



wwPDB Geometry-Only Validation Summary Report ⓘ

Aug 8, 2020 – 12:29 PM BST

PDB ID : 3IRJ
Title : Solution Structure of Heparin dp24
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

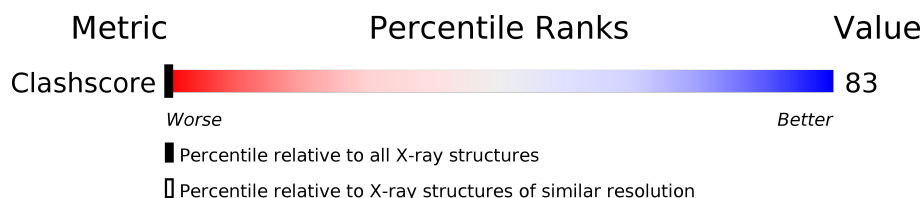
1 Overall quality at a glance

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	141614	-

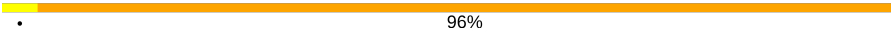




The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1-A	24	 17% 83%
1	10-A	24	 . 96%
1	11-A	24	 8% 92%
1	12-A	24	 21% 79%
1	13-A	24	 8% 92%
1	14-A	24	 13% 88%
1	15-A	24	 8% 92%
1	2-A	24	 13% 88%
1	3-A	24	 . 96%
1	4-A	24	 13% 88%

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Mol	Chain	Length	Quality of chain
1	5-A	24	 96%
1	6-A	24	 17% 83%
1	7-A	24	 33% 67%
1	8-A	24	 96%
1	9-A	24	 96%

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	14	-	-	X	-
1	IDS	1-A	6	-	-	X	-
1	SGN	1-A	7	-	-	X	-
1	SGN	10-A	1	-	-	X	-
1	IDS	10-A	2	-	-	X	-
1	SGN	10-A	3	-	-	X	-
1	IDS	10-A	4	-	-	X	-
1	SGN	11-A	23	-	-	X	-
1	IDS	11-A	24	-	-	X	-
1	IDS	12-A	6	-	-	X	-
1	IDS	13-A	14	-	-	X	-
1	SGN	13-A	15	-	-	X	-
1	SGN	13-A	17	-	-	X	-
1	IDS	13-A	18	-	-	X	-
1	SGN	13-A	19	-	-	X	-
1	IDS	14-A	20	-	-	X	-
1	IDS	15-A	22	-	-	X	-
1	SGN	15-A	23	-	-	X	-
1	IDS	15-A	24	-	-	X	-
1	SGN	15-A	5	-	-	X	-
1	IDS	15-A	6	-	-	X	-
1	SGN	15-A	7	-	-	X	-
1	IDS	15-A	8	-	-	X	-
1	SGN	15-A	9	-	-	X	-
1	IDS	2-A	12	-	-	X	-
1	SGN	2-A	13	-	-	X	-
1	IDS	2-A	16	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	IDS	2-A	20	-	-	X	-
1	IDS	3-A	12	-	-	X	-
1	SGN	3-A	13	-	-	X	-
1	SGN	3-A	17	-	-	X	-
1	IDS	3-A	18	-	-	X	-
1	IDS	3-A	24	-	-	X	-
1	IDS	3-A	4	-	-	X	-
1	SGN	3-A	5	-	-	X	-
1	IDS	3-A	8	-	-	X	-
1	SGN	4-A	21	-	-	X	-
1	IDS	4-A	22	-	-	X	-
1	IDS	5-A	10	-	-	X	-
1	IDS	5-A	6	-	-	X	-
1	SGN	5-A	7	-	-	X	-
1	IDS	6-A	10	-	-	X	-
1	IDS	6-A	12	-	-	X	-
1	SGN	6-A	13	-	-	X	-
1	IDS	6-A	14	-	-	X	-
1	IDS	6-A	2	-	-	X	-
1	SGN	6-A	21	-	-	X	-
1	IDS	6-A	22	-	-	X	-
1	SGN	6-A	5	-	-	X	-
1	IDS	6-A	6	-	-	X	-
1	SGN	6-A	7	X	-	X	-
1	SGN	6-A	9	-	-	X	-
1	SGN	8-A	15	-	-	X	-
1	IDS	8-A	16	-	-	X	-
1	SGN	8-A	17	-	-	X	-
1	IDS	8-A	18	-	-	X	-
1	SGN	8-A	19	-	-	X	-
1	IDS	8-A	2	-	-	X	-
1	IDS	8-A	20	-	-	X	-
1	SGN	8-A	3	-	-	X	-
1	IDS	8-A	4	-	-	X	-
1	SGN	8-A	5	-	-	X	-
1	IDS	8-A	6	-	-	X	-
1	IDS	9-A	10	-	-	X	-
1	SGN	9-A	15	-	-	X	-
1	IDS	9-A	16	-	-	X	-
1	SGN	9-A	17	-	-	X	-
1	IDS	9-A	2	-	-	X	-
1	IDS	9-A	20	-	-	X	-

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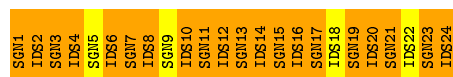
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	IDS	9-A	24	X	-	-	-
1	IDS	9-A	8	-	-	X	-
1	SGN	9-A	9	-	-	X	-

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	8-A	24	Total 420	C 144	N 12	O 228	S 36	0	0	0
1	9-A	24	Total 420	C 144	N 12	O 228	S 36	0	0	0
1	10-A	24	Total 420	C 144	N 12	O 228	S 36	0	0	0
1	11-A	24	Total 420	C 144	N 12	O 228	S 36	0	0	0
1	12-A	24	Total 420	C 144	N 12	O 228	S 36	0	0	0
1	13-A	24	Total 420	C 144	N 12	O 228	S 36	0	0	0
1	14-A	24	Total 420	C 144	N 12	O 228	S 36	0	0	0
1	15-A	24	Total 420	C 144	N 12	O 228	S 36	0	0	0

Note EDS was not executed.

Chain 1-A: 17% 83%

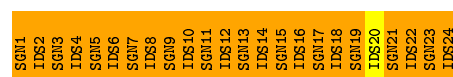


Chain 2-A:  13% 88%

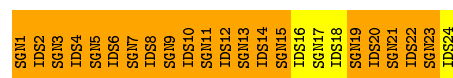
[illegible][illegible]

● 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

Chain 5-A: 96%



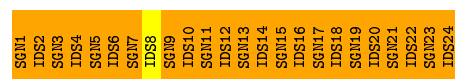
Chain 6-A:  17% 83%

[illegible]

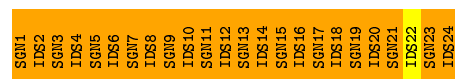
Chain 7-A:  33% 67%

[illegible]

Chain 8-A:  96%

[illegible]

Chain 9-A: 96%



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

[illegible]

Chain 10-A:  96%

SGN1
IDS2
SGN3
IDS4
SGN5
IDS6
SGN7
IDS8
SGN9
IDS10
SGN11
IDS12
SGN13
IDS14
SGN15
IDS16
SGN17
IDS18
SGN19
IDS20
SGN21
IDS22
SGN23
IDS24

[illegible]

Chain 11-A: 8% 92%

SGN1	IDS2	SGN3	IDS4	SGN5	IDS6	SGN7	IDS8	SGN9	IDS10	SGN11	IDS12	SGN13	IDS14	SGN15	IDS16	SGN17	IDS18	SGN19	IDS20	SGN21	IDS22	SGN23	IDS24
------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

[illegible]

WORLDWIDE
PDB
PROTEIN DATA BANK

[illegible]

SGN1
IDS2
SGN3
IDS4
SGN5
IDS6
SGN7
IDS8
SGN9
IDS10
SGN11
IDS12
SGN13
IDS14
SGN15
IDS16
SGN17
IDS18
SGN19
IDS20
SGN21
IDS22
SGN23
IDS24

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	420	0	133	43	0
1	2-A	420	0	131	49	0
1	3-A	420	0	132	52	0
1	4-A	420	0	129	36	0
1	5-A	420	0	132	35	0
1	6-A	420	0	131	63	0
1	7-A	420	0	128	22	0
1	8-A	420	0	129	72	0
1	9-A	420	0	132	60	0
1	10-A	420	0	130	48	0
1	11-A	420	0	132	47	0
1	12-A	420	0	132	26	0
1	13-A	420	0	130	46	0
1	14-A	420	0	129	33	0
1	15-A	420	0	127	51	0
All	All	6300	0	1957	683	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 83.

The worst 5 of 683 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:16:IDS:H3	1:A:17:SGN:N2	1.29	1.45
1:A:23:SGN:O4S	1:A:24:IDS:C6	1.66	1.42
1:A:10:IDS:H3	1:A:11:SGN:N2	1.17	1.40
1:A:7:SGN:C5	1:A:8:IDS:O2S	1.68	1.40
1:A:10:IDS:C3	1:A:11:SGN:N2	1.88	1.36

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](#)

360 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	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	1-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	1-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	1-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	1-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	1-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	1-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	1-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	1-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	1-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	1-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	10-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	10-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	10-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	10-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	10-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	10-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	10-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	10-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	10-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	10-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	10-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	10-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	10-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	11-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	11-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	11-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	11-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	11-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	11-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	11-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	11-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	11-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	11-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	11-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	11-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	11-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	11-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	11-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	11-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	11-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	11-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	12-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	12-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	12-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	12-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	12-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	12-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	12-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	12-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	12-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	12-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	12-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	12-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	12-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	12-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	12-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	12-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	12-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	13-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	13-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	13-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	13-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	13-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	13-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	13-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	13-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	13-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	13-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	13-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	13-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	13-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	13-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	13-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	13-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
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1	IDS	13-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	13-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	14-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	14-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	14-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	14-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
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1	SGN	14-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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1	SGN	14-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	14-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	14-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	15-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	15-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	15-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	15-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	15-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	15-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	15-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	15-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	15-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	2-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	2-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	2-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	2-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	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	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	2-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	2-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	2-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	2-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	2-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	2-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	2-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	2-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	3-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	3-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	3-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	3-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	3-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	3-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	3-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	3-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	3-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	3-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	3-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	3-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	3-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
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1	IDS	3-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	3-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	4-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	4-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	4-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	4-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
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1	SGN	4-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	5-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	5-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	5-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)

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1	IDS	5-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	5-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	5-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	5-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	5-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	5-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	5-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	5-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	5-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	5-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	5-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	5-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	5-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	5-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	5-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	6-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	6-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	6-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	6-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	6-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	6-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	6-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	6-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	6-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	6-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	6-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	6-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	6-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	6-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	6-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	6-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	6-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	7-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	7-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	7-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	7-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	7-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	7-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	7-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	7-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	7-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	7-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	7-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	7-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	7-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	7-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	7-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	7-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	7-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	8-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	8-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	8-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	8-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	8-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	8-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	8-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	8-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	8-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	8-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	8-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	8-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	8-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	9-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	9-A	10	1	13,16,17	1.45	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	9-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	12	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	9-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	9-A	14	1	13,16,17	1.45	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	9-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	16	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	9-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	9-A	20	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	9-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	9-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	9-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	24	1	12,15,17	1.49	2 (16%)	12,22,26	2.41	1 (8%)
1	SGN	9-A	3	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	6	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	8	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	9-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	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	-	0/5/26/29	0/1/1/1
1	SGN	1-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	1-A	12	1	-	3/5/26/29	0/1/1/1
1	SGN	1-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	14	1	-	0/5/26/29	0/1/1/1
1	SGN	1-A	15	1	-	2/11/28/31	0/1/1/1
1	IDS	1-A	16	1	-	5/5/26/29	0/1/1/1
1	SGN	1-A	17	1	-	5/11/28/31	0/1/1/1
1	IDS	1-A	18	1	-	3/5/26/29	0/1/1/1
1	SGN	1-A	19	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	2	1	-	1/5/26/29	0/1/1/1
1	IDS	1-A	20	1	-	3/5/26/29	0/1/1/1
1	SGN	1-A	21	1	-	9/11/28/31	0/1/1/1
1	IDS	1-A	22	1	-	1/5/26/29	0/1/1/1
1	SGN	1-A	23	1	-	8/11/28/31	0/1/1/1
1	IDS	1-A	24	1	-	0/5/22/29	0/1/1/1
1	SGN	1-A	3	1	-	3/11/28/31	0/1/1/1

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

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

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

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

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

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

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

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

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

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

The worst 5 of 720 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	14	IDS	O2-C2	-3.69	1.41	1.47
1	10-A	14	IDS	O2-C2	-3.69	1.41	1.47
1	5-A	14	IDS	O2-C2	-3.69	1.41	1.47
1	3-A	14	IDS	O2-C2	-3.69	1.41	1.47
1	15-A	14	IDS	O2-C2	-3.69	1.41	1.47

The worst 5 of 360 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	2	IDS	C2-O2-S	8.00	128.34	117.91
1	15-A	2	IDS	C2-O2-S	8.00	128.34	117.91
1	10-A	2	IDS	C2-O2-S	8.00	128.34	117.91
1	12-A	2	IDS	C2-O2-S	8.00	128.34	117.91
1	5-A	2	IDS	C2-O2-S	8.00	128.34	117.91

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	6-A	7	SGN	C1
1	9-A	24	IDS	C1

5 of 1080 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	15-A	7	SGN	C4-C5-C6-O6
1	15-A	7	SGN	C2-N2-S1-O1S
1	12-A	22	IDS	C1-C2-O2-S
1	1-A	7	SGN	C4-C5-C6-O6
1	1-A	7	SGN	C2-N2-S1-O1S

There are no ring outliers.

319 monomers are involved in 683 short contacts:

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

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5-A	11	SGN	3	0
1	13-A	7	SGN	2	0
1	8-A	5	SGN	9	0
1	11-A	20	IDS	4	0
1	11-A	8	IDS	5	0
1	5-A	8	IDS	3	0
1	14-A	17	SGN	2	0
1	9-A	7	SGN	3	0
1	7-A	3	SGN	2	0
1	4-A	12	IDS	4	0
1	9-A	4	IDS	1	0
1	1-A	21	SGN	1	0
1	15-A	21	SGN	6	0
1	10-A	16	IDS	1	0
1	15-A	4	IDS	4	0
1	5-A	4	IDS	3	0
1	6-A	5	SGN	7	0
1	10-A	17	SGN	4	0
1	9-A	1	SGN	4	0
1	15-A	3	SGN	1	0
1	10-A	9	SGN	3	0
1	3-A	14	IDS	1	0
1	7-A	21	SGN	2	0
1	2-A	4	IDS	3	0
1	11-A	17	SGN	3	0
1	12-A	17	SGN	1	0
1	9-A	13	SGN	1	0
1	2-A	10	IDS	4	0
1	6-A	9	SGN	8	0
1	1-A	3	SGN	4	0
1	5-A	2	IDS	2	0
1	15-A	14	IDS	2	0
1	10-A	1	SGN	13	0
1	3-A	12	IDS	7	0
1	7-A	11	SGN	1	0
1	1-A	8	IDS	5	0
1	14-A	7	SGN	5	0
1	13-A	12	IDS	4	0
1	12-A	21	SGN	1	0
1	8-A	7	SGN	4	0
1	2-A	3	SGN	5	0
1	14-A	15	SGN	4	0

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

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

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

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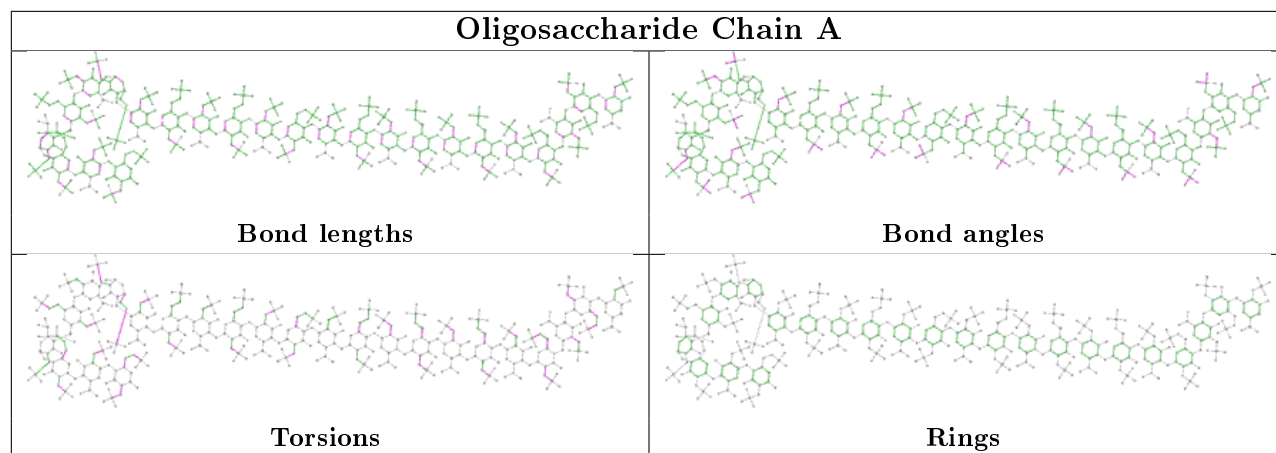
Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	4-A	14	IDS	5	0
1	11-A	14	IDS	1	0
1	4-A	7	SGN	6	0
1	11-A	21	SGN	3	0
1	5-A	17	SGN	1	0
1	12-A	5	SGN	6	0
1	8-A	12	IDS	2	0
1	5-A	16	IDS	2	0
1	9-A	6	IDS	2	0
1	3-A	4	IDS	6	0
1	15-A	22	IDS	6	0
1	9-A	21	SGN	6	0
1	15-A	17	SGN	2	0
1	14-A	6	IDS	4	0
1	13-A	21	SGN	2	0
1	14-A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

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