wwPDB Geometry-Only Validation Summary Report

Mar 9, 2026 – 11:00 PM UTC

PDB ID	:	3IRL / pdb_00003irl
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

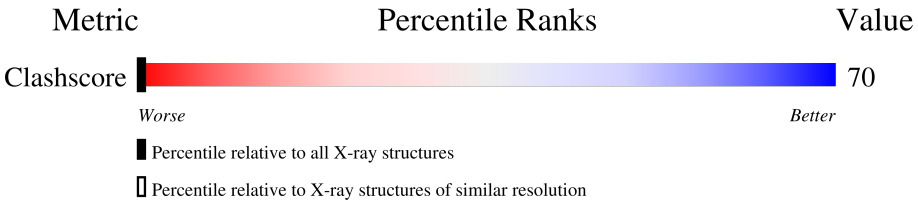
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION SCATTERING

The reported resolution of this entry is unknown.

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



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

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1-A	36	. 97%
1	10-A	36	100%
1	11-A	36	17% 83%
1	12-A	36	14% 86%
1	13-A	36	. 97%
1	14-A	36	100%
1	2-A	36	81% 19%
1	3-A	36	100%
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	14% 86%
1	7-A	36	17% 83%
1	8-A	36	14% 86%
1	9-A	36	14% 86%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SGN	1-A	13	-	-	X	-
1	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	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	-
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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	IDS	2-A	6	-	-	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	-
1	IDS	7-A	14	-	-	X	-
1	SGN	7-A	15	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8820 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	2-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	3-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	4-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	5-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			
1	6-A	36	Total	C	N	O	S	0	0	0
			630	216	18	342	54			

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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			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

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

Chain 1-A:



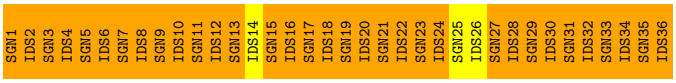


• Molecule 1: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic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

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

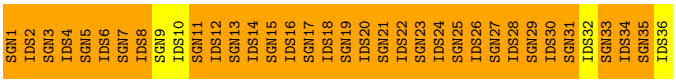
o-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deox y-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1 -4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuro nic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-id opyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyra nose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D -glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamin o)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopy ranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alp ha-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-glucopyrano se

Chain 4-A: 8% 92%



• Molecule 1: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alph a-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoa mino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulf o-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deox y-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-idopyranuro nic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-id opyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyra nose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D -glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamin o)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopy ranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alp ha-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-glucopyrano se

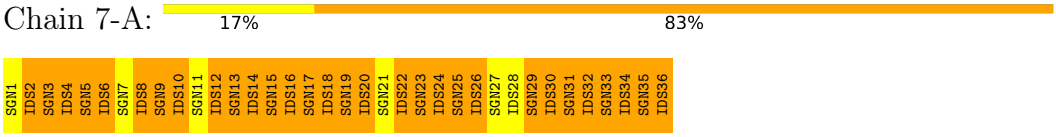
Chain 5-A: 11% 89%



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

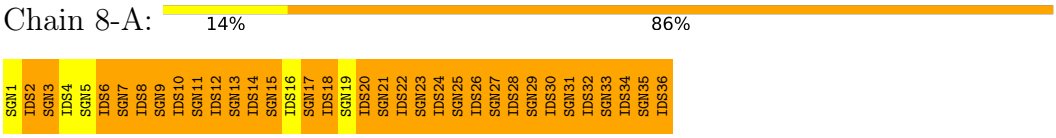
ranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain 7-A:



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

Chain 8-A:



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

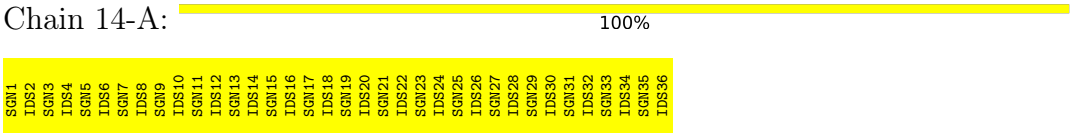
-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D

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

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

se

Chain 14-A:


100%
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

4 Model quality

4.1 Standard geometry

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	630	0	192	95	0
1	2-A	630	0	46	10	0
1	3-A	630	0	0	0	0
1	4-A	630	0	197	75	0
1	5-A	630	0	197	71	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	0	0	0
1	11-A	630	0	196	63	0
1	12-A	630	0	196	74	0
1	13-A	630	0	198	77	0
1	14-A	630	0	0	0	0
All	All	8820	0	2004	779	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 70.

The worst 5 of 779 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: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
1:A:28:IDS:H3	1:A:29:SGN:N2	1.30	1.41

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 Protein backbone

There are no protein molecules in this entry.

4.3.2 Protein sidechains

There are no protein molecules in this entry.

4.3.3 RNA

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates

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	20,20,20	1.13	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	1-A	10	1	16,16,17	1.41	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	1-A	11	1	19,19,20	1.26	2 (10%)	23,29,31	1.08	1 (4%)
1	IDS	1-A	12	1	16,16,17	1.41	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	1-A	13	1	19,19,20	1.27	2 (10%)	23,29,31	1.11	1 (4%)
1	IDS	1-A	14	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	15	1	19,19,20	1.26	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	16	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	17	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	18	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	19	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	2	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	IDS	1-A	20	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	1-A	21	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	22	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	23	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	24	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	25	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	1-A	26	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	1-A	27	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	1-A	28	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	29	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	1-A	3	1	19,19,20	1.24	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	1-A	30	1	16,16,17	1.43	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	1-A	31	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	32	1	16,16,17	1.40	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	33	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	34	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	35	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	36	1	15,15,17	1.55	2 (13%)	14,22,26	1.45	2 (14%)
1	IDS	1-A	4	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	5	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	1-A	6	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SGN	1-A	7	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	1-A	8	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	1-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.11	1 (4%)
1	SGN	10-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	10-A	10	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	11	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	10-A	12	1	16,16,17	1.40	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	10-A	14	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	10-A	15	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	16	1	16,16,17	1.40	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	17	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	18	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	10-A	19	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	IDS	10-A	20	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	21	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	22	1	16,16,17	1.39	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	10-A	23	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	10-A	24	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	10-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	26	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	10-A	28	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	10-A	29	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	10-A	3	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	10-A	30	1	16,16,17	1.44	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	31	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	32	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	10-A	33	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	34	1	16,16,17	1.45	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	10-A	35	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	36	1	15,15,17	1.52	2 (13%)	14,22,26	1.44	2 (14%)
1	IDS	10-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	5	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	IDS	10-A	6	1	16,16,17	1.40	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	7	1	19,19,20	1.30	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	10-A	8	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	10-A	9	1	19,19,20	1.26	2 (10%)	23,29,31	1.11	1 (4%)
1	SGN	11-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	11-A	10	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	11-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	11-A	12	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	13	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	14	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	15	1	19,19,20	1.26	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	17	1	19,19,20	1.29	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	11-A	18	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	19	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	2	1	16,16,17	1.42	3 (18%)	16,24,26	1.18	2 (12%)
1	IDS	11-A	20	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	11-A	21	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	11-A	22	1	16,16,17	1.43	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	23	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	24	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	26	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	11-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	28	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	11-A	29	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	11-A	3	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	11-A	30	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	31	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	32	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	11-A	33	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	34	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	11-A	35	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	36	1	15,15,17	1.53	2 (13%)	14,22,26	1.44	2 (14%)
1	IDS	11-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SGN	11-A	5	1	19,19,20	1.24	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	6	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	7	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	11-A	8	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	11-A	9	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	12-A	1	1	20,20,20	1.13	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	12-A	10	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	12-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	12-A	12	1	16,16,17	1.41	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	12-A	13	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	14	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	12-A	15	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	12-A	17	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	12-A	18	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	12-A	19	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	IDS	12-A	20	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	12-A	21	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	12-A	22	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	12-A	23	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	24	1	16,16,17	1.44	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	12-A	25	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	26	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	12-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	28	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	12-A	29	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	12-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	30	1	16,16,17	1.43	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	12-A	31	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	32	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	12-A	33	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	34	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	12-A	35	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	12-A	36	1	15,15,17	1.53	2 (13%)	14,22,26	1.45	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	IDS	12-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	12-A	5	1	19,19,20	1.24	2 (10%)	23,29,31	1.11	1 (4%)
1	IDS	12-A	6	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	12-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	12-A	8	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	12-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	13-A	1	1	20,20,20	1.15	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	13-A	10	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	13-A	11	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	13-A	12	1	16,16,17	1.39	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	13-A	13	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	14	1	16,16,17	1.44	2 (12%)	16,24,26	1.17	2 (12%)
1	SGN	13-A	15	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	13-A	17	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	18	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	13-A	19	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	2	1	16,16,17	1.40	3 (18%)	16,24,26	1.18	2 (12%)
1	IDS	13-A	20	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	13-A	21	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	22	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	13-A	23	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	24	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	13-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	13-A	26	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	13-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	13-A	28	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	13-A	29	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	13-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	30	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	13-A	31	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	13-A	32	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	13-A	33	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	34	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	13-A	35	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	IDS	13-A	36	1	15,15,17	1.54	2 (13%)	14,22,26	1.45	2 (14%)
1	IDS	13-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	13-A	5	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	6	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	13-A	7	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	13-A	8	1	16,16,17	1.44	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	13-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	14-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	14-A	10	1	16,16,17	1.44	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	11	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	14-A	12	1	16,16,17	1.41	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	14-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	14	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	15	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	17	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	14-A	18	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	14-A	19	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	2	1	16,16,17	1.42	3 (18%)	16,24,26	1.18	2 (12%)
1	IDS	14-A	20	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	21	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	14-A	22	1	16,16,17	1.40	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	14-A	23	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	14-A	24	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	14-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	26	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	14-A	27	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	28	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	29	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	14-A	3	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	30	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	31	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	14-A	32	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	33	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	34	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SGN	14-A	35	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	36	1	15,15,17	1.53	2 (13%)	14,22,26	1.44	2 (14%)
1	IDS	14-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	5	1	19,19,20	1.26	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	14-A	6	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	14-A	7	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	14-A	8	1	16,16,17	1.44	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	14-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	2-A	1	1	20,20,20	1.13	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	2-A	10	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	2-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	2-A	12	1	16,16,17	1.40	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	14	1	16,16,17	1.45	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	2-A	15	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	16	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	17	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	18	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	2-A	19	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	2	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	IDS	2-A	20	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	2-A	21	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	22	1	16,16,17	1.40	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	2-A	23	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	24	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	25	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	26	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	27	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	2-A	28	1	16,16,17	1.44	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	2-A	29	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	2-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	30	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	31	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	32	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	2-A	33	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	IDS	2-A	34	1	16,16,17	1.43	2 (12%)	16,24,26	1.17	2 (12%)
1	SGN	2-A	35	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	36	1	15,15,17	1.56	2 (13%)	14,22,26	1.44	2 (14%)
1	IDS	2-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	5	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	6	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	2-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	2-A	8	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	2-A	9	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	3-A	1	1	20,20,20	1.13	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	3-A	10	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	11	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	3-A	12	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	13	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	14	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	3-A	15	1	19,19,20	1.25	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	16	1	16,16,17	1.41	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	3-A	17	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	3-A	18	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	19	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	IDS	3-A	20	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	3-A	21	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	22	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	3-A	23	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	24	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	25	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	26	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	3-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	28	1	16,16,17	1.45	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	3-A	29	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	3-A	3	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	30	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	31	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	3-A	32	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SGN	3-A	33	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	34	1	16,16,17	1.44	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	3-A	35	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	3-A	36	1	15,15,17	1.53	2 (13%)	14,22,26	1.44	2 (14%)
1	IDS	3-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	5	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	3-A	6	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	3-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	3-A	8	1	16,16,17	1.43	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	3-A	9	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	4-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	4-A	10	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	4-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	4-A	12	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	14	1	16,16,17	1.45	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	4-A	15	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	16	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	4-A	17	1	19,19,20	1.28	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	4-A	18	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	19	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	2	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	IDS	4-A	20	1	16,16,17	1.43	2 (12%)	16,24,26	1.21	2 (12%)
1	SGN	4-A	21	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	4-A	22	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	4-A	23	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	24	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	26	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	4-A	28	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	29	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	4-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	30	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	31	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	IDS	4-A	32	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	33	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	34	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	4-A	35	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	36	1	15,15,17	1.56	3 (20%)	14,22,26	1.44	2 (14%)
1	IDS	4-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	4-A	5	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	4-A	6	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	4-A	7	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	4-A	8	1	16,16,17	1.44	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	4-A	9	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	5-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	5-A	10	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	11	1	19,19,20	1.28	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	5-A	12	1	16,16,17	1.41	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	5-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	14	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	15	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	16	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	17	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	5-A	18	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	19	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	2	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	IDS	5-A	20	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	5-A	21	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	5-A	22	1	16,16,17	1.39	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	23	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	24	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	26	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	27	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	5-A	28	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	29	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	5-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	30	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SGN	5-A	31	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	32	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	5-A	33	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	34	1	16,16,17	1.41	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	5-A	35	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	5-A	36	1	15,15,17	1.53	2 (13%)	14,22,26	1.45	2 (14%)
1	IDS	5-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	5-A	5	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	5-A	6	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	5-A	8	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	5-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	6-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	6-A	10	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	12	1	16,16,17	1.40	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	14	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	15	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	16	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	17	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	6-A	18	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	6-A	19	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	2	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	IDS	6-A	20	1	16,16,17	1.44	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	6-A	21	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	6-A	22	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	23	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	24	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	26	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	6-A	28	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	29	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	6-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	IDS	6-A	30	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	6-A	31	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	6-A	32	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	6-A	33	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	34	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	35	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	6-A	36	1	15,15,17	1.54	2 (13%)	14,22,26	1.45	2 (14%)
1	IDS	6-A	4	1	16,16,17	1.45	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	5	1	19,19,20	1.25	1 (5%)	23,29,31	1.09	1 (4%)
1	IDS	6-A	6	1	16,16,17	1.40	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	7	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	6-A	8	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	6-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	7-A	1	1	20,20,20	1.13	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	7-A	10	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	7-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	7-A	12	1	16,16,17	1.41	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	7-A	13	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	14	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	15	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	16	1	16,16,17	1.42	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	17	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	18	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	7-A	19	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	2	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	IDS	7-A	20	1	16,16,17	1.42	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	7-A	21	1	19,19,20	1.24	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	7-A	22	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	7-A	23	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	24	1	16,16,17	1.42	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	7-A	25	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	26	1	16,16,17	1.44	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	27	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	7-A	28	1	16,16,17	1.44	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	29	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SGN	7-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	30	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	31	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	7-A	32	1	16,16,17	1.40	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	33	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	7-A	34	1	16,16,17	1.44	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	7-A	35	1	19,19,20	1.24	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	7-A	36	1	15,15,17	1.54	2 (13%)	14,22,26	1.45	2 (14%)
1	IDS	7-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	5	1	19,19,20	1.25	2 (10%)	23,29,31	1.08	1 (4%)
1	IDS	7-A	6	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	7-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	7-A	8	1	16,16,17	1.44	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	7-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	8-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	8-A	10	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	8-A	12	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	13	1	19,19,20	1.26	2 (10%)	23,29,31	1.11	1 (4%)
1	IDS	8-A	14	1	16,16,17	1.45	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	8-A	15	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	17	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	18	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	19	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	IDS	8-A	20	1	16,16,17	1.45	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	8-A	21	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	8-A	22	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	8-A	23	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	8-A	24	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	26	1	16,16,17	1.43	2 (12%)	16,24,26	1.21	2 (12%)
1	SGN	8-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	28	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SGN	8-A	29	1	19,19,20	1.23	2 (10%)	23,29,31	1.09	1 (4%)
1	SGN	8-A	3	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	8-A	30	1	16,16,17	1.41	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	31	1	19,19,20	1.25	2 (10%)	23,29,31	1.08	1 (4%)
1	IDS	8-A	32	1	16,16,17	1.42	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	8-A	33	1	19,19,20	1.26	2 (10%)	23,29,31	1.11	1 (4%)
1	IDS	8-A	34	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	8-A	35	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	8-A	36	1	15,15,17	1.55	2 (13%)	14,22,26	1.44	2 (14%)
1	IDS	8-A	4	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	8-A	5	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	8-A	6	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	8-A	7	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	8-A	8	1	16,16,17	1.43	3 (18%)	16,24,26	1.18	2 (12%)
1	SGN	8-A	9	1	19,19,20	1.24	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	9-A	1	1	20,20,20	1.14	1 (5%)	25,31,31	1.00	1 (4%)
1	IDS	9-A	10	1	16,16,17	1.41	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	9-A	11	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	12	1	16,16,17	1.40	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	9-A	13	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	14	1	16,16,17	1.44	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	9-A	15	1	19,19,20	1.26	1 (5%)	23,29,31	1.09	1 (4%)
1	IDS	9-A	16	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	17	1	19,19,20	1.28	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	9-A	18	1	16,16,17	1.42	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	19	1	19,19,20	1.28	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	2	1	16,16,17	1.41	3 (18%)	16,24,26	1.18	2 (12%)
1	IDS	9-A	20	1	16,16,17	1.43	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	9-A	21	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	22	1	16,16,17	1.41	3 (18%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	23	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	24	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	25	1	19,19,20	1.26	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	9-A	26	1	16,16,17	1.43	2 (12%)	16,24,26	1.20	2 (12%)
1	SGN	9-A	27	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	IDS	9-A	28	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	29	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)
1	SGN	9-A	3	1	19,19,20	1.25	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	9-A	30	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	9-A	31	1	19,19,20	1.27	2 (10%)	23,29,31	1.09	1 (4%)
1	IDS	9-A	32	1	16,16,17	1.40	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	33	1	19,19,20	1.25	2 (10%)	23,29,31	1.11	1 (4%)
1	IDS	9-A	34	1	16,16,17	1.43	2 (12%)	16,24,26	1.18	2 (12%)
1	SGN	9-A	35	1	19,19,20	1.25	1 (5%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	36	1	15,15,17	1.52	2 (13%)	14,22,26	1.44	2 (14%)
1	IDS	9-A	4	1	16,16,17	1.44	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	5	1	19,19,20	1.26	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	6	1	16,16,17	1.41	3 (18%)	16,24,26	1.20	2 (12%)
1	SGN	9-A	7	1	19,19,20	1.27	2 (10%)	23,29,31	1.10	1 (4%)
1	IDS	9-A	8	1	16,16,17	1.43	2 (12%)	16,24,26	1.19	2 (12%)
1	SGN	9-A	9	1	19,19,20	1.25	2 (10%)	23,29,31	1.10	1 (4%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	1-A	21	1	-	8/11/28/31	0/1/1/1
1	IDS	1-A	22	1	-	0/9/26/29	0/1/1/1
1	SGN	1-A	23	1	-	4/11/28/31	0/1/1/1
1	IDS	1-A	24	1	-	0/9/26/29	0/1/1/1
1	SGN	1-A	25	1	-	1/11/28/31	0/1/1/1
1	IDS	1-A	26	1	-	2/9/26/29	0/1/1/1
1	SGN	1-A	27	1	-	4/11/28/31	0/1/1/1
1	IDS	1-A	28	1	-	5/9/26/29	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	-	3/9/26/29	0/1/1/1
1	SGN	1-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	1-A	32	1	-	6/9/26/29	0/1/1/1
1	SGN	1-A	33	1	-	4/11/28/31	0/1/1/1
1	IDS	1-A	34	1	-	1/9/26/29	0/1/1/1
1	SGN	1-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	1-A	36	1	-	3/9/22/29	0/1/1/1
1	IDS	1-A	4	1	-	4/9/26/29	0/1/1/1
1	SGN	1-A	5	1	-	4/11/28/31	0/1/1/1
1	IDS	1-A	6	1	-	3/9/26/29	0/1/1/1
1	SGN	1-A	7	1	-	1/11/28/31	0/1/1/1
1	IDS	1-A	8	1	-	1/9/26/29	0/1/1/1
1	SGN	1-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	10-A	1	1	-	5/11/31/31	0/1/1/1
1	IDS	10-A	10	1	-	5/9/26/29	0/1/1/1
1	SGN	10-A	11	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	12	1	-	3/9/26/29	0/1/1/1
1	SGN	10-A	13	1	-	6/11/28/31	0/1/1/1
1	IDS	10-A	14	1	-	3/9/26/29	0/1/1/1
1	SGN	10-A	15	1	-	5/11/28/31	0/1/1/1
1	IDS	10-A	16	1	-	0/9/26/29	0/1/1/1
1	SGN	10-A	17	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	18	1	-	6/9/26/29	0/1/1/1
1	SGN	10-A	19	1	-	6/11/28/31	0/1/1/1
1	IDS	10-A	2	1	-	0/9/26/29	0/1/1/1
1	IDS	10-A	20	1	-	0/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	10-A	21	1	-	4/11/28/31	0/1/1/1
1	IDS	10-A	22	1	-	2/9/26/29	0/1/1/1
1	SGN	10-A	23	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	24	1	-	2/9/26/29	0/1/1/1
1	SGN	10-A	25	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	26	1	-	2/9/26/29	0/1/1/1
1	SGN	10-A	27	1	-	5/11/28/31	0/1/1/1
1	IDS	10-A	28	1	-	4/9/26/29	0/1/1/1
1	SGN	10-A	29	1	-	2/11/28/31	0/1/1/1
1	SGN	10-A	3	1	-	5/11/28/31	0/1/1/1
1	IDS	10-A	30	1	-	3/9/26/29	0/1/1/1
1	SGN	10-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	10-A	32	1	-	2/9/26/29	0/1/1/1
1	SGN	10-A	33	1	-	1/11/28/31	0/1/1/1
1	IDS	10-A	34	1	-	3/9/26/29	0/1/1/1
1	SGN	10-A	35	1	-	2/11/28/31	0/1/1/1
1	IDS	10-A	36	1	-	1/9/22/29	0/1/1/1
1	IDS	10-A	4	1	-	3/9/26/29	0/1/1/1
1	SGN	10-A	5	1	-	1/11/28/31	0/1/1/1
1	IDS	10-A	6	1	-	4/9/26/29	0/1/1/1
1	SGN	10-A	7	1	-	0/11/28/31	0/1/1/1
1	IDS	10-A	8	1	-	6/9/26/29	0/1/1/1
1	SGN	10-A	9	1	-	7/11/28/31	0/1/1/1
1	SGN	11-A	1	1	-	7/11/31/31	0/1/1/1
1	IDS	11-A	10	1	-	2/9/26/29	0/1/1/1
1	SGN	11-A	11	1	-	2/11/28/31	0/1/1/1
1	IDS	11-A	12	1	-	2/9/26/29	0/1/1/1
1	SGN	11-A	13	1	-	1/11/28/31	0/1/1/1
1	IDS	11-A	14	1	-	1/9/26/29	0/1/1/1
1	SGN	11-A	15	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	16	1	-	3/9/26/29	0/1/1/1
1	SGN	11-A	17	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	18	1	-	1/9/26/29	0/1/1/1
1	SGN	11-A	19	1	-	6/11/28/31	0/1/1/1
1	IDS	11-A	2	1	-	2/9/26/29	0/1/1/1
1	IDS	11-A	20	1	-	0/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	11-A	21	1	-	5/11/28/31	0/1/1/1
1	IDS	11-A	22	1	-	0/9/26/29	0/1/1/1
1	SGN	11-A	23	1	-	4/11/28/31	0/1/1/1
1	IDS	11-A	24	1	-	3/9/26/29	0/1/1/1
1	SGN	11-A	25	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	26	1	-	2/9/26/29	0/1/1/1
1	SGN	11-A	27	1	-	2/11/28/31	0/1/1/1
1	IDS	11-A	28	1	-	4/9/26/29	0/1/1/1
1	SGN	11-A	29	1	-	6/11/28/31	0/1/1/1
1	SGN	11-A	3	1	-	6/11/28/31	0/1/1/1
1	IDS	11-A	30	1	-	0/9/26/29	0/1/1/1
1	SGN	11-A	31	1	-	2/11/28/31	0/1/1/1
1	IDS	11-A	32	1	-	3/9/26/29	0/1/1/1
1	SGN	11-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	11-A	34	1	-	7/9/26/29	0/1/1/1
1	SGN	11-A	35	1	-	2/11/28/31	0/1/1/1
1	IDS	11-A	36	1	-	0/9/22/29	0/1/1/1
1	IDS	11-A	4	1	-	5/9/26/29	0/1/1/1
1	SGN	11-A	5	1	-	4/11/28/31	0/1/1/1
1	IDS	11-A	6	1	-	3/9/26/29	0/1/1/1
1	SGN	11-A	7	1	-	3/11/28/31	0/1/1/1
1	IDS	11-A	8	1	-	7/9/26/29	0/1/1/1
1	SGN	11-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	12-A	1	1	-	5/11/31/31	0/1/1/1
1	IDS	12-A	10	1	-	0/9/26/29	0/1/1/1
1	SGN	12-A	11	1	-	5/11/28/31	0/1/1/1
1	IDS	12-A	12	1	-	5/9/26/29	0/1/1/1
1	SGN	12-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	14	1	-	0/9/26/29	0/1/1/1
1	SGN	12-A	15	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	16	1	-	4/9/26/29	0/1/1/1
1	SGN	12-A	17	1	-	5/11/28/31	0/1/1/1
1	IDS	12-A	18	1	-	3/9/26/29	0/1/1/1
1	SGN	12-A	19	1	-	8/11/28/31	0/1/1/1
1	IDS	12-A	2	1	-	4/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	12-A	20	1	-	3/9/26/29	0/1/1/1
1	SGN	12-A	21	1	-	5/11/28/31	0/1/1/1
1	IDS	12-A	22	1	-	0/9/26/29	0/1/1/1
1	SGN	12-A	23	1	-	6/11/28/31	0/1/1/1
1	IDS	12-A	24	1	-	0/9/26/29	0/1/1/1
1	SGN	12-A	25	1	-	6/11/28/31	0/1/1/1
1	IDS	12-A	26	1	-	2/9/26/29	0/1/1/1
1	SGN	12-A	27	1	-	4/11/28/31	0/1/1/1
1	IDS	12-A	28	1	-	1/9/26/29	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	-	0/9/26/29	0/1/1/1
1	SGN	12-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	32	1	-	2/9/26/29	0/1/1/1
1	SGN	12-A	33	1	-	4/11/28/31	0/1/1/1
1	IDS	12-A	34	1	-	2/9/26/29	0/1/1/1
1	SGN	12-A	35	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	36	1	-	1/9/22/29	0/1/1/1
1	IDS	12-A	4	1	-	2/9/26/29	0/1/1/1
1	SGN	12-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	12-A	6	1	-	3/9/26/29	0/1/1/1
1	SGN	12-A	7	1	-	7/11/28/31	0/1/1/1
1	IDS	12-A	8	1	-	0/9/26/29	0/1/1/1
1	SGN	12-A	9	1	-	4/11/28/31	0/1/1/1
1	SGN	13-A	1	1	-	6/11/31/31	0/1/1/1
1	IDS	13-A	10	1	-	3/9/26/29	0/1/1/1
1	SGN	13-A	11	1	-	6/11/28/31	0/1/1/1
1	IDS	13-A	12	1	-	2/9/26/29	0/1/1/1
1	SGN	13-A	13	1	-	4/11/28/31	0/1/1/1
1	IDS	13-A	14	1	-	0/9/26/29	0/1/1/1
1	SGN	13-A	15	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	16	1	-	3/9/26/29	0/1/1/1
1	SGN	13-A	17	1	-	1/11/28/31	0/1/1/1
1	IDS	13-A	18	1	-	0/9/26/29	0/1/1/1
1	SGN	13-A	19	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	2	1	-	0/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	13-A	20	1	-	7/9/26/29	0/1/1/1
1	SGN	13-A	21	1	-	1/11/28/31	0/1/1/1
1	IDS	13-A	22	1	-	0/9/26/29	0/1/1/1
1	SGN	13-A	23	1	-	8/11/28/31	0/1/1/1
1	IDS	13-A	24	1	-	1/9/26/29	0/1/1/1
1	SGN	13-A	25	1	-	6/11/28/31	0/1/1/1
1	IDS	13-A	26	1	-	0/9/26/29	0/1/1/1
1	SGN	13-A	27	1	-	8/11/28/31	0/1/1/1
1	IDS	13-A	28	1	-	4/9/26/29	0/1/1/1
1	SGN	13-A	29	1	-	3/11/28/31	0/1/1/1
1	SGN	13-A	3	1	-	5/11/28/31	0/1/1/1
1	IDS	13-A	30	1	-	5/9/26/29	0/1/1/1
1	SGN	13-A	31	1	-	5/11/28/31	0/1/1/1
1	IDS	13-A	32	1	-	5/9/26/29	0/1/1/1
1	SGN	13-A	33	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	34	1	-	1/9/26/29	0/1/1/1
1	SGN	13-A	35	1	-	3/11/28/31	0/1/1/1
1	IDS	13-A	36	1	-	0/9/22/29	0/1/1/1
1	IDS	13-A	4	1	-	5/9/26/29	0/1/1/1
1	SGN	13-A	5	1	-	4/11/28/31	0/1/1/1
1	IDS	13-A	6	1	-	0/9/26/29	0/1/1/1
1	SGN	13-A	7	1	-	4/11/28/31	0/1/1/1
1	IDS	13-A	8	1	-	1/9/26/29	0/1/1/1
1	SGN	13-A	9	1	-	8/11/28/31	0/1/1/1
1	SGN	14-A	1	1	-	3/11/31/31	0/1/1/1
1	IDS	14-A	10	1	-	1/9/26/29	0/1/1/1
1	SGN	14-A	11	1	-	6/11/28/31	0/1/1/1
1	IDS	14-A	12	1	-	3/9/26/29	0/1/1/1
1	SGN	14-A	13	1	-	1/11/28/31	0/1/1/1
1	IDS	14-A	14	1	-	0/9/26/29	0/1/1/1
1	SGN	14-A	15	1	-	3/11/28/31	0/1/1/1
1	IDS	14-A	16	1	-	1/9/26/29	0/1/1/1
1	SGN	14-A	17	1	-	1/11/28/31	0/1/1/1
1	IDS	14-A	18	1	-	2/9/26/29	0/1/1/1
1	SGN	14-A	19	1	-	5/11/28/31	0/1/1/1
1	IDS	14-A	2	1	-	2/9/26/29	0/1/1/1
1	IDS	14-A	20	1	-	2/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	14-A	21	1	-	5/11/28/31	0/1/1/1
1	IDS	14-A	22	1	-	0/9/26/29	0/1/1/1
1	SGN	14-A	23	1	-	6/11/28/31	0/1/1/1
1	IDS	14-A	24	1	-	4/9/26/29	0/1/1/1
1	SGN	14-A	25	1	-	4/11/28/31	0/1/1/1
1	IDS	14-A	26	1	-	2/9/26/29	0/1/1/1
1	SGN	14-A	27	1	-	6/11/28/31	0/1/1/1
1	IDS	14-A	28	1	-	0/9/26/29	0/1/1/1
1	SGN	14-A	29	1	-	8/11/28/31	0/1/1/1
1	SGN	14-A	3	1	-	2/11/28/31	0/1/1/1
1	IDS	14-A	30	1	-	0/9/26/29	0/1/1/1
1	SGN	14-A	31	1	-	5/11/28/31	0/1/1/1
1	IDS	14-A	32	1	-	3/9/26/29	0/1/1/1
1	SGN	14-A	33	1	-	8/11/28/31	0/1/1/1
1	IDS	14-A	34	1	-	4/9/26/29	0/1/1/1
1	SGN	14-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	14-A	36	1	-	6/9/22/29	0/1/1/1
1	IDS	14-A	4	1	-	2/9/26/29	0/1/1/1
1	SGN	14-A	5	1	-	10/11/28/31	0/1/1/1
1	IDS	14-A	6	1	-	1/9/26/29	0/1/1/1
1	SGN	14-A	7	1	-	3/11/28/31	0/1/1/1
1	IDS	14-A	8	1	-	6/9/26/29	0/1/1/1
1	SGN	14-A	9	1	-	2/11/28/31	0/1/1/1
1	SGN	2-A	1	1	-	1/11/31/31	0/1/1/1
1	IDS	2-A	10	1	-	5/9/26/29	0/1/1/1
1	SGN	2-A	11	1	-	5/11/28/31	0/1/1/1
1	IDS	2-A	12	1	-	1/9/26/29	0/1/1/1
1	SGN	2-A	13	1	-	6/11/28/31	0/1/1/1
1	IDS	2-A	14	1	-	2/9/26/29	0/1/1/1
1	SGN	2-A	15	1	-	8/11/28/31	0/1/1/1
1	IDS	2-A	16	1	-	3/9/26/29	0/1/1/1
1	SGN	2-A	17	1	-	0/11/28/31	0/1/1/1
1	IDS	2-A	18	1	-	1/9/26/29	0/1/1/1
1	SGN	2-A	19	1	-	6/11/28/31	0/1/1/1
1	IDS	2-A	2	1	-	4/9/26/29	0/1/1/1
1	IDS	2-A	20	1	-	4/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	2-A	21	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	22	1	-	2/9/26/29	0/1/1/1
1	SGN	2-A	23	1	-	6/11/28/31	0/1/1/1
1	IDS	2-A	24	1	-	0/9/26/29	0/1/1/1
1	SGN	2-A	25	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	26	1	-	2/9/26/29	0/1/1/1
1	SGN	2-A	27	1	-	1/11/28/31	0/1/1/1
1	IDS	2-A	28	1	-	5/9/26/29	0/1/1/1
1	SGN	2-A	29	1	-	6/11/28/31	0/1/1/1
1	SGN	2-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	30	1	-	1/9/26/29	0/1/1/1
1	SGN	2-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	32	1	-	4/9/26/29	0/1/1/1
1	SGN	2-A	33	1	-	4/11/28/31	0/1/1/1
1	IDS	2-A	34	1	-	7/9/26/29	0/1/1/1
1	SGN	2-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	2-A	36	1	-	0/9/22/29	0/1/1/1
1	IDS	2-A	4	1	-	0/9/26/29	0/1/1/1
1	SGN	2-A	5	1	-	1/11/28/31	0/1/1/1
1	IDS	2-A	6	1	-	3/9/26/29	0/1/1/1
1	SGN	2-A	7	1	-	3/11/28/31	0/1/1/1
1	IDS	2-A	8	1	-	3/9/26/29	0/1/1/1
1	SGN	2-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	3-A	1	1	-	6/11/31/31	0/1/1/1
1	IDS	3-A	10	1	-	0/9/26/29	0/1/1/1
1	SGN	3-A	11	1	-	6/11/28/31	0/1/1/1
1	IDS	3-A	12	1	-	0/9/26/29	0/1/1/1
1	SGN	3-A	13	1	-	8/11/28/31	0/1/1/1
1	IDS	3-A	14	1	-	6/9/26/29	0/1/1/1
1	SGN	3-A	15	1	-	1/11/28/31	0/1/1/1
1	IDS	3-A	16	1	-	1/9/26/29	0/1/1/1
1	SGN	3-A	17	1	-	3/11/28/31	0/1/1/1
1	IDS	3-A	18	1	-	3/9/26/29	0/1/1/1
1	SGN	3-A	19	1	-	6/11/28/31	0/1/1/1
1	IDS	3-A	2	1	-	3/9/26/29	0/1/1/1
1	IDS	3-A	20	1	-	1/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	3-A	21	1	-	1/11/28/31	0/1/1/1
1	IDS	3-A	22	1	-	5/9/26/29	0/1/1/1
1	SGN	3-A	23	1	-	6/11/28/31	0/1/1/1
1	IDS	3-A	24	1	-	4/9/26/29	0/1/1/1
1	SGN	3-A	25	1	-	4/11/28/31	0/1/1/1
1	IDS	3-A	26	1	-	7/9/26/29	0/1/1/1
1	SGN	3-A	27	1	-	2/11/28/31	0/1/1/1
1	IDS	3-A	28	1	-	0/9/26/29	0/1/1/1
1	SGN	3-A	29	1	-	4/11/28/31	0/1/1/1
1	SGN	3-A	3	1	-	7/11/28/31	0/1/1/1
1	IDS	3-A	30	1	-	0/9/26/29	0/1/1/1
1	SGN	3-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	3-A	32	1	-	2/9/26/29	0/1/1/1
1	SGN	3-A	33	1	-	6/11/28/31	0/1/1/1
1	IDS	3-A	34	1	-	3/9/26/29	0/1/1/1
1	SGN	3-A	35	1	-	5/11/28/31	0/1/1/1
1	IDS	3-A	36	1	-	0/9/22/29	0/1/1/1
1	IDS	3-A	4	1	-	2/9/26/29	0/1/1/1
1	SGN	3-A	5	1	-	5/11/28/31	0/1/1/1
1	IDS	3-A	6	1	-	2/9/26/29	0/1/1/1
1	SGN	3-A	7	1	-	2/11/28/31	0/1/1/1
1	IDS	3-A	8	1	-	1/9/26/29	0/1/1/1
1	SGN	3-A	9	1	-	8/11/28/31	0/1/1/1
1	SGN	4-A	1	1	-	6/11/31/31	0/1/1/1
1	IDS	4-A	10	1	-	1/9/26/29	0/1/1/1
1	SGN	4-A	11	1	-	6/11/28/31	0/1/1/1
1	IDS	4-A	12	1	-	1/9/26/29	0/1/1/1
1	SGN	4-A	13	1	-	8/11/28/31	0/1/1/1
1	IDS	4-A	14	1	-	0/9/26/29	0/1/1/1
1	SGN	4-A	15	1	-	4/11/28/31	0/1/1/1
1	IDS	4-A	16	1	-	3/9/26/29	0/1/1/1
1	SGN	4-A	17	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	18	1	-	5/9/26/29	0/1/1/1
1	SGN	4-A	19	1	-	8/11/28/31	0/1/1/1
1	IDS	4-A	2	1	-	3/9/26/29	0/1/1/1
1	IDS	4-A	20	1	-	2/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	4-A	21	1	-	10/11/28/31	0/1/1/1
1	IDS	4-A	22	1	-	0/9/26/29	0/1/1/1
1	SGN	4-A	23	1	-	7/11/28/31	0/1/1/1
1	IDS	4-A	24	1	-	0/9/26/29	0/1/1/1
1	SGN	4-A	25	1	-	6/11/28/31	0/1/1/1
1	IDS	4-A	26	1	-	0/9/26/29	0/1/1/1
1	SGN	4-A	27	1	-	4/11/28/31	0/1/1/1
1	IDS	4-A	28	1	-	5/9/26/29	0/1/1/1
1	SGN	4-A	29	1	-	6/11/28/31	0/1/1/1
1	SGN	4-A	3	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	30	1	-	3/9/26/29	0/1/1/1
1	SGN	4-A	31	1	-	5/11/28/31	0/1/1/1
1	IDS	4-A	32	1	-	0/9/26/29	0/1/1/1
1	SGN	4-A	33	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	34	1	-	5/9/26/29	0/1/1/1
1	SGN	4-A	35	1	-	3/11/28/31	0/1/1/1
1	IDS	4-A	36	1	-	1/9/22/29	0/1/1/1
1	IDS	4-A	4	1	-	0/9/26/29	0/1/1/1
1	SGN	4-A	5	1	-	5/11/28/31	0/1/1/1
1	IDS	4-A	6	1	-	4/9/26/29	0/1/1/1
1	SGN	4-A	7	1	-	5/11/28/31	0/1/1/1
1	IDS	4-A	8	1	-	2/9/26/29	0/1/1/1
1	SGN	4-A	9	1	-	4/11/28/31	0/1/1/1
1	SGN	5-A	1	1	-	4/11/31/31	0/1/1/1
1	IDS	5-A	10	1	-	4/9/26/29	0/1/1/1
1	SGN	5-A	11	1	-	8/11/28/31	0/1/1/1
1	IDS	5-A	12	1	-	2/9/26/29	0/1/1/1
1	SGN	5-A	13	1	-	3/11/28/31	0/1/1/1
1	IDS	5-A	14	1	-	1/9/26/29	0/1/1/1
1	SGN	5-A	15	1	-	7/11/28/31	0/1/1/1
1	IDS	5-A	16	1	-	3/9/26/29	0/1/1/1
1	SGN	5-A	17	1	-	6/11/28/31	0/1/1/1
1	IDS	5-A	18	1	-	1/9/26/29	0/1/1/1
1	SGN	5-A	19	1	-	1/11/28/31	0/1/1/1
1	IDS	5-A	2	1	-	3/9/26/29	0/1/1/1
1	IDS	5-A	20	1	-	2/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	5-A	21	1	-	4/11/28/31	0/1/1/1
1	IDS	5-A	22	1	-	0/9/26/29	0/1/1/1
1	SGN	5-A	23	1	-	1/11/28/31	0/1/1/1
1	IDS	5-A	24	1	-	1/9/26/29	0/1/1/1
1	SGN	5-A	25	1	-	2/11/28/31	0/1/1/1
1	IDS	5-A	26	1	-	0/9/26/29	0/1/1/1
1	SGN	5-A	27	1	-	1/11/28/31	0/1/1/1
1	IDS	5-A	28	1	-	2/9/26/29	0/1/1/1
1	SGN	5-A	29	1	-	5/11/28/31	0/1/1/1
1	SGN	5-A	3	1	-	4/11/28/31	0/1/1/1
1	IDS	5-A	30	1	-	3/9/26/29	0/1/1/1
1	SGN	5-A	31	1	-	6/11/28/31	0/1/1/1
1	IDS	5-A	32	1	-	4/9/26/29	0/1/1/1
1	SGN	5-A	33	1	-	0/11/28/31	0/1/1/1
1	IDS	5-A	34	1	-	0/9/26/29	0/1/1/1
1	SGN	5-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	5-A	36	1	-	3/9/22/29	0/1/1/1
1	IDS	5-A	4	1	-	4/9/26/29	0/1/1/1
1	SGN	5-A	5	1	-	6/11/28/31	0/1/1/1
1	IDS	5-A	6	1	-	0/9/26/29	0/1/1/1
1	SGN	5-A	7	1	-	3/11/28/31	0/1/1/1
1	IDS	5-A	8	1	-	1/9/26/29	0/1/1/1
1	SGN	5-A	9	1	-	1/11/28/31	0/1/1/1
1	SGN	6-A	1	1	-	1/11/31/31	0/1/1/1
1	IDS	6-A	10	1	-	0/9/26/29	0/1/1/1
1	SGN	6-A	11	1	-	5/11/28/31	0/1/1/1
1	IDS	6-A	12	1	-	4/9/26/29	0/1/1/1
1	SGN	6-A	13	1	-	4/11/28/31	0/1/1/1
1	IDS	6-A	14	1	-	2/9/26/29	0/1/1/1
1	SGN	6-A	15	1	-	2/11/28/31	0/1/1/1
1	IDS	6-A	16	1	-	0/9/26/29	0/1/1/1
1	SGN	6-A	17	1	-	4/11/28/31	0/1/1/1
1	IDS	6-A	18	1	-	0/9/26/29	0/1/1/1
1	SGN	6-A	19	1	-	4/11/28/31	0/1/1/1
1	IDS	6-A	2	1	-	3/9/26/29	0/1/1/1
1	IDS	6-A	20	1	-	3/9/26/29	0/1/1/1
1	SGN	6-A	21	1	-	3/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	6-A	22	1	-	1/9/26/29	0/1/1/1
1	SGN	6-A	23	1	-	6/11/28/31	0/1/1/1
1	IDS	6-A	24	1	-	1/9/26/29	0/1/1/1
1	SGN	6-A	25	1	-	8/11/28/31	0/1/1/1
1	IDS	6-A	26	1	-	3/9/26/29	0/1/1/1
1	SGN	6-A	27	1	-	1/11/28/31	0/1/1/1
1	IDS	6-A	28	1	-	2/9/26/29	0/1/1/1
1	SGN	6-A	29	1	-	8/11/28/31	0/1/1/1
1	SGN	6-A	3	1	-	6/11/28/31	0/1/1/1
1	IDS	6-A	30	1	-	4/9/26/29	0/1/1/1
1	SGN	6-A	31	1	-	5/11/28/31	0/1/1/1
1	IDS	6-A	32	1	-	2/9/26/29	0/1/1/1
1	SGN	6-A	33	1	-	4/11/28/31	0/1/1/1
1	IDS	6-A	34	1	-	0/9/26/29	0/1/1/1
1	SGN	6-A	35	1	-	4/11/28/31	0/1/1/1
1	IDS	6-A	36	1	-	0/9/22/29	0/1/1/1
1	IDS	6-A	4	1	-	3/9/26/29	0/1/1/1
1	SGN	6-A	5	1	-	4/11/28/31	0/1/1/1
1	IDS	6-A	6	1	-	1/9/26/29	0/1/1/1
1	SGN	6-A	7	1	-	2/11/28/31	0/1/1/1
1	IDS	6-A	8	1	-	0/9/26/29	0/1/1/1
1	SGN	6-A	9	1	-	3/11/28/31	0/1/1/1
1	SGN	7-A	1	1	-	6/11/31/31	0/1/1/1
1	IDS	7-A	10	1	-	3/9/26/29	0/1/1/1
1	SGN	7-A	11	1	-	5/11/28/31	0/1/1/1
1	IDS	7-A	12	1	-	0/9/26/29	0/1/1/1
1	SGN	7-A	13	1	-	5/11/28/31	0/1/1/1
1	IDS	7-A	14	1	-	1/9/26/29	0/1/1/1
1	SGN	7-A	15	1	-	5/11/28/31	0/1/1/1
1	IDS	7-A	16	1	-	6/9/26/29	0/1/1/1
1	SGN	7-A	17	1	-	5/11/28/31	0/1/1/1
1	IDS	7-A	18	1	-	5/9/26/29	0/1/1/1
1	SGN	7-A	19	1	-	2/11/28/31	0/1/1/1
1	IDS	7-A	2	1	-	3/9/26/29	0/1/1/1
1	IDS	7-A	20	1	-	0/9/26/29	0/1/1/1
1	SGN	7-A	21	1	-	8/11/28/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	IDS	7-A	22	1	-	0/9/26/29	0/1/1/1
1	SGN	7-A	23	1	-	8/11/28/31	0/1/1/1
1	IDS	7-A	24	1	-	7/9/26/29	0/1/1/1
1	SGN	7-A	25	1	-	6/11/28/31	0/1/1/1
1	IDS	7-A	26	1	-	0/9/26/29	0/1/1/1
1	SGN	7-A	27	1	-	1/11/28/31	0/1/1/1
1	IDS	7-A	28	1	-	2/9/26/29	0/1/1/1
1	SGN	7-A	29	1	-	5/11/28/31	0/1/1/1
1	SGN	7-A	3	1	-	6/11/28/31	0/1/1/1
1	IDS	7-A	30	1	-	0/9/26/29	0/1/1/1
1	SGN	7-A	31	1	-	6/11/28/31	0/1/1/1
1	IDS	7-A	32	1	-	2/9/26/29	0/1/1/1
1	SGN	7-A	33	1	-	4/11/28/31	0/1/1/1
1	IDS	7-A	34	1	-	0/9/26/29	0/1/1/1
1	SGN	7-A	35	1	-	6/11/28/31	0/1/1/1
1	IDS	7-A	36	1	-	0/9/22/29	0/1/1/1
1	IDS	7-A	4	1	-	1/9/26/29	0/1/1/1
1	SGN	7-A	5	1	-	7/11/28/31	0/1/1/1
1	IDS	7-A	6	1	-	1/9/26/29	0/1/1/1
1	SGN	7-A	7	1	-	6/11/28/31	0/1/1/1
1	IDS	7-A	8	1	-	0/9/26/29	0/1/1/1
1	SGN	7-A	9	1	-	5/11/28/31	0/1/1/1
1	SGN	8-A	1	1	-	2/11/31/31	0/1/1/1
1	IDS	8-A	10	1	-	2/9/26/29	0/1/1/1
1	SGN	8-A	11	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	12	1	-	3/9/26/29	0/1/1/1
1	SGN	8-A	13	1	-	1/11/28/31	0/1/1/1
1	IDS	8-A	14	1	-	2/9/26/29	0/1/1/1
1	SGN	8-A	15	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	16	1	-	0/9/26/29	0/1/1/1
1	SGN	8-A	17	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	18	1	-	4/9/26/29	0/1/1/1
1	SGN	8-A	19	1	-	5/11/28/31	0/1/1/1
1	IDS	8-A	2	1	-	0/9/26/29	0/1/1/1
1	IDS	8-A	20	1	-	3/9/26/29	0/1/1/1
1	SGN	8-A	21	1	-	8/11/28/31	0/1/1/1
1	IDS	8-A	22	1	-	1/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	8-A	23	1	-	6/11/28/31	0/1/1/1
1	IDS	8-A	24	1	-	2/9/26/29	0/1/1/1
1	SGN	8-A	25	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	26	1	-	3/9/26/29	0/1/1/1
1	SGN	8-A	27	1	-	5/11/28/31	0/1/1/1
1	IDS	8-A	28	1	-	5/9/26/29	0/1/1/1
1	SGN	8-A	29	1	-	5/11/28/31	0/1/1/1
1	SGN	8-A	3	1	-	1/11/28/31	0/1/1/1
1	IDS	8-A	30	1	-	4/9/26/29	0/1/1/1
1	SGN	8-A	31	1	-	4/11/28/31	0/1/1/1
1	IDS	8-A	32	1	-	3/9/26/29	0/1/1/1
1	SGN	8-A	33	1	-	4/11/28/31	0/1/1/1
1	IDS	8-A	34	1	-	1/9/26/29	0/1/1/1
1	SGN	8-A	35	1	-	3/11/28/31	0/1/1/1
1	IDS	8-A	36	1	-	0/9/22/29	0/1/1/1
1	IDS	8-A	4	1	-	0/9/26/29	0/1/1/1
1	SGN	8-A	5	1	-	6/11/28/31	0/1/1/1
1	IDS	8-A	6	1	-	0/9/26/29	0/1/1/1
1	SGN	8-A	7	1	-	5/11/28/31	0/1/1/1
1	IDS	8-A	8	1	-	2/9/26/29	0/1/1/1
1	SGN	8-A	9	1	-	4/11/28/31	0/1/1/1
1	SGN	9-A	1	1	-	6/11/31/31	0/1/1/1
1	IDS	9-A	10	1	-	2/9/26/29	0/1/1/1
1	SGN	9-A	11	1	-	4/11/28/31	0/1/1/1
1	IDS	9-A	12	1	-	2/9/26/29	0/1/1/1
1	SGN	9-A	13	1	-	8/11/28/31	0/1/1/1
1	IDS	9-A	14	1	-	1/9/26/29	0/1/1/1
1	SGN	9-A	15	1	-	0/11/28/31	0/1/1/1
1	IDS	9-A	16	1	-	3/9/26/29	0/1/1/1
1	SGN	9-A	17	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	18	1	-	2/9/26/29	0/1/1/1
1	SGN	9-A	19	1	-	1/11/28/31	0/1/1/1
1	IDS	9-A	2	1	-	0/9/26/29	0/1/1/1
1	IDS	9-A	20	1	-	1/9/26/29	0/1/1/1
1	SGN	9-A	21	1	-	4/11/28/31	0/1/1/1
1	IDS	9-A	22	1	-	3/9/26/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SGN	9-A	23	1	-	1/11/28/31	0/1/1/1
1	IDS	9-A	24	1	-	2/9/26/29	0/1/1/1
1	SGN	9-A	25	1	-	6/11/28/31	0/1/1/1
1	IDS	9-A	26	1	-	3/9/26/29	0/1/1/1
1	SGN	9-A	27	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	28	1	-	0/9/26/29	0/1/1/1
1	SGN	9-A	29	1	-	6/11/28/31	0/1/1/1
1	SGN	9-A	3	1	-	8/11/28/31	0/1/1/1
1	IDS	9-A	30	1	-	0/9/26/29	0/1/1/1
1	SGN	9-A	31	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	32	1	-	4/9/26/29	0/1/1/1
1	SGN	9-A	33	1	-	7/11/28/31	0/1/1/1
1	IDS	9-A	34	1	-	2/9/26/29	0/1/1/1
1	SGN	9-A	35	1	-	4/11/28/31	0/1/1/1
1	IDS	9-A	36	1	-	0/9/22/29	0/1/1/1
1	IDS	9-A	4	1	-	1/9/26/29	0/1/1/1
1	SGN	9-A	5	1	-	3/11/28/31	0/1/1/1
1	IDS	9-A	6	1	-	1/9/26/29	0/1/1/1
1	SGN	9-A	7	1	-	1/11/28/31	0/1/1/1
1	IDS	9-A	8	1	-	0/9/26/29	0/1/1/1
1	SGN	9-A	9	1	-	1/11/28/31	0/1/1/1

The worst 5 of 1046 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	4	IDS	O2-C2	-3.81	1.41	1.47
1	14-A	15	SGN	S1-N2	3.81	1.64	1.59
1	2-A	14	IDS	O2-C2	-3.81	1.41	1.47
1	4-A	14	IDS	O2-C2	-3.80	1.41	1.47
1	3-A	24	IDS	O2-C2	-3.80	1.41	1.47

The worst 5 of 756 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	13-A	36	IDS	O6B-C6-C5	3.46	121.71	112.71
1	1-A	36	IDS	O6B-C6-C5	3.46	121.70	112.71
1	12-A	36	IDS	O6B-C6-C5	3.46	121.70	112.71
1	5-A	36	IDS	O6B-C6-C5	3.45	121.69	112.71
1	6-A	36	IDS	O6B-C6-C5	3.45	121.69	112.71

There are no chirality outliers.

5 of 1597 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1-A	1	SGN	C2-N2-S1-O2S
1	3-A	1	SGN	C4-C5-C6-O6
1	3-A	1	SGN	O5-C5-C6-O6
1	4-A	1	SGN	C4-C5-C6-O6
1	4-A	1	SGN	O5-C5-C6-O6

There are no ring outliers.

326 monomers are involved in 779 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5-A	20	IDS	5	0
1	7-A	2	IDS	5	0
1	8-A	24	IDS	2	0
1	11-A	20	IDS	5	0
1	4-A	24	IDS	1	0
1	9-A	36	IDS	2	0
1	5-A	33	SGN	3	0
1	8-A	17	SGN	7	0
1	9-A	20	IDS	3	0
1	11-A	17	SGN	6	0
1	8-A	31	SGN	10	0
1	13-A	4	IDS	4	0
1	8-A	2	IDS	1	0
1	5-A	6	IDS	2	0
1	7-A	24	IDS	15	0
1	13-A	5	SGN	1	0
1	4-A	31	SGN	11	0
1	1-A	6	IDS	4	0
1	5-A	18	IDS	6	0
1	6-A	21	SGN	8	0
1	2-A	2	IDS	1	0
1	12-A	10	IDS	6	0
1	13-A	10	IDS	4	0
1	13-A	1	SGN	3	0
1	1-A	5	SGN	5	0
1	9-A	17	SGN	4	0
1	1-A	12	IDS	5	0
1	5-A	11	SGN	1	0
1	11-A	10	IDS	6	0
1	8-A	7	SGN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	4-A	19	SGN	3	0
1	8-A	13	SGN	6	0
1	7-A	20	IDS	4	0
1	11-A	34	IDS	7	0
1	1-A	24	IDS	10	0
1	1-A	29	SGN	7	0
1	5-A	13	SGN	6	0
1	5-A	7	SGN	1	0
1	6-A	26	IDS	7	0
1	6-A	29	SGN	8	0
1	1-A	25	SGN	4	0
1	2-A	6	IDS	6	0
1	11-A	8	IDS	3	0
1	11-A	29	SGN	1	0
1	5-A	1	SGN	3	0
1	1-A	2	IDS	2	0
1	13-A	30	IDS	2	0
1	13-A	15	SGN	14	0
1	1-A	20	IDS	2	0
1	6-A	27	SGN	11	0
1	4-A	13	SGN	2	0
1	11-A	25	SGN	2	0
1	5-A	19	SGN	6	0
1	8-A	11	SGN	7	0
1	4-A	11	SGN	2	0
1	12-A	24	IDS	5	0
1	6-A	22	IDS	14	0
1	4-A	30	IDS	9	0
1	11-A	24	IDS	1	0
1	6-A	25	SGN	5	0
1	6-A	34	IDS	1	0
1	9-A	5	SGN	1	0
1	4-A	15	SGN	3	0
1	6-A	24	IDS	4	0
1	9-A	28	IDS	5	0
1	13-A	32	IDS	2	0
1	9-A	29	SGN	3	0
1	12-A	26	IDS	2	0
1	13-A	23	SGN	3	0
1	9-A	35	SGN	2	0
1	12-A	11	SGN	7	0
1	1-A	18	IDS	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5-A	16	IDS	8	0
1	7-A	10	IDS	5	0
1	11-A	11	SGN	2	0
1	13-A	17	SGN	3	0
1	5-A	17	SGN	11	0
1	9-A	27	SGN	5	0
1	13-A	12	IDS	2	0
1	5-A	31	SGN	5	0
1	6-A	12	IDS	9	0
1	7-A	30	IDS	1	0
1	5-A	2	IDS	5	0
1	8-A	32	IDS	5	0
1	12-A	6	IDS	5	0
1	8-A	10	IDS	4	0
1	8-A	12	IDS	8	0
1	9-A	8	IDS	1	0
1	12-A	35	SGN	6	0
1	11-A	6	IDS	2	0
1	13-A	9	SGN	3	0
1	5-A	34	IDS	5	0
1	1-A	8	IDS	5	0
1	6-A	6	IDS	8	0
1	8-A	26	IDS	1	0
1	7-A	4	IDS	15	0
1	5-A	3	SGN	7	0
1	9-A	32	IDS	4	0
1	1-A	1	SGN	2	0
1	11-A	1	SGN	1	0
1	12-A	19	SGN	8	0
1	1-A	15	SGN	4	0
1	5-A	12	IDS	3	0
1	12-A	4	IDS	1	0
1	9-A	23	SGN	6	0
1	6-A	11	SGN	11	0
1	6-A	15	SGN	2	0
1	11-A	28	IDS	6	0
1	8-A	3	SGN	1	0
1	8-A	21	SGN	6	0
1	13-A	29	SGN	7	0
1	12-A	32	IDS	5	0
1	12-A	16	IDS	2	0
1	5-A	26	IDS	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	11-A	16	IDS	6	0
1	13-A	3	SGN	4	0
1	6-A	13	SGN	6	0
1	9-A	33	SGN	2	0
1	7-A	36	IDS	5	0
1	7-A	17	SGN	3	0
1	11-A	27	SGN	6	0
1	7-A	32	IDS	14	0
1	13-A	28	IDS	7	0
1	6-A	16	IDS	6	0
1	11-A	30	IDS	1	0
1	4-A	28	IDS	3	0
1	1-A	32	IDS	10	0
1	6-A	10	IDS	11	0
1	1-A	10	IDS	3	0
1	9-A	21	SGN	5	0
1	7-A	23	SGN	9	0
1	9-A	9	SGN	3	0
1	9-A	14	IDS	3	0
1	8-A	36	IDS	2	0
1	13-A	22	IDS	7	0
1	12-A	29	SGN	3	0
1	13-A	8	IDS	6	0
1	7-A	26	IDS	2	0
1	9-A	1	SGN	3	0
1	4-A	3	SGN	3	0
1	8-A	6	IDS	1	0
1	4-A	33	SGN	6	0
1	7-A	5	SGN	14	0
1	4-A	36	IDS	1	0
1	6-A	4	IDS	6	0
1	7-A	31	SGN	6	0
1	13-A	27	SGN	6	0
1	13-A	25	SGN	3	0
1	6-A	1	SGN	1	0
1	6-A	18	IDS	1	0
1	7-A	19	SGN	11	0
1	5-A	4	IDS	9	0
1	9-A	7	SGN	2	0
1	4-A	5	SGN	6	0
1	9-A	16	IDS	3	0
1	8-A	15	SGN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5-A	23	SGN	2	0
1	11-A	4	IDS	1	0
1	4-A	34	IDS	12	0
1	13-A	20	IDS	5	0
1	7-A	3	SGN	11	0
1	12-A	2	IDS	2	0
1	9-A	3	SGN	1	0
1	11-A	32	IDS	8	0
1	7-A	15	SGN	7	0
1	1-A	28	IDS	1	0
1	8-A	25	SGN	1	0
1	5-A	30	IDS	8	0
1	11-A	23	SGN	5	0
1	7-A	29	SGN	1	0
1	13-A	6	IDS	2	0
1	13-A	14	IDS	10	0
1	5-A	22	IDS	1	0
1	5-A	14	IDS	4	0
1	7-A	35	SGN	6	0
1	6-A	14	IDS	3	0
1	11-A	9	SGN	5	0
1	6-A	23	SGN	7	0
1	4-A	20	IDS	4	0
1	1-A	26	IDS	5	0
1	5-A	5	SGN	6	0
1	11-A	12	IDS	7	0
1	5-A	8	IDS	1	0
1	8-A	29	SGN	3	0
1	1-A	30	IDS	13	0
1	12-A	25	SGN	6	0
1	8-A	23	SGN	2	0
1	8-A	35	SGN	5	0
1	4-A	35	SGN	7	0
1	13-A	21	SGN	6	0
1	7-A	25	SGN	10	0
1	8-A	27	SGN	4	0
1	8-A	30	IDS	8	0
1	9-A	22	IDS	5	0
1	7-A	22	IDS	1	0
1	4-A	9	SGN	5	0
1	7-A	8	IDS	2	0
1	13-A	35	SGN	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	13-A	13	SGN	3	0
1	8-A	14	IDS	2	0
1	1-A	4	IDS	3	0
1	13-A	11	SGN	4	0
1	6-A	7	SGN	8	0
1	1-A	3	SGN	2	0
1	8-A	22	IDS	2	0
1	4-A	22	IDS	7	0
1	9-A	2	IDS	3	0
1	12-A	15	SGN	2	0
1	13-A	19	SGN	5	0
1	2-A	8	IDS	2	0
1	11-A	15	SGN	4	0
1	6-A	20	IDS	1	0
1	11-A	31	SGN	1	0
1	4-A	8	IDS	4	0
1	9-A	6	IDS	2	0
1	12-A	23	SGN	3	0
1	1-A	19	SGN	5	0
1	1-A	23	SGN	11	0
1	6-A	28	IDS	12	0
1	13-A	7	SGN	4	0
1	12-A	13	SGN	7	0
1	5-A	35	SGN	3	0
1	13-A	16	IDS	6	0
1	2-A	3	SGN	1	0
1	4-A	27	SGN	1	0
1	9-A	24	IDS	5	0
1	11-A	26	IDS	2	0
1	11-A	13	SGN	2	0
1	1-A	27	SGN	5	0
1	4-A	2	IDS	6	0
1	8-A	28	IDS	3	0
1	1-A	16	IDS	4	0
1	9-A	31	SGN	7	0
1	12-A	30	IDS	3	0
1	7-A	33	SGN	8	0
1	8-A	18	IDS	7	0
1	1-A	33	SGN	10	0
1	5-A	25	SGN	1	0
1	12-A	14	IDS	4	0
1	12-A	22	IDS	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1-A	35	SGN	3	0
1	9-A	13	SGN	7	0
1	7-A	9	SGN	7	0
1	11-A	22	IDS	6	0
1	7-A	6	IDS	5	0
1	7-A	14	IDS	6	0
1	4-A	7	SGN	6	0
1	13-A	34	IDS	3	0
1	8-A	33	SGN	1	0
1	1-A	9	SGN	3	0
1	6-A	30	IDS	1	0
1	1-A	14	IDS	4	0
1	12-A	8	IDS	9	0
1	1-A	7	SGN	5	0
1	13-A	18	IDS	2	0
1	9-A	11	SGN	5	0
1	12-A	17	SGN	5	0
1	6-A	8	IDS	4	0
1	4-A	29	SGN	6	0
1	1-A	21	SGN	3	0
1	2-A	9	SGN	1	0
1	8-A	8	IDS	5	0
1	1-A	17	SGN	7	0
1	6-A	2	IDS	1	0
1	4-A	6	IDS	8	0
1	9-A	19	SGN	4	0
1	12-A	21	SGN	3	0
1	4-A	1	SGN	3	0
1	2-A	5	SGN	6	0
1	2-A	7	SGN	2	0
1	5-A	28	IDS	5	0
1	6-A	5	SGN	7	0
1	4-A	18	IDS	1	0
1	5-A	15	SGN	1	0
1	12-A	34	IDS	3	0
1	7-A	13	SGN	10	0
1	8-A	34	IDS	4	0
1	5-A	29	SGN	9	0
1	1-A	13	SGN	7	0
1	13-A	31	SGN	1	0
1	12-A	33	SGN	7	0
1	13-A	2	IDS	3	0

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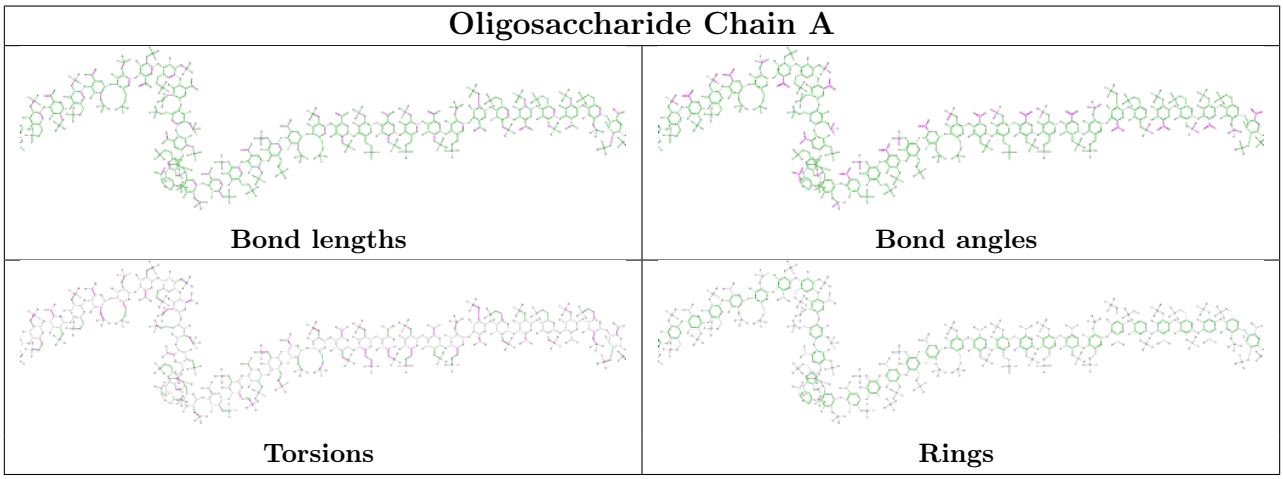
Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	9-A	12	IDS	6	0
1	1-A	31	SGN	12	0
1	12-A	36	IDS	4	0
1	1-A	36	IDS	3	0
1	6-A	33	SGN	2	0
1	1-A	22	IDS	7	0
1	11-A	14	IDS	4	0
1	7-A	16	IDS	8	0
1	4-A	16	IDS	4	0
1	12-A	9	SGN	9	0
1	8-A	20	IDS	5	0
1	12-A	1	SGN	1	0
1	9-A	18	IDS	3	0
1	1-A	34	IDS	5	0
1	12-A	18	IDS	13	0
1	5-A	24	IDS	1	0
1	6-A	9	SGN	5	0
1	4-A	23	SGN	3	0
1	9-A	10	IDS	5	0
1	12-A	3	SGN	2	0
1	7-A	18	IDS	8	0
1	11-A	5	SGN	2	0
1	12-A	12	IDS	4	0
1	5-A	27	SGN	5	0
1	13-A	33	SGN	2	0
1	9-A	30	IDS	8	0
1	8-A	9	SGN	4	0
1	7-A	12	IDS	5	0
1	4-A	4	IDS	4	0
1	6-A	32	IDS	1	0
1	11-A	33	SGN	14	0
1	13-A	26	IDS	7	0
1	7-A	34	IDS	3	0
1	5-A	21	SGN	1	0
1	12-A	7	SGN	5	0
1	6-A	17	SGN	7	0
1	11-A	21	SGN	7	0
1	4-A	32	IDS	4	0
1	4-A	10	IDS	5	0
1	11-A	7	SGN	2	0
1	4-A	12	IDS	2	0
1	4-A	21	SGN	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	4-A	17	SGN	1	0
1	13-A	36	IDS	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.