.64	1.59
1	4-A	2	IDS	O2-C2	-3.61	1.41	1.47
1	9-A	12	IDS	O2-C2	-3.61	1.41	1.47
1	2-A	3	SGN	S1-N2	3.61	1.64	1.59
1	7-A	8	IDS	O2-C2	-3.61	1.41	1.47
1	7-A	6	IDS	O2-C2	-3.61	1.41	1.47
1	1-A	13	SGN	S1-N2	3.61	1.64	1.59
1	6-A	16	IDS	O2-C2	-3.60	1.41	1.47
1	6-A	13	SGN	S1-N2	3.60	1.64	1.59
1	9-A	7	SGN	S1-N2	3.60	1.64	1.59
1	3-A	2	IDS	O2-C2	-3.60	1.41	1.47
1	3-A	13	SGN	S1-N2	3.60	1.64	1.59
1	9-A	2	IDS	O2-C2	-3.60	1.41	1.47
1	3-A	8	IDS	O2-C2	-3.60	1.41	1.47
1	3-A	6	IDS	O2-C2	-3.60	1.41	1.47
1	8-A	2	IDS	O2-C2	-3.60	1.41	1.47
1	9-A	6	IDS	O2-C2	-3.59	1.41	1.47
1	7-A	1	SGN	S1-N2	3.59	1.64	1.59
1	6-A	1	SGN	S1-N2	3.59	1.64	1.59
1	1-A	12	IDS	O2-C2	-3.59	1.41	1.47
1	6-A	7	SGN	S1-N2	3.59	1.64	1.59
1	9-A	3	SGN	S1-N2	3.59	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	7	SGN	S1-N2	3.58	1.64	1.59
1	2-A	1	SGN	S1-N2	3.58	1.64	1.59
1	3-A	16	IDS	O2-C2	-3.58	1.41	1.47
1	5-A	7	SGN	S1-N2	3.57	1.64	1.59
1	5-A	9	SGN	S1-N2	3.57	1.64	1.59
1	8-A	8	IDS	O2-C2	-3.57	1.42	1.47
1	3-A	7	SGN	S1-N2	3.57	1.64	1.59
1	8-A	7	SGN	S1-N2	3.56	1.64	1.59
1	5-A	13	SGN	S1-N2	3.56	1.63	1.59
1	6-A	11	SGN	S1-N2	3.56	1.63	1.59
1	3-A	1	SGN	S1-N2	3.56	1.63	1.59
1	8-A	16	IDS	O2-C2	-3.55	1.42	1.47
1	8-A	13	SGN	S1-N2	3.55	1.63	1.59
1	4-A	1	SGN	S1-N2	3.55	1.63	1.59
1	8-A	1	SGN	S1-N2	3.54	1.63	1.59
1	9-A	16	IDS	O2-C2	-3.54	1.42	1.47
1	1-A	6	IDS	O2-C2	-3.54	1.42	1.47
1	1-A	1	SGN	S1-N2	3.53	1.63	1.59
1	7-A	2	IDS	O2-C2	-3.53	1.42	1.47
1	5-A	1	SGN	S1-N2	3.51	1.63	1.59
1	1-A	9	SGN	S1-N2	3.51	1.63	1.59
1	4-A	9	SGN	S1-N2	3.51	1.63	1.59
1	8-A	9	SGN	S1-N2	3.51	1.63	1.59
1	7-A	3	SGN	S1-N2	3.50	1.63	1.59
1	7-A	9	SGN	S1-N2	3.50	1.63	1.59
1	2-A	9	SGN	S1-N2	3.48	1.63	1.59
1	6-A	9	SGN	S1-N2	3.47	1.63	1.59
1	9-A	9	SGN	S1-N2	3.45	1.63	1.59
1	3-A	9	SGN	S1-N2	3.43	1.63	1.59
1	5-A	8	IDS	O6B-C6	-2.97	1.21	1.30
1	1-A	8	IDS	O6B-C6	-2.97	1.21	1.30
1	3-A	8	IDS	O6B-C6	-2.96	1.21	1.30
1	9-A	8	IDS	O6B-C6	-2.95	1.21	1.30
1	8-A	8	IDS	O6B-C6	-2.94	1.21	1.30
1	4-A	18	IDS	O6B-C6	-2.94	1.21	1.30
1	6-A	8	IDS	O6B-C6	-2.94	1.21	1.30
1	8-A	16	IDS	O6B-C6	-2.93	1.21	1.30
1	2-A	8	IDS	O6B-C6	-2.93	1.21	1.30
1	4-A	10	IDS	O6B-C6	-2.92	1.21	1.30
1	7-A	8	IDS	O6B-C6	-2.92	1.21	1.30
1	1-A	18	IDS	O6B-C6	-2.92	1.21	1.30
1	5-A	14	IDS	O6B-C6	-2.92	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	10	IDS	O6B-C6	-2.92	1.21	1.30
1	6-A	14	IDS	O6B-C6	-2.92	1.21	1.30
1	6-A	4	IDS	O6B-C6	-2.92	1.21	1.30
1	4-A	8	IDS	O6B-C6	-2.91	1.21	1.30
1	4-A	6	IDS	O6B-C6	-2.91	1.21	1.30
1	8-A	4	IDS	O6B-C6	-2.91	1.21	1.30
1	9-A	14	IDS	O6B-C6	-2.91	1.21	1.30
1	9-A	18	IDS	O6B-C6	-2.91	1.21	1.30
1	7-A	18	IDS	O6B-C6	-2.90	1.21	1.30
1	5-A	12	IDS	O6B-C6	-2.90	1.21	1.30
1	5-A	16	IDS	O6B-C6	-2.90	1.21	1.30
1	2-A	18	IDS	O6B-C6	-2.90	1.21	1.30
1	3-A	6	IDS	O6B-C6	-2.90	1.21	1.30
1	2-A	14	IDS	O6B-C6	-2.90	1.21	1.30
1	2-A	2	IDS	O6B-C6	-2.90	1.21	1.30
1	9-A	2	IDS	O6B-C6	-2.90	1.21	1.30
1	1-A	10	IDS	O6B-C6	-2.90	1.21	1.30
1	8-A	14	IDS	O6B-C6	-2.90	1.21	1.30
1	1-A	6	IDS	O6B-C6	-2.90	1.21	1.30
1	6-A	10	IDS	O6B-C6	-2.89	1.21	1.30
1	3-A	18	IDS	O6B-C6	-2.89	1.21	1.30
1	5-A	4	IDS	O6B-C6	-2.89	1.21	1.30
1	3-A	2	IDS	O6B-C6	-2.89	1.21	1.30
1	7-A	14	IDS	O6B-C6	-2.89	1.21	1.30
1	3-A	12	IDS	O6B-C6	-2.89	1.21	1.30
1	1-A	16	IDS	O6B-C6	-2.89	1.21	1.30
1	7-A	6	IDS	O6B-C6	-2.89	1.21	1.30
1	4-A	14	IDS	O6B-C6	-2.89	1.21	1.30
1	6-A	16	IDS	O6B-C6	-2.89	1.21	1.30
1	3-A	4	IDS	O6B-C6	-2.89	1.21	1.30
1	2-A	6	IDS	O6B-C6	-2.89	1.21	1.30
1	9-A	4	IDS	O6B-C6	-2.88	1.21	1.30
1	7-A	10	IDS	O6B-C6	-2.88	1.21	1.30
1	6-A	18	IDS	O6B-C6	-2.88	1.21	1.30
1	5-A	18	IDS	O6B-C6	-2.88	1.21	1.30
1	9-A	6	IDS	O6B-C6	-2.88	1.21	1.30
1	8-A	18	IDS	O6B-C6	-2.88	1.21	1.30
1	7-A	4	IDS	O6B-C6	-2.88	1.21	1.30
1	7-A	12	IDS	O6B-C6	-2.88	1.21	1.30
1	3-A	14	IDS	O6B-C6	-2.88	1.21	1.30
1	5-A	6	IDS	O6B-C6	-2.88	1.21	1.30
1	5-A	10	IDS	O6B-C6	-2.88	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	10	IDS	O6B-C6	-2.88	1.21	1.30
1	4-A	4	IDS	O6B-C6	-2.88	1.21	1.30
1	4-A	16	IDS	O6B-C6	-2.87	1.21	1.30
1	3-A	16	IDS	O6B-C6	-2.87	1.21	1.30
1	9-A	12	IDS	O6B-C6	-2.87	1.21	1.30
1	8-A	2	IDS	O6B-C6	-2.87	1.21	1.30
1	9-A	10	IDS	O6B-C6	-2.87	1.21	1.30
1	4-A	12	IDS	O6B-C6	-2.87	1.21	1.30
1	7-A	16	IDS	O6B-C6	-2.87	1.21	1.30
1	5-A	2	IDS	O6B-C6	-2.87	1.21	1.30
1	2-A	12	IDS	O6B-C6	-2.86	1.21	1.30
1	1-A	12	IDS	O6B-C6	-2.86	1.21	1.30
1	9-A	16	IDS	O6B-C6	-2.86	1.21	1.30
1	4-A	2	IDS	O6B-C6	-2.86	1.21	1.30
1	1-A	2	IDS	O6B-C6	-2.86	1.21	1.30
1	2-A	4	IDS	O6B-C6	-2.86	1.21	1.30
1	6-A	6	IDS	O6B-C6	-2.86	1.21	1.30
1	2-A	10	IDS	O6B-C6	-2.86	1.21	1.30
1	6-A	12	IDS	O6B-C6	-2.86	1.21	1.30
1	1-A	4	IDS	O6B-C6	-2.85	1.21	1.30
1	1-A	14	IDS	O6B-C6	-2.85	1.21	1.30
1	7-A	2	IDS	O6B-C6	-2.85	1.21	1.30
1	8-A	6	IDS	O6B-C6	-2.85	1.21	1.30
1	2-A	16	IDS	O6B-C6	-2.85	1.21	1.30
1	8-A	12	IDS	O6B-C6	-2.85	1.21	1.30
1	6-A	2	IDS	O6B-C6	-2.84	1.21	1.30
1	8-A	17	SGN	O5-C1	-2.20	1.40	1.43
1	5-A	17	SGN	O5-C1	-2.18	1.40	1.43
1	4-A	17	SGN	O5-C1	-2.16	1.40	1.43
1	2-A	17	SGN	O5-C1	-2.15	1.40	1.43
1	2-A	7	SGN	O5-C1	-2.14	1.40	1.43
1	1-A	2	IDS	O5-C1	-2.13	1.40	1.43
1	6-A	3	SGN	O5-C1	-2.13	1.40	1.43
1	1-A	7	SGN	O5-C1	-2.13	1.40	1.43
1	9-A	17	SGN	O5-C1	-2.13	1.40	1.43
1	5-A	11	SGN	O5-C1	-2.12	1.40	1.43
1	2-A	13	SGN	O5-C1	-2.12	1.40	1.43
1	5-A	9	SGN	O5-C1	-2.12	1.40	1.43
1	6-A	9	SGN	O5-C1	-2.12	1.40	1.43
1	1-A	17	SGN	O5-C1	-2.11	1.40	1.43
1	4-A	7	SGN	O5-C1	-2.11	1.40	1.43
1	9-A	7	SGN	O5-C1	-2.11	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	3	SGN	O5-C1	-2.11	1.40	1.43
1	6-A	11	SGN	O5-C1	-2.11	1.40	1.43
1	3-A	17	SGN	O5-C1	-2.11	1.40	1.43
1	8-A	7	SGN	O5-C1	-2.11	1.40	1.43
1	7-A	2	IDS	O5-C1	-2.10	1.40	1.43
1	3-A	9	SGN	O5-C1	-2.10	1.40	1.43
1	7-A	17	SGN	O5-C1	-2.10	1.40	1.43
1	7-A	3	SGN	O5-C1	-2.10	1.40	1.43
1	8-A	11	SGN	O5-C1	-2.10	1.40	1.43
1	9-A	9	SGN	O5-C1	-2.09	1.40	1.43
1	7-A	9	SGN	O5-C1	-2.09	1.40	1.43
1	8-A	9	SGN	O5-C1	-2.09	1.40	1.43
1	3-A	7	SGN	O5-C1	-2.09	1.40	1.43
1	1-A	9	SGN	O5-C1	-2.09	1.40	1.43
1	6-A	17	SGN	O5-C1	-2.08	1.40	1.43
1	4-A	11	SGN	O5-C1	-2.08	1.40	1.43
1	6-A	13	SGN	O5-C1	-2.08	1.40	1.43
1	4-A	9	SGN	O5-C1	-2.08	1.40	1.43
1	5-A	7	SGN	O5-C1	-2.08	1.40	1.43
1	5-A	3	SGN	O5-C1	-2.08	1.40	1.43
1	6-A	7	SGN	O5-C1	-2.08	1.40	1.43
1	3-A	2	IDS	O5-C1	-2.07	1.40	1.43
1	1-A	11	SGN	O5-C1	-2.07	1.40	1.43
1	1-A	3	SGN	O5-C1	-2.07	1.40	1.43
1	9-A	5	SGN	O5-C1	-2.07	1.40	1.43
1	2-A	9	SGN	O5-C1	-2.07	1.40	1.43
1	7-A	11	SGN	O5-C1	-2.07	1.40	1.43
1	6-A	15	SGN	O5-C1	-2.07	1.40	1.43
1	8-A	13	SGN	O5-C1	-2.06	1.40	1.43
1	3-A	13	SGN	O5-C1	-2.06	1.40	1.43
1	5-A	13	SGN	O5-C1	-2.06	1.40	1.43
1	2-A	11	SGN	O5-C1	-2.06	1.40	1.43
1	4-A	3	SGN	O5-C1	-2.05	1.40	1.43
1	3-A	3	SGN	O5-C1	-2.05	1.40	1.43
1	8-A	5	SGN	O5-C1	-2.05	1.40	1.43
1	5-A	2	IDS	O5-C1	-2.05	1.40	1.43
1	1-A	13	SGN	O5-C1	-2.05	1.40	1.43
1	9-A	13	SGN	O5-C1	-2.05	1.40	1.43
1	9-A	11	SGN	O5-C1	-2.05	1.40	1.43
1	6-A	2	IDS	O5-C1	-2.05	1.40	1.43
1	9-A	16	IDS	O5-C1	-2.04	1.40	1.43
1	4-A	2	IDS	O5-C1	-2.04	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	3	SGN	O5-C1	-2.04	1.40	1.43
1	7-A	7	SGN	O5-C1	-2.04	1.40	1.43
1	4-A	13	SGN	O5-C1	-2.04	1.40	1.43
1	9-A	3	SGN	O5-C1	-2.04	1.40	1.43
1	6-A	12	IDS	O5-C1	-2.03	1.40	1.43
1	6-A	5	SGN	O5-C1	-2.03	1.40	1.43
1	5-A	12	IDS	O5-C1	-2.03	1.40	1.43
1	9-A	14	IDS	O5-C1	-2.03	1.40	1.43
1	7-A	13	SGN	O5-C1	-2.03	1.40	1.43
1	2-A	2	IDS	O5-C1	-2.03	1.40	1.43
1	4-A	8	IDS	O5-C1	-2.03	1.40	1.43
1	3-A	5	SGN	O5-C1	-2.02	1.40	1.43
1	3-A	11	SGN	O5-C1	-2.02	1.40	1.43
1	2-A	16	IDS	O5-C1	-2.02	1.40	1.43
1	4-A	5	SGN	O5-C1	-2.02	1.40	1.43
1	2-A	5	SGN	O5-C1	-2.02	1.40	1.43
1	8-A	2	IDS	O5-C1	-2.02	1.40	1.43
1	8-A	15	SGN	O5-C1	-2.01	1.40	1.43
1	5-A	5	SGN	O5-C1	-2.01	1.40	1.43
1	4-A	14	IDS	O5-C1	-2.01	1.40	1.43
1	4-A	15	SGN	O5-C1	-2.01	1.40	1.43
1	6-A	16	IDS	O5-C1	-2.01	1.40	1.43
1	1-A	5	SGN	O5-C1	-2.01	1.40	1.43

All (243) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	18	IDS	O6B-C6-C5	3.42	121.61	112.71
1	6-A	18	IDS	O6B-C6-C5	3.41	121.58	112.71
1	9-A	18	IDS	O6B-C6-C5	3.41	121.58	112.71
1	1-A	18	IDS	O6B-C6-C5	3.41	121.57	112.71
1	2-A	18	IDS	O6B-C6-C5	3.40	121.57	112.71
1	7-A	18	IDS	O6B-C6-C5	3.39	121.54	112.71
1	4-A	18	IDS	O6B-C6-C5	3.39	121.53	112.71
1	8-A	18	IDS	O6B-C6-C5	3.39	121.52	112.71
1	5-A	18	IDS	O6B-C6-C5	3.37	121.48	112.71
1	9-A	9	SGN	O1S-S1-O2S	-3.18	113.30	120.36
1	3-A	9	SGN	O1S-S1-O2S	-3.17	113.30	120.36
1	5-A	15	SGN	O1S-S1-O2S	-3.17	113.30	120.36
1	5-A	7	SGN	O1S-S1-O2S	-3.17	113.31	120.36
1	7-A	9	SGN	O1S-S1-O2S	-3.17	113.32	120.36
1	9-A	7	SGN	O1S-S1-O2S	-3.16	113.33	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	7	SGN	O1S-S1-O2S	-3.16	113.33	120.36
1	4-A	9	SGN	O1S-S1-O2S	-3.16	113.33	120.36
1	6-A	7	SGN	O1S-S1-O2S	-3.16	113.33	120.36
1	8-A	7	SGN	O1S-S1-O2S	-3.16	113.34	120.36
1	2-A	9	SGN	O1S-S1-O2S	-3.16	113.34	120.36
1	6-A	9	SGN	O1S-S1-O2S	-3.16	113.34	120.36
1	6-A	11	SGN	O1S-S1-O2S	-3.15	113.35	120.36
1	7-A	3	SGN	O1S-S1-O2S	-3.15	113.35	120.36
1	7-A	7	SGN	O1S-S1-O2S	-3.15	113.35	120.36
1	8-A	13	SGN	O1S-S1-O2S	-3.15	113.35	120.36
1	6-A	17	SGN	O1S-S1-O2S	-3.15	113.35	120.36
1	1-A	7	SGN	O1S-S1-O2S	-3.15	113.36	120.36
1	4-A	1	SGN	O1S-S1-O2S	-3.15	113.36	120.36
1	5-A	3	SGN	O1S-S1-O2S	-3.15	113.36	120.36
1	1-A	15	SGN	O1S-S1-O2S	-3.15	113.36	120.36
1	8-A	17	SGN	O1S-S1-O2S	-3.15	113.36	120.36
1	2-A	13	SGN	O1S-S1-O2S	-3.15	113.36	120.36
1	7-A	13	SGN	O1S-S1-O2S	-3.15	113.36	120.36
1	2-A	7	SGN	O1S-S1-O2S	-3.14	113.37	120.36
1	7-A	17	SGN	O1S-S1-O2S	-3.14	113.37	120.36
1	8-A	9	SGN	O1S-S1-O2S	-3.14	113.37	120.36
1	1-A	13	SGN	O1S-S1-O2S	-3.14	113.37	120.36
1	4-A	7	SGN	O1S-S1-O2S	-3.14	113.37	120.36
1	5-A	9	SGN	O1S-S1-O2S	-3.14	113.37	120.36
1	2-A	17	SGN	O1S-S1-O2S	-3.14	113.37	120.36
1	6-A	15	SGN	O1S-S1-O2S	-3.14	113.38	120.36
1	8-A	15	SGN	O1S-S1-O2S	-3.14	113.38	120.36
1	1-A	17	SGN	O1S-S1-O2S	-3.14	113.38	120.36
1	7-A	5	SGN	O1S-S1-O2S	-3.14	113.38	120.36
1	1-A	9	SGN	O1S-S1-O2S	-3.14	113.38	120.36
1	1-A	3	SGN	O1S-S1-O2S	-3.14	113.38	120.36
1	8-A	5	SGN	O1S-S1-O2S	-3.13	113.39	120.36
1	4-A	11	SGN	O1S-S1-O2S	-3.13	113.39	120.36
1	5-A	17	SGN	O1S-S1-O2S	-3.13	113.39	120.36
1	7-A	15	SGN	O1S-S1-O2S	-3.13	113.40	120.36
1	3-A	1	SGN	O1S-S1-O2S	-3.13	113.40	120.36
1	3-A	13	SGN	O1S-S1-O2S	-3.13	113.40	120.36
1	3-A	3	SGN	O1S-S1-O2S	-3.13	113.40	120.36
1	3-A	17	SGN	O1S-S1-O2S	-3.13	113.40	120.36
1	9-A	5	SGN	O1S-S1-O2S	-3.13	113.40	120.36
1	9-A	11	SGN	O1S-S1-O2S	-3.13	113.40	120.36
1	9-A	17	SGN	O1S-S1-O2S	-3.13	113.40	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	17	SGN	O1S-S1-O2S	-3.13	113.41	120.36
1	8-A	1	SGN	O1S-S1-O2S	-3.13	113.41	120.36
1	4-A	3	SGN	O1S-S1-O2S	-3.13	113.41	120.36
1	5-A	1	SGN	O1S-S1-O2S	-3.13	113.41	120.36
1	6-A	13	SGN	O1S-S1-O2S	-3.12	113.41	120.36
1	4-A	5	SGN	O1S-S1-O2S	-3.12	113.41	120.36
1	9-A	13	SGN	O1S-S1-O2S	-3.12	113.41	120.36
1	6-A	1	SGN	O1S-S1-O2S	-3.12	113.41	120.36
1	7-A	11	SGN	O1S-S1-O2S	-3.12	113.41	120.36
1	2-A	15	SGN	O1S-S1-O2S	-3.12	113.42	120.36
1	8-A	3	SGN	O1S-S1-O2S	-3.12	113.42	120.36
1	1-A	1	SGN	O1S-S1-O2S	-3.12	113.42	120.36
1	3-A	15	SGN	O1S-S1-O2S	-3.12	113.42	120.36
1	8-A	11	SGN	O1S-S1-O2S	-3.12	113.42	120.36
1	3-A	5	SGN	O1S-S1-O2S	-3.12	113.42	120.36
1	5-A	5	SGN	O1S-S1-O2S	-3.12	113.42	120.36
1	9-A	15	SGN	O1S-S1-O2S	-3.12	113.43	120.36
1	9-A	3	SGN	O1S-S1-O2S	-3.12	113.43	120.36
1	1-A	5	SGN	O1S-S1-O2S	-3.12	113.43	120.36
1	3-A	11	SGN	O1S-S1-O2S	-3.12	113.43	120.36
1	6-A	5	SGN	O1S-S1-O2S	-3.11	113.43	120.36
1	4-A	15	SGN	O1S-S1-O2S	-3.11	113.43	120.36
1	2-A	3	SGN	O1S-S1-O2S	-3.11	113.43	120.36
1	5-A	13	SGN	O1S-S1-O2S	-3.11	113.44	120.36
1	2-A	1	SGN	O1S-S1-O2S	-3.11	113.44	120.36
1	6-A	3	SGN	O1S-S1-O2S	-3.11	113.44	120.36
1	5-A	11	SGN	O1S-S1-O2S	-3.11	113.45	120.36
1	2-A	11	SGN	O1S-S1-O2S	-3.11	113.45	120.36
1	7-A	1	SGN	O1S-S1-O2S	-3.10	113.46	120.36
1	4-A	13	SGN	O1S-S1-O2S	-3.10	113.46	120.36
1	9-A	1	SGN	O1S-S1-O2S	-3.10	113.47	120.36
1	2-A	5	SGN	O1S-S1-O2S	-3.09	113.48	120.36
1	1-A	11	SGN	O1S-S1-O2S	-3.09	113.48	120.36
1	8-A	6	IDS	O6B-C6-O6A	-2.84	117.64	124.08
1	6-A	6	IDS	O6B-C6-O6A	-2.83	117.65	124.08
1	9-A	16	IDS	O6B-C6-O6A	-2.83	117.65	124.08
1	2-A	6	IDS	O6B-C6-O6A	-2.83	117.66	124.08
1	2-A	16	IDS	O6B-C6-O6A	-2.83	117.67	124.08
1	7-A	10	IDS	O6B-C6-O6A	-2.82	117.69	124.08
1	5-A	10	IDS	O6B-C6-O6A	-2.81	117.70	124.08
1	5-A	6	IDS	O6B-C6-O6A	-2.81	117.70	124.08
1	4-A	16	IDS	O6B-C6-O6A	-2.81	117.70	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	6	IDS	O6B-C6-O6A	-2.81	117.70	124.08
1	7-A	16	IDS	O6B-C6-O6A	-2.81	117.71	124.08
1	3-A	6	IDS	O6B-C6-O6A	-2.81	117.71	124.08
1	2-A	10	IDS	O6B-C6-O6A	-2.81	117.72	124.08
1	1-A	6	IDS	O6B-C6-O6A	-2.80	117.73	124.08
1	9-A	6	IDS	O6B-C6-O6A	-2.80	117.73	124.08
1	8-A	12	IDS	O6B-C6-O6A	-2.80	117.73	124.08
1	1-A	16	IDS	O6B-C6-O6A	-2.79	117.74	124.08
1	2-A	8	IDS	O6B-C6-O6A	-2.79	117.74	124.08
1	7-A	12	IDS	O6B-C6-O6A	-2.79	117.74	124.08
1	9-A	12	IDS	O6B-C6-O6A	-2.79	117.74	124.08
1	9-A	4	IDS	O6B-C6-O6A	-2.79	117.75	124.08
1	3-A	4	IDS	O6B-C6-O6A	-2.79	117.75	124.08
1	1-A	12	IDS	O6B-C6-O6A	-2.79	117.75	124.08
1	7-A	4	IDS	O6B-C6-O6A	-2.79	117.75	124.08
1	3-A	16	IDS	O6B-C6-O6A	-2.79	117.75	124.08
1	3-A	14	IDS	O6B-C6-O6A	-2.79	117.76	124.08
1	1-A	10	IDS	O6B-C6-O6A	-2.79	117.76	124.08
1	3-A	18	IDS	O6B-C6-O6A	-2.79	117.76	124.08
1	5-A	16	IDS	O6B-C6-O6A	-2.79	117.76	124.08
1	2-A	4	IDS	O6B-C6-O6A	-2.78	117.76	124.08
1	8-A	16	IDS	O6B-C6-O6A	-2.78	117.76	124.08
1	1-A	2	IDS	O6B-C6-O6A	-2.78	117.77	124.08
1	7-A	8	IDS	O6B-C6-O6A	-2.78	117.77	124.08
1	7-A	2	IDS	O6B-C6-O6A	-2.78	117.77	124.08
1	1-A	4	IDS	O6B-C6-O6A	-2.78	117.77	124.08
1	6-A	8	IDS	O6B-C6-O6A	-2.78	117.77	124.08
1	4-A	10	IDS	O6B-C6-O6A	-2.78	117.77	124.08
1	6-A	16	IDS	O6B-C6-O6A	-2.78	117.78	124.08
1	2-A	14	IDS	O6B-C6-O6A	-2.78	117.78	124.08
1	9-A	10	IDS	O6B-C6-O6A	-2.78	117.78	124.08
1	3-A	10	IDS	O6B-C6-O6A	-2.77	117.79	124.08
1	6-A	4	IDS	O6B-C6-O6A	-2.77	117.79	124.08
1	4-A	8	IDS	O6B-C6-O6A	-2.77	117.79	124.08
1	5-A	8	IDS	O6B-C6-O6A	-2.77	117.79	124.08
1	8-A	10	IDS	O6B-C6-O6A	-2.77	117.79	124.08
1	2-A	12	IDS	O6B-C6-O6A	-2.77	117.79	124.08
1	6-A	2	IDS	O6B-C6-O6A	-2.77	117.79	124.08
1	4-A	6	IDS	O6B-C6-O6A	-2.77	117.80	124.08
1	3-A	8	IDS	O6B-C6-O6A	-2.77	117.80	124.08
1	5-A	12	IDS	O6B-C6-O6A	-2.77	117.80	124.08
1	4-A	2	IDS	O6B-C6-O6A	-2.77	117.80	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	2	IDS	O6B-C6-O6A	-2.76	117.82	124.08
1	6-A	10	IDS	O6B-C6-O6A	-2.76	117.82	124.08
1	3-A	12	IDS	O6B-C6-O6A	-2.76	117.82	124.08
1	8-A	2	IDS	O6B-C6-O6A	-2.76	117.83	124.08
1	7-A	14	IDS	O6B-C6-O6A	-2.75	117.83	124.08
1	9-A	18	IDS	O6B-C6-O6A	-2.75	117.83	124.08
1	4-A	4	IDS	O6B-C6-O6A	-2.75	117.83	124.08
1	1-A	8	IDS	O6B-C6-O6A	-2.75	117.84	124.08
1	6-A	18	IDS	O6B-C6-O6A	-2.75	117.84	124.08
1	5-A	18	IDS	O6B-C6-O6A	-2.75	117.84	124.08
1	8-A	14	IDS	O6B-C6-O6A	-2.75	117.85	124.08
1	5-A	4	IDS	O6B-C6-O6A	-2.75	117.85	124.08
1	1-A	14	IDS	O6B-C6-O6A	-2.75	117.85	124.08
1	4-A	14	IDS	O6B-C6-O6A	-2.75	117.85	124.08
1	5-A	14	IDS	O6B-C6-O6A	-2.75	117.85	124.08
1	8-A	8	IDS	O6B-C6-O6A	-2.74	117.85	124.08
1	2-A	18	IDS	O6B-C6-O6A	-2.74	117.86	124.08
1	3-A	2	IDS	O6B-C6-O6A	-2.74	117.86	124.08
1	9-A	2	IDS	O6B-C6-O6A	-2.74	117.86	124.08
1	8-A	18	IDS	O6B-C6-O6A	-2.74	117.86	124.08
1	2-A	2	IDS	O6B-C6-O6A	-2.74	117.87	124.08
1	6-A	14	IDS	O6B-C6-O6A	-2.74	117.87	124.08
1	4-A	18	IDS	O6B-C6-O6A	-2.74	117.87	124.08
1	4-A	12	IDS	O6B-C6-O6A	-2.73	117.88	124.08
1	6-A	12	IDS	O6B-C6-O6A	-2.73	117.88	124.08
1	9-A	14	IDS	O6B-C6-O6A	-2.73	117.88	124.08
1	9-A	8	IDS	O6B-C6-O6A	-2.73	117.89	124.08
1	8-A	4	IDS	O6B-C6-O6A	-2.72	117.91	124.08
1	7-A	18	IDS	O6B-C6-O6A	-2.72	117.92	124.08
1	1-A	18	IDS	O6B-C6-O6A	-2.71	117.93	124.08
1	1-A	6	IDS	O6B-C6-C5	2.25	121.76	113.64
1	4-A	16	IDS	O6B-C6-C5	2.25	121.76	113.64
1	3-A	6	IDS	O6B-C6-C5	2.25	121.76	113.64
1	7-A	6	IDS	O6B-C6-C5	2.25	121.75	113.64
1	6-A	6	IDS	O6B-C6-C5	2.25	121.75	113.64
1	5-A	8	IDS	O6B-C6-C5	2.25	121.75	113.64
1	3-A	8	IDS	O6B-C6-C5	2.24	121.74	113.64
1	8-A	6	IDS	O6B-C6-C5	2.24	121.74	113.64
1	8-A	16	IDS	O6B-C6-C5	2.24	121.73	113.64
1	2-A	6	IDS	O6B-C6-C5	2.24	121.71	113.64
1	9-A	16	IDS	O6B-C6-C5	2.24	121.71	113.64
1	7-A	12	IDS	O6B-C6-C5	2.23	121.70	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-A	6	IDS	O6B-C6-C5	2.23	121.69	113.64
1	7-A	10	IDS	O6B-C6-C5	2.23	121.69	113.64
1	9-A	6	IDS	O6B-C6-C5	2.23	121.69	113.64
1	2-A	8	IDS	O6B-C6-C5	2.23	121.69	113.64
1	1-A	12	IDS	O6B-C6-C5	2.23	121.69	113.64
1	8-A	10	IDS	O6B-C6-C5	2.23	121.69	113.64
1	3-A	16	IDS	O6B-C6-C5	2.23	121.69	113.64
1	5-A	6	IDS	O6B-C6-C5	2.23	121.69	113.64
1	7-A	8	IDS	O6B-C6-C5	2.23	121.68	113.64
1	3-A	12	IDS	O6B-C6-C5	2.23	121.68	113.64
1	1-A	8	IDS	O6B-C6-C5	2.23	121.68	113.64
1	5-A	12	IDS	O6B-C6-C5	2.23	121.68	113.64
1	2-A	10	IDS	O6B-C6-C5	2.23	121.67	113.64
1	2-A	16	IDS	O6B-C6-C5	2.23	121.67	113.64
1	5-A	10	IDS	O6B-C6-C5	2.23	121.67	113.64
1	5-A	16	IDS	O6B-C6-C5	2.23	121.67	113.64
1	3-A	10	IDS	O6B-C6-C5	2.22	121.67	113.64
1	4-A	10	IDS	O6B-C6-C5	2.22	121.67	113.64
1	1-A	16	IDS	O6B-C6-C5	2.22	121.66	113.64
1	6-A	16	IDS	O6B-C6-C5	2.22	121.66	113.64
1	1-A	10	IDS	O6B-C6-C5	2.22	121.66	113.64
1	7-A	16	IDS	O6B-C6-C5	2.22	121.65	113.64
1	2-A	12	IDS	O6B-C6-C5	2.22	121.65	113.64
1	9-A	10	IDS	O6B-C6-C5	2.22	121.64	113.64
1	9-A	12	IDS	O6B-C6-C5	2.21	121.63	113.64
1	4-A	2	IDS	O6B-C6-C5	2.21	121.63	113.64
1	1-A	2	IDS	O6B-C6-C5	2.21	121.63	113.64
1	6-A	12	IDS	O6B-C6-C5	2.21	121.62	113.64
1	6-A	10	IDS	O6B-C6-C5	2.21	121.62	113.64
1	6-A	2	IDS	O6B-C6-C5	2.21	121.61	113.64
1	4-A	8	IDS	O6B-C6-C5	2.21	121.61	113.64
1	6-A	8	IDS	O6B-C6-C5	2.21	121.61	113.64
1	8-A	12	IDS	O6B-C6-C5	2.21	121.61	113.64
1	2-A	2	IDS	O6B-C6-C5	2.21	121.61	113.64
1	5-A	2	IDS	O6B-C6-C5	2.21	121.61	113.64
1	9-A	4	IDS	O6B-C6-C5	2.21	121.61	113.64
1	3-A	2	IDS	O6B-C6-C5	2.21	121.61	113.64
1	9-A	8	IDS	O6B-C6-C5	2.21	121.60	113.64
1	6-A	4	IDS	O6B-C6-C5	2.20	121.60	113.64
1	9-A	2	IDS	O6B-C6-C5	2.20	121.59	113.64
1	7-A	2	IDS	O6B-C6-C5	2.20	121.59	113.64
1	8-A	2	IDS	O6B-C6-C5	2.20	121.59	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	8	IDS	O6B-C6-C5	2.20	121.59	113.64
1	4-A	12	IDS	O6B-C6-C5	2.20	121.58	113.64
1	3-A	4	IDS	O6B-C6-C5	2.20	121.58	113.64
1	5-A	14	IDS	O6B-C6-C5	2.20	121.57	113.64
1	7-A	4	IDS	O6B-C6-C5	2.19	121.56	113.64
1	1-A	4	IDS	O6B-C6-C5	2.19	121.55	113.64
1	5-A	4	IDS	O6B-C6-C5	2.19	121.55	113.64
1	2-A	4	IDS	O6B-C6-C5	2.19	121.55	113.64
1	3-A	14	IDS	O6B-C6-C5	2.19	121.54	113.64
1	2-A	14	IDS	O6B-C6-C5	2.19	121.54	113.64
1	1-A	14	IDS	O6B-C6-C5	2.19	121.53	113.64
1	8-A	4	IDS	O6B-C6-C5	2.19	121.53	113.64
1	8-A	14	IDS	O6B-C6-C5	2.19	121.53	113.64
1	6-A	14	IDS	O6B-C6-C5	2.18	121.52	113.64
1	4-A	14	IDS	O6B-C6-C5	2.18	121.51	113.64
1	4-A	4	IDS	O6B-C6-C5	2.18	121.51	113.64
1	9-A	14	IDS	O6B-C6-C5	2.18	121.50	113.64
1	7-A	14	IDS	O6B-C6-C5	2.18	121.49	113.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	8-A	11	SGN	C1

All (530) 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	2-A	1	SGN	C1-C2-N2-S1
1	2-A	1	SGN	C3-C2-N2-S1
1	2-A	1	SGN	C4-C5-C6-O6
1	2-A	1	SGN	O5-C5-C6-O6
1	2-A	1	SGN	C2-N2-S1-O2S
1	5-A	1	SGN	C2-N2-S1-O2S
1	6-A	1	SGN	O5-C5-C6-O6
1	8-A	1	SGN	C1-C2-N2-S1
1	8-A	1	SGN	C3-C2-N2-S1
1	8-A	1	SGN	C4-C5-C6-O6
1	8-A	1	SGN	O5-C5-C6-O6
1	8-A	1	SGN	C2-N2-S1-O2S
1	8-A	1	SGN	C2-N2-S1-O3S

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Mol	Chain	Res	Type	Atoms
1	9-A	1	SGN	C1-C2-N2-S1
1	9-A	1	SGN	C3-C2-N2-S1
1	9-A	1	SGN	C2-N2-S1-O2S
1	3-A	2	IDS	C1-C2-O2-S
1	3-A	2	IDS	C3-C2-O2-S
1	3-A	2	IDS	C2-O2-S-O1S
1	3-A	2	IDS	C2-O2-S-O2S
1	3-A	2	IDS	C2-O2-S-O3S
1	5-A	2	IDS	C1-C2-O2-S
1	5-A	2	IDS	C4-C5-C6-O6A
1	5-A	2	IDS	C4-C5-C6-O6B
1	1-A	3	SGN	C4-C5-C6-O6
1	1-A	3	SGN	O5-C5-C6-O6
1	1-A	3	SGN	C2-N2-S1-O2S
1	1-A	3	SGN	C2-N2-S1-O3S
1	2-A	3	SGN	O5-C5-C6-O6
1	2-A	3	SGN	C2-N2-S1-O2S
1	3-A	3	SGN	C4-C5-C6-O6
1	3-A	3	SGN	O5-C5-C6-O6
1	3-A	3	SGN	C2-N2-S1-O2S
1	3-A	3	SGN	C2-N2-S1-O3S
1	4-A	3	SGN	C4-C5-C6-O6
1	5-A	3	SGN	O5-C5-C6-O6
1	5-A	3	SGN	C2-N2-S1-O2S
1	6-A	3	SGN	C4-C5-C6-O6
1	6-A	3	SGN	O5-C5-C6-O6
1	6-A	3	SGN	C2-N2-S1-O2S
1	6-A	3	SGN	C2-N2-S1-O3S
1	7-A	3	SGN	C4-C5-C6-O6
1	7-A	3	SGN	O5-C5-C6-O6
1	7-A	3	SGN	C2-N2-S1-O2S
1	8-A	3	SGN	C4-C5-C6-O6
1	8-A	3	SGN	O5-C5-C6-O6
1	8-A	3	SGN	C2-N2-S1-O2S
1	8-A	3	SGN	C2-N2-S1-O3S
1	1-A	4	IDS	C2-O2-S-O2S
1	1-A	4	IDS	C2-O2-S-O3S
1	4-A	4	IDS	C2-O2-S-O3S
1	5-A	4	IDS	C1-C2-O2-S
1	5-A	4	IDS	C3-C2-O2-S
1	5-A	4	IDS	C4-C5-C6-O6A
1	5-A	4	IDS	C4-C5-C6-O6B

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Mol	Chain	Res	Type	Atoms
1	7-A	4	IDS	C4-C5-C6-O6A
1	7-A	4	IDS	C4-C5-C6-O6B
1	9-A	4	IDS	C2-O2-S-O2S
1	1-A	5	SGN	O5-C5-C6-O6
1	2-A	5	SGN	O5-C5-C6-O6
1	2-A	5	SGN	C2-N2-S1-O2S
1	2-A	5	SGN	C2-N2-S1-O3S
1	3-A	5	SGN	O5-C5-C6-O6
1	4-A	5	SGN	C4-C5-C6-O6
1	4-A	5	SGN	O5-C5-C6-O6
1	4-A	5	SGN	C2-N2-S1-O1S
1	5-A	5	SGN	C4-C5-C6-O6
1	5-A	5	SGN	O5-C5-C6-O6
1	5-A	5	SGN	C2-N2-S1-O2S
1	5-A	5	SGN	C2-N2-S1-O3S
1	6-A	5	SGN	C2-N2-S1-O2S
1	7-A	5	SGN	C4-C5-C6-O6
1	7-A	5	SGN	O5-C5-C6-O6
1	8-A	5	SGN	C2-N2-S1-O1S
1	9-A	5	SGN	O5-C5-C6-O6
1	9-A	5	SGN	C2-N2-S1-O2S
1	2-A	6	IDS	C2-O2-S-O1S
1	2-A	6	IDS	C2-O2-S-O2S
1	2-A	6	IDS	C2-O2-S-O3S
1	9-A	6	IDS	C4-C5-C6-O6A
1	9-A	6	IDS	C4-C5-C6-O6B
1	9-A	6	IDS	C2-O2-S-O2S
1	2-A	7	SGN	C2-N2-S1-O1S
1	3-A	7	SGN	C2-N2-S1-O2S
1	4-A	7	SGN	C4-C5-C6-O6
1	4-A	7	SGN	O5-C5-C6-O6
1	4-A	7	SGN	C2-N2-S1-O2S
1	4-A	7	SGN	C2-N2-S1-O3S
1	5-A	7	SGN	C4-C5-C6-O6
1	5-A	7	SGN	O5-C5-C6-O6
1	5-A	7	SGN	C2-N2-S1-O2S
1	5-A	7	SGN	C2-N2-S1-O3S
1	6-A	7	SGN	C4-C5-C6-O6
1	6-A	7	SGN	O5-C5-C6-O6
1	7-A	7	SGN	O5-C5-C6-O6
1	8-A	7	SGN	C4-C5-C6-O6
1	8-A	7	SGN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
1	8-A	7	SGN	C2-N2-S1-O2S
1	9-A	7	SGN	C4-C5-C6-O6
1	9-A	7	SGN	O5-C5-C6-O6
1	4-A	8	IDS	C1-C2-O2-S
1	4-A	8	IDS	C3-C2-O2-S
1	5-A	8	IDS	C4-C5-C6-O6A
1	5-A	8	IDS	C4-C5-C6-O6B
1	6-A	8	IDS	C2-O2-S-O3S
1	7-A	8	IDS	C1-C2-O2-S
1	9-A	8	IDS	C1-C2-O2-S
1	9-A	8	IDS	C3-C2-O2-S
1	1-A	9	SGN	C4-C5-C6-O6
1	1-A	9	SGN	O5-C5-C6-O6
1	1-A	9	SGN	C2-N2-S1-O2S
1	1-A	9	SGN	C2-N2-S1-O3S
1	2-A	9	SGN	C2-N2-S1-O2S
1	3-A	9	SGN	C4-C5-C6-O6
1	3-A	9	SGN	O5-C5-C6-O6
1	4-A	9	SGN	O5-C5-C6-O6
1	4-A	9	SGN	C2-N2-S1-O2S
1	5-A	9	SGN	C2-N2-S1-O1S
1	6-A	9	SGN	C4-C5-C6-O6
1	6-A	9	SGN	O5-C5-C6-O6
1	6-A	9	SGN	C2-N2-S1-O2S
1	7-A	9	SGN	C4-C5-C6-O6
1	7-A	9	SGN	O5-C5-C6-O6
1	7-A	9	SGN	C2-N2-S1-O2S
1	7-A	9	SGN	C2-N2-S1-O3S
1	8-A	9	SGN	C4-C5-C6-O6
1	8-A	9	SGN	O5-C5-C6-O6
1	9-A	9	SGN	O5-C5-C6-O6
1	9-A	9	SGN	C2-N2-S1-O2S
1	4-A	10	IDS	C2-O2-S-O1S
1	4-A	10	IDS	C2-O2-S-O2S
1	4-A	10	IDS	C2-O2-S-O3S
1	7-A	10	IDS	C2-O2-S-O3S
1	9-A	10	IDS	C2-O2-S-O2S
1	9-A	10	IDS	C2-O2-S-O3S
1	1-A	11	SGN	C2-N2-S1-O2S
1	2-A	11	SGN	O5-C5-C6-O6
1	3-A	11	SGN	C2-N2-S1-O1S
1	4-A	11	SGN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
1	4-A	11	SGN	O5-C5-C6-O6
1	5-A	11	SGN	C2-N2-S1-O2S
1	5-A	11	SGN	C2-N2-S1-O3S
1	7-A	11	SGN	O5-C5-C6-O6
1	7-A	11	SGN	C2-N2-S1-O2S
1	7-A	11	SGN	C2-N2-S1-O3S
1	8-A	11	SGN	O5-C5-C6-O6
1	9-A	11	SGN	C4-C5-C6-O6
1	9-A	11	SGN	O5-C5-C6-O6
1	9-A	11	SGN	C2-N2-S1-O2S
1	2-A	12	IDS	C1-C2-O2-S
1	2-A	12	IDS	C3-C2-O2-S
1	5-A	12	IDS	C2-O2-S-O1S
1	5-A	12	IDS	C2-O2-S-O2S
1	5-A	12	IDS	C2-O2-S-O3S
1	6-A	12	IDS	C4-C5-C6-O6A
1	6-A	12	IDS	C4-C5-C6-O6B
1	2-A	13	SGN	O5-C5-C6-O6
1	3-A	13	SGN	O5-C5-C6-O6
1	4-A	13	SGN	C2-N2-S1-O2S
1	4-A	13	SGN	C2-N2-S1-O3S
1	5-A	13	SGN	C4-C5-C6-O6
1	5-A	13	SGN	O5-C5-C6-O6
1	5-A	13	SGN	C2-N2-S1-O2S
1	6-A	13	SGN	O5-C5-C6-O6
1	8-A	13	SGN	O5-C5-C6-O6
1	9-A	13	SGN	O5-C5-C6-O6
1	9-A	13	SGN	C2-N2-S1-O2S
1	9-A	13	SGN	C2-N2-S1-O3S
1	1-A	14	IDS	C4-C5-C6-O6A
1	1-A	14	IDS	C4-C5-C6-O6B
1	1-A	14	IDS	C2-O2-S-O1S
1	1-A	14	IDS	C2-O2-S-O2S
1	1-A	14	IDS	C2-O2-S-O3S
1	2-A	14	IDS	C4-C5-C6-O6A
1	2-A	14	IDS	C4-C5-C6-O6B
1	7-A	14	IDS	C1-C2-O2-S
1	7-A	14	IDS	C3-C2-O2-S
1	8-A	14	IDS	C1-C2-O2-S
1	1-A	15	SGN	C4-C5-C6-O6
1	1-A	15	SGN	O5-C5-C6-O6
1	2-A	15	SGN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
1	2-A	15	SGN	O5-C5-C6-O6
1	3-A	15	SGN	C2-N2-S1-O1S
1	4-A	15	SGN	O5-C5-C6-O6
1	5-A	15	SGN	C4-C5-C6-O6
1	5-A	15	SGN	O5-C5-C6-O6
1	5-A	15	SGN	C2-N2-S1-O2S
1	5-A	15	SGN	C2-N2-S1-O3S
1	6-A	15	SGN	C4-C5-C6-O6
1	6-A	15	SGN	O5-C5-C6-O6
1	6-A	15	SGN	C2-N2-S1-O2S
1	7-A	15	SGN	C2-N2-S1-O1S
1	9-A	15	SGN	C4-C5-C6-O6
1	9-A	15	SGN	O5-C5-C6-O6
1	1-A	16	IDS	C1-C2-O2-S
1	1-A	16	IDS	C3-C2-O2-S
1	2-A	16	IDS	C1-C2-O2-S
1	2-A	16	IDS	C3-C2-O2-S
1	2-A	16	IDS	C4-C5-C6-O6A
1	2-A	16	IDS	C4-C5-C6-O6B
1	5-A	16	IDS	C1-C2-O2-S
1	5-A	16	IDS	C3-C2-O2-S
1	6-A	16	IDS	C4-C5-C6-O6A
1	6-A	16	IDS	C4-C5-C6-O6B
1	7-A	16	IDS	C1-C2-O2-S
1	7-A	16	IDS	C3-C2-O2-S
1	2-A	17	SGN	C2-N2-S1-O1S
1	3-A	17	SGN	C4-C5-C6-O6
1	3-A	17	SGN	O5-C5-C6-O6
1	3-A	17	SGN	C2-N2-S1-O1S
1	4-A	17	SGN	C2-N2-S1-O2S
1	4-A	17	SGN	C2-N2-S1-O3S
1	5-A	17	SGN	C4-C5-C6-O6
1	5-A	17	SGN	O5-C5-C6-O6
1	5-A	17	SGN	C2-N2-S1-O2S
1	5-A	17	SGN	C2-N2-S1-O3S
1	6-A	17	SGN	C2-N2-S1-O1S
1	7-A	17	SGN	C4-C5-C6-O6
1	7-A	17	SGN	O5-C5-C6-O6
1	8-A	17	SGN	O5-C5-C6-O6
1	8-A	17	SGN	C2-N2-S1-O2S
1	8-A	17	SGN	C2-N2-S1-O3S
1	9-A	17	SGN	C2-N2-S1-O2S

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Mol	Chain	Res	Type	Atoms
1	1-A	18	IDS	C1-C2-O2-S
1	1-A	18	IDS	C3-C2-O2-S
1	5-A	18	IDS	C1-C2-O2-S
1	5-A	18	IDS	C3-C2-O2-S
1	3-A	13	SGN	C6-O6-S2-O4S
1	6-A	13	SGN	C6-O6-S2-O5S
1	7-A	15	SGN	C6-O6-S2-O5S
1	1-A	1	SGN	C6-O6-S2-O4S
1	3-A	1	SGN	C6-O6-S2-O5S
1	4-A	1	SGN	C6-O6-S2-O4S
1	8-A	1	SGN	C6-O6-S2-O4S
1	3-A	7	SGN	C6-O6-S2-O4S
1	8-A	7	SGN	C6-O6-S2-O5S
1	1-A	4	IDS	C2-O2-S-O1S
1	4-A	4	IDS	C2-O2-S-O1S
1	4-A	4	IDS	C2-O2-S-O2S
1	9-A	4	IDS	C2-O2-S-O1S
1	1-A	6	IDS	C2-O2-S-O1S
1	8-A	6	IDS	C2-O2-S-O1S
1	8-A	6	IDS	C2-O2-S-O2S
1	9-A	6	IDS	C2-O2-S-O1S
1	6-A	8	IDS	C2-O2-S-O1S
1	6-A	8	IDS	C2-O2-S-O2S
1	1-A	10	IDS	C2-O2-S-O1S
1	1-A	10	IDS	C2-O2-S-O2S
1	7-A	10	IDS	C2-O2-S-O1S
1	7-A	10	IDS	C2-O2-S-O2S
1	9-A	10	IDS	C2-O2-S-O1S
1	4-A	14	IDS	C2-O2-S-O1S
1	4-A	14	IDS	C2-O2-S-O2S
1	7-A	16	IDS	C2-O2-S-O1S
1	7-A	16	IDS	C2-O2-S-O2S
1	9-A	16	IDS	C2-O2-S-O1S
1	9-A	16	IDS	C2-O2-S-O2S
1	1-A	1	SGN	C6-O6-S2-O6S
1	4-A	1	SGN	C6-O6-S2-O6S
1	8-A	1	SGN	C6-O6-S2-O6S
1	4-A	3	SGN	C6-O6-S2-O6S
1	3-A	7	SGN	C6-O6-S2-O6S
1	7-A	7	SGN	C6-O6-S2-O6S
1	1-A	9	SGN	C6-O6-S2-O6S
1	3-A	9	SGN	C6-O6-S2-O6S

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Mol	Chain	Res	Type	Atoms
1	1-A	11	SGN	C6-O6-S2-O6S
1	5-A	11	SGN	C6-O6-S2-O6S
1	9-A	11	SGN	C6-O6-S2-O6S
1	3-A	13	SGN	C6-O6-S2-O6S
1	5-A	13	SGN	C6-O6-S2-O6S
1	9-A	15	SGN	C6-O6-S2-O6S
1	4-A	17	SGN	C6-O6-S2-O6S
1	8-A	17	SGN	C6-O6-S2-O6S
1	7-A	15	SGN	C1-C2-N2-S1
1	3-A	1	SGN	C6-O6-S2-O4S
1	6-A	1	SGN	C6-O6-S2-O4S
1	6-A	1	SGN	C6-O6-S2-O5S
1	4-A	3	SGN	C6-O6-S2-O4S
1	9-A	3	SGN	C6-O6-S2-O4S
1	9-A	3	SGN	C6-O6-S2-O5S
1	3-A	5	SGN	C6-O6-S2-O4S
1	3-A	5	SGN	C6-O6-S2-O5S
1	5-A	5	SGN	C6-O6-S2-O4S
1	5-A	5	SGN	C6-O6-S2-O5S
1	8-A	7	SGN	C6-O6-S2-O4S
1	9-A	9	SGN	C6-O6-S2-O4S
1	9-A	9	SGN	C6-O6-S2-O5S
1	4-A	11	SGN	C6-O6-S2-O4S
1	6-A	13	SGN	C6-O6-S2-O4S
1	5-A	15	SGN	C6-O6-S2-O4S
1	5-A	15	SGN	C6-O6-S2-O5S
1	7-A	15	SGN	C6-O6-S2-O4S
1	4-A	17	SGN	C6-O6-S2-O4S
1	4-A	9	SGN	C3-C2-N2-S1
1	5-A	9	SGN	C3-C2-N2-S1
1	7-A	15	SGN	C3-C2-N2-S1
1	8-A	17	SGN	C3-C2-N2-S1
1	4-A	3	SGN	C6-O6-S2-O5S
1	5-A	3	SGN	C6-O6-S2-O5S
1	8-A	5	SGN	C6-O6-S2-O5S
1	9-A	5	SGN	C6-O6-S2-O5S
1	4-A	7	SGN	C6-O6-S2-O5S
1	7-A	7	SGN	C6-O6-S2-O4S
1	4-A	9	SGN	C6-O6-S2-O5S
1	4-A	11	SGN	C6-O6-S2-O5S
1	5-A	11	SGN	C6-O6-S2-O5S
1	6-A	11	SGN	C6-O6-S2-O5S

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Mol	Chain	Res	Type	Atoms
1	1-A	15	SGN	C6-O6-S2-O5S
1	4-A	17	SGN	C6-O6-S2-O5S
1	1-A	3	SGN	C2-N2-S1-O1S
1	1-A	9	SGN	C2-N2-S1-O1S
1	1-A	13	SGN	C2-N2-S1-O2S
1	9-A	13	SGN	C2-N2-S1-O1S
1	1-A	15	SGN	C2-N2-S1-O2S
1	4-A	15	SGN	C2-N2-S1-O2S
1	5-A	15	SGN	C2-N2-S1-O1S
1	7-A	2	IDS	C2-O2-S-O3S
1	9-A	4	IDS	C2-O2-S-O3S
1	1-A	6	IDS	C2-O2-S-O3S
1	8-A	6	IDS	C2-O2-S-O3S
1	9-A	6	IDS	C2-O2-S-O3S
1	1-A	10	IDS	C2-O2-S-O3S
1	4-A	14	IDS	C2-O2-S-O3S
1	9-A	14	IDS	C2-O2-S-O3S
1	1-A	16	IDS	C2-O2-S-O3S
1	7-A	16	IDS	C2-O2-S-O3S
1	9-A	16	IDS	C2-O2-S-O3S
1	3-A	18	IDS	C2-O2-S-O1S
1	3-A	18	IDS	C2-O2-S-O3S
1	6-A	18	IDS	C2-O2-S-O1S
1	6-A	18	IDS	C2-O2-S-O3S
1	8-A	18	IDS	O5-C5-C6-O6A
1	3-A	1	SGN	C6-O6-S2-O6S
1	6-A	1	SGN	C6-O6-S2-O6S
1	9-A	3	SGN	C6-O6-S2-O6S
1	8-A	7	SGN	C6-O6-S2-O6S
1	2-A	9	SGN	C6-O6-S2-O6S
1	6-A	13	SGN	C6-O6-S2-O6S
1	1-A	15	SGN	C6-O6-S2-O6S
1	7-A	15	SGN	C6-O6-S2-O6S
1	4-A	9	SGN	C1-C2-N2-S1
1	5-A	9	SGN	C1-C2-N2-S1
1	6-A	13	SGN	C1-C2-N2-S1
1	1-A	1	SGN	C6-O6-S2-O5S
1	4-A	1	SGN	C6-O6-S2-O5S
1	8-A	1	SGN	C6-O6-S2-O5S
1	1-A	3	SGN	C6-O6-S2-O5S
1	3-A	7	SGN	C6-O6-S2-O5S
1	7-A	7	SGN	C6-O6-S2-O5S

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Mol	Chain	Res	Type	Atoms
1	1-A	11	SGN	C6-O6-S2-O4S
1	1-A	11	SGN	C6-O6-S2-O5S
1	3-A	13	SGN	C6-O6-S2-O5S
1	9-A	15	SGN	C6-O6-S2-O4S
1	9-A	15	SGN	C6-O6-S2-O5S
1	1-A	3	SGN	C6-O6-S2-O4S
1	5-A	3	SGN	C6-O6-S2-O4S
1	8-A	5	SGN	C6-O6-S2-O4S
1	9-A	5	SGN	C6-O6-S2-O4S
1	4-A	7	SGN	C6-O6-S2-O4S
1	2-A	9	SGN	C6-O6-S2-O4S
1	4-A	9	SGN	C6-O6-S2-O4S
1	6-A	9	SGN	C6-O6-S2-O5S
1	5-A	11	SGN	C6-O6-S2-O4S
1	6-A	11	SGN	C6-O6-S2-O4S
1	1-A	15	SGN	C6-O6-S2-O4S
1	5-A	17	SGN	C6-O6-S2-O5S
1	5-A	2	IDS	C3-C2-O2-S
1	8-A	14	IDS	C3-C2-O2-S
1	1-A	6	IDS	C2-O2-S-O2S
1	1-A	16	IDS	C2-O2-S-O1S
1	1-A	16	IDS	C2-O2-S-O2S
1	3-A	18	IDS	C2-O2-S-O2S
1	6-A	18	IDS	C2-O2-S-O2S
1	9-A	3	SGN	C3-C2-N2-S1
1	3-A	9	SGN	C3-C2-N2-S1
1	5-A	11	SGN	C3-C2-N2-S1
1	5-A	3	SGN	C6-O6-S2-O6S
1	3-A	5	SGN	C6-O6-S2-O6S
1	5-A	5	SGN	C6-O6-S2-O6S
1	8-A	5	SGN	C6-O6-S2-O6S
1	4-A	7	SGN	C6-O6-S2-O6S
1	4-A	9	SGN	C6-O6-S2-O6S
1	9-A	9	SGN	C6-O6-S2-O6S
1	6-A	11	SGN	C6-O6-S2-O6S
1	5-A	15	SGN	C6-O6-S2-O6S
1	9-A	3	SGN	C1-C2-N2-S1
1	3-A	9	SGN	C1-C2-N2-S1
1	5-A	11	SGN	C1-C2-N2-S1
1	3-A	13	SGN	C1-C2-N2-S1
1	8-A	17	SGN	C1-C2-N2-S1
1	7-A	2	IDS	C4-C5-C6-O6B

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Mol	Chain	Res	Type	Atoms
1	2-A	6	IDS	C4-C5-C6-O6A
1	2-A	6	IDS	C4-C5-C6-O6B
1	1-A	10	IDS	C4-C5-C6-O6A
1	3-A	12	IDS	C4-C5-C6-O6A
1	3-A	12	IDS	C4-C5-C6-O6B
1	5-A	12	IDS	C4-C5-C6-O6B
1	7-A	16	IDS	C4-C5-C6-O6A
1	1-A	4	IDS	C1-C2-O2-S
1	4-A	14	IDS	C1-C2-O2-S
1	1-A	9	SGN	C6-O6-S2-O4S
1	2-A	9	SGN	C6-O6-S2-O5S
1	1-A	1	SGN	C2-N2-S1-O1S
1	8-A	1	SGN	C2-N2-S1-O1S
1	3-A	3	SGN	C2-N2-S1-O1S
1	4-A	3	SGN	O5-C5-C6-O6
1	6-A	3	SGN	C2-N2-S1-O1S
1	8-A	3	SGN	C2-N2-S1-O1S
1	2-A	5	SGN	C2-N2-S1-O1S
1	5-A	5	SGN	C2-N2-S1-O1S
1	7-A	5	SGN	C2-N2-S1-O1S
1	1-A	7	SGN	C2-N2-S1-O1S
1	4-A	7	SGN	C2-N2-S1-O1S
1	5-A	7	SGN	C2-N2-S1-O1S
1	7-A	7	SGN	C2-N2-S1-O1S
1	5-A	11	SGN	C2-N2-S1-O1S
1	6-A	11	SGN	C2-N2-S1-O2S
1	4-A	13	SGN	C2-N2-S1-O1S
1	1-A	17	SGN	C2-N2-S1-O1S
1	4-A	17	SGN	C2-N2-S1-O1S
1	5-A	17	SGN	C2-N2-S1-O1S
1	8-A	17	SGN	C2-N2-S1-O1S
1	2-A	3	SGN	C4-C5-C6-O6
1	2-A	5	SGN	C4-C5-C6-O6
1	7-A	7	SGN	C4-C5-C6-O6
1	2-A	11	SGN	C4-C5-C6-O6
1	3-A	11	SGN	C4-C5-C6-O6
1	7-A	11	SGN	C4-C5-C6-O6
1	8-A	11	SGN	C4-C5-C6-O6
1	6-A	13	SGN	C4-C5-C6-O6
1	9-A	13	SGN	C4-C5-C6-O6
1	3-A	4	IDS	C2-O2-S-O3S
1	5-A	4	IDS	C2-O2-S-O3S

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Mol	Chain	Res	Type	Atoms
1	6-A	4	IDS	C2-O2-S-O3S
1	7-A	6	IDS	C2-O2-S-O3S
1	1-A	8	IDS	C2-O2-S-O3S
1	7-A	8	IDS	C2-O2-S-O1S
1	7-A	8	IDS	C2-O2-S-O3S
1	5-A	10	IDS	C2-O2-S-O3S
1	7-A	12	IDS	C2-O2-S-O3S
1	2-A	14	IDS	C2-O2-S-O3S
1	4-A	16	IDS	C2-O2-S-O3S
1	7-A	18	IDS	C2-O2-S-O3S
1	9-A	7	SGN	C6-O6-S2-O5S
1	1-A	3	SGN	C6-O6-S2-O6S
1	9-A	5	SGN	C6-O6-S2-O6S
1	4-A	11	SGN	C6-O6-S2-O6S
1	2-A	7	SGN	C1-C2-N2-S1
1	5-A	17	SGN	C1-C2-N2-S1
1	6-A	3	SGN	C6-O6-S2-O5S
1	5-A	7	SGN	C6-O6-S2-O5S
1	1-A	9	SGN	C6-O6-S2-O5S
1	3-A	9	SGN	C6-O6-S2-O5S
1	9-A	11	SGN	C6-O6-S2-O4S
1	9-A	11	SGN	C6-O6-S2-O5S
1	5-A	13	SGN	C6-O6-S2-O4S
1	5-A	13	SGN	C6-O6-S2-O5S
1	2-A	15	SGN	C6-O6-S2-O5S
1	8-A	17	SGN	C6-O6-S2-O5S
1	2-A	7	SGN	C3-C2-N2-S1
1	3-A	13	SGN	C3-C2-N2-S1
1	6-A	13	SGN	C3-C2-N2-S1
1	7-A	2	IDS	C2-O2-S-O1S
1	3-A	4	IDS	C2-O2-S-O1S
1	1-A	8	IDS	C2-O2-S-O1S
1	5-A	10	IDS	C2-O2-S-O1S
1	9-A	14	IDS	C2-O2-S-O1S
1	3-A	9	SGN	C6-O6-S2-O4S
1	6-A	9	SGN	C6-O6-S2-O4S
1	5-A	17	SGN	C6-O6-S2-O4S
1	8-A	17	SGN	C6-O6-S2-O4S
1	3-A	1	SGN	C2-N2-S1-O1S
1	4-A	1	SGN	C2-N2-S1-O1S
1	6-A	1	SGN	C2-N2-S1-O2S
1	7-A	1	SGN	C2-N2-S1-O2S

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Mol	Chain	Res	Type	Atoms
1	4-A	3	SGN	C2-N2-S1-O1S
1	6-A	7	SGN	C2-N2-S1-O1S
1	3-A	9	SGN	C2-N2-S1-O2S
1	4-A	11	SGN	C2-N2-S1-O1S
1	8-A	11	SGN	C2-N2-S1-O1S
1	2-A	13	SGN	C2-N2-S1-O1S
1	3-A	13	SGN	C2-N2-S1-O1S
1	6-A	13	SGN	C2-N2-S1-O2S
1	7-A	13	SGN	C2-N2-S1-O2S
1	8-A	13	SGN	C2-N2-S1-O2S
1	9-A	15	SGN	C2-N2-S1-O2S
1	7-A	17	SGN	C2-N2-S1-O1S
1	8-A	14	IDS	C2-O2-S-O1S
1	8-A	14	IDS	C2-O2-S-O3S
1	4-A	18	IDS	O5-C5-C6-O6A
1	5-A	17	SGN	C3-C2-N2-S1
1	7-A	2	IDS	C2-O2-S-O2S
1	1-A	8	IDS	C2-O2-S-O2S
1	7-A	8	IDS	C2-O2-S-O2S
1	9-A	14	IDS	C2-O2-S-O2S
1	4-A	2	IDS	O5-C5-C6-O6B
1	8-A	2	IDS	O5-C5-C6-O6A
1	8-A	2	IDS	O5-C5-C6-O6B
1	9-A	2	IDS	O5-C5-C6-O6B
1	3-A	4	IDS	O5-C5-C6-O6B
1	9-A	4	IDS	O5-C5-C6-O6B
1	1-A	8	IDS	O5-C5-C6-O6B
1	3-A	8	IDS	O5-C5-C6-O6B
1	9-A	8	IDS	O5-C5-C6-O6B
1	2-A	10	IDS	O5-C5-C6-O6B
1	4-A	10	IDS	O5-C5-C6-O6B
1	7-A	12	IDS	O5-C5-C6-O6B
1	3-A	16	IDS	O5-C5-C6-O6A
1	3-A	16	IDS	O5-C5-C6-O6B
1	5-A	16	IDS	O5-C5-C6-O6B
1	1-A	5	SGN	C1-C2-N2-S1
1	1-A	4	IDS	C4-C5-C6-O6B
1	3-A	4	IDS	C4-C5-C6-O6B
1	2-A	8	IDS	C4-C5-C6-O6B
1	6-A	8	IDS	C4-C5-C6-O6A
1	4-A	10	IDS	C4-C5-C6-O6B
1	6-A	14	IDS	C4-C5-C6-O6B

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Mol	Chain	Res	Type	Atoms
1	1-A	16	IDS	C4-C5-C6-O6B
1	7-A	16	IDS	C4-C5-C6-O6B
1	8-A	16	IDS	C4-C5-C6-O6B
1	6-A	9	SGN	C6-O6-S2-O6S
1	5-A	17	SGN	C6-O6-S2-O6S
1	9-A	7	SGN	C6-O6-S2-O4S
1	1-A	5	SGN	C2-N2-S1-O2S
1	3-A	5	SGN	C2-N2-S1-O1S
1	8-A	9	SGN	C2-N2-S1-O1S
1	7-A	11	SGN	C2-N2-S1-O1S
1	2-A	15	SGN	C2-N2-S1-O1S

There are no ring outliers.

138 monomers are involved in 274 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	8-A	8	IDS	4	0
1	7-A	17	SGN	3	0
1	5-A	3	SGN	1	0
1	7-A	5	SGN	2	0
1	5-A	17	SGN	1	0
1	4-A	8	IDS	13	0
1	1-A	14	IDS	5	0
1	1-A	12	IDS	2	0
1	6-A	7	SGN	1	0
1	6-A	10	IDS	7	0
1	6-A	14	IDS	6	0
1	2-A	2	IDS	10	0
1	6-A	1	SGN	1	0
1	8-A	7	SGN	7	0
1	4-A	7	SGN	12	0
1	9-A	11	SGN	3	0
1	8-A	2	IDS	3	0
1	2-A	4	IDS	4	0
1	2-A	15	SGN	1	0
1	4-A	18	IDS	1	0
1	3-A	14	IDS	4	0
1	3-A	6	IDS	8	0
1	7-A	15	SGN	5	0
1	3-A	1	SGN	5	0
1	6-A	16	IDS	1	0
1	5-A	15	SGN	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	9-A	15	SGN	1	0
1	6-A	2	IDS	1	0
1	6-A	8	IDS	2	0
1	4-A	12	IDS	1	0
1	2-A	14	IDS	1	0
1	3-A	17	SGN	10	0
1	8-A	16	IDS	4	0
1	9-A	17	SGN	2	0
1	7-A	4	IDS	5	0
1	3-A	18	IDS	8	0
1	3-A	4	IDS	1	0
1	2-A	11	SGN	7	0
1	2-A	16	IDS	2	0
1	9-A	4	IDS	1	0
1	1-A	11	SGN	2	0
1	9-A	16	IDS	3	0
1	2-A	8	IDS	1	0
1	3-A	8	IDS	4	0
1	7-A	13	SGN	1	0
1	4-A	9	SGN	6	0
1	4-A	2	IDS	4	0
1	9-A	5	SGN	1	0
1	9-A	1	SGN	5	0
1	5-A	10	IDS	2	0
1	3-A	11	SGN	5	0
1	6-A	18	IDS	2	0
1	1-A	15	SGN	6	0
1	6-A	3	SGN	6	0
1	5-A	5	SGN	1	0
1	7-A	12	IDS	1	0
1	4-A	1	SGN	1	0
1	8-A	6	IDS	5	0
1	1-A	17	SGN	8	0
1	1-A	18	IDS	4	0
1	3-A	9	SGN	7	0
1	8-A	12	IDS	1	0
1	5-A	7	SGN	2	0
1	9-A	2	IDS	10	0
1	4-A	3	SGN	3	0
1	4-A	17	SGN	1	0
1	2-A	1	SGN	5	0
1	6-A	13	SGN	12	0

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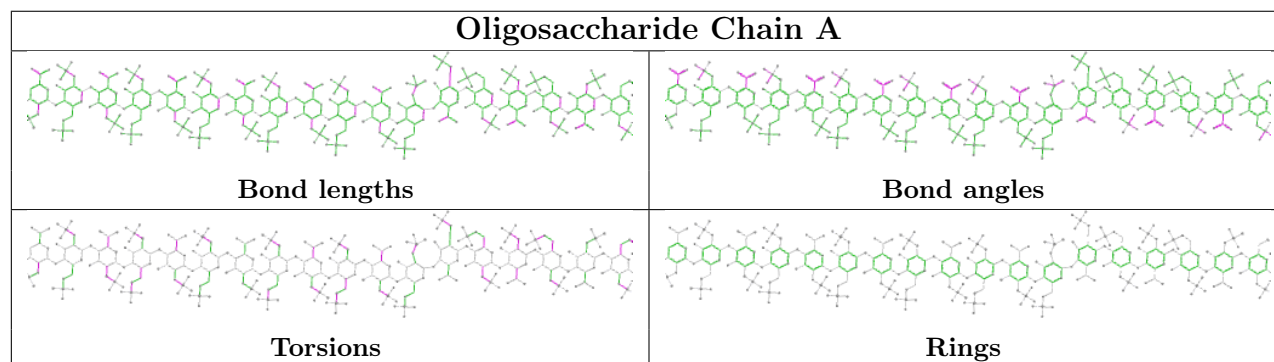
Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5-A	16	IDS	3	0
1	5-A	13	SGN	3	0
1	2-A	9	SGN	7	0
1	3-A	5	SGN	2	0
1	6-A	9	SGN	6	0
1	1-A	5	SGN	8	0
1	2-A	10	IDS	11	0
1	5-A	12	IDS	6	0
1	2-A	18	IDS	2	0
1	3-A	13	SGN	6	0
1	2-A	3	SGN	10	0
1	1-A	2	IDS	3	0
1	9-A	10	IDS	2	0
1	9-A	13	SGN	2	0
1	9-A	3	SGN	6	0
1	2-A	6	IDS	6	0
1	1-A	7	SGN	3	0
1	1-A	10	IDS	2	0
1	8-A	9	SGN	2	0
1	8-A	14	IDS	5	0
1	2-A	17	SGN	4	0
1	5-A	14	IDS	3	0
1	1-A	1	SGN	3	0
1	4-A	6	IDS	5	0
1	6-A	12	IDS	11	0
1	9-A	7	SGN	6	0
1	7-A	7	SGN	1	0
1	9-A	8	IDS	5	0
1	8-A	11	SGN	1	0
1	5-A	6	IDS	1	0
1	9-A	6	IDS	5	0
1	1-A	16	IDS	8	0
1	2-A	12	IDS	2	0
1	5-A	18	IDS	1	0
1	3-A	12	IDS	5	0
1	5-A	4	IDS	1	0
1	3-A	15	SGN	3	0
1	6-A	11	SGN	7	0
1	1-A	8	IDS	1	0
1	9-A	12	IDS	3	0
1	6-A	17	SGN	2	0
1	4-A	13	SGN	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5-A	8	IDS	2	0
1	4-A	14	IDS	1	0
1	2-A	7	SGN	5	0
1	2-A	5	SGN	1	0
1	1-A	4	IDS	1	0
1	4-A	5	SGN	1	0
1	7-A	8	IDS	1	0
1	6-A	15	SGN	1	0
1	3-A	2	IDS	5	0
1	5-A	11	SGN	5	0
1	4-A	11	SGN	1	0
1	7-A	6	IDS	1	0
1	8-A	15	SGN	8	0
1	3-A	10	IDS	5	0
1	6-A	4	IDS	6	0
1	7-A	9	SGN	1	0
1	7-A	16	IDS	8	0
1	5-A	9	SGN	1	0
1	9-A	9	SGN	5	0
1	8-A	1	SGN	5	0
1	1-A	13	SGN	7	0
1	9-A	14	IDS	1	0
1	7-A	10	IDS	1	0
1	8-A	17	SGN	1	0
1	3-A	7	SGN	7	0
1	1-A	6	IDS	9	0
1	3-A	16	IDS	5	0
1	7-A	3	SGN	4	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

There are no ligands in this entry.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.