



wwPDB Geometry-Only Validation Summary Report ⓘ

Aug 10, 2020 – 12:57 AM BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

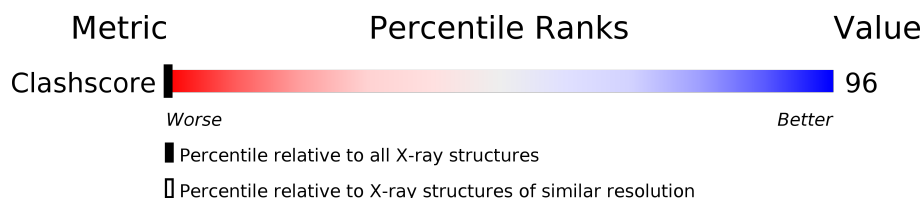
1 Overall quality at a glance

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	30	 10% 90%
1	10-A	30	 7% 93%
1	11-A	30	 13% 87%
1	12-A	30	 20% 80%
1	13-A	30	 . 97%
1	14-A	30	 17% 83%
1	2-A	30	 . 97%
1	3-A	30	 13% 87%
1	4-A	30	 . 97%
1	5-A	30	 17% 83%

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Mol	Chain	Length	Quality of chain
1	6-A	30	 7% 93%
1	7-A	30	 3% 97%
1	8-A	30	 13% 87%
1	9-A	30	 10% 90%

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

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

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

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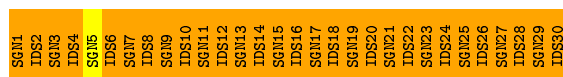
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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	IDS	6-A	12	-	-	X	-
1	SGN	6-A	13	-	-	X	-
1	SGN	6-A	15	-	-	X	-
1	IDS	6-A	16	-	-	X	-
1	IDS	6-A	18	-	-	X	-
1	IDS	6-A	24	-	-	X	-
1	IDS	6-A	30	-	-	X	-
1	IDS	7-A	10	-	-	X	-
1	IDS	7-A	16	-	-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

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

Chain 2-A:  97%



- [illegible]



- [illegible]

Chain 4-A: 97%

SGM1	IDS2	SGN3	IDS4	SGN5	IDS6	SGN7	IDS8	SGN9	IDS10	SGN11	IDS12	SGN13	IDS14	SGN15	IDS16	SGN17	IDS18	SGN19	IDS20	SGM21	IDS22	SGM23	IDS24	SGM25	IDS26	SGM27	IDS28	SGM29	IDS30
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- [illegible]

Chain 5-A: 17% 83%

SGN1	IDS2	SGN3	IDS4	SGN5	IDS6	SGN7	IDS8	SGN9	IDS10	SGN11	IDS12	SGN13	IDS14	SGN15	IDS16	SGN17	IDS18	SGN19	IDS20	SGN21	IDS22	SGN23	IDS24	SGN25	IDS26	SGN27	IDS28	SGN29	IDS30
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- [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	SGN25	IDS26	SGN27	IDS28	SGN29	IDS30
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SGN1	IDS2	SGN3	IDS4	SGN5	IDS6	SGN7	IDS8	SGN9	IDS10	SGN11	IDS12	SGN13	IDS14	SGN15	IDS16	SGN17	IDS18	SGN19	IDS20	SGN21	IDS22	SGN23	IDS24	SGN25	IDS26	SGN27	IDS28	SGN29	IDS30
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WORLD WIDE
PDB
PROTEIN DATA BANK





WORLD WIDE
PDB
PROTEIN DATA BANK

SGM1	IDS10
IDS2	SGM11
SGM3	IDS12
IDS4	SGM13
SGM5	IDS14
IDS6	SGM15
SGM7	IDS16
IDS8	SGM17
SGM9	IDS18
	SGM19
	IDS20
	SGM21
	IDS22
	SGM23
	IDS24
	SGM25
	IDS26
	SGM27
	IDS28
	SGM29
	IDS30

4 Model quality

4.1 Standard geometry

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	525	0	162	51	0
1	2-A	525	0	164	50	0
1	3-A	525	0	164	79	0
1	4-A	525	0	164	105	0
1	5-A	525	0	163	47	0
1	6-A	525	0	162	64	0
1	7-A	525	0	161	73	0
1	8-A	525	0	165	53	0
1	9-A	525	0	165	110	0
1	10-A	525	0	163	44	0
1	11-A	525	0	162	60	0
1	12-A	525	0	163	56	0
1	13-A	525	0	163	73	0
1	14-A	525	0	164	57	0
All	All	7350	0	2285	922	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 96.

The worst 5 of 922 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

4.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

420 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SGN	1-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	1-A	10	1	13,16,17	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	1-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	1-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	1-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	1-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	1-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	1-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	1-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	1-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	1-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	1-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	11	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
1	IDS	10-A	12	1	13,16,17	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	10-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	10-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	10-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	10-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	10-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	10-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	10-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	10-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	10-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	10-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	10-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	10-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	10-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	10-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	11-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	14	1	13,16,17	1.44	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	1.40	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	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	2.22	1 (6%)
1	SGN	11-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	11-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	11-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	11-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	11-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	11-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	11-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	11-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	11-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	11-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	11-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	11-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	11-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	12-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	12-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	12-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	12-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	12-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	12-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	12-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	12-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	12-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	12-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	12-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	12-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	12-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	12-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	13-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	14	1	13,16,17	1.44	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%)
1	IDS	13-A	16	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	13-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	13-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	13-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	13-A	25	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	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	13-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	13-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	13-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	13-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	13-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	13-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	13-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	13-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	13-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	14-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	14	1	13,16,17	1.44	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	14-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	16	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	14-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	14-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	IDS	14-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	14-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	14-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	24	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	14-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	14-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	14-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	14-A	3	1	18,19,20	1.21	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	14-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	14-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	14-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	14-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	14-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	2-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	2-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	2-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	2-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	2-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	2-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	2-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	2-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	2-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	2-A	7	1	18,19,20	1.23	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	2-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	2-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	3-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	3-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	3-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	3-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
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1	SGN	3-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	3-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
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1	SGN	3-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	3-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	3-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	3-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	3-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	3-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	4-A	11	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
1	IDS	4-A	12	1	13,16,17	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	4-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	14	1	13,16,17	1.44	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	4-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	16	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	4-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	4-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	4-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	2	1	13,16,17	1.41	2 (15%)	15,24,26	2.21	1 (6%)
1	IDS	4-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	4-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	4-A	22	1	13,16,17	1.41	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	4-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	24	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	4-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	4-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	4-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	4-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	4-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	4-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	4-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	4-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	4-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	4-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	5-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	12	1	13,16,17	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	5-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	14	1	13,16,17	1.44	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	1.40	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	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	2.22	1 (6%)
1	SGN	5-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	5-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	5-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	5-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	5-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	5-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	5-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	5-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	5-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	5-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	5-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	5-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	5-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	6-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	6-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	6-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	6-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	6-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	6-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	6-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	6-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	6-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	6-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	6-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	6-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	6-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	6-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	7-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	7-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	7-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	7-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	7-A	25	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	7-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	7-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	7-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	7-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	7-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	7-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	7-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	7-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	7-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	7-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	1 (4%)
1	SGN	8-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	8-A	10	1	13,16,17	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	8-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	8-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	8-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	8-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	8-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	8-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	8-A	3	1	18,19,20	1.21	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	8-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	8-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	8-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	8-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	8-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	8-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	1.40	2 (15%)	15,24,26	2.21	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	1.39	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	9-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	14	1	13,16,17	1.44	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	1.40	2 (15%)	15,24,26	2.23	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	2.22	1 (6%)
1	SGN	9-A	19	1	18,19,20	1.23	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	2.21	1 (6%)
1	IDS	9-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	21	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	26	1	13,16,17	1.43	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	9-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	9-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	9-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	9-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	30	1	12,15,17	1.47	2 (16%)	12,22,26	2.41	1 (8%)
1	IDS	9-A	4	1	13,16,17	1.46	3 (23%)	15,24,26	2.22	1 (6%)
1	SGN	9-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	6	1	13,16,17	1.42	2 (15%)	15,24,26	2.19	1 (6%)
1	SGN	9-A	7	1	18,19,20	1.23	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	9-A	8	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	9-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	1 (4%)

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

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

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

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

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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	9-A	17	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	18	1	-	3/5/26/29	0/1/1/1
1	SGN	9-A	19	1	-	1/11/28/31	0/1/1/1
1	IDS	9-A	2	1	-	2/5/26/29	0/1/1/1
1	IDS	9-A	20	1	-	3/5/26/29	0/1/1/1
1	SGN	9-A	21	1	-	1/11/28/31	0/1/1/1
1	IDS	9-A	22	1	-	2/5/26/29	0/1/1/1
1	SGN	9-A	23	1	-	4/11/28/31	0/1/1/1
1	IDS	9-A	24	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	25	1	-	2/11/28/31	0/1/1/1
1	IDS	9-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	27	1	-	6/11/28/31	0/1/1/1
1	IDS	9-A	28	1	-	1/5/26/29	0/1/1/1
1	SGN	9-A	29	1	-	5/11/28/31	0/1/1/1
1	SGN	9-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	30	1	-	0/5/22/29	0/1/1/1
1	IDS	9-A	4	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	5	1	-	2/11/28/31	0/1/1/1
1	IDS	9-A	6	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	7	1	-	3/11/28/31	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 840 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	4	IDS	O2-C2	-3.64	1.41	1.47
1	8-A	4	IDS	O2-C2	-3.64	1.41	1.47
1	6-A	4	IDS	O2-C2	-3.64	1.41	1.47
1	7-A	4	IDS	O2-C2	-3.64	1.41	1.47
1	13-A	4	IDS	O2-C2	-3.64	1.41	1.47

The worst 5 of 420 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	16	IDS	C2-O2-S	8.02	128.37	117.91
1	2-A	16	IDS	C2-O2-S	8.02	128.37	117.91
1	5-A	16	IDS	C2-O2-S	8.02	128.37	117.91
1	4-A	16	IDS	C2-O2-S	8.02	128.37	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	16	IDS	C2-O2-S	8.02	128.37	117.91

There are no chirality outliers.

5 of 1036 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2-A	3	SGN	C4-C5-C6-O6
1	2-A	3	SGN	O5-C5-C6-O6
1	2-A	3	SGN	C2-N2-S1-O2S
1	3-A	27	SGN	C4-C5-C6-O6
1	3-A	27	SGN	O5-C5-C6-O6

There are no ring outliers.

378 monomers are involved in 922 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	9-A	24	IDS	18	0
1	3-A	12	IDS	2	0
1	14-A	25	SGN	6	0
1	11-A	4	IDS	4	0
1	2-A	3	SGN	2	0
1	7-A	23	SGN	6	0
1	7-A	9	SGN	9	0
1	8-A	13	SGN	5	0
1	5-A	17	SGN	2	0
1	7-A	16	IDS	7	0
1	14-A	22	IDS	5	0
1	6-A	3	SGN	4	0
1	8-A	20	IDS	1	0
1	9-A	27	SGN	2	0
1	5-A	11	SGN	1	0
1	14-A	5	SGN	2	0
1	11-A	19	SGN	4	0
1	8-A	4	IDS	1	0
1	11-A	8	IDS	2	0
1	6-A	22	IDS	4	0
1	3-A	18	IDS	1	0
1	13-A	30	IDS	1	0
1	6-A	6	IDS	2	0
1	3-A	20	IDS	13	0
1	11-A	3	SGN	1	0

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	9-A	14	IDS	11	0
1	5-A	13	SGN	3	0
1	5-A	14	IDS	9	0
1	3-A	14	IDS	6	0
1	11-A	5	SGN	7	0
1	4-A	17	SGN	4	0
1	2-A	21	SGN	5	0
1	12-A	24	IDS	7	0
1	11-A	28	IDS	2	0
1	9-A	12	IDS	7	0
1	9-A	22	IDS	7	0
1	11-A	25	SGN	2	0
1	3-A	21	SGN	13	0
1	4-A	9	SGN	14	0
1	9-A	21	SGN	8	0
1	1-A	27	SGN	2	0
1	1-A	22	IDS	5	0
1	10-A	2	IDS	3	0
1	14-A	1	SGN	3	0
1	5-A	24	IDS	1	0
1	3-A	25	SGN	5	0
1	12-A	30	IDS	1	0
1	4-A	29	SGN	1	0
1	13-A	8	IDS	1	0
1	5-A	27	SGN	4	0
1	10-A	6	IDS	3	0
1	12-A	14	IDS	4	0
1	2-A	26	IDS	10	0
1	5-A	18	IDS	2	0
1	12-A	13	SGN	5	0
1	2-A	23	SGN	9	0
1	6-A	29	SGN	6	0
1	9-A	19	SGN	17	0
1	1-A	28	IDS	3	0
1	4-A	15	SGN	6	0
1	2-A	10	IDS	3	0
1	7-A	18	IDS	2	0
1	13-A	1	SGN	3	0
1	13-A	4	IDS	7	0
1	11-A	26	IDS	1	0
1	5-A	28	IDS	6	0
1	5-A	2	IDS	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	12-A	6	IDS	7	0
1	13-A	2	IDS	3	0
1	2-A	6	IDS	3	0
1	13-A	27	SGN	5	0
1	12-A	15	SGN	6	0
1	11-A	17	SGN	7	0
1	3-A	27	SGN	1	0
1	7-A	19	SGN	1	0
1	6-A	8	IDS	5	0
1	13-A	13	SGN	12	0
1	1-A	5	SGN	2	0
1	14-A	13	SGN	6	0
1	11-A	22	IDS	3	0
1	5-A	16	IDS	1	0
1	7-A	28	IDS	3	0
1	9-A	23	SGN	9	0
1	3-A	6	IDS	5	0
1	11-A	18	IDS	6	0
1	11-A	12	IDS	8	0
1	11-A	24	IDS	7	0
1	5-A	21	SGN	5	0
1	5-A	10	IDS	1	0
1	12-A	19	SGN	3	0
1	3-A	29	SGN	11	0
1	7-A	20	IDS	1	0
1	14-A	24	IDS	10	0
1	1-A	6	IDS	3	0
1	10-A	15	SGN	4	0
1	14-A	21	SGN	2	0
1	7-A	25	SGN	4	0
1	3-A	17	SGN	5	0
1	9-A	1	SGN	2	0
1	14-A	9	SGN	1	0
1	2-A	25	SGN	3	0
1	1-A	24	IDS	6	0
1	11-A	9	SGN	2	0
1	7-A	13	SGN	2	0
1	6-A	25	SGN	5	0
1	12-A	10	IDS	5	0
1	2-A	1	SGN	1	0
1	2-A	12	IDS	1	0
1	5-A	22	IDS	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	14-A	19	SGN	5	0
1	4-A	18	IDS	7	0
1	14-A	15	SGN	3	0
1	4-A	16	IDS	8	0
1	10-A	24	IDS	3	0
1	13-A	20	IDS	3	0
1	8-A	18	IDS	7	0
1	14-A	3	SGN	3	0
1	5-A	30	IDS	1	0
1	4-A	4	IDS	2	0
1	7-A	5	SGN	2	0
1	4-A	23	SGN	9	0
1	4-A	26	IDS	3	0
1	3-A	16	IDS	6	0
1	9-A	29	SGN	1	0
1	9-A	18	IDS	12	0
1	8-A	15	SGN	3	0
1	3-A	22	IDS	10	0
1	4-A	3	SGN	4	0
1	2-A	30	IDS	4	0
1	5-A	15	SGN	7	0
1	9-A	20	IDS	15	0
1	4-A	24	IDS	10	0
1	9-A	7	SGN	4	0
1	11-A	21	SGN	6	0
1	4-A	22	IDS	4	0
1	13-A	18	IDS	6	0
1	9-A	17	SGN	12	0
1	3-A	23	SGN	6	0
1	3-A	15	SGN	2	0
1	2-A	4	IDS	2	0
1	10-A	5	SGN	4	0
1	14-A	18	IDS	1	0
1	10-A	12	IDS	1	0
1	4-A	21	SGN	5	0
1	11-A	10	IDS	2	0
1	13-A	7	SGN	2	0
1	9-A	2	IDS	5	0
1	1-A	13	SGN	2	0
1	7-A	24	IDS	8	0
1	13-A	24	IDS	1	0
1	6-A	2	IDS	2	0

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	9-A	15	SGN	11	0
1	4-A	27	SGN	4	0
1	14-A	11	SGN	4	0
1	4-A	2	IDS	4	0
1	5-A	25	SGN	9	0
1	11-A	6	IDS	7	0
1	10-A	8	IDS	3	0
1	11-A	15	SGN	7	0
1	11-A	23	SGN	9	0
1	5-A	9	SGN	1	0
1	13-A	16	IDS	7	0
1	4-A	14	IDS	3	0
1	2-A	19	SGN	1	0
1	6-A	19	SGN	2	0
1	10-A	7	SGN	2	0
1	6-A	30	IDS	6	0
1	8-A	7	SGN	1	0
1	4-A	5	SGN	1	0
1	9-A	28	IDS	2	0
1	14-A	20	IDS	6	0
1	10-A	18	IDS	4	0
1	10-A	4	IDS	4	0
1	9-A	26	IDS	13	0
1	4-A	25	SGN	8	0
1	9-A	16	IDS	11	0
1	13-A	23	SGN	1	0
1	6-A	24	IDS	6	0
1	8-A	25	SGN	6	0
1	1-A	17	SGN	3	0
1	13-A	14	IDS	3	0
1	1-A	10	IDS	11	0
1	8-A	19	SGN	5	0
1	6-A	12	IDS	10	0
1	8-A	1	SGN	1	0
1	6-A	27	SGN	1	0
1	1-A	8	IDS	4	0
1	3-A	5	SGN	11	0
1	5-A	23	SGN	5	0
1	5-A	26	IDS	9	0
1	10-A	30	IDS	2	0
1	2-A	15	SGN	2	0
1	2-A	29	SGN	5	0

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

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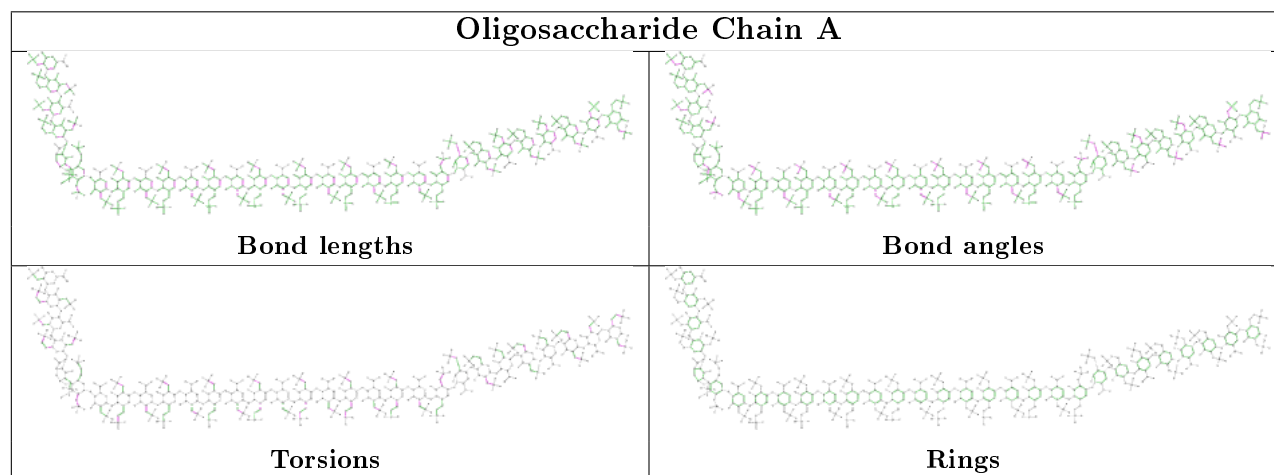
Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	14-A	23	SGN	8	0
1	7-A	6	IDS	1	0
1	6-A	14	IDS	4	0
1	8-A	14	IDS	3	0
1	13-A	15	SGN	7	0
1	1-A	25	SGN	7	0
1	6-A	7	SGN	2	0
1	8-A	2	IDS	1	0
1	7-A	10	IDS	14	0
1	14-A	8	IDS	4	0
1	10-A	19	SGN	4	0
1	2-A	24	IDS	10	0
1	8-A	28	IDS	5	0
1	1-A	14	IDS	2	0
1	14-A	14	IDS	5	0
1	12-A	18	IDS	1	0
1	13-A	10	IDS	5	0
1	8-A	11	SGN	2	0
1	5-A	3	SGN	2	0
1	9-A	6	IDS	6	0
1	3-A	24	IDS	3	0
1	2-A	9	SGN	1	0
1	10-A	22	IDS	2	0
1	1-A	21	SGN	2	0
1	8-A	17	SGN	2	0
1	12-A	16	IDS	6	0
1	12-A	27	SGN	13	0
1	5-A	20	IDS	1	0
1	4-A	28	IDS	4	0
1	11-A	13	SGN	7	0
1	12-A	28	IDS	13	0
1	6-A	20	IDS	1	0
1	1-A	26	IDS	3	0
1	7-A	15	SGN	2	0
1	8-A	5	SGN	3	0
1	12-A	22	IDS	2	0
1	7-A	1	SGN	5	0
1	2-A	8	IDS	1	0
1	4-A	6	IDS	12	0
1	2-A	18	IDS	3	0
1	11-A	27	SGN	2	0
1	12-A	20	IDS	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	10-A	16	IDS	2	0
1	7-A	27	SGN	6	0
1	1-A	16	IDS	2	0
1	8-A	10	IDS	11	0
1	4-A	7	SGN	11	0
1	5-A	29	SGN	3	0
1	1-A	11	SGN	8	0
1	12-A	11	SGN	6	0
1	10-A	28	IDS	7	0
1	1-A	9	SGN	4	0
1	2-A	14	IDS	2	0
1	7-A	11	SGN	6	0
1	1-A	3	SGN	2	0
1	8-A	16	IDS	2	0
1	2-A	17	SGN	2	0
1	1-A	1	SGN	5	0
1	13-A	19	SGN	6	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 ⓘ

There are no chain breaks in this entry.