



# wwPDB Geometry-Only Validation Summary Report ⓘ

Aug 9, 2020 – 01:37 PM BST

PDB ID : 3IRL  
Title : Solution Structure of Heparin dp36  
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](mailto: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.

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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

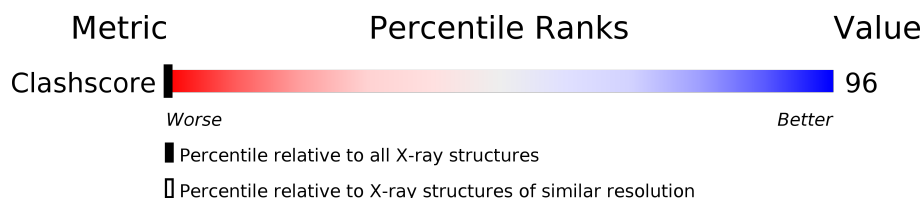
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION SCATTERING*

The reported resolution of this entry is unknown.

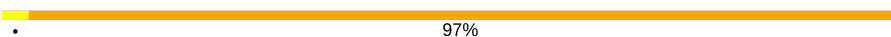



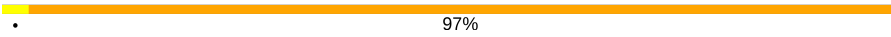





Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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  $\geq 3$ , 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	36	 97%
1	10-A	36	 11% 89%
1	11-A	36	 17% 83%
1	12-A	36	 14% 86%
1	13-A	36	 97%
1	14-A	36	 14% 86%
1	2-A	36	 6% 94%
1	3-A	36	 17% 83%
1	4-A	36	 8% 92%
1	5-A	36	 11% 89%

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Mol	Chain	Length	Quality of chain
1	6-A	36	
1	7-A	36	
1	8-A	36	
1	9-A	36	

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	17	-	-	X	-
1	IDS	1-A	18	-	-	X	-
1	IDS	1-A	22	-	-	X	-
1	SGN	1-A	23	-	-	X	-
1	IDS	1-A	24	-	-	X	-
1	SGN	1-A	29	-	-	X	-
1	IDS	1-A	30	-	-	X	-
1	SGN	1-A	31	-	-	X	-
1	IDS	1-A	32	-	-	X	-
1	SGN	1-A	33	-	-	X	-
1	IDS	10-A	10	-	-	X	-
1	SGN	10-A	11	-	-	X	-
1	IDS	10-A	12	-	-	X	-
1	SGN	10-A	19	-	-	X	-
1	IDS	10-A	20	-	-	X	-
1	SGN	10-A	21	-	-	X	-
1	IDS	10-A	22	-	-	X	-
1	SGN	10-A	27	-	-	X	-
1	IDS	10-A	28	-	-	X	-
1	IDS	10-A	6	-	-	X	-
1	SGN	10-A	9	-	-	X	-
1	IDS	11-A	10	-	-	X	-
1	IDS	11-A	12	-	-	X	-
1	IDS	11-A	16	-	-	X	-
1	SGN	11-A	21	-	-	X	-
1	IDS	11-A	22	-	-	X	-
1	IDS	11-A	28	-	-	X	-
1	IDS	11-A	32	-	-	X	-
1	SGN	11-A	33	-	-	X	-
1	IDS	11-A	34	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	IDS	12-A	10	-	-	X	-
1	SGN	12-A	11	-	-	X	-
1	SGN	12-A	13	-	-	X	-
1	IDS	12-A	18	-	-	X	-
1	SGN	12-A	19	-	-	X	-
1	SGN	12-A	33	-	-	X	-
1	IDS	12-A	8	-	-	X	-
1	SGN	12-A	9	-	-	X	-
1	IDS	13-A	14	-	-	X	-
1	SGN	13-A	15	-	-	X	-
1	IDS	13-A	16	-	-	X	-
1	IDS	13-A	22	-	-	X	-
1	IDS	13-A	26	-	-	X	-
1	IDS	13-A	28	-	-	X	-
1	SGN	13-A	29	-	-	X	-
1	IDS	13-A	8	-	-	X	-
1	SGN	14-A	1	-	-	X	-
1	SGN	14-A	17	-	-	X	-
1	IDS	14-A	18	-	-	X	-
1	IDS	14-A	2	-	-	X	-
1	IDS	14-A	20	-	-	X	-
1	SGN	14-A	25	-	-	X	-
1	IDS	14-A	26	-	-	X	-
1	SGN	14-A	3	-	-	X	-
1	IDS	14-A	4	-	-	X	-
1	SGN	14-A	5	-	-	X	-
1	IDS	14-A	6	-	-	X	-
1	IDS	14-A	8	-	-	X	-
1	IDS	2-A	10	-	-	X	-
1	IDS	2-A	12	-	-	X	-
1	SGN	2-A	13	-	-	X	-
1	IDS	2-A	14	-	-	X	-
1	IDS	2-A	18	-	-	X	-
1	SGN	2-A	19	-	-	X	-
1	IDS	2-A	20	-	-	X	-
1	SGN	2-A	21	-	-	X	-
1	IDS	2-A	22	-	-	X	-
1	SGN	2-A	23	-	-	X	-
1	IDS	2-A	28	-	-	X	-
1	SGN	2-A	29	-	-	X	-
1	IDS	2-A	30	-	-	X	-
1	IDS	2-A	32	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SGN	2-A	33	-	-	X	-
1	IDS	2-A	36	-	-	X	-
1	IDS	2-A	6	-	-	X	-
1	SGN	2-A	9	-	-	X	-
1	IDS	3-A	22	-	-	X	-
1	SGN	3-A	25	-	-	X	-
1	IDS	3-A	26	-	-	X	-
1	IDS	3-A	30	-	-	X	-
1	SGN	3-A	31	-	-	X	-
1	IDS	4-A	2	-	-	X	-
1	SGN	4-A	21	-	-	X	-
1	IDS	4-A	22	-	-	X	-
1	IDS	4-A	30	-	-	X	-
1	SGN	4-A	31	-	-	X	-
1	IDS	4-A	34	-	-	X	-
1	SGN	4-A	35	-	-	X	-
1	IDS	4-A	6	-	-	X	-
1	IDS	5-A	16	-	-	X	-
1	SGN	5-A	17	-	-	X	-
1	IDS	5-A	18	-	-	X	-
1	IDS	5-A	26	-	-	X	-
1	SGN	5-A	29	-	-	X	-
1	SGN	5-A	3	-	-	X	-
1	IDS	5-A	30	-	-	X	-
1	IDS	5-A	4	-	-	X	-
1	IDS	6-A	10	-	-	X	-
1	SGN	6-A	11	-	-	X	-
1	IDS	6-A	12	-	-	X	-
1	IDS	6-A	16	-	-	X	-
1	SGN	6-A	17	-	-	X	-
1	SGN	6-A	21	-	-	X	-
1	IDS	6-A	22	-	-	X	-
1	SGN	6-A	23	-	-	X	-
1	IDS	6-A	26	-	-	X	-
1	SGN	6-A	27	-	-	X	-
1	IDS	6-A	28	-	-	X	-
1	SGN	6-A	29	-	-	X	-
1	IDS	6-A	4	-	-	X	-
1	SGN	6-A	5	-	-	X	-
1	IDS	6-A	6	-	-	X	-
1	SGN	6-A	7	-	-	X	-
1	SGN	7-A	13	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	IDS	7-A	14	-	-	X	-
1	SGN	7-A	15	-	-	X	-
1	IDS	7-A	16	-	-	X	-
1	IDS	7-A	18	-	-	X	-
1	SGN	7-A	19	-	-	X	-
1	SGN	7-A	23	-	-	X	-
1	IDS	7-A	24	-	-	X	-
1	SGN	7-A	25	-	-	X	-
1	SGN	7-A	3	-	-	X	-
1	IDS	7-A	32	-	-	X	-
1	SGN	7-A	33	-	-	X	-
1	IDS	7-A	4	-	-	X	-
1	SGN	7-A	5	-	-	X	-
1	SGN	7-A	9	-	-	X	-
1	SGN	8-A	11	-	-	X	-
1	IDS	8-A	12	-	-	X	-
1	SGN	8-A	17	-	-	X	-
1	IDS	8-A	18	-	-	X	-
1	IDS	8-A	30	-	-	X	-
1	SGN	8-A	31	-	-	X	-
1	IDS	9-A	12	-	-	X	-
1	SGN	9-A	13	-	-	X	-
1	IDS	9-A	30	-	-	X	-
1	SGN	9-A	31	-	-	X	-



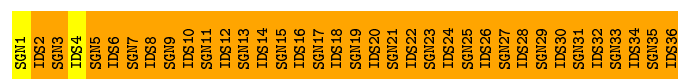
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	7-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	8-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	9-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	10-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	11-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	12-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	13-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	14-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			





Chain 2-A:  6% 94%



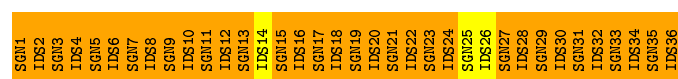
Chain 3-A:  17% 83%



- 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

[illegible]

Chain 4-A:  8% 92%

[illegible]

Chain 5-A:  11% 89%

[illegible][illegible]







[illegible]

Chain 13-A:  97%

SGN1  
IDS2  
SGN3  
IDS4  
SGN5  
IDS6  
SGN7  
IDS8  
SGN9  
IDS10  
SGN11  
IDS12  
SGN13  
IDS14  
SGN15  
IDS16  
SGN17  
IDS18  
SGN19  
IDS20  
SGN21  
IDS22  
SGN23  
IDS24  
SGN25  
IDS26  
SGN27  
IDS28  
SGN29  
IDS30  
SGN31  
IDS32  
SGN33  
IDS34  
SGN35  
IDS36

[illegible]



se



## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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 [i](#)

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	630	0	192	95	0
1	2-A	630	0	196	99	0
1	3-A	630	0	198	60	0
1	4-A	630	0	197	76	0
1	5-A	630	0	197	72	0
1	6-A	630	0	195	89	0
1	7-A	630	0	196	104	0
1	8-A	630	0	194	61	0
1	9-A	630	0	197	60	0
1	10-A	630	0	192	97	0
1	11-A	630	0	196	63	0
1	12-A	630	0	196	75	0
1	13-A	630	0	198	77	0
1	14-A	630	0	195	84	0
All	All	8820	0	2739	1112	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 1112 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:24:IDS:H3	1:A:25:SGN:N2	1.23	1.51
1:A:32:IDS:H3	1:A:33:SGN:N2	1.20	1.51
1:A:16:IDS:H3	1:A:17:SGN:S1	1.47	1.50
1:A:30:IDS:H3	1:A:31:SGN:N2	1.20	1.47
1:A:18:IDS:H3	1:A:19:SGN:N2	1.30	1.45

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](#)

504 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	0.97	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	1.07	1 (4%)
1	IDS	1-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	1-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	1-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	1-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	1-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	1-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	1-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	1-A	29	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	1-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	1-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	1-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	1-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SGN	1-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	10-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	10-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	10-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	10-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	10-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	10-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	10-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	10-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	10-A	29	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	10-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	10-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	10-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	10-A	5	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	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	10-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	10-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	11-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	11-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	11-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	11-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	11-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	11-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	11-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	11-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	11-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	11-A	29	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	11-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	11-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	11-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	11-A	4	1	13,16,17	1.41	1 (7%)	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	11-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	11-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	11-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	12-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	12-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	12-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	12-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	12-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	12-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	12-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	12-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	12-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	12-A	29	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	12-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	12-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	12-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	IDS	12-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	12-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	12-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	12-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	13-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	13-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	13-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	13-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	13-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	13-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	13-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	13-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	13-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	13-A	29	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	13-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	13-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	13-A	35	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	13-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	13-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	13-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	13-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	13-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	14-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	14-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	14-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	14-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	14-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	14-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	18	1	13,16,17	1.42	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	14-A	19	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	14-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	14-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	14-A	25	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	14-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	14-A	29	1	18,19,20	1.23	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%)
1	IDS	14-A	30	1	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	14-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	14-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	34	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	14-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	14-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	14-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	14-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	2-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	2-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	2-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	2-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	2-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	2-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	2-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	2-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	2-A	29	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	2-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	2-A	33	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	2-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	2-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	2-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	2-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	2-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	3-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	3-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	3-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	3-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	3-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	3-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	3-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	3-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	3-A	29	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	3-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SGN	3-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	3-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	3-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	3-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	3-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	3-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	4-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	4-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
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1	SGN	4-A	19	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	4-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
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1	SGN	4-A	25	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	4-A	29	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	4-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)

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1	SGN	4-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	4-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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1	IDS	4-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	4-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	4-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	4-A	8	1	13,16,17	1.41	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	4-A	9	1	18,19,20	1.22	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	0.97	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	1.07	1 (4%)
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1	SGN	5-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	5-A	19	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	5-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	5-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	5-A	29	1	18,19,20	1.23	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	13,16,17	1.42	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	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
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1	SGN	5-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
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1	IDS	5-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	5-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	5-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
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1	SGN	5-A	9	1	18,19,20	1.22	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	0.97	1 (4%)
1	IDS	6-A	10	1	13,16,17	1.40	2 (15%)	15,24,26	2.21	1 (6%)
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1	SGN	6-A	9	1	18,19,20	1.22	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	0.97	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	1.07	1 (4%)
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1	SGN	7-A	19	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	7-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	7-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	7-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	7-A	29	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	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	7-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	7-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	7-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	7-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	7-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	7-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	7-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	8-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	8-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	8-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	8-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	8-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	8-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	8-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	8-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	28	1	13,16,17	1.43	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	8-A	29	1	18,19,20	1.23	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%)
1	IDS	8-A	30	1	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	8-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	8-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	8-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	8-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	8-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	8-A	8	1	13,16,17	1.41	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	1.09	1 (4%)
1	SGN	9-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.97	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	1.07	1 (4%)
1	IDS	9-A	12	1	13,16,17	1.41	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	9-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	9-A	14	1	13,16,17	1.43	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	16	1	13,16,17	1.42	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	9-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	2	1	13,16,17	1.40	2 (15%)	15,24,26	2.23	1 (6%)
1	IDS	9-A	20	1	13,16,17	1.43	2 (15%)	15,24,26	2.22	1 (6%)
1	SGN	9-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	22	1	13,16,17	1.40	2 (15%)	15,24,26	2.22	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	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	26	1	13,16,17	1.42	2 (15%)	15,24,26	2.20	1 (6%)
1	SGN	9-A	27	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	9-A	28	1	13,16,17	1.43	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	9-A	29	1	18,19,20	1.23	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	13,16,17	1.42	2 (15%)	15,24,26	2.23	1 (6%)
1	SGN	9-A	31	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	32	1	13,16,17	1.39	2 (15%)	15,24,26	2.24	1 (6%)
1	SGN	9-A	33	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	34	1	13,16,17	1.43	2 (15%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	35	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	36	1	12,15,17	1.48	2 (16%)	12,22,26	2.42	1 (8%)
1	IDS	9-A	4	1	13,16,17	1.41	1 (7%)	15,24,26	2.21	1 (6%)
1	SGN	9-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	6	1	13,16,17	1.42	1 (7%)	15,24,26	2.20	1 (6%)
1	SGN	9-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	9-A	8	1	13,16,17	1.41	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	1.09	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	-	2/11/31/31	0/1/1/1
1	IDS	1-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	1-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	1-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	1-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	1-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	1-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	1-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	1-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	1-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	1-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	1-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	1-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	1-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	1-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	1-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	1-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	1-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	1-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	1-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	1-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	1-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	1-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	1-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	1-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	1-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	1-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	1-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	10-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	10-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	10-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	10-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	10-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	10-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	10-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	10-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	10-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	10-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	10-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	10-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	10-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	10-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	10-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	10-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	10-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	10-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	10-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	10-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	10-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	10-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	10-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	10-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	10-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	10-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	10-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	10-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	11-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	11-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	11-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	11-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	11-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	11-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	11-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	11-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	11-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	11-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	11-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	11-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	11-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	11-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	11-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	11-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	11-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	11-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	11-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	11-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	11-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	11-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	11-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	11-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	11-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	11-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	11-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	11-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	12-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	12-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	12-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	12-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	12-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	12-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	12-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	12-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	12-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	12-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	12-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	12-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	12-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	12-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	12-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	12-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	12-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	12-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	12-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	12-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	12-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	12-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	12-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	12-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	12-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	12-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	12-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	12-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	13-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	13-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	13-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	13-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	13-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	13-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	13-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	13-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	13-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	13-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	13-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	13-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	13-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	13-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	13-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	13-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	13-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	13-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	13-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	13-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	13-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	13-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	13-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	13-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	13-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	13-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	13-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	13-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	14-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	14-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	14-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	14-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	14-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	14-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	14-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	14-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	14-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	14-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	14-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	14-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	14-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	14-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	14-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	14-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	14-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	14-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	14-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	14-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	14-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	14-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	14-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	14-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	14-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	14-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	14-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	14-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	14-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	14-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	14-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	14-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	14-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	2-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	2-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	2-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	2-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	2-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	2-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	2-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	2-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	2-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	2-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	2-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	2-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	2-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	2-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	2-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	2-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	2-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	2-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	2-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	2-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	2-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	2-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	2-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	2-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	2-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	2-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	2-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	2-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	3-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	3-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	3-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	3-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	3-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	3-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	3-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	3-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	3-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	3-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	3-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	3-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	3-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	3-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	3-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	3-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	3-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	3-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	3-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	3-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	3-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	3-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	3-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	3-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	3-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	3-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	3-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	3-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	3-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	3-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	3-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	3-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	3-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	4-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	4-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	4-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	4-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	4-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	4-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	4-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	4-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	4-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	4-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	4-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	4-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	4-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	4-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	4-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	4-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	4-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	4-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	4-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	4-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	4-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	4-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	4-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	4-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	4-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	4-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	4-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	4-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	5-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	5-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	5-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	5-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	5-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	5-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	5-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	5-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	5-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	5-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	5-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	5-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	5-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	5-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	5-A	22	1	-	1/5/26/29	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
1	SGN	5-A	25	1	-	1/11/28/31	0/1/1/1
1	IDS	5-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	5-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	5-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	5-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	5-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	5-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	5-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	5-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	5-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	5-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	5-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	5-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	5-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	5-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	5-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	5-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	5-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	5-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	6-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	6-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	6-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	6-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	6-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	6-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	6-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	6-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	6-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	6-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	6-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	6-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	6-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	6-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	6-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	6-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	6-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	6-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	6-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	6-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	6-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	6-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	6-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	6-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	6-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	6-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	6-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	6-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	6-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	6-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	6-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	6-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	6-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	7-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	7-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	7-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	7-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	7-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	7-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	7-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	7-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	7-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	7-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	7-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	7-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	7-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	7-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	7-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	7-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	7-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	7-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	7-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	7-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	7-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	7-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	7-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	7-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	7-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	7-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	7-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	7-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	7-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	7-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	7-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	7-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	7-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	8-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	8-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	8-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	8-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	8-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	8-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	8-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	8-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	8-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	8-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	8-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	8-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	8-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	8-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	8-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	8-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	8-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	8-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	8-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	8-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	8-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	8-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	8-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	8-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	8-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	8-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	8-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	8-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	9-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	9-A	10	1	-	3/5/26/29	0/1/1/1
1	SGN	9-A	11	1	-	1/11/28/31	0/1/1/1
1	IDS	9-A	12	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	14	1	-	3/5/26/29	0/1/1/1
1	SGN	9-A	15	1	-	6/11/28/31	0/1/1/1
1	IDS	9-A	16	1	-	3/5/26/29	0/1/1/1
1	SGN	9-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	9-A	18	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	9-A	2	1	-	3/5/26/29	0/1/1/1
1	IDS	9-A	20	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	9-A	22	1	-	1/5/26/29	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	-	1/11/28/31	0/1/1/1
1	IDS	9-A	26	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	28	1	-	4/5/26/29	0/1/1/1
1	SGN	9-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	9-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	30	1	-	2/5/26/29	0/1/1/1
1	SGN	9-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	32	1	-	5/5/26/29	0/1/1/1
1	SGN	9-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	9-A	34	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	9-A	36	1	-	3/5/22/29	0/1/1/1
1	IDS	9-A	4	1	-	3/5/26/29	0/1/1/1
1	SGN	9-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	6	1	-	3/5/26/29	0/1/1/1
1	SGN	9-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	9-A	8	1	-	0/5/26/29	0/1/1/1
1	SGN	9-A	9	1	-	3/11/28/31	0/1/1/1

The worst 5 of 952 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	20	IDS	O2-C2	-3.62	1.41	1.47
1	14-A	20	IDS	O2-C2	-3.62	1.41	1.47
1	6-A	20	IDS	O2-C2	-3.62	1.41	1.47
1	4-A	20	IDS	O2-C2	-3.62	1.41	1.47
1	8-A	20	IDS	O2-C2	-3.62	1.41	1.47

The worst 5 of 504 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	32	IDS	C2-O2-S	8.02	128.37	117.91
1	9-A	32	IDS	C2-O2-S	8.02	128.37	117.91
1	11-A	32	IDS	C2-O2-S	8.02	128.37	117.91
1	4-A	32	IDS	C2-O2-S	8.02	128.37	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	32	IDS	C2-O2-S	8.02	128.37	117.91

There are no chirality outliers.

5 of 1358 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	3-A	32	IDS	C1-C2-O2-S
1	3-A	32	IDS	C3-C2-O2-S
1	3-A	14	IDS	C2-O2-S-O1S
1	3-A	14	IDS	C2-O2-S-O3S
1	6-A	28	IDS	C1-C2-O2-S

There are no ring outliers.

446 monomers are involved in 1112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	3-A	32	IDS	3	0
1	3-A	14	IDS	1	0
1	6-A	28	IDS	12	0
1	5-A	31	SGN	5	0
1	1-A	22	IDS	7	0
1	2-A	19	SGN	7	0
1	3-A	31	SGN	15	0
1	5-A	25	SGN	1	0
1	12-A	17	SGN	5	0
1	2-A	9	SGN	7	0
1	9-A	20	IDS	3	0
1	11-A	12	IDS	7	0
1	7-A	19	SGN	11	0
1	10-A	30	IDS	3	0
1	1-A	23	SGN	11	0
1	1-A	9	SGN	3	0
1	11-A	31	SGN	1	0
1	10-A	7	SGN	5	0
1	8-A	22	IDS	2	0
1	6-A	18	IDS	1	0
1	6-A	16	IDS	6	0
1	9-A	5	SGN	1	0
1	10-A	17	SGN	5	0
1	11-A	7	SGN	2	0
1	9-A	7	SGN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	3-A	2	IDS	2	0
1	1-A	1	SGN	2	0
1	14-A	35	SGN	1	0
1	14-A	4	IDS	9	0
1	8-A	36	IDS	2	0
1	13-A	27	SGN	6	0
1	8-A	31	SGN	10	0
1	5-A	33	SGN	3	0
1	13-A	15	SGN	14	0
1	6-A	22	IDS	14	0
1	6-A	5	SGN	7	0
1	8-A	25	SGN	1	0
1	6-A	13	SGN	6	0
1	3-A	34	IDS	3	0
1	6-A	15	SGN	2	0
1	12-A	29	SGN	4	0
1	13-A	10	IDS	4	0
1	5-A	27	SGN	5	0
1	7-A	8	IDS	2	0
1	8-A	26	IDS	1	0
1	5-A	29	SGN	9	0
1	13-A	12	IDS	2	0
1	13-A	28	IDS	7	0
1	5-A	30	IDS	8	0
1	14-A	8	IDS	7	0
1	2-A	2	IDS	1	0
1	7-A	23	SGN	9	0
1	9-A	8	IDS	1	0
1	4-A	19	SGN	3	0
1	13-A	3	SGN	4	0
1	9-A	29	SGN	3	0
1	4-A	31	SGN	11	0
1	9-A	2	IDS	3	0
1	14-A	23	SGN	6	0
1	7-A	29	SGN	1	0
1	8-A	27	SGN	4	0
1	7-A	26	IDS	2	0
1	2-A	3	SGN	1	0
1	6-A	26	IDS	7	0
1	13-A	11	SGN	4	0
1	6-A	11	SGN	11	0
1	14-A	20	IDS	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	7-A	4	IDS	15	0
1	4-A	34	IDS	12	0
1	6-A	9	SGN	5	0
1	9-A	23	SGN	6	0
1	14-A	17	SGN	8	0
1	10-A	5	SGN	6	0
1	8-A	13	SGN	6	0
1	5-A	17	SGN	11	0
1	13-A	34	IDS	3	0
1	4-A	12	IDS	2	0
1	1-A	18	IDS	9	0
1	5-A	18	IDS	6	0
1	13-A	21	SGN	6	0
1	11-A	29	SGN	1	0
1	8-A	15	SGN	2	0
1	1-A	19	SGN	5	0
1	1-A	27	SGN	5	0
1	6-A	23	SGN	7	0
1	9-A	32	IDS	4	0
1	7-A	9	SGN	7	0
1	3-A	3	SGN	4	0
1	8-A	12	IDS	8	0
1	11-A	32	IDS	8	0
1	3-A	8	IDS	2	0
1	6-A	27	SGN	11	0
1	14-A	5	SGN	10	0
1	1-A	21	SGN	3	0
1	3-A	24	IDS	3	0
1	8-A	24	IDS	2	0
1	10-A	24	IDS	5	0
1	6-A	20	IDS	1	0
1	14-A	3	SGN	10	0
1	4-A	20	IDS	5	0
1	3-A	22	IDS	7	0
1	3-A	12	IDS	4	0
1	14-A	16	IDS	2	0
1	2-A	34	IDS	2	0
1	1-A	24	IDS	10	0
1	10-A	6	IDS	9	0
1	8-A	9	SGN	4	0
1	3-A	11	SGN	5	0
1	9-A	9	SGN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	6-A	21	SGN	8	0
1	8-A	11	SGN	7	0
1	10-A	18	IDS	4	0
1	8-A	28	IDS	3	0
1	1-A	31	SGN	12	0
1	2-A	8	IDS	2	0
1	5-A	14	IDS	5	0
1	13-A	22	IDS	7	0
1	1-A	16	IDS	5	0
1	7-A	18	IDS	8	0
1	8-A	33	SGN	1	0
1	6-A	1	SGN	1	0
1	9-A	16	IDS	3	0
1	5-A	1	SGN	3	0
1	9-A	28	IDS	5	0
1	7-A	34	IDS	3	0
1	11-A	25	SGN	2	0
1	12-A	1	SGN	1	0
1	12-A	8	IDS	9	0
1	11-A	23	SGN	5	0
1	14-A	22	IDS	3	0
1	14-A	25	SGN	8	0
1	5-A	34	IDS	5	0
1	1-A	2	IDS	2	0
1	13-A	8	IDS	6	0
1	13-A	4	IDS	4	0
1	10-A	11	SGN	16	0
1	14-A	11	SGN	6	0
1	10-A	14	IDS	5	0
1	1-A	3	SGN	2	0
1	13-A	18	IDS	2	0
1	14-A	9	SGN	6	0
1	4-A	21	SGN	8	0
1	13-A	19	SGN	5	0
1	6-A	10	IDS	11	0
1	2-A	28	IDS	6	0
1	10-A	36	IDS	2	0
1	5-A	22	IDS	1	0
1	1-A	35	SGN	3	0
1	9-A	33	SGN	2	0
1	12-A	13	SGN	7	0
1	12-A	16	IDS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	9-A	19	SGN	4	0
1	7-A	33	SGN	8	0
1	2-A	11	SGN	4	0
1	9-A	6	IDS	2	0
1	12-A	14	IDS	4	0
1	12-A	3	SGN	2	0
1	3-A	13	SGN	1	0
1	14-A	13	SGN	1	0
1	14-A	1	SGN	10	0
1	9-A	35	SGN	2	0
1	14-A	15	SGN	2	0
1	6-A	6	IDS	8	0
1	14-A	36	IDS	1	0
1	9-A	18	IDS	3	0
1	12-A	21	SGN	3	0
1	13-A	33	SGN	2	0
1	4-A	7	SGN	6	0
1	14-A	7	SGN	3	0
1	5-A	24	IDS	1	0
1	5-A	19	SGN	6	0
1	13-A	26	IDS	7	0
1	7-A	17	SGN	3	0
1	8-A	7	SGN	2	0
1	14-A	12	IDS	5	0
1	1-A	26	IDS	5	0
1	6-A	7	SGN	8	0
1	12-A	33	SGN	7	0
1	2-A	31	SGN	1	0
1	3-A	33	SGN	1	0
1	4-A	36	IDS	1	0
1	4-A	9	SGN	5	0
1	4-A	13	SGN	2	0
1	13-A	36	IDS	4	0
1	2-A	26	IDS	3	0
1	7-A	24	IDS	15	0
1	4-A	3	SGN	3	0
1	14-A	24	IDS	3	0
1	5-A	13	SGN	6	0
1	4-A	32	IDS	4	0
1	10-A	9	SGN	7	0
1	6-A	4	IDS	6	0
1	10-A	34	IDS	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1-A	10	IDS	3	0
1	2-A	30	IDS	7	0
1	4-A	1	SGN	3	0
1	14-A	21	SGN	5	0
1	7-A	32	IDS	14	0
1	10-A	16	IDS	2	0
1	2-A	17	SGN	6	0
1	7-A	3	SGN	11	0
1	3-A	19	SGN	3	0
1	11-A	21	SGN	7	0
1	2-A	16	IDS	1	0
1	8-A	30	IDS	8	0
1	11-A	4	IDS	1	0
1	11-A	26	IDS	2	0
1	3-A	10	IDS	3	0
1	10-A	21	SGN	11	0
1	3-A	4	IDS	3	0
1	5-A	6	IDS	2	0
1	4-A	22	IDS	7	0
1	3-A	6	IDS	2	0
1	10-A	15	SGN	4	0
1	14-A	10	IDS	3	0
1	8-A	3	SGN	1	0
1	1-A	4	IDS	3	0
1	1-A	33	SGN	10	0
1	10-A	10	IDS	16	0
1	5-A	23	SGN	2	0
1	8-A	6	IDS	1	0
1	11-A	16	IDS	6	0
1	11-A	30	IDS	1	0
1	5-A	5	SGN	6	0
1	6-A	14	IDS	3	0
1	4-A	29	SGN	6	0
1	2-A	5	SGN	6	0
1	11-A	28	IDS	6	0
1	11-A	15	SGN	4	0
1	12-A	30	IDS	4	0
1	2-A	22	IDS	17	0
1	10-A	12	IDS	8	0
1	8-A	20	IDS	5	0
1	6-A	8	IDS	4	0
1	2-A	23	SGN	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	11-A	33	SGN	14	0
1	3-A	15	SGN	6	0
1	3-A	23	SGN	1	0
1	10-A	32	IDS	4	0
1	12-A	10	IDS	6	0
1	12-A	32	IDS	5	0
1	4-A	10	IDS	5	0
1	12-A	26	IDS	2	0
1	4-A	17	SGN	1	0
1	2-A	27	SGN	2	0
1	4-A	30	IDS	9	0
1	12-A	24	IDS	5	0
1	1-A	8	IDS	5	0
1	2-A	21	SGN	12	0
1	13-A	17	SGN	3	0
1	12-A	15	SGN	2	0
1	9-A	17	SGN	4	0
1	2-A	33	SGN	8	0
1	12-A	4	IDS	1	0
1	8-A	8	IDS	5	0
1	6-A	2	IDS	1	0
1	12-A	19	SGN	8	0
1	6-A	25	SGN	5	0
1	1-A	7	SGN	5	0
1	7-A	25	SGN	10	0
1	12-A	2	IDS	2	0
1	13-A	35	SGN	6	0
1	12-A	36	IDS	4	0
1	9-A	3	SGN	1	0
1	7-A	35	SGN	6	0
1	2-A	32	IDS	6	0
1	11-A	5	SGN	2	0
1	11-A	24	IDS	1	0
1	14-A	26	IDS	9	0
1	10-A	13	SGN	5	0
1	13-A	23	SGN	3	0
1	9-A	31	SGN	7	0
1	1-A	29	SGN	7	0
1	3-A	9	SGN	3	0
1	5-A	21	SGN	1	0
1	5-A	11	SGN	1	0
1	1-A	32	IDS	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	11-A	13	SGN	2	0
1	7-A	5	SGN	14	0
1	12-A	18	IDS	13	0
1	8-A	17	SGN	7	0
1	9-A	22	IDS	5	0
1	6-A	34	IDS	1	0
1	11-A	22	IDS	6	0
1	14-A	32	IDS	1	0
1	4-A	2	IDS	6	0
1	12-A	7	SGN	5	0
1	11-A	1	SGN	1	0
1	3-A	25	SGN	9	0
1	4-A	4	IDS	4	0
1	13-A	2	IDS	3	0
1	4-A	28	IDS	3	0
1	2-A	18	IDS	12	0
1	1-A	17	SGN	7	0
1	4-A	11	SGN	2	0
1	4-A	35	SGN	7	0
1	2-A	20	IDS	8	0
1	13-A	7	SGN	4	0
1	14-A	28	IDS	3	0
1	8-A	34	IDS	4	0
1	2-A	29	SGN	10	0
1	11-A	10	IDS	6	0
1	4-A	33	SGN	6	0
1	5-A	35	SGN	3	0
1	13-A	6	IDS	2	0
1	8-A	32	IDS	5	0
1	3-A	18	IDS	2	0
1	7-A	16	IDS	8	0
1	2-A	15	SGN	2	0
1	13-A	1	SGN	3	0
1	5-A	12	IDS	3	0
1	14-A	18	IDS	8	0
1	3-A	16	IDS	5	0
1	5-A	26	IDS	6	0
1	12-A	9	SGN	9	0
1	3-A	26	IDS	6	0
1	2-A	24	IDS	2	0
1	6-A	30	IDS	1	0
1	2-A	14	IDS	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	7-A	2	IDS	5	0
1	11-A	20	IDS	5	0
1	13-A	25	SGN	3	0
1	9-A	36	IDS	2	0
1	9-A	1	SGN	3	0
1	11-A	27	SGN	6	0
1	13-A	9	SGN	3	0
1	9-A	12	IDS	6	0
1	5-A	8	IDS	1	0
1	9-A	30	IDS	8	0
1	5-A	7	SGN	1	0
1	13-A	32	IDS	2	0
1	9-A	11	SGN	5	0
1	10-A	4	IDS	1	0
1	10-A	19	SGN	8	0
1	2-A	10	IDS	7	0
1	12-A	35	SGN	6	0
1	2-A	13	SGN	8	0
1	4-A	15	SGN	3	0
1	7-A	36	IDS	5	0
1	3-A	1	SGN	2	0
1	10-A	8	IDS	1	0
1	10-A	28	IDS	14	0
1	5-A	3	SGN	7	0
1	13-A	14	IDS	10	0
1	2-A	35	SGN	6	0
1	4-A	23	SGN	3	0
1	7-A	12	IDS	5	0
1	13-A	29	SGN	7	0
1	1-A	15	SGN	5	0
1	6-A	17	SGN	7	0
1	1-A	34	IDS	5	0
1	7-A	13	SGN	10	0
1	3-A	21	SGN	6	0
1	1-A	25	SGN	4	0
1	13-A	5	SGN	1	0
1	4-A	5	SGN	6	0
1	14-A	19	SGN	5	0
1	6-A	12	IDS	9	0
1	3-A	7	SGN	2	0
1	9-A	14	IDS	3	0
1	5-A	2	IDS	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	14-A	27	SGN	4	0
1	5-A	28	IDS	5	0
1	10-A	27	SGN	11	0
1	14-A	6	IDS	7	0
1	4-A	8	IDS	4	0
1	4-A	24	IDS	1	0
1	1-A	5	SGN	5	0
1	12-A	22	IDS	4	0
1	13-A	13	SGN	3	0
1	2-A	7	SGN	2	0
1	2-A	6	IDS	6	0
1	7-A	10	IDS	5	0
1	1-A	28	IDS	1	0
1	7-A	31	SGN	6	0
1	2-A	12	IDS	6	0
1	8-A	2	IDS	1	0
1	10-A	26	IDS	2	0
1	7-A	14	IDS	6	0
1	12-A	34	IDS	3	0
1	13-A	30	IDS	2	0
1	2-A	36	IDS	6	0
1	1-A	13	SGN	6	0
1	9-A	10	IDS	5	0
1	12-A	12	IDS	4	0
1	10-A	35	SGN	3	0
1	10-A	31	SGN	5	0
1	5-A	4	IDS	9	0
1	4-A	27	SGN	1	0
1	8-A	18	IDS	7	0
1	2-A	25	SGN	5	0
1	1-A	6	IDS	4	0
1	8-A	29	SGN	3	0
1	1-A	30	IDS	13	0
1	10-A	25	SGN	6	0
1	3-A	20	IDS	1	0
1	11-A	6	IDS	2	0
1	12-A	11	SGN	7	0
1	5-A	15	SGN	2	0
1	8-A	23	SGN	2	0
1	9-A	24	IDS	5	0
1	11-A	17	SGN	6	0
1	7-A	6	IDS	5	0

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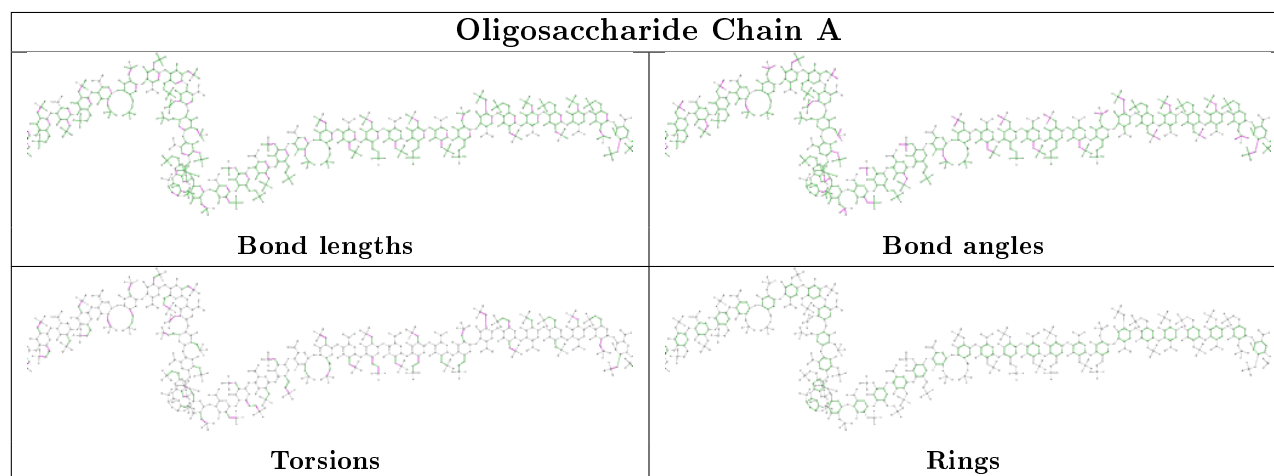
Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	8-A	10	IDS	4	0
1	13-A	16	IDS	6	0
1	8-A	35	SGN	5	0
1	12-A	25	SGN	6	0
1	6-A	29	SGN	8	0
1	7-A	20	IDS	4	0
1	4-A	18	IDS	1	0
1	9-A	21	SGN	5	0
1	5-A	20	IDS	5	0
1	8-A	14	IDS	2	0
1	14-A	2	IDS	11	0
1	11-A	8	IDS	3	0
1	4-A	6	IDS	8	0
1	1-A	36	IDS	3	0
1	5-A	16	IDS	8	0
1	13-A	31	SGN	1	0
1	10-A	33	SGN	3	0
1	1-A	20	IDS	2	0
1	10-A	29	SGN	3	0
1	6-A	33	SGN	2	0
1	3-A	35	SGN	2	0
1	14-A	31	SGN	1	0
1	12-A	23	SGN	3	0
1	7-A	15	SGN	7	0
1	7-A	30	IDS	1	0
1	6-A	24	IDS	4	0
1	3-A	30	IDS	12	0
1	8-A	21	SGN	6	0
1	12-A	6	IDS	5	0
1	13-A	20	IDS	5	0
1	4-A	16	IDS	4	0
1	1-A	14	IDS	4	0
1	7-A	22	IDS	1	0
1	11-A	34	IDS	7	0
1	9-A	13	SGN	7	0
1	6-A	32	IDS	1	0
1	9-A	27	SGN	5	0
1	10-A	20	IDS	10	0
1	11-A	11	SGN	2	0
1	1-A	12	IDS	4	0
1	11-A	14	IDS	4	0
1	11-A	9	SGN	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	10-A	22	IDS	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 [i](#)

There are no chain breaks in this entry.