



Full wwPDB Geometry-Only Validation Report ⓘ

Feb 13, 2024 – 09:38 AM EST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-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) : 2.36

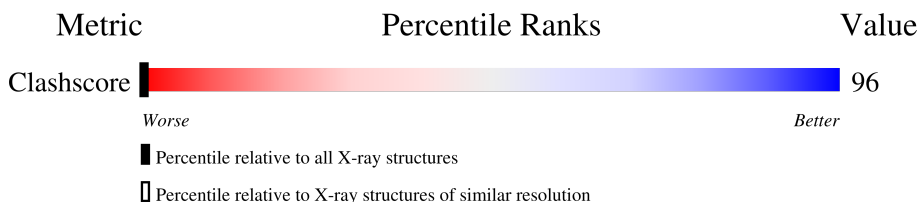
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

SOLUTION SCATTERING

The reported resolution of this entry is unknown.




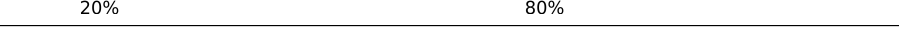
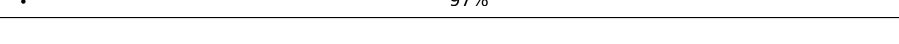





Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued from previous page...

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

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-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:  10% 90%

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

- 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

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

● 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

Chain 9-A:  10% 90%

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

● 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

Chain 10-A:  7% 93%

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

4 Model quality

4.1 Standard geometry

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-close contacts

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

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 96.

All (922) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SGN:H61	1:A:28:IDS:S	1.48	1.51
1:A:17:SGN:C6	1:A:18:IDS:O2S	1.65	1.45
1:A:28:IDS:H3	1:A:29:SGN:N2	1.21	1.44
1:A:18:IDS:H3	1:A:19:SGN:N2	1.29	1.43
1:A:6:IDS:H3	1:A:7:SGN:N2	1.13	1.42
1:A:10:IDS:H3	1:A:11:SGN:N2	1.21	1.41
1:A:18:IDS:H3	1:A:19:SGN:N2	1.25	1.41
1:A:4:IDS:H3	1:A:5:SGN:N2	1.41	1.36
1:A:18:IDS:O6A	1:A:19:SGN:C5	1.74	1.36
1:A:12:IDS:O6A	1:A:13:SGN:C5	1.75	1.35
1:A:12:IDS:H3	1:A:13:SGN:N2	1.05	1.34
1:A:23:SGN:C5	1:A:24:IDS:O2S	1.73	1.34
1:A:22:IDS:O6A	1:A:23:SGN:C5	1.76	1.33
1:A:9:SGN:C6	1:A:10:IDS:O2S	1.75	1.33
1:A:14:IDS:H3	1:A:15:SGN:N2	1.32	1.32
1:A:6:IDS:C3	1:A:7:SGN:N2	1.91	1.32
1:A:1:SGN:O3	1:A:2:IDS:H5	1.28	1.32
1:A:23:SGN:C6	1:A:24:IDS:O2S	1.77	1.31
1:A:6:IDS:H3	1:A:7:SGN:N2	1.44	1.31
1:A:14:IDS:H3	1:A:15:SGN:N2	1.44	1.31
1:A:10:IDS:C3	1:A:11:SGN:O1S	1.76	1.31
1:A:7:SGN:H61	1:A:8:IDS:O2S	1.26	1.31
1:A:18:IDS:H3	1:A:19:SGN:N2	1.43	1.31
1:A:19:SGN:H61	1:A:20:IDS:S	1.69	1.30
1:A:19:SGN:O5S	1:A:20:IDS:C6	1.79	1.30
1:A:12:IDS:H3	1:A:13:SGN:N2	1.44	1.29
1:A:10:IDS:O6A	1:A:11:SGN:H5	1.20	1.29
1:A:4:IDS:C3	1:A:5:SGN:N2	1.95	1.29
1:A:4:IDS:H3	1:A:5:SGN:N2	0.99	1.28
1:A:17:SGN:H61	1:A:18:IDS:O2S	1.21	1.28
1:A:24:IDS:O6A	1:A:25:SGN:H5	1.20	1.27
1:A:18:IDS:O6A	1:A:19:SGN:H5	1.26	1.27
1:A:16:IDS:C3	1:A:17:SGN:O1S	1.81	1.26
1:A:24:IDS:H3	1:A:25:SGN:N2	1.49	1.26
1:A:19:SGN:O5S	1:A:20:IDS:O6B	1.53	1.26
1:A:27:SGN:C6	1:A:28:IDS:O2S	1.84	1.26
1:A:18:IDS:C3	1:A:19:SGN:N2	1.97	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SGN:C6	1:A:28:IDS:S	2.23	1.25
1:A:16:IDS:H3	1:A:17:SGN:O1S	1.26	1.25
1:A:23:SGN:O5S	1:A:24:IDS:O5	1.53	1.25
1:A:10:IDS:C3	1:A:11:SGN:O1S	1.84	1.24
1:A:23:SGN:H5	1:A:24:IDS:O2S	1.22	1.24
1:A:24:IDS:O3	1:A:25:SGN:O1S	1.55	1.23
1:A:11:SGN:H61	1:A:12:IDS:O2S	1.10	1.23
1:A:12:IDS:C3	1:A:13:SGN:N2	2.01	1.22
1:A:8:IDS:H3	1:A:9:SGN:N2	1.50	1.22
1:A:21:SGN:O4S	1:A:22:IDS:O1S	1.53	1.22
1:A:12:IDS:H3	1:A:13:SGN:N2	1.53	1.21
1:A:14:IDS:C3	1:A:15:SGN:N2	2.03	1.21
1:A:13:SGN:H61	1:A:14:IDS:O2S	1.04	1.21
1:A:28:IDS:O2	1:A:29:SGN:O3S	1.55	1.21
1:A:25:SGN:C6	1:A:26:IDS:O2S	1.89	1.20
1:A:23:SGN:O3	1:A:24:IDS:C5	1.90	1.20
1:A:9:SGN:H61	1:A:10:IDS:O2S	1.37	1.20
1:A:16:IDS:O3	1:A:17:SGN:S1	1.99	1.20
1:A:12:IDS:O6A	1:A:13:SGN:H62	1.40	1.20
1:A:27:SGN:C5	1:A:28:IDS:O2S	1.91	1.19
1:A:22:IDS:O6A	1:A:23:SGN:C5	1.89	1.19
1:A:23:SGN:O3	1:A:24:IDS:C5	1.91	1.18
1:A:22:IDS:O6A	1:A:24:IDS:S	2.01	1.18
1:A:8:IDS:O3	1:A:9:SGN:O3S	1.61	1.18
1:A:24:IDS:O6A	1:A:25:SGN:C5	1.90	1.18
1:A:2:IDS:H3	1:A:3:SGN:N2	1.58	1.18
1:A:14:IDS:H3	1:A:15:SGN:N2	1.52	1.17
1:A:22:IDS:O6A	1:A:23:SGN:H5	1.01	1.17
1:A:1:SGN:O3	1:A:2:IDS:C5	1.93	1.17
1:A:27:SGN:C6	1:A:28:IDS:O1S	1.92	1.17
1:A:1:SGN:O4S	1:A:2:IDS:O2	1.62	1.17
1:A:10:IDS:O6A	1:A:11:SGN:C5	1.92	1.17
1:A:24:IDS:H3	1:A:25:SGN:N2	1.57	1.16
1:A:10:IDS:O3	1:A:11:SGN:N2	1.79	1.16
1:A:27:SGN:O3	1:A:28:IDS:H5	1.43	1.16
1:A:11:SGN:C6	1:A:12:IDS:O2S	1.91	1.16
1:A:10:IDS:H3	1:A:11:SGN:O1S	1.43	1.16
1:A:13:SGN:O5S	1:A:14:IDS:O2	1.62	1.16
1:A:15:SGN:O4S	1:A:16:IDS:S	2.04	1.16
1:A:16:IDS:O3	1:A:17:SGN:O3S	1.60	1.15
1:A:25:SGN:O5S	1:A:26:IDS:O6B	1.63	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:IDS:H3	1:A:11:SGN:O1S	0.99	1.15
1:A:5:SGN:H61	1:A:6:IDS:O2S	1.41	1.15
1:A:9:SGN:C6	1:A:10:IDS:O2S	1.95	1.15
1:A:22:IDS:O6A	1:A:23:SGN:H5	0.98	1.15
1:A:10:IDS:C3	1:A:11:SGN:N2	2.10	1.15
1:A:27:SGN:O3	1:A:28:IDS:C5	1.94	1.15
1:A:3:SGN:S2	1:A:4:IDS:O5	2.04	1.14
1:A:13:SGN:O3	1:A:14:IDS:C5	1.95	1.14
1:A:22:IDS:O3	1:A:23:SGN:O1S	1.61	1.14
1:A:20:IDS:H3	1:A:21:SGN:S1	1.86	1.14
1:A:23:SGN:O3	1:A:24:IDS:H5	1.48	1.13
1:A:20:IDS:H3	1:A:21:SGN:N2	1.64	1.13
1:A:12:IDS:O6A	1:A:13:SGN:C6	1.97	1.13
1:A:3:SGN:O4S	1:A:4:IDS:O5	1.66	1.13
1:A:16:IDS:O6A	1:A:17:SGN:C5	1.96	1.13
1:A:19:SGN:H61	1:A:20:IDS:O2S	1.47	1.12
1:A:16:IDS:H3	1:A:17:SGN:O1S	0.96	1.12
1:A:23:SGN:O4S	1:A:24:IDS:O5	1.63	1.12
1:A:24:IDS:O3	1:A:25:SGN:S1	2.06	1.12
1:A:20:IDS:O3	1:A:21:SGN:O1S	1.66	1.11
1:A:19:SGN:C6	1:A:20:IDS:O2S	1.97	1.11
1:A:14:IDS:C3	1:A:15:SGN:N2	2.05	1.11
1:A:15:SGN:O5S	1:A:16:IDS:C6	1.99	1.11
1:A:9:SGN:H61	1:A:10:IDS:O2S	0.94	1.11
1:A:16:IDS:O6A	1:A:17:SGN:H5	1.50	1.11
1:A:19:SGN:O3	1:A:20:IDS:C5	1.98	1.10
1:A:25:SGN:H62	1:A:26:IDS:O2S	1.48	1.10
1:A:29:SGN:O6	1:A:30:IDS:O5	1.70	1.10
1:A:6:IDS:H3	1:A:7:SGN:N2	1.67	1.09
1:A:24:IDS:C3	1:A:25:SGN:N2	2.15	1.09
1:A:27:SGN:H61	1:A:28:IDS:O1S	1.46	1.09
1:A:16:IDS:C3	1:A:17:SGN:N2	2.16	1.09
1:A:16:IDS:H3	1:A:17:SGN:N2	1.62	1.08
1:A:16:IDS:O6A	1:A:17:SGN:H5	1.51	1.08
1:A:23:SGN:O3	1:A:24:IDS:C6	2.02	1.08
1:A:13:SGN:C6	1:A:14:IDS:O2S	2.00	1.08
1:A:23:SGN:HO3	1:A:24:IDS:C5	1.66	1.08
1:A:18:IDS:C3	1:A:19:SGN:N2	2.16	1.08
1:A:28:IDS:H3	1:A:29:SGN:N2	1.69	1.08
1:A:28:IDS:C3	1:A:29:SGN:N2	2.17	1.07
1:A:24:IDS:O6A	1:A:25:SGN:C5	2.02	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:SGN:H5	1:A:28:IDS:O2S	1.54	1.07
1:A:24:IDS:O3	1:A:25:SGN:O1S	1.73	1.07
1:A:18:IDS:C3	1:A:19:SGN:N2	2.17	1.07
1:A:13:SGN:H61	1:A:14:IDS:O2S	1.52	1.06
1:A:19:SGN:O3	1:A:20:IDS:H5	1.55	1.06
1:A:23:SGN:O3	1:A:24:IDS:H5	1.54	1.06
1:A:12:IDS:C6	1:A:13:SGN:H5	1.85	1.05
1:A:24:IDS:C3	1:A:25:SGN:N2	2.19	1.05
1:A:28:IDS:C3	1:A:29:SGN:N2	2.20	1.05
1:A:22:IDS:H4	1:A:23:SGN:O1S	1.53	1.05
1:A:5:SGN:O3	1:A:6:IDS:H5	1.57	1.05
1:A:18:IDS:O3	1:A:19:SGN:N2	1.89	1.04
1:A:28:IDS:H3	1:A:29:SGN:S1	1.97	1.04
1:A:18:IDS:O6A	1:A:19:SGN:C6	2.05	1.04
1:A:19:SGN:O5S	1:A:20:IDS:C5	2.04	1.04
1:A:15:SGN:H61	1:A:16:IDS:O1S	1.57	1.04
1:A:9:SGN:O4S	1:A:10:IDS:C1	2.05	1.04
1:A:25:SGN:O4S	1:A:26:IDS:O2	1.76	1.03
1:A:7:SGN:C6	1:A:8:IDS:O2S	2.06	1.03
1:A:6:IDS:C3	1:A:7:SGN:N2	2.20	1.03
1:A:16:IDS:O6A	1:A:17:SGN:H5	1.58	1.03
1:A:12:IDS:O6A	1:A:13:SGN:C5	2.05	1.03
1:A:6:IDS:O3	1:A:7:SGN:O1S	1.75	1.03
1:A:10:IDS:C3	1:A:11:SGN:N2	2.21	1.03
1:A:23:SGN:O3	1:A:24:IDS:C6	2.07	1.03
1:A:23:SGN:O4S	1:A:24:IDS:C1	2.06	1.03
1:A:13:SGN:O5S	1:A:14:IDS:O6B	1.76	1.03
1:A:24:IDS:O3	1:A:25:SGN:N2	1.91	1.02
1:A:16:IDS:O3	1:A:17:SGN:N2	1.92	1.02
1:A:13:SGN:O3	1:A:14:IDS:C6	2.06	1.02
1:A:28:IDS:O3	1:A:29:SGN:O1S	1.78	1.02
1:A:12:IDS:C3	1:A:13:SGN:N2	2.23	1.02
1:A:29:SGN:O3	1:A:30:IDS:C5	2.06	1.02
1:A:27:SGN:O3	1:A:28:IDS:H5	1.59	1.02
1:A:23:SGN:HO3	1:A:24:IDS:C6	1.71	1.02
1:A:22:IDS:O6A	1:A:24:IDS:O2S	1.78	1.01
1:A:1:SGN:HO3	1:A:2:IDS:H5	1.25	1.01
1:A:24:IDS:O6A	1:A:25:SGN:H5	1.60	1.01
1:A:19:SGN:H61	1:A:20:IDS:O2S	1.59	1.01
1:A:10:IDS:O6A	1:A:11:SGN:H5	1.61	1.01
1:A:6:IDS:H3	1:A:7:SGN:O1S	1.59	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:IDS:O6A	1:A:13:SGN:H5	1.56	1.01
1:A:19:SGN:O6S	1:A:20:IDS:O1S	1.79	1.00
1:A:2:IDS:C3	1:A:3:SGN:N2	2.19	1.00
1:A:19:SGN:S2	1:A:20:IDS:O5	2.18	1.00
1:A:27:SGN:O3	1:A:28:IDS:O6B	1.80	1.00
1:A:17:SGN:C6	1:A:18:IDS:O2S	2.08	1.00
1:A:18:IDS:O3	1:A:19:SGN:S1	2.19	1.00
1:A:18:IDS:C3	1:A:19:SGN:N2	2.24	1.00
1:A:11:SGN:O6	1:A:12:IDS:O5	1.78	1.00
1:A:7:SGN:H61	1:A:8:IDS:O2S	1.61	1.00
1:A:15:SGN:O4S	1:A:16:IDS:O2S	1.79	1.00
1:A:25:SGN:H61	1:A:26:IDS:O1S	1.61	0.99
1:A:9:SGN:C6	1:A:10:IDS:O2S	2.10	0.99
1:A:4:IDS:H3	1:A:5:SGN:N2	1.77	0.99
1:A:16:IDS:H3	1:A:17:SGN:N2	1.77	0.99
1:A:23:SGN:S2	1:A:24:IDS:O5	2.21	0.99
1:A:28:IDS:O3	1:A:29:SGN:S1	2.20	0.99
1:A:24:IDS:O3	1:A:25:SGN:S1	2.20	0.99
1:A:29:SGN:O3	1:A:30:IDS:C6	2.11	0.99
1:A:12:IDS:O6A	1:A:13:SGN:C6	2.10	0.99
1:A:12:IDS:S	1:A:13:SGN:O3S	2.20	0.98
1:A:17:SGN:O4S	1:A:18:IDS:O5	1.81	0.98
1:A:13:SGN:O3	1:A:14:IDS:H5	1.59	0.98
1:A:18:IDS:O3	1:A:19:SGN:N2	1.96	0.98
1:A:28:IDS:C3	1:A:29:SGN:O3S	2.12	0.98
1:A:22:IDS:O3	1:A:23:SGN:O3S	1.81	0.98
1:A:26:IDS:O6A	1:A:27:SGN:C5	2.12	0.98
1:A:10:IDS:O3	1:A:11:SGN:O1S	1.81	0.97
1:A:27:SGN:O3	1:A:28:IDS:C5	2.12	0.97
1:A:23:SGN:HO3	1:A:24:IDS:C6	1.74	0.97
1:A:16:IDS:H3	1:A:17:SGN:S1	2.04	0.97
1:A:24:IDS:O3	1:A:25:SGN:O3S	1.79	0.97
1:A:27:SGN:O6	1:A:28:IDS:O5	1.82	0.97
1:A:10:IDS:H3	1:A:11:SGN:N2	1.79	0.97
1:A:22:IDS:C3	1:A:23:SGN:N2	2.27	0.96
1:A:16:IDS:C3	1:A:17:SGN:N2	2.26	0.96
1:A:23:SGN:O3	1:A:24:IDS:C5	2.14	0.96
1:A:9:SGN:O6	1:A:10:IDS:O2S	1.74	0.96
1:A:22:IDS:O3	1:A:23:SGN:O1S	1.83	0.96
1:A:13:SGN:HO3	1:A:14:IDS:C6	1.77	0.96
1:A:20:IDS:C3	1:A:21:SGN:N2	2.28	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SGN:H61	1:A:10:IDS:O5	1.65	0.96
1:A:9:SGN:H61	1:A:10:IDS:S	2.05	0.96
1:A:16:IDS:O6A	1:A:17:SGN:C5	2.14	0.95
1:A:9:SGN:O4S	1:A:10:IDS:O1S	1.84	0.95
1:A:19:SGN:O3	1:A:20:IDS:C6	2.13	0.95
1:A:29:SGN:H61	1:A:30:IDS:O2S	1.65	0.95
1:A:10:IDS:O3	1:A:11:SGN:O1S	1.83	0.95
1:A:14:IDS:C3	1:A:15:SGN:N2	2.28	0.95
1:A:18:IDS:H3	1:A:19:SGN:N2	1.80	0.95
1:A:20:IDS:H3	1:A:21:SGN:O1S	1.66	0.94
1:A:19:SGN:H61	1:A:20:IDS:O1S	1.65	0.94
1:A:4:IDS:O3	1:A:5:SGN:O1S	1.81	0.94
1:A:9:SGN:H61	1:A:10:IDS:O2S	1.67	0.94
1:A:19:SGN:C6	1:A:20:IDS:S	2.53	0.94
1:A:22:IDS:O3	1:A:23:SGN:N2	2.00	0.94
1:A:1:SGN:H61	1:A:2:IDS:O2S	1.68	0.94
1:A:7:SGN:O3	1:A:8:IDS:O6B	1.86	0.93
1:A:27:SGN:O3	1:A:28:IDS:C6	2.15	0.93
1:A:12:IDS:O6A	1:A:13:SGN:O5	1.85	0.93
1:A:6:IDS:O6A	1:A:7:SGN:H62	1.67	0.93
1:A:4:IDS:C3	1:A:5:SGN:N2	2.31	0.93
1:A:13:SGN:H61	1:A:14:IDS:O2S	1.69	0.93
1:A:2:IDS:H3	1:A:3:SGN:N2	1.81	0.93
1:A:23:SGN:H62	1:A:24:IDS:O2S	1.66	0.93
1:A:28:IDS:H3	1:A:29:SGN:N2	1.84	0.92
1:A:20:IDS:C3	1:A:21:SGN:N2	2.33	0.92
1:A:28:IDS:C3	1:A:29:SGN:S1	2.58	0.92
1:A:15:SGN:O3	1:A:16:IDS:H5	1.68	0.92
1:A:18:IDS:C6	1:A:19:SGN:H5	1.99	0.92
1:A:24:IDS:O3	1:A:25:SGN:O3S	1.88	0.91
1:A:28:IDS:C3	1:A:29:SGN:N2	2.34	0.91
1:A:19:SGN:O6	1:A:20:IDS:O5	1.87	0.91
1:A:10:IDS:O3	1:A:11:SGN:O1S	1.87	0.91
1:A:27:SGN:H61	1:A:28:IDS:O2S	1.51	0.91
1:A:13:SGN:O4S	1:A:14:IDS:O2	1.89	0.90
1:A:22:IDS:C4	1:A:23:SGN:O1S	2.17	0.90
1:A:29:SGN:S2	1:A:30:IDS:O6B	2.29	0.90
1:A:25:SGN:O4S	1:A:26:IDS:O1S	1.90	0.90
1:A:18:IDS:O6A	1:A:19:SGN:H62	1.69	0.90
1:A:24:IDS:O3	1:A:25:SGN:O3S	1.89	0.90
1:A:5:SGN:C6	1:A:6:IDS:O2S	2.18	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:IDS:H3	1:A:9:SGN:N2	1.87	0.90
1:A:10:IDS:C3	1:A:11:SGN:N2	2.34	0.90
1:A:29:SGN:O5S	1:A:30:IDS:C6	2.19	0.89
1:A:9:SGN:O4S	1:A:10:IDS:O1S	1.89	0.89
1:A:12:IDS:O2	1:A:13:SGN:O3S	1.89	0.89
1:A:15:SGN:O5S	1:A:16:IDS:O6B	1.89	0.89
1:A:20:IDS:O3	1:A:21:SGN:N2	2.06	0.89
1:A:6:IDS:O2	1:A:7:SGN:O3S	1.85	0.89
1:A:23:SGN:O3	1:A:24:IDS:C6	2.19	0.89
1:A:9:SGN:O4S	1:A:10:IDS:O5	1.91	0.89
1:A:15:SGN:O3	1:A:16:IDS:O6B	1.91	0.89
1:A:24:IDS:H3	1:A:25:SGN:N2	1.84	0.89
1:A:25:SGN:O3	1:A:26:IDS:H5	1.72	0.88
1:A:20:IDS:C3	1:A:21:SGN:O1S	2.21	0.88
1:A:5:SGN:H61	1:A:6:IDS:O2S	1.71	0.88
1:A:24:IDS:O6A	1:A:25:SGN:C6	2.22	0.88
1:A:9:SGN:H61	1:A:10:IDS:O2S	1.72	0.88
1:A:6:IDS:O3	1:A:7:SGN:S1	2.29	0.88
1:A:18:IDS:O3	1:A:19:SGN:S1	2.32	0.88
1:A:20:IDS:H3	1:A:21:SGN:N2	1.87	0.88
1:A:3:SGN:O4S	1:A:4:IDS:C1	2.21	0.88
1:A:23:SGN:O5S	1:A:24:IDS:C5	2.22	0.87
1:A:10:IDS:H3	1:A:11:SGN:S1	2.14	0.87
1:A:25:SGN:O4S	1:A:26:IDS:C1	2.22	0.87
1:A:14:IDS:H3	1:A:15:SGN:N2	1.90	0.87
1:A:25:SGN:C5	1:A:26:IDS:O2S	2.22	0.87
1:A:12:IDS:O3	1:A:13:SGN:S1	2.30	0.87
1:A:24:IDS:C3	1:A:25:SGN:N2	2.38	0.87
1:A:26:IDS:C6	1:A:27:SGN:H5	2.05	0.87
1:A:27:SGN:HO3	1:A:28:IDS:C6	1.87	0.86
1:A:23:SGN:H61	1:A:24:IDS:O2S	1.74	0.86
1:A:6:IDS:C6	1:A:7:SGN:H5	2.05	0.86
1:A:16:IDS:C3	1:A:17:SGN:N2	2.38	0.86
1:A:6:IDS:O3	1:A:7:SGN:S1	2.33	0.86
1:A:22:IDS:H3	1:A:23:SGN:N2	1.90	0.86
1:A:10:IDS:H3	1:A:11:SGN:S1	2.15	0.86
1:A:25:SGN:O4S	1:A:26:IDS:C2	2.22	0.86
1:A:15:SGN:O6	1:A:16:IDS:O5	1.92	0.86
1:A:20:IDS:O3	1:A:21:SGN:O3S	1.93	0.86
1:A:19:SGN:C6	1:A:20:IDS:O2S	2.23	0.86
1:A:9:SGN:H61	1:A:10:IDS:S	2.16	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:IDS:O3	1:A:17:SGN:N2	2.09	0.85
1:A:15:SGN:O3	1:A:16:IDS:C5	2.24	0.85
1:A:1:SGN:O3	1:A:2:IDS:C6	2.25	0.85
1:A:28:IDS:C2	1:A:29:SGN:O3S	2.24	0.85
1:A:14:IDS:C3	1:A:15:SGN:N2	2.39	0.85
1:A:28:IDS:O3	1:A:29:SGN:O1S	1.93	0.85
1:A:22:IDS:O6A	1:A:23:SGN:H5	1.75	0.85
1:A:20:IDS:O3	1:A:21:SGN:S1	2.34	0.84
1:A:5:SGN:S2	1:A:6:IDS:O5	2.36	0.84
1:A:25:SGN:C6	1:A:26:IDS:S	2.66	0.84
1:A:5:SGN:O3	1:A:6:IDS:C5	2.26	0.84
1:A:26:IDS:O6A	1:A:27:SGN:H62	1.78	0.84
1:A:19:SGN:C6	1:A:20:IDS:O1S	2.26	0.84
1:A:12:IDS:C6	1:A:13:SGN:C5	2.54	0.84
1:A:23:SGN:H61	1:A:24:IDS:C1	2.08	0.84
1:A:12:IDS:H3	1:A:13:SGN:S1	2.17	0.84
1:A:24:IDS:O6A	1:A:25:SGN:H62	1.78	0.84
1:A:5:SGN:O3	1:A:6:IDS:O6B	1.96	0.83
1:A:1:SGN:O4S	1:A:2:IDS:S	2.36	0.83
1:A:19:SGN:H5	1:A:20:IDS:O2S	1.78	0.83
1:A:27:SGN:H62	1:A:28:IDS:O1S	1.75	0.83
1:A:25:SGN:H61	1:A:26:IDS:S	2.18	0.83
1:A:17:SGN:H61	1:A:18:IDS:C1	2.07	0.83
1:A:20:IDS:H3	1:A:21:SGN:N2	1.94	0.83
1:A:11:SGN:H61	1:A:12:IDS:O2S	1.79	0.83
1:A:15:SGN:O4S	1:A:16:IDS:O2	1.96	0.83
1:A:23:SGN:O3	1:A:24:IDS:C6	2.27	0.83
1:A:13:SGN:C6	1:A:14:IDS:O2S	2.25	0.83
1:A:28:IDS:O3	1:A:29:SGN:N2	2.11	0.83
1:A:10:IDS:O3	1:A:11:SGN:O1S	1.96	0.82
1:A:22:IDS:O6A	1:A:24:IDS:O2S	1.95	0.82
1:A:29:SGN:O3	1:A:30:IDS:H5	1.79	0.82
1:A:29:SGN:HO3	1:A:30:IDS:C6	1.91	0.82
1:A:12:IDS:H3	1:A:13:SGN:S1	2.20	0.82
1:A:25:SGN:H62	1:A:26:IDS:S	2.19	0.82
1:A:10:IDS:O3	1:A:11:SGN:S1	2.37	0.82
1:A:26:IDS:O6B	1:A:27:SGN:H5	1.80	0.81
1:A:14:IDS:H3	1:A:15:SGN:N2	1.95	0.81
1:A:5:SGN:O3	1:A:6:IDS:C6	2.29	0.81
1:A:19:SGN:H61	1:A:20:IDS:O1S	1.80	0.81
1:A:24:IDS:O3	1:A:25:SGN:S1	2.38	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:SGN:H61	1:A:26:IDS:C1	2.11	0.81
1:A:19:SGN:O5S	1:A:20:IDS:O5	1.99	0.81
1:A:1:SGN:O5S	1:A:2:IDS:O5	1.98	0.81
1:A:10:IDS:O2	1:A:11:SGN:O3S	1.99	0.81
1:A:25:SGN:H61	1:A:26:IDS:O2S	1.81	0.81
1:A:8:IDS:O3	1:A:9:SGN:O1S	1.98	0.81
1:A:23:SGN:O3	1:A:24:IDS:H5	1.81	0.80
1:A:15:SGN:O3	1:A:16:IDS:C6	2.29	0.80
1:A:22:IDS:O3	1:A:23:SGN:S1	2.39	0.80
1:A:23:SGN:H61	1:A:24:IDS:C1	2.11	0.80
1:A:27:SGN:O3	1:A:28:IDS:C6	2.30	0.80
1:A:15:SGN:S2	1:A:16:IDS:O5	2.39	0.80
1:A:24:IDS:H3	1:A:25:SGN:N2	1.97	0.80
1:A:24:IDS:O3	1:A:25:SGN:N2	2.14	0.80
1:A:3:SGN:H5	1:A:4:IDS:O2S	1.80	0.80
1:A:1:SGN:H61	1:A:2:IDS:C1	2.11	0.79
1:A:12:IDS:O3S	1:A:13:SGN:O3S	1.99	0.79
1:A:19:SGN:H61	1:A:20:IDS:C1	2.11	0.79
1:A:25:SGN:H5	1:A:26:IDS:O2S	1.82	0.79
1:A:4:IDS:H3	1:A:5:SGN:S1	2.21	0.79
1:A:23:SGN:H61	1:A:24:IDS:C1	2.13	0.79
1:A:21:SGN:H61	1:A:22:IDS:C1	2.13	0.79
1:A:23:SGN:H5	1:A:24:IDS:S	2.23	0.79
1:A:24:IDS:O3	1:A:25:SGN:N2	2.16	0.79
1:A:9:SGN:H61	1:A:10:IDS:C1	2.11	0.79
1:A:24:IDS:O2	1:A:25:SGN:O3S	2.01	0.79
1:A:15:SGN:H61	1:A:16:IDS:O5	1.83	0.79
1:A:27:SGN:O3	1:A:28:IDS:C6	2.30	0.79
1:A:29:SGN:HO3	1:A:30:IDS:C5	1.96	0.78
1:A:29:SGN:H61	1:A:30:IDS:O3S	1.80	0.78
1:A:22:IDS:O6A	1:A:24:IDS:O3S	2.01	0.78
1:A:23:SGN:O3	1:A:24:IDS:C5	2.31	0.78
1:A:14:IDS:O3	1:A:15:SGN:O3S	2.01	0.78
1:A:27:SGN:H61	1:A:28:IDS:C1	2.14	0.78
1:A:10:IDS:H3	1:A:11:SGN:S1	2.23	0.78
1:A:21:SGN:O3	1:A:22:IDS:O6B	2.02	0.78
1:A:7:SGN:O3	1:A:8:IDS:C6	2.31	0.78
1:A:23:SGN:O3	1:A:24:IDS:O6B	2.00	0.78
1:A:15:SGN:H61	1:A:16:IDS:O2S	1.83	0.78
1:A:18:IDS:H3	1:A:19:SGN:S1	2.24	0.78
1:A:26:IDS:H3	1:A:27:SGN:N2	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:IDS:O6A	1:A:17:SGN:C5	2.32	0.77
1:A:10:IDS:H3	1:A:11:SGN:N2	1.98	0.77
1:A:12:IDS:O6A	1:A:13:SGN:H62	1.84	0.77
1:A:5:SGN:C6	1:A:6:IDS:O2S	2.33	0.77
1:A:9:SGN:O5S	1:A:10:IDS:O6B	2.03	0.77
1:A:22:IDS:H3	1:A:23:SGN:S1	2.25	0.76
1:A:10:IDS:C3	1:A:11:SGN:S1	2.73	0.76
1:A:15:SGN:O4S	1:A:16:IDS:O2S	2.02	0.76
1:A:13:SGN:HO3	1:A:14:IDS:C5	1.87	0.76
1:A:8:IDS:C3	1:A:9:SGN:O1S	2.33	0.76
1:A:5:SGN:H61	1:A:6:IDS:C1	2.16	0.76
1:A:10:IDS:O3	1:A:11:SGN:S1	2.44	0.76
1:A:23:SGN:O6	1:A:24:IDS:O5	2.04	0.76
1:A:8:IDS:O6A	1:A:9:SGN:C5	2.34	0.76
1:A:17:SGN:S2	1:A:18:IDS:O2S	2.43	0.76
1:A:23:SGN:S2	1:A:24:IDS:C1	2.75	0.75
1:A:4:IDS:O2	1:A:5:SGN:O3S	2.04	0.75
1:A:24:IDS:O6A	1:A:25:SGN:C6	2.34	0.75
1:A:14:IDS:O3	1:A:15:SGN:N2	2.19	0.75
1:A:15:SGN:O3	1:A:16:IDS:C5	2.34	0.75
1:A:20:IDS:O3	1:A:21:SGN:O3S	2.03	0.75
1:A:13:SGN:S2	1:A:14:IDS:O2	2.44	0.75
1:A:16:IDS:O6A	1:A:17:SGN:C6	2.34	0.75
1:A:19:SGN:C5	1:A:20:IDS:O2S	2.34	0.75
1:A:24:IDS:C6	1:A:25:SGN:H5	2.14	0.74
1:A:23:SGN:O3	1:A:24:IDS:H5	1.86	0.74
1:A:27:SGN:O3	1:A:28:IDS:C5	2.35	0.74
1:A:14:IDS:O3S	1:A:15:SGN:O3S	2.04	0.74
1:A:25:SGN:S2	1:A:26:IDS:C1	2.75	0.74
1:A:16:IDS:H3	1:A:17:SGN:N2	2.02	0.74
1:A:28:IDS:O3	1:A:29:SGN:N2	2.21	0.74
1:A:9:SGN:S2	1:A:10:IDS:O6B	2.46	0.74
1:A:22:IDS:O6A	1:A:23:SGN:C6	2.36	0.73
1:A:27:SGN:O6S	1:A:28:IDS:O1S	2.07	0.73
1:A:14:IDS:O2	1:A:15:SGN:O3S	2.06	0.73
1:A:20:IDS:O3	1:A:21:SGN:N2	2.21	0.73
1:A:7:SGN:O3	1:A:8:IDS:C5	2.36	0.73
1:A:5:SGN:O4S	1:A:6:IDS:O1S	2.06	0.73
1:A:22:IDS:O6A	1:A:23:SGN:C5	2.36	0.73
1:A:24:IDS:C6	1:A:25:SGN:H5	2.17	0.73
1:A:7:SGN:H61	1:A:8:IDS:C1	2.19	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:SGN:S2	1:A:20:IDS:O6B	2.46	0.73
1:A:13:SGN:O4S	1:A:14:IDS:O1S	2.07	0.73
1:A:25:SGN:H61	1:A:26:IDS:C1	2.19	0.73
1:A:14:IDS:H3	1:A:15:SGN:S1	2.30	0.72
1:A:16:IDS:C3	1:A:17:SGN:O1S	2.23	0.72
1:A:26:IDS:O6A	1:A:27:SGN:H5	1.88	0.72
1:A:29:SGN:O5S	1:A:30:IDS:O6B	2.06	0.72
1:A:22:IDS:H3	1:A:23:SGN:N2	2.04	0.72
1:A:28:IDS:O3	1:A:29:SGN:O3S	2.06	0.72
1:A:12:IDS:O3S	1:A:13:SGN:O3S	2.07	0.72
1:A:17:SGN:H61	1:A:18:IDS:C1	2.20	0.72
1:A:2:IDS:H3	1:A:3:SGN:N2	2.05	0.72
1:A:4:IDS:C6	1:A:5:SGN:H5	2.19	0.72
1:A:8:IDS:O6A	1:A:9:SGN:H5	1.90	0.72
1:A:15:SGN:O5S	1:A:16:IDS:O6A	2.05	0.72
1:A:8:IDS:C6	1:A:9:SGN:H5	2.19	0.72
1:A:1:SGN:O5S	1:A:2:IDS:C1	2.38	0.72
1:A:6:IDS:C3	1:A:7:SGN:S1	2.78	0.72
1:A:5:SGN:H61	1:A:6:IDS:C1	2.20	0.72
1:A:5:SGN:O3	1:A:6:IDS:C5	2.36	0.72
1:A:26:IDS:C6	1:A:27:SGN:C5	2.68	0.71
1:A:20:IDS:O3	1:A:21:SGN:O1S	2.07	0.71
1:A:2:IDS:H3	1:A:3:SGN:O1S	1.90	0.71
1:A:12:IDS:H3	1:A:13:SGN:C2	2.09	0.71
1:A:23:SGN:HO3	1:A:24:IDS:C5	1.89	0.71
1:A:23:SGN:H61	1:A:24:IDS:O2S	1.89	0.71
1:A:24:IDS:O3	1:A:25:SGN:N2	2.24	0.71
1:A:26:IDS:O6A	1:A:27:SGN:C6	2.38	0.71
1:A:8:IDS:O6A	1:A:9:SGN:C6	2.39	0.71
1:A:23:SGN:O3	1:A:24:IDS:O6B	2.09	0.71
1:A:20:IDS:C3	1:A:21:SGN:N2	2.54	0.71
1:A:5:SGN:H61	1:A:6:IDS:C1	2.19	0.71
1:A:17:SGN:O3	1:A:18:IDS:C6	2.39	0.71
1:A:17:SGN:O4S	1:A:18:IDS:O5	2.08	0.70
1:A:6:IDS:H3	1:A:7:SGN:O1S	1.92	0.70
1:A:11:SGN:O4S	1:A:12:IDS:C1	2.39	0.70
1:A:14:IDS:O6A	1:A:15:SGN:H5	1.90	0.70
1:A:25:SGN:H61	1:A:26:IDS:O5	1.90	0.70
1:A:18:IDS:H3	1:A:19:SGN:S1	2.31	0.70
1:A:24:IDS:C3	1:A:25:SGN:N2	2.44	0.70
1:A:29:SGN:O6	1:A:30:IDS:O5	2.08	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:SGN:O3	1:A:26:IDS:C5	2.39	0.70
1:A:10:IDS:O6A	1:A:11:SGN:C6	2.40	0.69
1:A:25:SGN:H61	1:A:26:IDS:S	2.31	0.69
1:A:7:SGN:H61	1:A:8:IDS:S	2.32	0.69
1:A:8:IDS:O6A	1:A:9:SGN:H62	1.92	0.69
1:A:3:SGN:O4S	1:A:4:IDS:C1	2.41	0.69
1:A:11:SGN:O3	1:A:12:IDS:H5	1.92	0.69
1:A:26:IDS:O6A	1:A:27:SGN:O5	2.10	0.69
1:A:9:SGN:C4	1:A:10:IDS:O2S	2.40	0.69
1:A:4:IDS:O6A	1:A:5:SGN:C6	2.40	0.69
1:A:19:SGN:HO3	1:A:20:IDS:H5	1.58	0.69
1:A:9:SGN:H61	1:A:10:IDS:O3S	1.93	0.69
1:A:6:IDS:H3	1:A:7:SGN:S1	2.31	0.69
1:A:18:IDS:O3	1:A:19:SGN:O1S	2.10	0.69
1:A:6:IDS:O6A	1:A:7:SGN:C6	2.38	0.69
1:A:15:SGN:H61	1:A:16:IDS:C1	2.23	0.69
1:A:9:SGN:O4S	1:A:10:IDS:C5	2.41	0.68
1:A:11:SGN:H61	1:A:12:IDS:C1	2.23	0.68
1:A:22:IDS:O6A	1:A:23:SGN:H5	1.93	0.68
1:A:11:SGN:S2	1:A:12:IDS:O5	2.52	0.68
1:A:17:SGN:O3	1:A:18:IDS:C5	2.41	0.68
1:A:24:IDS:O3	1:A:25:SGN:N2	2.26	0.68
1:A:7:SGN:O3	1:A:8:IDS:H5	1.94	0.68
1:A:29:SGN:O5S	1:A:30:IDS:C5	2.42	0.67
1:A:6:IDS:O3	1:A:7:SGN:N2	2.26	0.67
1:A:8:IDS:H3	1:A:9:SGN:S1	2.34	0.67
1:A:29:SGN:O6	1:A:30:IDS:C1	2.42	0.67
1:A:29:SGN:S2	1:A:30:IDS:O5	2.52	0.67
1:A:22:IDS:C6	1:A:23:SGN:H5	2.25	0.67
1:A:29:SGN:O5S	1:A:30:IDS:O5	2.13	0.67
1:A:14:IDS:H3	1:A:15:SGN:N2	2.08	0.67
1:A:9:SGN:C5	1:A:10:IDS:O2S	2.42	0.67
1:A:23:SGN:O5S	1:A:24:IDS:C4	2.43	0.67
1:A:25:SGN:O4S	1:A:26:IDS:C1	2.43	0.66
1:A:21:SGN:O4S	1:A:22:IDS:S	2.52	0.66
1:A:12:IDS:C3	1:A:13:SGN:S1	2.83	0.66
1:A:16:IDS:C2	1:A:17:SGN:O1S	2.43	0.66
1:A:17:SGN:H5	1:A:18:IDS:O2S	1.96	0.66
1:A:11:SGN:H61	1:A:12:IDS:C1	2.25	0.66
1:A:12:IDS:H4	1:A:13:SGN:O1S	1.94	0.66
1:A:26:IDS:O6A	1:A:27:SGN:C6	2.42	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:IDS:H3	1:A:29:SGN:N2	2.11	0.66
1:A:21:SGN:O4S	1:A:22:IDS:S	2.54	0.66
1:A:7:SGN:O3	1:A:8:IDS:C5	2.44	0.66
1:A:6:IDS:C6	1:A:7:SGN:C5	2.74	0.66
1:A:1:SGN:S2	1:A:2:IDS:C1	2.84	0.66
1:A:22:IDS:H3	1:A:23:SGN:N2	2.10	0.66
1:A:9:SGN:O4S	1:A:10:IDS:C6	2.44	0.66
1:A:9:SGN:O5S	1:A:10:IDS:O6B	2.13	0.66
1:A:19:SGN:S2	1:A:20:IDS:O1S	2.54	0.66
1:A:11:SGN:O4S	1:A:12:IDS:O2S	2.09	0.65
1:A:15:SGN:O3	1:A:16:IDS:C6	2.43	0.65
1:A:24:IDS:O3	1:A:25:SGN:S1	2.53	0.65
1:A:27:SGN:H62	1:A:28:IDS:S	2.27	0.65
1:A:18:IDS:C3	1:A:19:SGN:S1	2.85	0.65
1:A:25:SGN:H5	1:A:26:IDS:O2S	1.95	0.65
1:A:14:IDS:O2	1:A:15:SGN:S1	2.49	0.65
1:A:6:IDS:H3	1:A:7:SGN:C2	2.18	0.65
1:A:1:SGN:H61	1:A:2:IDS:O2	1.96	0.65
1:A:18:IDS:O2	1:A:19:SGN:O3S	2.14	0.65
1:A:6:IDS:O2	1:A:7:SGN:O3S	2.15	0.65
1:A:10:IDS:O3	1:A:11:SGN:N2	2.29	0.65
1:A:19:SGN:H61	1:A:20:IDS:S	2.36	0.65
1:A:11:SGN:O5S	1:A:12:IDS:O5	2.15	0.65
1:A:18:IDS:O3	1:A:19:SGN:O1S	2.09	0.65
1:A:13:SGN:S2	1:A:14:IDS:C1	2.85	0.64
1:A:5:SGN:O3	1:A:6:IDS:C6	2.45	0.64
1:A:17:SGN:O4S	1:A:18:IDS:C1	2.45	0.64
1:A:29:SGN:O6S	1:A:30:IDS:O6B	2.15	0.64
1:A:23:SGN:O6	1:A:24:IDS:C1	2.45	0.64
1:A:27:SGN:O3	1:A:28:IDS:H5	1.98	0.64
1:A:8:IDS:H3	1:A:9:SGN:O1S	1.97	0.64
1:A:26:IDS:O6A	1:A:27:SGN:H62	1.97	0.64
1:A:12:IDS:O2	1:A:13:SGN:O3S	2.16	0.64
1:A:7:SGN:O3	1:A:8:IDS:O6B	2.14	0.64
1:A:5:SGN:O3	1:A:6:IDS:H5	1.95	0.64
1:A:17:SGN:O6	1:A:18:IDS:O2S	2.16	0.63
1:A:13:SGN:O5S	1:A:14:IDS:C1	2.46	0.63
1:A:10:IDS:H3	1:A:11:SGN:N2	2.12	0.63
1:A:22:IDS:O6A	1:A:24:IDS:S	2.57	0.63
1:A:23:SGN:O5S	1:A:24:IDS:C1	2.46	0.63
1:A:5:SGN:O3	1:A:6:IDS:O5	2.15	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:SGN:O6	1:A:12:IDS:C1	2.47	0.63
1:A:9:SGN:O4S	1:A:10:IDS:S	2.55	0.63
1:A:7:SGN:H61	1:A:8:IDS:C1	2.28	0.63
1:A:22:IDS:H3	1:A:23:SGN:N2	2.14	0.62
1:A:23:SGN:S2	1:A:24:IDS:C1	2.87	0.62
1:A:6:IDS:O6B	1:A:7:SGN:H5	1.99	0.62
1:A:12:IDS:C3	1:A:13:SGN:S1	2.81	0.62
1:A:22:IDS:C3	1:A:23:SGN:O1S	2.46	0.62
1:A:9:SGN:H61	1:A:10:IDS:C1	2.29	0.62
1:A:16:IDS:O6A	1:A:17:SGN:O5	2.16	0.62
1:A:24:IDS:O6A	1:A:25:SGN:H62	2.00	0.62
1:A:15:SGN:H61	1:A:16:IDS:C1	2.30	0.62
1:A:20:IDS:H3	1:A:21:SGN:N2	2.14	0.62
1:A:15:SGN:S2	1:A:16:IDS:O2S	2.57	0.62
1:A:24:IDS:C3	1:A:25:SGN:S1	2.88	0.62
1:A:2:IDS:H3	1:A:3:SGN:S1	2.39	0.62
1:A:28:IDS:O3	1:A:29:SGN:S1	2.57	0.62
1:A:12:IDS:C3	1:A:13:SGN:O3S	2.47	0.62
1:A:1:SGN:O6	1:A:2:IDS:C1	2.48	0.62
1:A:8:IDS:H3	1:A:9:SGN:S1	2.39	0.62
1:A:14:IDS:O3	1:A:15:SGN:S1	2.57	0.61
1:A:15:SGN:S2	1:A:16:IDS:C6	2.87	0.61
1:A:21:SGN:O3	1:A:22:IDS:O5	2.17	0.61
1:A:12:IDS:O3	1:A:13:SGN:O1S	2.16	0.61
1:A:19:SGN:C5	1:A:20:IDS:O2S	2.48	0.61
1:A:17:SGN:O4S	1:A:18:IDS:O2	2.18	0.61
1:A:15:SGN:O3	1:A:16:IDS:O5	2.17	0.61
1:A:1:SGN:O6	1:A:2:IDS:C1	2.49	0.61
1:A:4:IDS:C6	1:A:5:SGN:C5	2.78	0.61
1:A:15:SGN:HO3	1:A:16:IDS:C5	2.13	0.61
1:A:4:IDS:H3	1:A:5:SGN:C2	2.02	0.61
1:A:22:IDS:O6A	1:A:23:SGN:H5	2.01	0.61
1:A:3:SGN:O6	1:A:4:IDS:C1	2.49	0.60
1:A:21:SGN:O4S	1:A:22:IDS:O1S	2.18	0.60
1:A:9:SGN:H5	1:A:10:IDS:O2S	2.00	0.60
1:A:10:IDS:O3	1:A:11:SGN:O1S	2.17	0.60
1:A:14:IDS:O6A	1:A:15:SGN:O5	2.20	0.60
1:A:9:SGN:S2	1:A:10:IDS:O6B	2.59	0.60
1:A:13:SGN:O6	1:A:14:IDS:O5	2.20	0.60
1:A:12:IDS:O3	1:A:13:SGN:O3S	2.14	0.60
1:A:15:SGN:O6	1:A:16:IDS:O2S	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:SGN:O3	1:A:6:IDS:C5	2.50	0.59
1:A:18:IDS:H3	1:A:19:SGN:O1S	2.02	0.59
1:A:3:SGN:O4S	1:A:4:IDS:O5	2.20	0.59
1:A:24:IDS:H3	1:A:25:SGN:N2	2.17	0.59
1:A:26:IDS:O3	1:A:27:SGN:O1S	2.10	0.59
1:A:12:IDS:O6B	1:A:13:SGN:H5	2.03	0.59
1:A:4:IDS:O6A	1:A:5:SGN:C5	2.51	0.59
1:A:3:SGN:O6	1:A:4:IDS:O5	2.21	0.59
1:A:9:SGN:C4	1:A:10:IDS:O2S	2.50	0.58
1:A:24:IDS:C3	1:A:25:SGN:N2	2.59	0.58
1:A:12:IDS:O6B	1:A:13:SGN:H5	2.03	0.58
1:A:20:IDS:H3	1:A:21:SGN:O3S	2.02	0.58
1:A:10:IDS:O3	1:A:11:SGN:O1S	2.21	0.58
1:A:18:IDS:O6B	1:A:20:IDS:O1S	2.21	0.58
1:A:2:IDS:C3	1:A:3:SGN:N2	2.66	0.58
1:A:17:SGN:HO3	1:A:18:IDS:C5	2.15	0.58
1:A:25:SGN:S2	1:A:26:IDS:O6B	2.60	0.58
1:A:29:SGN:H61	1:A:30:IDS:C1	2.34	0.58
1:A:27:SGN:C6	1:A:28:IDS:O5	2.51	0.58
1:A:23:SGN:H61	1:A:24:IDS:O5	2.04	0.58
1:A:12:IDS:H3	1:A:13:SGN:S1	2.44	0.58
1:A:7:SGN:O3	1:A:8:IDS:O5	2.22	0.57
1:A:3:SGN:O6	1:A:4:IDS:C1	2.52	0.57
1:A:6:IDS:H3	1:A:7:SGN:O1S	2.05	0.57
1:A:20:IDS:C3	1:A:21:SGN:S1	2.76	0.57
1:A:12:IDS:H3	1:A:13:SGN:N2	2.19	0.57
1:A:9:SGN:C5	1:A:10:IDS:O2S	2.50	0.57
1:A:6:IDS:C3	1:A:7:SGN:O1S	2.44	0.57
1:A:23:SGN:HO3	1:A:24:IDS:C5	2.13	0.57
1:A:24:IDS:O6B	1:A:26:IDS:O1S	2.23	0.57
1:A:10:IDS:O3	1:A:11:SGN:S1	2.50	0.57
1:A:14:IDS:S	1:A:15:SGN:O3S	2.63	0.57
1:A:6:IDS:C3	1:A:7:SGN:S1	2.88	0.57
1:A:27:SGN:C6	1:A:28:IDS:C1	2.82	0.57
1:A:9:SGN:S2	1:A:10:IDS:C1	2.93	0.57
1:A:21:SGN:O6	1:A:22:IDS:C1	2.53	0.57
1:A:22:IDS:O6A	1:A:23:SGN:C6	2.53	0.56
1:A:12:IDS:C4	1:A:13:SGN:O1S	2.46	0.56
1:A:15:SGN:O3	1:A:16:IDS:O6B	2.20	0.56
1:A:1:SGN:O1S	1:A:1:SGN:H1	2.05	0.56
1:A:3:SGN:O5S	1:A:4:IDS:O5	2.22	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SGN:C6	1:A:10:IDS:S	2.83	0.56
1:A:25:SGN:C5	1:A:26:IDS:O2S	2.54	0.56
1:A:17:SGN:HO3	1:A:18:IDS:C6	2.18	0.56
1:A:27:SGN:O3	1:A:28:IDS:O5	2.24	0.56
1:A:6:IDS:O3S	1:A:7:SGN:O3S	2.24	0.56
1:A:11:SGN:O3	1:A:12:IDS:O5	2.20	0.56
1:A:29:SGN:C1	1:A:29:SGN:O1S	2.53	0.56
1:A:23:SGN:O3	1:A:24:IDS:O6B	2.07	0.56
1:A:13:SGN:O5S	1:A:14:IDS:C2	2.52	0.56
1:A:9:SGN:O1S	1:A:9:SGN:C1	2.53	0.56
1:A:23:SGN:O5S	1:A:24:IDS:O4	2.24	0.56
1:A:13:SGN:O4S	1:A:14:IDS:S	2.63	0.56
1:A:24:IDS:O3S	1:A:25:SGN:O3S	2.24	0.56
1:A:6:IDS:O6A	1:A:7:SGN:C5	2.54	0.56
1:A:1:SGN:O1S	1:A:1:SGN:H1	2.06	0.55
1:A:6:IDS:S	1:A:7:SGN:O3S	2.65	0.55
1:A:5:SGN:O6	1:A:6:IDS:O5	2.25	0.55
1:A:15:SGN:O5S	1:A:16:IDS:O5	2.23	0.55
1:A:6:IDS:O3	1:A:7:SGN:O3S	2.16	0.55
1:A:29:SGN:C6	1:A:30:IDS:C1	2.85	0.55
1:A:15:SGN:C6	1:A:16:IDS:C1	2.84	0.55
1:A:24:IDS:O6A	1:A:25:SGN:H5	2.06	0.55
1:A:23:SGN:H5	1:A:24:IDS:O2S	2.07	0.55
1:A:10:IDS:C6	1:A:11:SGN:H5	2.20	0.55
1:A:20:IDS:H3	1:A:21:SGN:N2	2.20	0.55
1:A:12:IDS:O3	1:A:13:SGN:O3S	2.22	0.55
1:A:25:SGN:H61	1:A:26:IDS:S	2.46	0.55
1:A:6:IDS:O3	1:A:7:SGN:N2	2.39	0.55
1:A:13:SGN:O6	1:A:14:IDS:S	2.65	0.55
1:A:1:SGN:S2	1:A:2:IDS:C1	2.94	0.55
1:A:6:IDS:C3	1:A:7:SGN:O1S	2.54	0.55
1:A:13:SGN:O1S	1:A:13:SGN:C1	2.55	0.55
1:A:19:SGN:O5S	1:A:20:IDS:O4	2.25	0.55
1:A:1:SGN:H61	1:A:2:IDS:C1	2.37	0.55
1:A:25:SGN:O4S	1:A:26:IDS:S	2.65	0.55
1:A:3:SGN:O6	1:A:4:IDS:C1	2.54	0.55
1:A:14:IDS:O6A	1:A:15:SGN:H5	2.07	0.54
1:A:11:SGN:H61	1:A:12:IDS:O2S	2.08	0.54
1:A:15:SGN:S2	1:A:16:IDS:O2S	2.65	0.54
1:A:17:SGN:O4S	1:A:18:IDS:O2S	2.26	0.54
1:A:21:SGN:O4S	1:A:22:IDS:H3	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:IDS:C3	1:A:9:SGN:O1S	2.55	0.54
1:A:19:SGN:O3	1:A:20:IDS:O5	2.23	0.54
1:A:17:SGN:H61	1:A:18:IDS:C1	2.38	0.54
1:A:7:SGN:O3	1:A:8:IDS:C6	2.56	0.54
1:A:21:SGN:H61	1:A:22:IDS:O2S	2.08	0.54
1:A:24:IDS:C3	1:A:25:SGN:O3S	2.50	0.54
1:A:29:SGN:S2	1:A:30:IDS:O5	2.66	0.54
1:A:10:IDS:O6A	1:A:11:SGN:C5	2.47	0.53
1:A:21:SGN:O4	1:A:22:IDS:O2S	2.26	0.53
1:A:12:IDS:C6	1:A:13:SGN:H5	2.38	0.53
1:A:25:SGN:C6	1:A:26:IDS:C1	2.86	0.53
1:A:15:SGN:C6	1:A:16:IDS:O2S	2.56	0.53
1:A:20:IDS:O3	1:A:21:SGN:S1	2.66	0.53
1:A:29:SGN:O5S	1:A:30:IDS:O5	2.27	0.53
1:A:9:SGN:O4	1:A:10:IDS:O2S	2.26	0.53
1:A:7:SGN:C6	1:A:8:IDS:O2S	2.47	0.53
1:A:17:SGN:O4S	1:A:18:IDS:S	2.66	0.53
1:A:12:IDS:C6	1:A:13:SGN:H5	2.33	0.53
1:A:17:SGN:C6	1:A:18:IDS:C1	2.86	0.53
1:A:9:SGN:H4	1:A:10:IDS:O2S	2.07	0.53
1:A:13:SGN:H61	1:A:14:IDS:C1	2.39	0.53
1:A:9:SGN:O4S	1:A:10:IDS:O6B	2.27	0.53
1:A:3:SGN:O4S	1:A:4:IDS:C1	2.57	0.53
1:A:6:IDS:H3	1:A:7:SGN:O1S	2.09	0.53
1:A:6:IDS:H3	1:A:7:SGN:S1	2.49	0.53
1:A:8:IDS:H3	1:A:9:SGN:O1S	2.09	0.52
1:A:21:SGN:C6	1:A:22:IDS:C1	2.87	0.52
1:A:2:IDS:O2	1:A:3:SGN:O3S	2.28	0.52
1:A:28:IDS:C3	1:A:29:SGN:N2	2.73	0.52
1:A:20:IDS:C3	1:A:21:SGN:O1S	2.57	0.52
1:A:11:SGN:C6	1:A:12:IDS:C1	2.88	0.52
1:A:15:SGN:S2	1:A:16:IDS:O6B	2.67	0.52
1:A:29:SGN:O6	1:A:30:IDS:C1	2.58	0.52
1:A:1:SGN:O5S	1:A:2:IDS:O5	2.27	0.52
1:A:4:IDS:O3	1:A:5:SGN:O3S	2.24	0.52
1:A:23:SGN:O3	1:A:24:IDS:O5	2.27	0.52
1:A:2:IDS:C3	1:A:3:SGN:O1S	2.57	0.52
1:A:4:IDS:C3	1:A:5:SGN:N2	2.63	0.52
1:A:15:SGN:C6	1:A:16:IDS:O5	2.57	0.52
1:A:6:IDS:H3	1:A:7:SGN:S1	2.50	0.52
1:A:23:SGN:O3	1:A:24:IDS:O5	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:SGN:C6	1:A:20:IDS:C1	2.87	0.52
1:A:27:SGN:O3	1:A:28:IDS:O6B	2.28	0.52
1:A:20:IDS:C3	1:A:21:SGN:S1	2.98	0.52
1:A:9:SGN:O4	1:A:10:IDS:O2S	2.27	0.52
1:A:21:SGN:O4S	1:A:22:IDS:C1	2.58	0.51
1:A:25:SGN:H61	1:A:26:IDS:O2S	2.11	0.51
1:A:7:SGN:O4S	1:A:8:IDS:O1S	2.29	0.51
1:A:20:IDS:C3	1:A:21:SGN:N2	2.73	0.51
1:A:17:SGN:H61	1:A:18:IDS:C1	2.40	0.51
1:A:9:SGN:C5	1:A:10:IDS:O2S	2.57	0.51
1:A:21:SGN:H61	1:A:22:IDS:O2S	2.10	0.51
1:A:7:SGN:C6	1:A:8:IDS:C1	2.87	0.51
1:A:5:SGN:O4	1:A:6:IDS:O2S	2.29	0.51
1:A:23:SGN:H61	1:A:24:IDS:C1	2.40	0.51
1:A:20:IDS:H3	1:A:21:SGN:N2	2.26	0.51
1:A:2:IDS:C3	1:A:3:SGN:N2	2.73	0.51
1:A:1:SGN:O4	1:A:2:IDS:O2S	2.29	0.51
1:A:21:SGN:O3	1:A:22:IDS:C6	2.59	0.51
1:A:15:SGN:O3	1:A:16:IDS:O5	2.29	0.51
1:A:19:SGN:C6	1:A:20:IDS:O1S	2.55	0.51
1:A:29:SGN:C6	1:A:30:IDS:C1	2.88	0.51
1:A:22:IDS:C3	1:A:23:SGN:N2	2.74	0.51
1:A:11:SGN:H61	1:A:12:IDS:O5	2.11	0.51
1:A:19:SGN:H62	1:A:20:IDS:O2S	2.02	0.51
1:A:5:SGN:O3	1:A:6:IDS:O6B	2.28	0.50
1:A:6:IDS:C3	1:A:7:SGN:O1S	2.59	0.50
1:A:17:SGN:H61	1:A:18:IDS:C1	2.42	0.50
1:A:17:SGN:O4	1:A:18:IDS:O2S	2.29	0.50
1:A:15:SGN:H61	1:A:16:IDS:S	2.50	0.50
1:A:18:IDS:H3	1:A:19:SGN:O3S	2.11	0.50
1:A:16:IDS:O6A	1:A:17:SGN:O5	2.27	0.50
1:A:20:IDS:H3	1:A:21:SGN:S1	2.51	0.50
1:A:24:IDS:C3	1:A:25:SGN:S1	2.93	0.50
1:A:20:IDS:H3	1:A:21:SGN:S1	2.51	0.50
1:A:23:SGN:C6	1:A:24:IDS:C1	2.90	0.50
1:A:1:SGN:O3	1:A:2:IDS:O6B	2.30	0.50
1:A:15:SGN:O4S	1:A:16:IDS:O5	2.29	0.50
1:A:10:IDS:O3	1:A:11:SGN:O3S	2.29	0.50
1:A:23:SGN:C6	1:A:24:IDS:C1	2.83	0.50
1:A:4:IDS:C3	1:A:5:SGN:S1	2.89	0.50
1:A:25:SGN:H61	1:A:26:IDS:O2S	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SGN:C6	1:A:10:IDS:C1	2.90	0.50
1:A:14:IDS:H3	1:A:15:SGN:O1S	2.12	0.50
1:A:27:SGN:O3	1:A:28:IDS:H5	2.11	0.50
1:A:12:IDS:C3	1:A:13:SGN:S1	2.98	0.49
1:A:2:IDS:H3	1:A:3:SGN:N2	2.27	0.49
1:A:23:SGN:HO3	1:A:24:IDS:C6	2.23	0.49
1:A:5:SGN:O4S	1:A:6:IDS:O5	2.30	0.49
1:A:1:SGN:H61	1:A:2:IDS:O5	2.12	0.49
1:A:16:IDS:O6A	1:A:17:SGN:C6	2.61	0.49
1:A:15:SGN:O5S	1:A:16:IDS:O6B	2.27	0.49
1:A:25:SGN:H61	1:A:26:IDS:C1	2.43	0.49
1:A:21:SGN:H61	1:A:22:IDS:C1	2.43	0.49
1:A:3:SGN:H61	1:A:4:IDS:C1	2.43	0.49
1:A:11:SGN:O3	1:A:12:IDS:O6B	2.30	0.49
1:A:13:SGN:O3	1:A:14:IDS:O5	2.30	0.49
1:A:3:SGN:O3	1:A:4:IDS:O6B	2.31	0.49
1:A:4:IDS:O6A	1:A:5:SGN:H62	2.13	0.49
1:A:21:SGN:S2	1:A:22:IDS:C1	3.01	0.49
1:A:8:IDS:O3	1:A:9:SGN:O1S	2.26	0.49
1:A:21:SGN:O3	1:A:22:IDS:C5	2.61	0.49
1:A:15:SGN:O4S	1:A:16:IDS:C1	2.60	0.49
1:A:16:IDS:O3S	1:A:17:SGN:O3S	2.31	0.49
1:A:28:IDS:O6A	1:A:29:SGN:H5	2.13	0.48
1:A:15:SGN:H61	1:A:16:IDS:O2S	2.13	0.48
1:A:5:SGN:H61	1:A:6:IDS:C1	2.43	0.48
1:A:5:SGN:O4	1:A:6:IDS:O2S	2.31	0.48
1:A:14:IDS:C3	1:A:15:SGN:O1S	2.62	0.48
1:A:14:IDS:S	1:A:15:SGN:O3S	2.71	0.48
1:A:23:SGN:C6	1:A:24:IDS:C1	2.91	0.48
1:A:25:SGN:H5	1:A:26:IDS:O2S	2.13	0.48
1:A:27:SGN:H61	1:A:28:IDS:O2S	2.13	0.48
1:A:18:IDS:O6A	1:A:19:SGN:O5	2.28	0.48
1:A:27:SGN:H61	1:A:28:IDS:S	2.54	0.48
1:A:11:SGN:O1S	1:A:11:SGN:C1	2.61	0.48
1:A:12:IDS:C3	1:A:13:SGN:O3S	2.62	0.48
1:A:13:SGN:O4S	1:A:14:IDS:O1S	2.32	0.48
1:A:21:SGN:O6	1:A:22:IDS:C1	2.61	0.48
1:A:20:IDS:O3	1:A:21:SGN:N2	2.46	0.48
1:A:3:SGN:O6	1:A:4:IDS:O5	2.31	0.48
1:A:21:SGN:O3	1:A:22:IDS:C6	2.62	0.48
1:A:25:SGN:H61	1:A:26:IDS:O2S	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:IDS:O3	1:A:17:SGN:S1	2.68	0.48
1:A:22:IDS:C3	1:A:23:SGN:S1	2.98	0.48
1:A:14:IDS:O3S	1:A:15:SGN:O3S	2.32	0.48
1:A:2:IDS:O3	1:A:3:SGN:S1	2.68	0.48
1:A:18:IDS:H3	1:A:19:SGN:N2	2.29	0.47
1:A:24:IDS:C3	1:A:25:SGN:N2	2.76	0.47
1:A:1:SGN:S2	1:A:2:IDS:C1	3.02	0.47
1:A:9:SGN:S2	1:A:10:IDS:O5	2.72	0.47
1:A:4:IDS:O6A	1:A:5:SGN:O5	2.33	0.47
1:A:5:SGN:O5S	1:A:6:IDS:O5	2.31	0.47
1:A:3:SGN:O3	1:A:4:IDS:O5	2.29	0.47
1:A:3:SGN:O4S	1:A:4:IDS:O5	2.32	0.47
1:A:29:SGN:O6	1:A:30:IDS:C1	2.59	0.47
1:A:3:SGN:O3	1:A:4:IDS:C6	2.63	0.47
1:A:3:SGN:S2	1:A:4:IDS:C5	3.00	0.47
1:A:25:SGN:H61	1:A:26:IDS:O2	2.13	0.47
1:A:27:SGN:C4	1:A:28:IDS:O2S	2.60	0.47
1:A:20:IDS:O2	1:A:21:SGN:O3S	2.33	0.47
1:A:19:SGN:O3	1:A:20:IDS:C6	2.63	0.47
1:A:6:IDS:O3	1:A:7:SGN:N2	2.46	0.47
1:A:12:IDS:O6A	1:A:13:SGN:C5	2.63	0.47
1:A:27:SGN:O4S	1:A:28:IDS:O1S	2.33	0.47
1:A:25:SGN:H61	1:A:26:IDS:O2S	1.99	0.46
1:A:15:SGN:HO3	1:A:16:IDS:H5	1.76	0.46
1:A:22:IDS:O6A	1:A:23:SGN:C6	2.61	0.46
1:A:24:IDS:C3	1:A:25:SGN:N2	2.78	0.46
1:A:9:SGN:O4	1:A:10:IDS:O2S	2.34	0.46
1:A:17:SGN:C6	1:A:18:IDS:C1	2.89	0.46
1:A:16:IDS:O6A	1:A:17:SGN:C1	2.64	0.46
1:A:20:IDS:H3	1:A:21:SGN:N2	2.31	0.46
1:A:6:IDS:S	1:A:7:SGN:O3S	2.73	0.46
1:A:10:IDS:O3	1:A:11:SGN:S1	2.65	0.46
1:A:23:SGN:C6	1:A:24:IDS:C1	2.94	0.46
1:A:3:SGN:C5	1:A:4:IDS:O2S	2.59	0.46
1:A:7:SGN:HO3	1:A:8:IDS:C6	2.28	0.46
1:A:15:SGN:O4S	1:A:16:IDS:C1	2.64	0.46
1:A:11:SGN:O5S	1:A:12:IDS:O6B	2.34	0.46
1:A:25:SGN:O6	1:A:26:IDS:O5	2.34	0.45
1:A:24:IDS:C3	1:A:25:SGN:O3S	2.63	0.45
1:A:11:SGN:H61	1:A:12:IDS:C1	2.46	0.45
1:A:26:IDS:O6A	1:A:27:SGN:C5	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:IDS:C3	1:A:5:SGN:O1S	2.63	0.45
1:A:7:SGN:O3	1:A:8:IDS:C5	2.64	0.45
1:A:13:SGN:O6	1:A:14:IDS:C1	2.65	0.45
1:A:27:SGN:O4	1:A:28:IDS:O2S	2.35	0.45
1:A:3:SGN:O5S	1:A:4:IDS:O5	2.35	0.45
1:A:9:SGN:O1S	1:A:9:SGN:C1	2.65	0.45
1:A:3:SGN:C6	1:A:4:IDS:C1	2.95	0.45
1:A:20:IDS:O3	1:A:21:SGN:S1	2.55	0.45
1:A:3:SGN:H61	1:A:4:IDS:O2	2.17	0.45
1:A:25:SGN:C6	1:A:26:IDS:C1	2.87	0.45
1:A:27:SGN:HO3	1:A:28:IDS:C6	2.29	0.45
1:A:3:SGN:S2	1:A:4:IDS:C1	3.05	0.45
1:A:12:IDS:O2	1:A:13:SGN:O3S	2.34	0.45
1:A:4:IDS:O6B	1:A:5:SGN:H5	2.17	0.45
1:A:1:SGN:H61	1:A:2:IDS:C1	2.47	0.45
1:A:13:SGN:O3	1:A:14:IDS:O5	2.35	0.44
1:A:18:IDS:O3	1:A:19:SGN:O1S	2.34	0.44
1:A:21:SGN:H5	1:A:22:IDS:O2S	2.18	0.44
1:A:13:SGN:C6	1:A:14:IDS:C1	2.95	0.44
1:A:9:SGN:O4S	1:A:10:IDS:O2S	2.35	0.44
1:A:25:SGN:O4	1:A:26:IDS:O2S	2.35	0.44
1:A:15:SGN:O3	1:A:16:IDS:O6B	2.35	0.44
1:A:3:SGN:O3	1:A:4:IDS:C5	2.66	0.44
1:A:14:IDS:O6A	1:A:15:SGN:H5	2.18	0.44
1:A:27:SGN:H61	1:A:28:IDS:C1	2.48	0.44
1:A:27:SGN:O3	1:A:28:IDS:C5	2.65	0.44
1:A:12:IDS:C2	1:A:13:SGN:O3S	2.66	0.44
1:A:21:SGN:O6	1:A:22:IDS:C1	2.66	0.44
1:A:21:SGN:H61	1:A:22:IDS:C1	2.48	0.44
1:A:13:SGN:O3	1:A:14:IDS:C5	2.66	0.44
1:A:21:SGN:O3	1:A:22:IDS:C5	2.65	0.44
1:A:1:SGN:S2	1:A:2:IDS:O5	2.76	0.44
1:A:20:IDS:O3	1:A:21:SGN:S1	2.74	0.44
1:A:2:IDS:H4	1:A:3:SGN:O1S	2.18	0.44
1:A:18:IDS:H3	1:A:19:SGN:C2	2.38	0.43
1:A:27:SGN:S2	1:A:28:IDS:O5	2.75	0.43
1:A:4:IDS:H3	1:A:5:SGN:N2	2.33	0.43
1:A:6:IDS:C3	1:A:7:SGN:O3S	2.66	0.43
1:A:29:SGN:H5	1:A:30:IDS:O2S	2.18	0.43
1:A:19:SGN:O3	1:A:20:IDS:C5	2.66	0.43
1:A:13:SGN:O4S	1:A:14:IDS:O2	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:SGN:C6	1:A:4:IDS:C1	2.96	0.43
1:A:20:IDS:O6B	1:A:21:SGN:H5	2.18	0.43
1:A:13:SGN:O4	1:A:14:IDS:O2S	2.33	0.43
1:A:16:IDS:O6A	1:A:17:SGN:H62	2.15	0.43
1:A:28:IDS:O3	1:A:29:SGN:N2	2.51	0.43
1:A:3:SGN:H61	1:A:4:IDS:C1	2.48	0.43
1:A:25:SGN:O3	1:A:26:IDS:C6	2.66	0.43
1:A:3:SGN:C6	1:A:4:IDS:C1	2.97	0.43
1:A:13:SGN:O4S	1:A:14:IDS:S	2.76	0.43
1:A:13:SGN:O3	1:A:14:IDS:C6	2.67	0.43
1:A:15:SGN:C6	1:A:16:IDS:C1	2.97	0.43
1:A:17:SGN:O3	1:A:18:IDS:O6B	2.37	0.42
1:A:22:IDS:O6A	1:A:23:SGN:H62	2.18	0.42
1:A:21:SGN:HO3	1:A:22:IDS:C5	2.32	0.42
1:A:21:SGN:C6	1:A:22:IDS:C1	2.87	0.42
1:A:23:SGN:O1S	1:A:23:SGN:C1	2.66	0.42
1:A:26:IDS:C3	1:A:27:SGN:N2	2.83	0.42
1:A:4:IDS:H3	1:A:5:SGN:S1	2.53	0.42
1:A:27:SGN:O4S	1:A:28:IDS:O5	2.38	0.42
1:A:21:SGN:C6	1:A:22:IDS:O2S	2.66	0.42
1:A:29:SGN:S2	1:A:30:IDS:C6	2.98	0.42
1:A:3:SGN:O3	1:A:4:IDS:H5	2.19	0.42
1:A:18:IDS:H3	1:A:19:SGN:N2	2.34	0.42
1:A:19:SGN:O5S	1:A:20:IDS:C4	2.63	0.42
1:A:23:SGN:O3	1:A:24:IDS:O5	2.38	0.42
1:A:14:IDS:O3S	1:A:15:SGN:O3S	2.37	0.42
1:A:12:IDS:C6	1:A:13:SGN:H5	2.49	0.42
1:A:28:IDS:C3	1:A:29:SGN:O1S	2.62	0.42
1:A:14:IDS:O3	1:A:15:SGN:O1S	2.29	0.42
1:A:19:SGN:C6	1:A:20:IDS:C1	2.98	0.42
1:A:7:SGN:O3	1:A:8:IDS:H5	2.20	0.42
1:A:27:SGN:H61	1:A:28:IDS:O2S	2.19	0.42
1:A:10:IDS:C2	1:A:11:SGN:O1S	2.61	0.42
1:A:18:IDS:O6A	1:A:20:IDS:O2S	2.38	0.42
1:A:11:SGN:H61	1:A:12:IDS:C1	2.50	0.42
1:A:1:SGN:O5S	1:A:2:IDS:C1	2.68	0.42
1:A:12:IDS:O6A	1:A:13:SGN:O5	2.36	0.42
1:A:29:SGN:O3	1:A:30:IDS:O5	2.29	0.41
1:A:18:IDS:C3	1:A:19:SGN:S1	3.01	0.41
1:A:17:SGN:O3	1:A:18:IDS:H5	2.20	0.41
1:A:3:SGN:O3	1:A:4:IDS:C5	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SGN:C6	1:A:10:IDS:O5	2.51	0.41
1:A:12:IDS:O6A	1:A:13:SGN:C1	2.67	0.41
1:A:15:SGN:O4S	1:A:16:IDS:C1	2.67	0.41
1:A:8:IDS:O3	1:A:9:SGN:N2	2.53	0.41
1:A:20:IDS:O3	1:A:21:SGN:O1S	2.30	0.41
1:A:21:SGN:HO3	1:A:22:IDS:C6	2.34	0.41
1:A:25:SGN:C6	1:A:26:IDS:O2S	2.69	0.41
1:A:12:IDS:O6A	1:A:13:SGN:H5	2.19	0.41
1:A:1:SGN:C6	1:A:2:IDS:C1	2.99	0.41
1:A:25:SGN:O4	1:A:26:IDS:O2S	2.37	0.41
1:A:6:IDS:C6	1:A:7:SGN:H5	2.51	0.41
1:A:27:SGN:H61	1:A:28:IDS:O1S	2.21	0.41
1:A:17:SGN:O4S	1:A:19:SGN:O3S	2.39	0.41
1:A:16:IDS:C6	1:A:17:SGN:H5	2.51	0.41
1:A:20:IDS:H3	1:A:21:SGN:N2	2.36	0.41
1:A:10:IDS:C2	1:A:11:SGN:O1S	2.62	0.40
1:A:21:SGN:C6	1:A:22:IDS:C1	2.99	0.40
1:A:12:IDS:C6	1:A:13:SGN:C5	2.99	0.40
1:A:28:IDS:O6A	1:A:29:SGN:H5	2.22	0.40
1:A:19:SGN:HO3	1:A:20:IDS:C6	2.27	0.40
1:A:25:SGN:O1S	1:A:25:SGN:C1	2.69	0.40
1:A:7:SGN:O4	1:A:8:IDS:O2S	2.40	0.40
1:A:21:SGN:O4	1:A:22:IDS:O2S	2.40	0.40
1:A:15:SGN:H61	1:A:16:IDS:C1	2.52	0.40

There are no symmetry-related clashes.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

4.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

420 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	1-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	1-A	10	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	1-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	12	1	16,16,17	1.39	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	1-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	1-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	16	1	16,16,17	1.39	3 (18%)	17,24,26	2.28	3 (17%)
1	SGN	1-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	18	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	1-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	2	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	1-A	20	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	1-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	22	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	1-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	26	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	1-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	28	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	1-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	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	15,15,17	1.51	3 (20%)	15,22,26	2.45	3 (20%)
1	IDS	1-A	4	1	16,16,17	1.43	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	1-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	1-A	6	1	16,16,17	1.40	3 (18%)	17,24,26	2.24	3 (17%)
1	SGN	1-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	1-A	8	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	1-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	1 (4%)
1	SGN	10-A	1	1	19,20,20	1.07	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	10-A	10	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	10-A	11	1	18,19,20	1.24	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	10-A	12	1	16,16,17	1.37	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	10-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.41	3 (18%)	17,24,26	2.28	3 (17%)
1	SGN	10-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	18	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	10-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	2	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	10-A	20	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	10-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	10-A	22	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	10-A	25	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	26	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	10-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	1 (4%)
1	SGN	10-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	10-A	30	1	15,15,17	1.54	3 (20%)	15,22,26	2.46	3 (20%)
1	IDS	10-A	4	1	16,16,17	1.42	2 (12%)	17,24,26	2.25	3 (17%)
1	SGN	10-A	5	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	6	1	16,16,17	1.39	3 (18%)	17,24,26	2.25	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	10-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	10-A	8	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	10-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	11-A	1	1	19,20,20	1.10	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	11-A	10	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
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	16,16,17	1.39	3 (18%)	17,24,26	2.28	3 (17%)
1	SGN	11-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	14	1	16,16,17	1.44	3 (18%)	17,24,26	2.25	3 (17%)
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	16,16,17	1.40	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	11-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	11-A	18	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	11-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	11-A	2	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	11-A	20	1	16,16,17	1.40	3 (18%)	17,24,26	2.24	3 (17%)
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	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	11-A	23	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	24	1	16,16,17	1.41	2 (12%)	17,24,26	2.26	3 (17%)
1	SGN	11-A	25	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	11-A	26	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	11-A	27	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	28	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	11-A	29	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	11-A	3	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	30	1	15,15,17	1.51	3 (20%)	15,22,26	2.45	3 (20%)
1	IDS	11-A	4	1	16,16,17	1.42	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	11-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	6	1	16,16,17	1.41	3 (18%)	17,24,26	2.24	3 (17%)
1	SGN	11-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	11-A	8	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
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	0.98	1 (4%)
1	IDS	12-A	10	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	16,16,17	1.38	3 (18%)	17,24,26	2.28	3 (17%)
1	SGN	12-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	12-A	15	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	12-A	16	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	12-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	12-A	18	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	12-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	2	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	12-A	20	1	16,16,17	1.43	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	12-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	12-A	26	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.42	3 (18%)	17,24,26	2.27	3 (17%)
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	1.07	1 (4%)
1	IDS	12-A	30	1	15,15,17	1.50	3 (20%)	15,22,26	2.46	3 (20%)
1	IDS	12-A	4	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	12-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	6	1	16,16,17	1.39	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	12-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	12-A	8	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	12-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	13-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	13-A	10	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	13-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	12	1	16,16,17	1.37	3 (18%)	17,24,26	2.28	3 (17%)
1	SGN	13-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	14	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	13-A	15	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	16	1	16,16,17	1.40	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	13-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	18	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	13-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	13-A	2	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	13-A	20	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	13-A	23	1	18,19,20	1.26	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	13-A	24	1	16,16,17	1.42	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	13-A	25	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	26	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	13-A	27	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	28	1	16,16,17	1.43	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	13-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	13-A	3	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	30	1	15,15,17	1.52	3 (20%)	15,22,26	2.46	3 (20%)
1	IDS	13-A	4	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	13-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	13-A	6	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	13-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	13-A	8	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	13-A	9	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	14-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	14-A	10	1	16,16,17	1.42	3 (18%)	17,24,26	2.24	3 (17%)
1	SGN	14-A	11	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	12	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	14-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	14-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	16	1	16,16,17	1.41	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	14-A	17	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	18	1	16,16,17	1.40	3 (18%)	17,24,26	2.24	3 (17%)
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	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	14-A	20	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	14-A	21	1	18,19,20	1.21	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	22	1	16,16,17	1.41	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	14-A	23	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	24	1	16,16,17	1.41	2 (12%)	17,24,26	2.25	3 (17%)
1	SGN	14-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	26	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
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	16,16,17	1.42	3 (18%)	17,24,26	2.27	3 (17%)
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	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	30	1	15,15,17	1.53	3 (20%)	15,22,26	2.45	3 (20%)
1	IDS	14-A	4	1	16,16,17	1.41	2 (12%)	17,24,26	2.26	3 (17%)
1	SGN	14-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	14-A	6	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	14-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	14-A	8	1	16,16,17	1.41	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	14-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	2-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	2-A	10	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	2-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	12	1	16,16,17	1.38	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	2-A	13	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.24	3 (17%)
1	SGN	2-A	15	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	16	1	16,16,17	1.40	3 (18%)	17,24,26	2.27	3 (17%)
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	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
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	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	2-A	20	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	2-A	21	1	18,19,20	1.21	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	2-A	22	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	2-A	25	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	26	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	2-A	27	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	28	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	2-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	1 (4%)
1	SGN	2-A	3	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	2-A	30	1	15,15,17	1.52	3 (20%)	15,22,26	2.45	3 (20%)
1	IDS	2-A	4	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	2-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	2-A	6	1	16,16,17	1.39	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	2-A	7	1	18,19,20	1.24	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	2-A	8	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	2-A	9	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	3-A	1	1	19,20,20	1.10	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	3-A	10	1	16,16,17	1.41	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	3-A	11	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	12	1	16,16,17	1.38	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	3-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	3-A	17	1	18,19,20	1.24	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	3-A	18	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	3-A	19	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	2	1	16,16,17	1.38	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	3-A	20	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	3-A	21	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	22	1	16,16,17	1.40	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	3-A	23	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	24	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	3-A	25	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	26	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	3-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	28	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	3-A	29	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	SGN	3-A	3	1	18,19,20	1.21	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	3-A	30	1	15,15,17	1.51	3 (20%)	15,22,26	2.45	3 (20%)
1	IDS	3-A	4	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	3-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	3-A	6	1	16,16,17	1.38	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	3-A	7	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	3-A	8	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	3-A	9	1	18,19,20	1.23	2 (11%)	22,29,31	1.10	1 (4%)
1	SGN	4-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	4-A	10	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	4-A	11	1	18,19,20	1.24	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	4-A	12	1	16,16,17	1.39	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	4-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	4-A	15	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	16	1	16,16,17	1.38	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	4-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	18	1	16,16,17	1.40	3 (18%)	17,24,26	2.24	3 (17%)
1	SGN	4-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	2	1	16,16,17	1.38	3 (18%)	17,24,26	2.25	3 (17%)
1	IDS	4-A	20	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	4-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	22	1	16,16,17	1.38	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	4-A	23	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	24	1	16,16,17	1.40	2 (12%)	17,24,26	2.26	3 (17%)
1	SGN	4-A	25	1	18,19,20	1.21	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	4-A	26	1	16,16,17	1.40	3 (18%)	17,24,26	2.28	3 (17%)
1	SGN	4-A	27	1	18,19,20	1.26	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	28	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	4-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	15,15,17	1.53	3 (20%)	15,22,26	2.45	3 (20%)
1	IDS	4-A	4	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	4-A	5	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	6	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	4-A	7	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	4-A	8	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	4-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	5-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	5-A	10	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	5-A	11	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	5-A	12	1	16,16,17	1.38	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	5-A	13	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	5-A	15	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	16	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	5-A	17	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	18	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	5-A	19	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	2	1	16,16,17	1.42	3 (18%)	17,24,26	2.27	3 (17%)
1	IDS	5-A	20	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	5-A	21	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	22	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	5-A	25	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	26	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	5-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	28	1	16,16,17	1.42	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	5-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	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	15,15,17	1.52	3 (20%)	15,22,26	2.47	3 (20%)
1	IDS	5-A	4	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	5-A	5	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	6	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	5-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	5-A	8	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	5-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	1 (4%)
1	SGN	6-A	1	1	19,20,20	1.09	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	6-A	10	1	16,16,17	1.39	3 (18%)	17,24,26	2.25	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	6-A	11	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	6-A	12	1	16,16,17	1.38	3 (18%)	17,24,26	2.28	3 (17%)
1	SGN	6-A	13	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	6-A	15	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	16	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	6-A	17	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	18	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	6-A	19	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	2	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	6-A	20	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	6-A	21	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	22	1	16,16,17	1.38	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	6-A	23	1	18,19,20	1.25	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	24	1	16,16,17	1.40	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	6-A	25	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	26	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	6-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	6-A	28	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	6-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	6-A	3	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	30	1	15,15,17	1.51	3 (20%)	15,22,26	2.45	3 (20%)
1	IDS	6-A	4	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	6-A	5	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	6	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	6-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	6-A	8	1	16,16,17	1.41	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	6-A	9	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	7-A	1	1	19,20,20	1.10	1 (5%)	24,31,31	0.97	1 (4%)
1	IDS	7-A	10	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	7-A	11	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	7-A	12	1	16,16,17	1.39	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	7-A	13	1	18,19,20	1.21	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	7-A	14	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	7-A	15	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	7-A	16	1	16,16,17	1.39	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	7-A	17	1	18,19,20	1.26	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	7-A	18	1	16,16,17	1.40	3 (18%)	17,24,26	2.24	3 (17%)
1	SGN	7-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	2	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	7-A	20	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	7-A	21	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	22	1	16,16,17	1.38	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	7-A	23	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	24	1	16,16,17	1.41	2 (12%)	17,24,26	2.25	3 (17%)
1	SGN	7-A	25	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	26	1	16,16,17	1.40	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	7-A	27	1	18,19,20	1.22	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	7-A	28	1	16,16,17	1.43	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	7-A	29	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	7-A	3	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	30	1	15,15,17	1.53	3 (20%)	15,22,26	2.46	3 (20%)
1	IDS	7-A	4	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	7-A	5	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	6	1	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	7-A	7	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	7-A	8	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	7-A	9	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	8-A	1	1	19,20,20	1.08	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	8-A	10	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	8-A	11	1	18,19,20	1.25	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	8-A	12	1	16,16,17	1.39	3 (18%)	17,24,26	2.27	3 (17%)
1	SGN	8-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.25	3 (17%)
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	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	8-A	17	1	18,19,20	1.26	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	18	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	8-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	2	1	16,16,17	1.40	3 (18%)	17,24,26	2.27	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	IDS	8-A	20	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	8-A	21	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	22	1	16,16,17	1.39	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	8-A	23	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	24	1	16,16,17	1.42	2 (12%)	17,24,26	2.25	3 (17%)
1	SGN	8-A	25	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	8-A	26	1	16,16,17	1.42	3 (18%)	17,24,26	2.27	3 (17%)
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	16,16,17	1.40	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	8-A	29	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	8-A	3	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	30	1	15,15,17	1.50	3 (20%)	15,22,26	2.47	3 (20%)
1	IDS	8-A	4	1	16,16,17	1.41	2 (12%)	17,24,26	2.26	3 (17%)
1	SGN	8-A	5	1	18,19,20	1.20	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	8-A	6	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	8-A	7	1	18,19,20	1.24	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	8-A	8	1	16,16,17	1.43	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	8-A	9	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	SGN	9-A	1	1	19,20,20	1.08	1 (5%)	24,31,31	0.98	1 (4%)
1	IDS	9-A	10	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
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	16,16,17	1.40	3 (18%)	17,24,26	2.29	3 (17%)
1	SGN	9-A	13	1	18,19,20	1.23	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	9-A	14	1	16,16,17	1.42	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	9-A	15	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	16	1	16,16,17	1.39	3 (18%)	17,24,26	2.27	3 (17%)
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	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	9-A	19	1	18,19,20	1.23	2 (11%)	22,29,31	1.07	1 (4%)
1	IDS	9-A	2	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	IDS	9-A	20	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	9-A	21	1	18,19,20	1.24	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	22	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	9-A	23	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	24	1	16,16,17	1.40	3 (18%)	17,24,26	2.25	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SGN	9-A	25	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	26	1	16,16,17	1.41	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	9-A	27	1	18,19,20	1.23	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	28	1	16,16,17	1.41	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	9-A	29	1	18,19,20	1.21	2 (11%)	22,29,31	1.08	1 (4%)
1	SGN	9-A	3	1	18,19,20	1.22	2 (11%)	22,29,31	1.09	1 (4%)
1	IDS	9-A	30	1	15,15,17	1.51	3 (20%)	15,22,26	2.46	3 (20%)
1	IDS	9-A	4	1	16,16,17	1.43	2 (12%)	17,24,26	2.27	3 (17%)
1	SGN	9-A	5	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	6	1	16,16,17	1.39	3 (18%)	17,24,26	2.26	3 (17%)
1	SGN	9-A	7	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)
1	IDS	9-A	8	1	16,16,17	1.42	3 (18%)	17,24,26	2.25	3 (17%)
1	SGN	9-A	9	1	18,19,20	1.22	2 (11%)	22,29,31	1.08	1 (4%)

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

All (1027) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-A	4	IDS	O2-C2	-3.70	1.41	1.47
1	9-A	4	IDS	O2-C2	-3.70	1.41	1.47
1	11-A	14	IDS	O2-C2	-3.69	1.41	1.47
1	10-A	4	IDS	O2-C2	-3.69	1.41	1.47
1	13-A	24	IDS	O2-C2	-3.68	1.41	1.47
1	8-A	4	IDS	O2-C2	-3.68	1.41	1.47
1	5-A	4	IDS	O2-C2	-3.67	1.41	1.47
1	10-A	30	IDS	O2-C2	-3.66	1.41	1.47
1	8-A	24	IDS	O2-C2	-3.66	1.41	1.47
1	3-A	4	IDS	O2-C2	-3.66	1.41	1.47
1	8-A	14	IDS	O2-C2	-3.66	1.41	1.47
1	12-A	20	IDS	O2-C2	-3.66	1.41	1.47
1	3-A	14	IDS	O2-C2	-3.65	1.41	1.47
1	4-A	10	IDS	O2-C2	-3.65	1.41	1.47
1	5-A	24	IDS	O2-C2	-3.65	1.41	1.47
1	1-A	4	IDS	O2-C2	-3.64	1.41	1.47
1	2-A	14	IDS	O2-C2	-3.64	1.41	1.47
1	11-A	4	IDS	O2-C2	-3.64	1.41	1.47
1	4-A	14	IDS	O2-C2	-3.64	1.41	1.47
1	5-A	14	IDS	O2-C2	-3.63	1.41	1.47
1	9-A	14	IDS	O2-C2	-3.63	1.41	1.47
1	10-A	14	IDS	O2-C2	-3.63	1.41	1.47
1	14-A	30	IDS	O2-C2	-3.63	1.41	1.47
1	9-A	10	IDS	O2-C2	-3.63	1.41	1.47
1	7-A	20	IDS	O2-C2	-3.63	1.41	1.47
1	14-A	28	IDS	O2-C2	-3.63	1.41	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	18	IDS	O2-C2	-3.63	1.41	1.47
1	4-A	20	IDS	O2-C2	-3.63	1.41	1.47
1	6-A	14	IDS	O2-C2	-3.63	1.41	1.47
1	14-A	4	IDS	O2-C2	-3.62	1.41	1.47
1	1-A	18	IDS	O2-C2	-3.62	1.41	1.47
1	12-A	14	IDS	O2-C2	-3.62	1.41	1.47
1	14-A	24	IDS	O2-C2	-3.62	1.41	1.47
1	2-A	10	IDS	O2-C2	-3.62	1.41	1.47
1	14-A	14	IDS	O2-C2	-3.62	1.41	1.47
1	13-A	20	IDS	O2-C2	-3.61	1.41	1.47
1	7-A	14	IDS	O2-C2	-3.61	1.41	1.47
1	2-A	20	IDS	O2-C2	-3.61	1.41	1.47
1	8-A	6	IDS	O2-C2	-3.61	1.41	1.47
1	3-A	10	IDS	O2-C2	-3.61	1.41	1.47
1	14-A	20	IDS	O2-C2	-3.61	1.41	1.47
1	5-A	10	IDS	O2-C2	-3.61	1.41	1.47
1	1-A	14	IDS	O2-C2	-3.61	1.41	1.47
1	4-A	24	IDS	O2-C2	-3.60	1.41	1.47
1	5-A	30	IDS	O2-C2	-3.60	1.41	1.47
1	7-A	30	IDS	O2-C2	-3.60	1.41	1.47
1	4-A	12	IDS	O2-C2	-3.60	1.41	1.47
1	11-A	24	IDS	O2-C2	-3.60	1.41	1.47
1	13-A	14	IDS	O2-C2	-3.60	1.41	1.47
1	9-A	20	IDS	O2-C2	-3.60	1.41	1.47
1	3-A	24	IDS	O2-C2	-3.60	1.41	1.47
1	13-A	8	IDS	O2-C2	-3.60	1.41	1.47
1	4-A	30	IDS	O2-C2	-3.60	1.41	1.47
1	6-A	24	IDS	O2-C2	-3.59	1.41	1.47
1	6-A	4	IDS	O2-C2	-3.59	1.41	1.47
1	12-A	24	IDS	O2-C2	-3.59	1.41	1.47
1	3-A	20	IDS	O2-C2	-3.59	1.41	1.47
1	11-A	30	IDS	O2-C2	-3.59	1.41	1.47
1	7-A	4	IDS	O2-C2	-3.59	1.41	1.47
1	8-A	8	IDS	O2-C2	-3.59	1.41	1.47
1	11-A	18	IDS	O2-C2	-3.59	1.41	1.47
1	1-A	30	IDS	O2-C2	-3.59	1.41	1.47
1	6-A	20	IDS	O2-C2	-3.59	1.41	1.47
1	2-A	30	IDS	O2-C2	-3.59	1.41	1.47
1	7-A	24	IDS	O2-C2	-3.59	1.41	1.47
1	11-A	8	IDS	O2-C2	-3.59	1.41	1.47
1	12-A	4	IDS	O2-C2	-3.58	1.41	1.47
1	4-A	4	IDS	O2-C2	-3.58	1.41	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	28	IDS	O2-C2	-3.58	1.41	1.47
1	11-A	2	IDS	O2-C2	-3.58	1.41	1.47
1	1-A	28	IDS	O2-C2	-3.58	1.41	1.47
1	2-A	28	IDS	O2-C2	-3.58	1.41	1.47
1	13-A	28	IDS	O2-C2	-3.58	1.41	1.47
1	1-A	24	IDS	O2-C2	-3.58	1.41	1.47
1	5-A	28	IDS	O2-C2	-3.58	1.41	1.47
1	5-A	22	IDS	O2-C2	-3.58	1.41	1.47
1	9-A	22	IDS	O2-C2	-3.58	1.41	1.47
1	5-A	20	IDS	O2-C2	-3.58	1.41	1.47
1	2-A	24	IDS	O2-C2	-3.58	1.41	1.47
1	3-A	30	IDS	O2-C2	-3.57	1.41	1.47
1	14-A	10	IDS	O2-C2	-3.57	1.41	1.47
1	9-A	18	IDS	O2-C2	-3.57	1.41	1.47
1	10-A	28	IDS	O2-C2	-3.57	1.41	1.47
1	12-A	30	IDS	O2-C2	-3.57	1.41	1.47
1	12-A	10	IDS	O2-C2	-3.57	1.41	1.47
1	14-A	22	IDS	O2-C2	-3.57	1.41	1.47
1	6-A	30	IDS	O2-C2	-3.57	1.41	1.47
1	12-A	28	IDS	O2-C2	-3.57	1.41	1.47
1	5-A	2	IDS	O2-C2	-3.57	1.41	1.47
1	8-A	20	IDS	O2-C2	-3.57	1.41	1.47
1	13-A	18	IDS	O2-C2	-3.57	1.41	1.47
1	13-A	30	IDS	O2-C2	-3.57	1.41	1.47
1	2-A	12	IDS	O2-C2	-3.57	1.41	1.47
1	1-A	20	IDS	O2-C2	-3.57	1.41	1.47
1	13-A	4	IDS	O2-C2	-3.57	1.41	1.47
1	3-A	22	IDS	O2-C2	-3.56	1.41	1.47
1	10-A	18	IDS	O2-C2	-3.56	1.41	1.47
1	13-A	26	IDS	O2-C2	-3.56	1.41	1.47
1	5-A	18	IDS	O2-C2	-3.56	1.41	1.47
1	14-A	12	IDS	O2-C2	-3.56	1.41	1.47
1	11-A	28	IDS	O2-C2	-3.56	1.41	1.47
1	10-A	16	IDS	O2-C2	-3.56	1.41	1.47
1	9-A	28	IDS	O2-C2	-3.56	1.41	1.47
1	6-A	18	IDS	O2-C2	-3.55	1.41	1.47
1	11-A	6	IDS	O2-C2	-3.55	1.41	1.47
1	10-A	10	IDS	O2-C2	-3.55	1.41	1.47
1	3-A	18	IDS	O2-C2	-3.55	1.41	1.47
1	5-A	8	IDS	O2-C2	-3.55	1.41	1.47
1	10-A	26	IDS	O2-C2	-3.55	1.41	1.47
1	7-A	8	IDS	O2-C2	-3.55	1.41	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	22	IDS	O2-C2	-3.55	1.41	1.47
1	6-A	12	IDS	O2-C2	-3.55	1.41	1.47
1	10-A	24	IDS	O2-C2	-3.55	1.41	1.47
1	7-A	26	IDS	O2-C2	-3.55	1.41	1.47
1	9-A	12	IDS	O2-C2	-3.55	1.41	1.47
1	8-A	30	IDS	O2-C2	-3.55	1.41	1.47
1	2-A	26	IDS	O2-C2	-3.55	1.41	1.47
1	1-A	8	IDS	O2-C2	-3.55	1.41	1.47
1	9-A	24	IDS	O2-C2	-3.55	1.41	1.47
1	9-A	2	IDS	O2-C2	-3.55	1.41	1.47
1	9-A	8	IDS	O2-C2	-3.54	1.41	1.47
1	11-A	12	IDS	O2-C2	-3.54	1.41	1.47
1	8-A	26	IDS	O2-C2	-3.54	1.41	1.47
1	5-A	6	IDS	O2-C2	-3.54	1.41	1.47
1	3-A	8	IDS	O2-C2	-3.54	1.41	1.47
1	14-A	26	IDS	O2-C2	-3.54	1.41	1.47
1	8-A	2	IDS	O2-C2	-3.54	1.41	1.47
1	5-A	26	IDS	O2-C2	-3.54	1.41	1.47
1	13-A	10	IDS	O2-C2	-3.54	1.41	1.47
1	10-A	22	IDS	O2-C2	-3.54	1.41	1.47
1	12-A	22	IDS	O2-C2	-3.53	1.41	1.47
1	1-A	26	IDS	O2-C2	-3.53	1.41	1.47
1	9-A	30	IDS	O2-C2	-3.53	1.41	1.47
1	6-A	28	IDS	O2-C2	-3.53	1.41	1.47
1	13-A	6	IDS	O2-C2	-3.53	1.41	1.47
1	10-A	8	IDS	O2-C2	-3.53	1.41	1.47
1	13-A	16	IDS	O2-C2	-3.53	1.41	1.47
1	7-A	10	IDS	O2-C2	-3.53	1.41	1.47
1	7-A	18	IDS	O2-C2	-3.53	1.41	1.47
1	13-A	22	IDS	O2-C2	-3.53	1.41	1.47
1	6-A	6	IDS	O2-C2	-3.53	1.41	1.47
1	12-A	12	IDS	O2-C2	-3.53	1.41	1.47
1	7-A	6	IDS	O2-C2	-3.53	1.41	1.47
1	6-A	10	IDS	O2-C2	-3.53	1.41	1.47
1	12-A	18	IDS	O2-C2	-3.53	1.41	1.47
1	14-A	16	IDS	O2-C2	-3.53	1.41	1.47
1	5-A	16	IDS	O2-C2	-3.53	1.41	1.47
1	12-A	26	IDS	O2-C2	-3.52	1.41	1.47
1	4-A	28	IDS	O2-C2	-3.52	1.41	1.47
1	2-A	18	IDS	O2-C2	-3.52	1.41	1.47
1	10-A	20	IDS	O2-C2	-3.52	1.41	1.47
1	3-A	26	IDS	O2-C2	-3.52	1.41	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	12	IDS	O2-C2	-3.52	1.41	1.47
1	6-A	26	IDS	O2-C2	-3.52	1.41	1.47
1	11-A	16	IDS	O2-C2	-3.52	1.41	1.47
1	4-A	18	IDS	O2-C2	-3.52	1.41	1.47
1	11-A	20	IDS	O2-C2	-3.52	1.41	1.47
1	9-A	26	IDS	O2-C2	-3.52	1.41	1.47
1	2-A	6	IDS	O2-C2	-3.52	1.41	1.47
1	14-A	6	IDS	O2-C2	-3.52	1.41	1.47
1	8-A	12	IDS	O2-C2	-3.52	1.41	1.47
1	4-A	26	IDS	O2-C2	-3.52	1.41	1.47
1	6-A	8	IDS	O2-C2	-3.52	1.41	1.47
1	4-A	27	SGN	S1-N2	3.52	1.64	1.59
1	11-A	10	IDS	O2-C2	-3.51	1.41	1.47
1	14-A	18	IDS	O2-C2	-3.51	1.41	1.47
1	14-A	8	IDS	O2-C2	-3.51	1.41	1.47
1	6-A	16	IDS	O2-C2	-3.51	1.41	1.47
1	3-A	28	IDS	O2-C2	-3.51	1.41	1.47
1	12-A	2	IDS	O2-C2	-3.51	1.41	1.47
1	8-A	10	IDS	O2-C2	-3.51	1.41	1.47
1	1-A	2	IDS	O2-C2	-3.51	1.41	1.47
1	1-A	6	IDS	O2-C2	-3.51	1.41	1.47
1	2-A	16	IDS	O2-C2	-3.51	1.41	1.47
1	1-A	10	IDS	O2-C2	-3.50	1.41	1.47
1	7-A	17	SGN	S1-N2	3.50	1.64	1.59
1	8-A	17	SGN	S1-N2	3.50	1.64	1.59
1	13-A	12	IDS	O2-C2	-3.50	1.41	1.47
1	3-A	12	IDS	O2-C2	-3.50	1.41	1.47
1	10-A	2	IDS	O2-C2	-3.50	1.41	1.47
1	9-A	6	IDS	O2-C2	-3.50	1.41	1.47
1	12-A	6	IDS	O2-C2	-3.50	1.41	1.47
1	11-A	22	IDS	O2-C2	-3.50	1.41	1.47
1	11-A	26	IDS	O2-C2	-3.50	1.41	1.47
1	12-A	8	IDS	O2-C2	-3.49	1.41	1.47
1	7-A	22	IDS	O2-C2	-3.49	1.41	1.47
1	6-A	2	IDS	O2-C2	-3.49	1.41	1.47
1	8-A	28	IDS	O2-C2	-3.49	1.41	1.47
1	7-A	16	IDS	O2-C2	-3.49	1.41	1.47
1	13-A	2	IDS	O2-C2	-3.49	1.41	1.47
1	9-A	16	IDS	O2-C2	-3.49	1.41	1.47
1	7-A	12	IDS	O2-C2	-3.48	1.41	1.47
1	2-A	15	SGN	S1-N2	3.48	1.64	1.59
1	4-A	6	IDS	O2-C2	-3.48	1.41	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	12-A	16	IDS	O2-C2	-3.48	1.41	1.47
1	6-A	22	IDS	O2-C2	-3.48	1.41	1.47
1	4-A	2	IDS	O2-C2	-3.48	1.41	1.47
1	4-A	22	IDS	O2-C2	-3.48	1.41	1.47
1	1-A	16	IDS	O2-C2	-3.48	1.41	1.47
1	4-A	8	IDS	O2-C2	-3.47	1.41	1.47
1	10-A	12	IDS	O2-C2	-3.47	1.41	1.47
1	10-A	6	IDS	O2-C2	-3.47	1.41	1.47
1	3-A	16	IDS	O2-C2	-3.47	1.41	1.47
1	2-A	8	IDS	O2-C2	-3.47	1.41	1.47
1	14-A	2	IDS	O2-C2	-3.47	1.41	1.47
1	2-A	2	IDS	O2-C2	-3.47	1.41	1.47
1	2-A	22	IDS	O2-C2	-3.47	1.41	1.47
1	8-A	16	IDS	O2-C2	-3.47	1.41	1.47
1	3-A	6	IDS	O2-C2	-3.47	1.41	1.47
1	7-A	2	IDS	O2-C2	-3.47	1.41	1.47
1	5-A	12	IDS	O2-C2	-3.47	1.41	1.47
1	8-A	22	IDS	O2-C2	-3.47	1.41	1.47
1	8-A	15	SGN	S1-N2	3.46	1.64	1.59
1	5-A	11	SGN	S1-N2	3.45	1.64	1.59
1	2-A	27	SGN	S1-N2	3.45	1.64	1.59
1	4-A	11	SGN	S1-N2	3.45	1.64	1.59
1	8-A	25	SGN	S1-N2	3.45	1.64	1.59
1	1-A	17	SGN	S1-N2	3.45	1.64	1.59
1	7-A	15	SGN	S1-N2	3.45	1.64	1.59
1	12-A	27	SGN	S1-N2	3.44	1.64	1.59
1	10-A	5	SGN	S1-N2	3.44	1.64	1.59
1	3-A	17	SGN	S1-N2	3.44	1.64	1.59
1	4-A	16	IDS	O2-C2	-3.43	1.42	1.47
1	3-A	2	IDS	O2-C2	-3.43	1.42	1.47
1	10-A	17	SGN	S1-N2	3.43	1.64	1.59
1	3-A	11	SGN	S1-N2	3.43	1.64	1.59
1	12-A	17	SGN	S1-N2	3.43	1.64	1.59
1	9-A	5	SGN	S1-N2	3.42	1.64	1.59
1	12-A	15	SGN	S1-N2	3.42	1.64	1.59
1	11-A	15	SGN	S1-N2	3.42	1.64	1.59
1	6-A	11	SGN	S1-N2	3.42	1.64	1.59
1	1-A	27	SGN	S1-N2	3.41	1.64	1.59
1	12-A	5	SGN	S1-N2	3.41	1.64	1.59
1	3-A	15	SGN	S1-N2	3.41	1.64	1.59
1	6-A	15	SGN	S1-N2	3.41	1.64	1.59
1	4-A	15	SGN	S1-N2	3.41	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	17	SGN	S1-N2	3.40	1.64	1.59
1	12-A	11	SGN	S1-N2	3.40	1.64	1.59
1	1-A	5	SGN	S1-N2	3.40	1.64	1.59
1	7-A	25	SGN	S1-N2	3.40	1.64	1.59
1	11-A	11	SGN	S1-N2	3.40	1.64	1.59
1	10-A	25	SGN	S1-N2	3.40	1.64	1.59
1	13-A	23	SGN	S1-N2	3.39	1.64	1.59
1	3-A	27	SGN	S1-N2	3.39	1.64	1.59
1	8-A	27	SGN	S1-N2	3.39	1.64	1.59
1	14-A	27	SGN	S1-N2	3.39	1.64	1.59
1	13-A	27	SGN	S1-N2	3.39	1.64	1.59
1	13-A	5	SGN	S1-N2	3.39	1.64	1.59
1	7-A	11	SGN	S1-N2	3.39	1.64	1.59
1	2-A	5	SGN	S1-N2	3.39	1.64	1.59
1	4-A	17	SGN	S1-N2	3.39	1.64	1.59
1	5-A	27	SGN	S1-N2	3.39	1.64	1.59
1	9-A	15	SGN	S1-N2	3.38	1.64	1.59
1	14-A	15	SGN	S1-N2	3.38	1.64	1.59
1	5-A	17	SGN	S1-N2	3.38	1.64	1.59
1	6-A	23	SGN	S1-N2	3.38	1.64	1.59
1	2-A	7	SGN	S1-N2	3.38	1.64	1.59
1	11-A	25	SGN	S1-N2	3.38	1.64	1.59
1	11-A	27	SGN	S1-N2	3.38	1.64	1.59
1	9-A	21	SGN	S1-N2	3.38	1.64	1.59
1	3-A	5	SGN	S1-N2	3.38	1.64	1.59
1	5-A	21	SGN	S1-N2	3.38	1.64	1.59
1	3-A	7	SGN	S1-N2	3.38	1.64	1.59
1	1-A	11	SGN	S1-N2	3.38	1.64	1.59
1	8-A	11	SGN	S1-N2	3.38	1.64	1.59
1	6-A	25	SGN	S1-N2	3.38	1.64	1.59
1	1-A	7	SGN	S1-N2	3.37	1.64	1.59
1	7-A	3	SGN	S1-N2	3.37	1.64	1.59
1	13-A	15	SGN	S1-N2	3.37	1.64	1.59
1	3-A	13	SGN	S1-N2	3.37	1.64	1.59
1	3-A	25	SGN	S1-N2	3.37	1.64	1.59
1	8-A	3	SGN	S1-N2	3.37	1.64	1.59
1	14-A	5	SGN	S1-N2	3.37	1.64	1.59
1	2-A	25	SGN	S1-N2	3.37	1.64	1.59
1	10-A	27	SGN	S1-N2	3.37	1.64	1.59
1	2-A	17	SGN	S1-N2	3.36	1.64	1.59
1	6-A	17	SGN	S1-N2	3.36	1.64	1.59
1	14-A	23	SGN	S1-N2	3.36	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	14-A	25	SGN	S1-N2	3.36	1.64	1.59
1	14-A	17	SGN	S1-N2	3.36	1.64	1.59
1	7-A	1	SGN	S1-N2	3.36	1.64	1.59
1	3-A	19	SGN	S1-N2	3.36	1.64	1.59
1	2-A	11	SGN	S1-N2	3.35	1.64	1.59
1	9-A	25	SGN	S1-N2	3.35	1.64	1.59
1	11-A	5	SGN	S1-N2	3.35	1.64	1.59
1	10-A	15	SGN	S1-N2	3.35	1.64	1.59
1	4-A	7	SGN	S1-N2	3.35	1.64	1.59
1	13-A	17	SGN	S1-N2	3.35	1.64	1.59
1	10-A	21	SGN	S1-N2	3.35	1.64	1.59
1	10-A	23	SGN	S1-N2	3.35	1.64	1.59
1	2-A	23	SGN	S1-N2	3.35	1.64	1.59
1	11-A	7	SGN	S1-N2	3.35	1.64	1.59
1	6-A	19	SGN	S1-N2	3.35	1.64	1.59
1	11-A	1	SGN	S1-N2	3.34	1.64	1.59
1	6-A	5	SGN	S1-N2	3.34	1.64	1.59
1	9-A	27	SGN	S1-N2	3.34	1.64	1.59
1	11-A	17	SGN	S1-N2	3.34	1.64	1.59
1	10-A	3	SGN	S1-N2	3.34	1.64	1.59
1	3-A	1	SGN	S1-N2	3.34	1.64	1.59
1	8-A	13	SGN	S1-N2	3.34	1.64	1.59
1	10-A	11	SGN	S1-N2	3.34	1.64	1.59
1	1-A	15	SGN	S1-N2	3.34	1.64	1.59
1	7-A	7	SGN	S1-N2	3.33	1.64	1.59
1	12-A	13	SGN	S1-N2	3.33	1.64	1.59
1	13-A	3	SGN	S1-N2	3.33	1.64	1.59
1	14-A	19	SGN	S1-N2	3.33	1.64	1.59
1	12-A	25	SGN	S1-N2	3.33	1.64	1.59
1	13-A	19	SGN	S1-N2	3.33	1.64	1.59
1	4-A	23	SGN	S1-N2	3.33	1.64	1.59
1	11-A	23	SGN	S1-N2	3.32	1.64	1.59
1	3-A	23	SGN	S1-N2	3.32	1.64	1.59
1	12-A	21	SGN	S1-N2	3.32	1.64	1.59
1	8-A	7	SGN	S1-N2	3.32	1.64	1.59
1	3-A	21	SGN	S1-N2	3.32	1.64	1.59
1	14-A	11	SGN	S1-N2	3.32	1.64	1.59
1	6-A	7	SGN	S1-N2	3.32	1.64	1.59
1	7-A	27	SGN	S1-N2	3.32	1.64	1.59
1	2-A	13	SGN	S1-N2	3.32	1.64	1.59
1	13-A	25	SGN	S1-N2	3.32	1.64	1.59
1	5-A	3	SGN	S1-N2	3.32	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	13	SGN	S1-N2	3.32	1.64	1.59
1	1-A	13	SGN	S1-N2	3.31	1.64	1.59
1	10-A	19	SGN	S1-N2	3.31	1.64	1.59
1	11-A	3	SGN	S1-N2	3.31	1.64	1.59
1	10-A	7	SGN	S1-N2	3.31	1.64	1.59
1	6-A	13	SGN	S1-N2	3.31	1.64	1.59
1	4-A	25	SGN	S1-N2	3.31	1.64	1.59
1	1-A	25	SGN	S1-N2	3.31	1.64	1.59
1	9-A	11	SGN	S1-N2	3.31	1.64	1.59
1	5-A	15	SGN	S1-N2	3.31	1.64	1.59
1	7-A	5	SGN	S1-N2	3.30	1.64	1.59
1	4-A	13	SGN	S1-N2	3.30	1.64	1.59
1	7-A	23	SGN	S1-N2	3.30	1.64	1.59
1	1-A	3	SGN	S1-N2	3.30	1.64	1.59
1	6-A	27	SGN	S1-N2	3.30	1.64	1.59
1	14-A	13	SGN	S1-N2	3.30	1.64	1.59
1	11-A	21	SGN	S1-N2	3.30	1.64	1.59
1	13-A	7	SGN	S1-N2	3.30	1.64	1.59
1	9-A	19	SGN	S1-N2	3.30	1.64	1.59
1	10-A	13	SGN	S1-N2	3.30	1.64	1.59
1	1-A	21	SGN	S1-N2	3.30	1.64	1.59
1	2-A	1	SGN	S1-N2	3.30	1.64	1.59
1	5-A	23	SGN	S1-N2	3.30	1.64	1.59
1	14-A	7	SGN	S1-N2	3.29	1.64	1.59
1	12-A	7	SGN	S1-N2	3.29	1.64	1.59
1	5-A	25	SGN	S1-N2	3.29	1.64	1.59
1	12-A	3	SGN	S1-N2	3.29	1.64	1.59
1	13-A	13	SGN	S1-N2	3.29	1.64	1.59
1	5-A	5	SGN	S1-N2	3.29	1.64	1.59
1	9-A	13	SGN	S1-N2	3.29	1.64	1.59
1	13-A	21	SGN	S1-N2	3.29	1.64	1.59
1	1-A	23	SGN	S1-N2	3.29	1.64	1.59
1	12-A	23	SGN	S1-N2	3.29	1.64	1.59
1	13-A	11	SGN	S1-N2	3.29	1.64	1.59
1	14-A	1	SGN	S1-N2	3.28	1.64	1.59
1	8-A	5	SGN	S1-N2	3.28	1.64	1.59
1	14-A	3	SGN	S1-N2	3.28	1.64	1.59
1	4-A	5	SGN	S1-N2	3.28	1.64	1.59
1	11-A	19	SGN	S1-N2	3.28	1.64	1.59
1	8-A	29	SGN	S1-N2	3.28	1.64	1.59
1	2-A	3	SGN	S1-N2	3.28	1.64	1.59
1	7-A	19	SGN	S1-N2	3.27	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	1	SGN	S1-N2	3.27	1.64	1.59
1	2-A	19	SGN	S1-N2	3.27	1.64	1.59
1	12-A	29	SGN	S1-N2	3.27	1.64	1.59
1	2-A	21	SGN	S1-N2	3.27	1.64	1.59
1	4-A	21	SGN	S1-N2	3.27	1.64	1.59
1	7-A	29	SGN	S1-N2	3.26	1.64	1.59
1	4-A	19	SGN	S1-N2	3.26	1.64	1.59
1	12-A	19	SGN	S1-N2	3.26	1.64	1.59
1	2-A	29	SGN	S1-N2	3.26	1.64	1.59
1	6-A	21	SGN	S1-N2	3.26	1.64	1.59
1	6-A	29	SGN	S1-N2	3.26	1.64	1.59
1	5-A	9	SGN	S1-N2	3.26	1.64	1.59
1	1-A	19	SGN	S1-N2	3.26	1.64	1.59
1	5-A	7	SGN	S1-N2	3.26	1.63	1.59
1	9-A	23	SGN	S1-N2	3.25	1.63	1.59
1	12-A	1	SGN	S1-N2	3.25	1.63	1.59
1	3-A	3	SGN	S1-N2	3.25	1.63	1.59
1	4-A	9	SGN	S1-N2	3.25	1.63	1.59
1	8-A	23	SGN	S1-N2	3.25	1.63	1.59
1	5-A	29	SGN	S1-N2	3.25	1.63	1.59
1	11-A	29	SGN	S1-N2	3.24	1.63	1.59
1	3-A	9	SGN	S1-N2	3.24	1.63	1.59
1	8-A	1	SGN	S1-N2	3.24	1.63	1.59
1	9-A	7	SGN	S1-N2	3.24	1.63	1.59
1	7-A	21	SGN	S1-N2	3.24	1.63	1.59
1	8-A	19	SGN	S1-N2	3.24	1.63	1.59
1	9-A	3	SGN	S1-N2	3.24	1.63	1.59
1	13-A	29	SGN	S1-N2	3.24	1.63	1.59
1	7-A	13	SGN	S1-N2	3.23	1.63	1.59
1	1-A	29	SGN	S1-N2	3.23	1.63	1.59
1	14-A	29	SGN	S1-N2	3.23	1.63	1.59
1	1-A	1	SGN	S1-N2	3.23	1.63	1.59
1	5-A	1	SGN	S1-N2	3.23	1.63	1.59
1	14-A	21	SGN	S1-N2	3.22	1.63	1.59
1	12-A	9	SGN	S1-N2	3.22	1.63	1.59
1	3-A	29	SGN	S1-N2	3.22	1.63	1.59
1	6-A	1	SGN	S1-N2	3.22	1.63	1.59
1	13-A	1	SGN	S1-N2	3.22	1.63	1.59
1	2-A	9	SGN	S1-N2	3.22	1.63	1.59
1	4-A	3	SGN	S1-N2	3.22	1.63	1.59
1	13-A	9	SGN	S1-N2	3.21	1.63	1.59
1	5-A	13	SGN	S1-N2	3.20	1.63	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	9	SGN	S1-N2	3.19	1.63	1.59
1	1-A	9	SGN	S1-N2	3.19	1.63	1.59
1	8-A	21	SGN	S1-N2	3.19	1.63	1.59
1	6-A	3	SGN	S1-N2	3.19	1.63	1.59
1	7-A	9	SGN	S1-N2	3.19	1.63	1.59
1	11-A	9	SGN	S1-N2	3.18	1.63	1.59
1	9-A	9	SGN	S1-N2	3.18	1.63	1.59
1	10-A	1	SGN	S1-N2	3.18	1.63	1.59
1	9-A	1	SGN	S1-N2	3.18	1.63	1.59
1	10-A	9	SGN	S1-N2	3.18	1.63	1.59
1	9-A	29	SGN	S1-N2	3.17	1.63	1.59
1	5-A	19	SGN	S1-N2	3.15	1.63	1.59
1	10-A	29	SGN	S1-N2	3.15	1.63	1.59
1	14-A	9	SGN	S1-N2	3.15	1.63	1.59
1	4-A	29	SGN	S1-N2	3.14	1.63	1.59
1	6-A	9	SGN	S1-N2	3.14	1.63	1.59
1	8-A	8	IDS	O6B-C6	-2.87	1.21	1.30
1	5-A	8	IDS	O6B-C6	-2.86	1.21	1.30
1	13-A	8	IDS	O6B-C6	-2.85	1.21	1.30
1	14-A	8	IDS	O6B-C6	-2.85	1.21	1.30
1	9-A	8	IDS	O6B-C6	-2.85	1.21	1.30
1	6-A	8	IDS	O6B-C6	-2.85	1.21	1.30
1	7-A	8	IDS	O6B-C6	-2.85	1.21	1.30
1	2-A	8	IDS	O6B-C6	-2.84	1.21	1.30
1	1-A	8	IDS	O6B-C6	-2.84	1.21	1.30
1	12-A	8	IDS	O6B-C6	-2.84	1.21	1.30
1	1-A	24	IDS	O6B-C6	-2.83	1.21	1.30
1	11-A	8	IDS	O6B-C6	-2.83	1.21	1.30
1	10-A	8	IDS	O6B-C6	-2.83	1.21	1.30
1	8-A	26	IDS	O6B-C6	-2.83	1.21	1.30
1	9-A	30	IDS	O6B-C6	-2.82	1.21	1.30
1	2-A	22	IDS	O6B-C6	-2.82	1.21	1.30
1	14-A	28	IDS	O6B-C6	-2.82	1.21	1.30
1	6-A	18	IDS	O6B-C6	-2.82	1.21	1.30
1	3-A	8	IDS	O6B-C6	-2.82	1.21	1.30
1	7-A	26	IDS	O6B-C6	-2.82	1.21	1.30
1	4-A	18	IDS	O6B-C6	-2.82	1.21	1.30
1	13-A	30	IDS	O6B-C6	-2.82	1.21	1.30
1	11-A	24	IDS	O6B-C6	-2.82	1.21	1.30
1	1-A	28	IDS	O6B-C6	-2.81	1.21	1.30
1	14-A	14	IDS	O6B-C6	-2.81	1.21	1.30
1	5-A	26	IDS	O6B-C6	-2.81	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	10-A	4	IDS	O6B-C6	-2.81	1.21	1.30
1	9-A	26	IDS	O6B-C6	-2.81	1.21	1.30
1	5-A	24	IDS	O6B-C6	-2.81	1.21	1.30
1	6-A	30	IDS	O6B-C6	-2.81	1.21	1.30
1	14-A	4	IDS	O6B-C6	-2.81	1.21	1.30
1	7-A	30	IDS	O6B-C6	-2.81	1.21	1.30
1	9-A	14	IDS	O6B-C6	-2.81	1.21	1.30
1	14-A	18	IDS	O6B-C6	-2.81	1.21	1.30
1	4-A	8	IDS	O6B-C6	-2.80	1.21	1.30
1	10-A	26	IDS	O6B-C6	-2.80	1.21	1.30
1	10-A	30	IDS	O6B-C6	-2.80	1.21	1.30
1	3-A	18	IDS	O6B-C6	-2.80	1.21	1.30
1	13-A	26	IDS	O6B-C6	-2.80	1.21	1.30
1	8-A	18	IDS	O6B-C6	-2.80	1.21	1.30
1	3-A	28	IDS	O6B-C6	-2.80	1.21	1.30
1	12-A	20	IDS	O6B-C6	-2.80	1.21	1.30
1	2-A	28	IDS	O6B-C6	-2.80	1.21	1.30
1	2-A	14	IDS	O6B-C6	-2.80	1.21	1.30
1	3-A	30	IDS	O6B-C6	-2.80	1.21	1.30
1	11-A	18	IDS	O6B-C6	-2.80	1.21	1.30
1	12-A	26	IDS	O6B-C6	-2.80	1.21	1.30
1	3-A	22	IDS	O6B-C6	-2.80	1.21	1.30
1	9-A	4	IDS	O6B-C6	-2.80	1.21	1.30
1	5-A	10	IDS	O6B-C6	-2.80	1.21	1.30
1	5-A	14	IDS	O6B-C6	-2.80	1.21	1.30
1	7-A	28	IDS	O6B-C6	-2.80	1.21	1.30
1	3-A	26	IDS	O6B-C6	-2.80	1.21	1.30
1	13-A	28	IDS	O6B-C6	-2.80	1.21	1.30
1	11-A	14	IDS	O6B-C6	-2.80	1.21	1.30
1	5-A	12	IDS	O6B-C6	-2.80	1.21	1.30
1	1-A	4	IDS	O6B-C6	-2.79	1.21	1.30
1	5-A	16	IDS	O6B-C6	-2.79	1.21	1.30
1	11-A	30	IDS	O6B-C6	-2.79	1.21	1.30
1	11-A	20	IDS	O6B-C6	-2.79	1.21	1.30
1	1-A	26	IDS	O6B-C6	-2.79	1.21	1.30
1	10-A	18	IDS	O6B-C6	-2.79	1.21	1.30
1	10-A	28	IDS	O6B-C6	-2.79	1.21	1.30
1	6-A	2	IDS	O6B-C6	-2.79	1.21	1.30
1	11-A	10	IDS	O6B-C6	-2.79	1.21	1.30
1	13-A	10	IDS	O6B-C6	-2.79	1.21	1.30
1	3-A	12	IDS	O6B-C6	-2.79	1.21	1.30
1	3-A	24	IDS	O6B-C6	-2.79	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-A	24	IDS	O6B-C6	-2.79	1.21	1.30
1	14-A	30	IDS	O6B-C6	-2.79	1.21	1.30
1	4-A	6	IDS	O6B-C6	-2.79	1.21	1.30
1	9-A	22	IDS	O6B-C6	-2.79	1.21	1.30
1	12-A	4	IDS	O6B-C6	-2.79	1.21	1.30
1	10-A	6	IDS	O6B-C6	-2.79	1.21	1.30
1	10-A	14	IDS	O6B-C6	-2.79	1.21	1.30
1	7-A	4	IDS	O6B-C6	-2.79	1.21	1.30
1	1-A	14	IDS	O6B-C6	-2.79	1.21	1.30
1	12-A	28	IDS	O6B-C6	-2.79	1.21	1.30
1	1-A	30	IDS	O6B-C6	-2.79	1.21	1.30
1	4-A	28	IDS	O6B-C6	-2.79	1.21	1.30
1	13-A	4	IDS	O6B-C6	-2.79	1.21	1.30
1	1-A	22	IDS	O6B-C6	-2.79	1.21	1.30
1	9-A	24	IDS	O6B-C6	-2.79	1.21	1.30
1	7-A	24	IDS	O6B-C6	-2.79	1.21	1.30
1	2-A	18	IDS	O6B-C6	-2.79	1.21	1.30
1	7-A	2	IDS	O6B-C6	-2.79	1.21	1.30
1	5-A	28	IDS	O6B-C6	-2.79	1.21	1.30
1	14-A	6	IDS	O6B-C6	-2.79	1.21	1.30
1	9-A	10	IDS	O6B-C6	-2.79	1.21	1.30
1	7-A	14	IDS	O6B-C6	-2.79	1.21	1.30
1	8-A	28	IDS	O6B-C6	-2.79	1.21	1.30
1	1-A	12	IDS	O6B-C6	-2.79	1.21	1.30
1	11-A	26	IDS	O6B-C6	-2.79	1.21	1.30
1	6-A	28	IDS	O6B-C6	-2.79	1.21	1.30
1	12-A	24	IDS	O6B-C6	-2.79	1.21	1.30
1	3-A	20	IDS	O6B-C6	-2.78	1.21	1.30
1	5-A	6	IDS	O6B-C6	-2.78	1.21	1.30
1	7-A	18	IDS	O6B-C6	-2.78	1.21	1.30
1	10-A	22	IDS	O6B-C6	-2.78	1.21	1.30
1	10-A	10	IDS	O6B-C6	-2.78	1.21	1.30
1	12-A	14	IDS	O6B-C6	-2.78	1.21	1.30
1	2-A	4	IDS	O6B-C6	-2.78	1.21	1.30
1	3-A	6	IDS	O6B-C6	-2.78	1.21	1.30
1	9-A	18	IDS	O6B-C6	-2.78	1.21	1.30
1	2-A	26	IDS	O6B-C6	-2.78	1.21	1.30
1	6-A	26	IDS	O6B-C6	-2.78	1.21	1.30
1	14-A	24	IDS	O6B-C6	-2.78	1.21	1.30
1	4-A	14	IDS	O6B-C6	-2.78	1.21	1.30
1	12-A	6	IDS	O6B-C6	-2.78	1.21	1.30
1	14-A	10	IDS	O6B-C6	-2.78	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	11-A	6	IDS	O6B-C6	-2.78	1.21	1.30
1	5-A	18	IDS	O6B-C6	-2.78	1.21	1.30
1	13-A	6	IDS	O6B-C6	-2.78	1.21	1.30
1	6-A	24	IDS	O6B-C6	-2.78	1.21	1.30
1	8-A	10	IDS	O6B-C6	-2.78	1.21	1.30
1	4-A	30	IDS	O6B-C6	-2.78	1.21	1.30
1	12-A	30	IDS	O6B-C6	-2.78	1.21	1.30
1	1-A	16	IDS	O6B-C6	-2.78	1.21	1.30
1	1-A	10	IDS	O6B-C6	-2.78	1.21	1.30
1	8-A	22	IDS	O6B-C6	-2.78	1.21	1.30
1	12-A	10	IDS	O6B-C6	-2.78	1.21	1.30
1	6-A	14	IDS	O6B-C6	-2.78	1.21	1.30
1	14-A	22	IDS	O6B-C6	-2.78	1.21	1.30
1	12-A	16	IDS	O6B-C6	-2.78	1.21	1.30
1	4-A	24	IDS	O6B-C6	-2.78	1.21	1.30
1	2-A	2	IDS	O6B-C6	-2.78	1.21	1.30
1	6-A	6	IDS	O6B-C6	-2.78	1.21	1.30
1	12-A	18	IDS	O6B-C6	-2.78	1.21	1.30
1	2-A	30	IDS	O6B-C6	-2.77	1.21	1.30
1	3-A	4	IDS	O6B-C6	-2.77	1.21	1.30
1	9-A	12	IDS	O6B-C6	-2.77	1.21	1.30
1	5-A	2	IDS	O6B-C6	-2.77	1.21	1.30
1	4-A	22	IDS	O6B-C6	-2.77	1.21	1.30
1	7-A	10	IDS	O6B-C6	-2.77	1.21	1.30
1	7-A	20	IDS	O6B-C6	-2.77	1.21	1.30
1	4-A	4	IDS	O6B-C6	-2.77	1.21	1.30
1	9-A	28	IDS	O6B-C6	-2.77	1.21	1.30
1	10-A	20	IDS	O6B-C6	-2.77	1.21	1.30
1	1-A	6	IDS	O6B-C6	-2.77	1.21	1.30
1	7-A	6	IDS	O6B-C6	-2.77	1.21	1.30
1	2-A	10	IDS	O6B-C6	-2.77	1.21	1.30
1	2-A	6	IDS	O6B-C6	-2.77	1.21	1.30
1	8-A	14	IDS	O6B-C6	-2.77	1.21	1.30
1	4-A	26	IDS	O6B-C6	-2.77	1.21	1.30
1	14-A	16	IDS	O6B-C6	-2.77	1.21	1.30
1	13-A	14	IDS	O6B-C6	-2.77	1.21	1.30
1	11-A	12	IDS	O6B-C6	-2.77	1.21	1.30
1	3-A	14	IDS	O6B-C6	-2.77	1.21	1.30
1	6-A	22	IDS	O6B-C6	-2.77	1.21	1.30
1	13-A	24	IDS	O6B-C6	-2.77	1.21	1.30
1	11-A	28	IDS	O6B-C6	-2.77	1.21	1.30
1	1-A	20	IDS	O6B-C6	-2.77	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	30	IDS	O6B-C6	-2.77	1.21	1.30
1	8-A	6	IDS	O6B-C6	-2.77	1.21	1.30
1	1-A	18	IDS	O6B-C6	-2.77	1.21	1.30
1	8-A	12	IDS	O6B-C6	-2.77	1.21	1.30
1	7-A	22	IDS	O6B-C6	-2.77	1.21	1.30
1	12-A	2	IDS	O6B-C6	-2.77	1.21	1.30
1	9-A	2	IDS	O6B-C6	-2.77	1.21	1.30
1	8-A	4	IDS	O6B-C6	-2.77	1.21	1.30
1	2-A	24	IDS	O6B-C6	-2.77	1.21	1.30
1	11-A	16	IDS	O6B-C6	-2.76	1.21	1.30
1	7-A	16	IDS	O6B-C6	-2.76	1.21	1.30
1	13-A	18	IDS	O6B-C6	-2.76	1.21	1.30
1	13-A	22	IDS	O6B-C6	-2.76	1.21	1.30
1	14-A	26	IDS	O6B-C6	-2.76	1.21	1.30
1	7-A	12	IDS	O6B-C6	-2.76	1.21	1.30
1	13-A	16	IDS	O6B-C6	-2.76	1.21	1.30
1	8-A	20	IDS	O6B-C6	-2.76	1.21	1.30
1	6-A	20	IDS	O6B-C6	-2.76	1.21	1.30
1	11-A	4	IDS	O6B-C6	-2.76	1.21	1.30
1	11-A	2	IDS	O6B-C6	-2.76	1.21	1.30
1	9-A	6	IDS	O6B-C6	-2.76	1.21	1.30
1	6-A	16	IDS	O6B-C6	-2.76	1.21	1.30
1	3-A	2	IDS	O6B-C6	-2.76	1.21	1.30
1	6-A	10	IDS	O6B-C6	-2.76	1.21	1.30
1	4-A	2	IDS	O6B-C6	-2.76	1.21	1.30
1	14-A	2	IDS	O6B-C6	-2.76	1.21	1.30
1	12-A	12	IDS	O6B-C6	-2.76	1.21	1.30
1	5-A	4	IDS	O6B-C6	-2.76	1.21	1.30
1	9-A	16	IDS	O6B-C6	-2.75	1.21	1.30
1	5-A	22	IDS	O6B-C6	-2.75	1.21	1.30
1	10-A	16	IDS	O6B-C6	-2.75	1.21	1.30
1	10-A	24	IDS	O6B-C6	-2.75	1.21	1.30
1	13-A	20	IDS	O6B-C6	-2.75	1.21	1.30
1	8-A	16	IDS	O6B-C6	-2.75	1.21	1.30
1	1-A	2	IDS	O6B-C6	-2.75	1.21	1.30
1	14-A	12	IDS	O6B-C6	-2.75	1.21	1.30
1	4-A	10	IDS	O6B-C6	-2.75	1.21	1.30
1	3-A	10	IDS	O6B-C6	-2.75	1.21	1.30
1	8-A	30	IDS	O6B-C6	-2.75	1.21	1.30
1	2-A	20	IDS	O6B-C6	-2.75	1.21	1.30
1	9-A	20	IDS	O6B-C6	-2.75	1.21	1.30
1	11-A	22	IDS	O6B-C6	-2.75	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	16	IDS	O6B-C6	-2.75	1.21	1.30
1	5-A	20	IDS	O6B-C6	-2.75	1.21	1.30
1	8-A	2	IDS	O6B-C6	-2.75	1.21	1.30
1	10-A	12	IDS	O6B-C6	-2.74	1.21	1.30
1	4-A	12	IDS	O6B-C6	-2.74	1.21	1.30
1	14-A	20	IDS	O6B-C6	-2.74	1.21	1.30
1	3-A	16	IDS	O6B-C6	-2.74	1.21	1.30
1	12-A	22	IDS	O6B-C6	-2.74	1.21	1.30
1	13-A	2	IDS	O6B-C6	-2.74	1.21	1.30
1	6-A	4	IDS	O6B-C6	-2.74	1.21	1.30
1	10-A	2	IDS	O6B-C6	-2.74	1.21	1.30
1	2-A	16	IDS	O6B-C6	-2.73	1.21	1.30
1	13-A	12	IDS	O6B-C6	-2.73	1.21	1.30
1	4-A	20	IDS	O6B-C6	-2.73	1.21	1.30
1	2-A	12	IDS	O6B-C6	-2.72	1.21	1.30
1	6-A	12	IDS	O6B-C6	-2.72	1.21	1.30
1	12-A	29	SGN	O5-C1	-2.36	1.39	1.43
1	14-A	29	SGN	O5-C1	-2.35	1.40	1.43
1	9-A	9	SGN	O5-C1	-2.32	1.40	1.43
1	3-A	29	SGN	O5-C1	-2.32	1.40	1.43
1	1-A	27	SGN	O5-C1	-2.30	1.40	1.43
1	10-A	13	SGN	O5-C1	-2.30	1.40	1.43
1	4-A	27	SGN	O5-C1	-2.30	1.40	1.43
1	11-A	29	SGN	O5-C1	-2.29	1.40	1.43
1	7-A	29	SGN	O5-C1	-2.29	1.40	1.43
1	13-A	17	SGN	O5-C1	-2.28	1.40	1.43
1	9-A	29	SGN	O5-C1	-2.28	1.40	1.43
1	4-A	29	SGN	O5-C1	-2.28	1.40	1.43
1	11-A	17	SGN	O5-C1	-2.28	1.40	1.43
1	4-A	25	SGN	O5-C1	-2.27	1.40	1.43
1	2-A	27	SGN	O5-C1	-2.27	1.40	1.43
1	10-A	9	SGN	O5-C1	-2.27	1.40	1.43
1	1-A	29	SGN	O5-C1	-2.26	1.40	1.43
1	8-A	17	SGN	O5-C1	-2.26	1.40	1.43
1	14-A	9	SGN	O5-C1	-2.26	1.40	1.43
1	4-A	17	SGN	O5-C1	-2.26	1.40	1.43
1	11-A	21	SGN	O5-C1	-2.26	1.40	1.43
1	6-A	19	SGN	O5-C1	-2.26	1.40	1.43
1	12-A	19	SGN	O5-C1	-2.26	1.40	1.43
1	5-A	13	SGN	O5-C1	-2.25	1.40	1.43
1	2-A	17	SGN	O5-C1	-2.25	1.40	1.43
1	8-A	13	SGN	O5-C1	-2.25	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	27	SGN	O5-C1	-2.25	1.40	1.43
1	14-A	7	SGN	O5-C1	-2.25	1.40	1.43
1	2-A	19	SGN	O5-C1	-2.25	1.40	1.43
1	1-A	17	SGN	O5-C1	-2.25	1.40	1.43
1	6-A	23	SGN	O5-C1	-2.25	1.40	1.43
1	11-A	27	SGN	O5-C1	-2.25	1.40	1.43
1	13-A	9	SGN	O5-C1	-2.25	1.40	1.43
1	9-A	17	SGN	O5-C1	-2.25	1.40	1.43
1	13-A	27	SGN	O5-C1	-2.25	1.40	1.43
1	1-A	7	SGN	O5-C1	-2.24	1.40	1.43
1	1-A	19	SGN	O5-C1	-2.24	1.40	1.43
1	11-A	25	SGN	O5-C1	-2.24	1.40	1.43
1	7-A	17	SGN	O5-C1	-2.24	1.40	1.43
1	7-A	25	SGN	O5-C1	-2.24	1.40	1.43
1	2-A	13	SGN	O5-C1	-2.24	1.40	1.43
1	10-A	27	SGN	O5-C1	-2.24	1.40	1.43
1	14-A	3	SGN	O5-C1	-2.24	1.40	1.43
1	6-A	9	SGN	O5-C1	-2.24	1.40	1.43
1	9-A	7	SGN	O5-C1	-2.24	1.40	1.43
1	5-A	7	SGN	O5-C1	-2.24	1.40	1.43
1	2-A	9	SGN	O5-C1	-2.24	1.40	1.43
1	5-A	21	SGN	O5-C1	-2.24	1.40	1.43
1	8-A	7	SGN	O5-C1	-2.24	1.40	1.43
1	8-A	29	SGN	O5-C1	-2.24	1.40	1.43
1	13-A	25	SGN	O5-C1	-2.24	1.40	1.43
1	1-A	23	SGN	O5-C1	-2.24	1.40	1.43
1	5-A	23	SGN	O5-C1	-2.24	1.40	1.43
1	6-A	7	SGN	O5-C1	-2.23	1.40	1.43
1	6-A	25	SGN	O5-C1	-2.23	1.40	1.43
1	2-A	7	SGN	O5-C1	-2.23	1.40	1.43
1	3-A	25	SGN	O5-C1	-2.23	1.40	1.43
1	8-A	27	SGN	O5-C1	-2.23	1.40	1.43
1	6-A	29	SGN	O5-C1	-2.23	1.40	1.43
1	9-A	19	SGN	O5-C1	-2.23	1.40	1.43
1	7-A	7	SGN	O5-C1	-2.23	1.40	1.43
1	6-A	17	SGN	O5-C1	-2.23	1.40	1.43
1	8-A	25	SGN	O5-C1	-2.23	1.40	1.43
1	10-A	25	SGN	O5-C1	-2.23	1.40	1.43
1	13-A	7	SGN	O5-C1	-2.23	1.40	1.43
1	1-A	13	SGN	O5-C1	-2.23	1.40	1.43
1	6-A	27	SGN	O5-C1	-2.23	1.40	1.43
1	7-A	27	SGN	O5-C1	-2.23	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	17	SGN	O5-C1	-2.23	1.40	1.43
1	4-A	19	SGN	O5-C1	-2.23	1.40	1.43
1	1-A	21	SGN	O5-C1	-2.23	1.40	1.43
1	2-A	29	SGN	O5-C1	-2.23	1.40	1.43
1	13-A	21	SGN	O5-C1	-2.23	1.40	1.43
1	10-A	29	SGN	O5-C1	-2.23	1.40	1.43
1	8-A	21	SGN	O5-C1	-2.23	1.40	1.43
1	14-A	21	SGN	O5-C1	-2.23	1.40	1.43
1	11-A	22	IDS	O5-C1	-2.22	1.40	1.43
1	3-A	27	SGN	O5-C1	-2.22	1.40	1.43
1	5-A	29	SGN	O5-C1	-2.22	1.40	1.43
1	10-A	5	SGN	O5-C1	-2.22	1.40	1.43
1	14-A	17	SGN	O5-C1	-2.22	1.40	1.43
1	12-A	25	SGN	O5-C1	-2.22	1.40	1.43
1	13-A	3	SGN	O5-C1	-2.22	1.40	1.43
1	3-A	7	SGN	O5-C1	-2.22	1.40	1.43
1	4-A	21	SGN	O5-C1	-2.22	1.40	1.43
1	8-A	23	SGN	O5-C1	-2.22	1.40	1.43
1	7-A	21	SGN	O5-C1	-2.22	1.40	1.43
1	10-A	7	SGN	O5-C1	-2.22	1.40	1.43
1	10-A	17	SGN	O5-C1	-2.22	1.40	1.43
1	3-A	9	SGN	O5-C1	-2.22	1.40	1.43
1	10-A	11	SGN	O5-C1	-2.22	1.40	1.43
1	9-A	25	SGN	O5-C1	-2.22	1.40	1.43
1	14-A	22	IDS	O5-C1	-2.22	1.40	1.43
1	13-A	23	SGN	O5-C1	-2.22	1.40	1.43
1	4-A	7	SGN	O5-C1	-2.22	1.40	1.43
1	11-A	9	SGN	O5-C1	-2.22	1.40	1.43
1	3-A	2	IDS	O5-C1	-2.21	1.40	1.43
1	4-A	11	SGN	O5-C1	-2.21	1.40	1.43
1	11-A	3	SGN	O5-C1	-2.21	1.40	1.43
1	2-A	25	SGN	O5-C1	-2.21	1.40	1.43
1	12-A	2	IDS	O5-C1	-2.21	1.40	1.43
1	11-A	19	SGN	O5-C1	-2.21	1.40	1.43
1	9-A	27	SGN	O5-C1	-2.21	1.40	1.43
1	3-A	19	SGN	O5-C1	-2.21	1.40	1.43
1	10-A	19	SGN	O5-C1	-2.21	1.40	1.43
1	8-A	9	SGN	O5-C1	-2.21	1.40	1.43
1	3-A	17	SGN	O5-C1	-2.21	1.40	1.43
1	9-A	3	SGN	O5-C1	-2.21	1.40	1.43
1	11-A	7	SGN	O5-C1	-2.21	1.40	1.43
1	13-A	29	SGN	O5-C1	-2.20	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-A	11	SGN	O5-C1	-2.20	1.40	1.43
1	7-A	19	SGN	O5-C1	-2.20	1.40	1.43
1	12-A	23	SGN	O5-C1	-2.20	1.40	1.43
1	11-A	23	SGN	O5-C1	-2.20	1.40	1.43
1	11-A	13	SGN	O5-C1	-2.20	1.40	1.43
1	8-A	2	IDS	O5-C1	-2.20	1.40	1.43
1	2-A	3	SGN	O5-C1	-2.20	1.40	1.43
1	7-A	9	SGN	O5-C1	-2.20	1.40	1.43
1	7-A	12	IDS	O5-C1	-2.20	1.40	1.43
1	9-A	2	IDS	O5-C1	-2.20	1.40	1.43
1	6-A	11	SGN	O5-C1	-2.20	1.40	1.43
1	9-A	13	SGN	O5-C1	-2.20	1.40	1.43
1	5-A	2	IDS	O5-C1	-2.19	1.40	1.43
1	14-A	11	SGN	O5-C1	-2.19	1.40	1.43
1	5-A	19	SGN	O5-C1	-2.19	1.40	1.43
1	4-A	13	SGN	O5-C1	-2.19	1.40	1.43
1	6-A	13	SGN	O5-C1	-2.19	1.40	1.43
1	12-A	17	SGN	O5-C1	-2.19	1.40	1.43
1	7-A	3	SGN	O5-C1	-2.19	1.40	1.43
1	8-A	19	SGN	O5-C1	-2.19	1.40	1.43
1	14-A	27	SGN	O5-C1	-2.19	1.40	1.43
1	2-A	21	SGN	O5-C1	-2.19	1.40	1.43
1	10-A	21	SGN	O5-C1	-2.19	1.40	1.43
1	14-A	13	SGN	O5-C1	-2.19	1.40	1.43
1	5-A	25	SGN	O5-C1	-2.19	1.40	1.43
1	14-A	19	SGN	O5-C1	-2.19	1.40	1.43
1	3-A	21	SGN	O5-C1	-2.19	1.40	1.43
1	12-A	21	SGN	O5-C1	-2.18	1.40	1.43
1	12-A	9	SGN	O5-C1	-2.18	1.40	1.43
1	3-A	11	SGN	O5-C1	-2.18	1.40	1.43
1	9-A	21	SGN	O5-C1	-2.18	1.40	1.43
1	1-A	25	SGN	O5-C1	-2.18	1.40	1.43
1	13-A	19	SGN	O5-C1	-2.18	1.40	1.43
1	13-A	13	SGN	O5-C1	-2.18	1.40	1.43
1	8-A	3	SGN	O5-C1	-2.18	1.40	1.43
1	8-A	11	SGN	O5-C1	-2.18	1.40	1.43
1	7-A	2	IDS	O5-C1	-2.18	1.40	1.43
1	6-A	15	SGN	O5-C1	-2.18	1.40	1.43
1	6-A	22	IDS	O5-C1	-2.18	1.40	1.43
1	3-A	13	SGN	O5-C1	-2.18	1.40	1.43
1	3-A	23	SGN	O5-C1	-2.18	1.40	1.43
1	13-A	15	SGN	O5-C1	-2.17	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	28	IDS	O5-C1	-2.17	1.40	1.43
1	12-A	7	SGN	O5-C1	-2.17	1.40	1.43
1	1-A	9	SGN	O5-C1	-2.17	1.40	1.43
1	14-A	2	IDS	O5-C1	-2.17	1.40	1.43
1	10-A	3	SGN	O5-C1	-2.17	1.40	1.43
1	7-A	13	SGN	O5-C1	-2.17	1.40	1.43
1	10-A	23	SGN	O5-C1	-2.17	1.40	1.43
1	3-A	22	IDS	O5-C1	-2.17	1.40	1.43
1	8-A	12	IDS	O5-C1	-2.17	1.40	1.43
1	1-A	22	IDS	O5-C1	-2.17	1.40	1.43
1	6-A	21	SGN	O5-C1	-2.17	1.40	1.43
1	13-A	11	SGN	O5-C1	-2.17	1.40	1.43
1	9-A	12	IDS	O5-C1	-2.17	1.40	1.43
1	13-A	2	IDS	O5-C1	-2.16	1.40	1.43
1	4-A	20	IDS	O5-C1	-2.16	1.40	1.43
1	12-A	27	SGN	O5-C1	-2.16	1.40	1.43
1	6-A	2	IDS	O5-C1	-2.16	1.40	1.43
1	4-A	9	SGN	O5-C1	-2.16	1.40	1.43
1	14-A	25	SGN	O5-C1	-2.16	1.40	1.43
1	2-A	23	SGN	O5-C1	-2.16	1.40	1.43
1	10-A	15	SGN	O5-C1	-2.16	1.40	1.43
1	6-A	3	SGN	O5-C1	-2.16	1.40	1.43
1	9-A	23	SGN	O5-C1	-2.16	1.40	1.43
1	8-A	26	IDS	O5-C1	-2.16	1.40	1.43
1	3-A	3	SGN	O5-C1	-2.16	1.40	1.43
1	4-A	3	SGN	O5-C1	-2.16	1.40	1.43
1	7-A	22	IDS	O5-C1	-2.16	1.40	1.43
1	4-A	23	SGN	O5-C1	-2.16	1.40	1.43
1	13-A	20	IDS	O5-C1	-2.15	1.40	1.43
1	9-A	22	IDS	O5-C1	-2.15	1.40	1.43
1	1-A	3	SGN	O5-C1	-2.15	1.40	1.43
1	12-A	13	SGN	O5-C1	-2.15	1.40	1.43
1	4-A	15	SGN	O5-C1	-2.15	1.40	1.43
1	1-A	5	SGN	O5-C1	-2.15	1.40	1.43
1	13-A	28	IDS	O5-C1	-2.15	1.40	1.43
1	5-A	26	IDS	O5-C1	-2.15	1.40	1.43
1	12-A	11	SGN	O5-C1	-2.15	1.40	1.43
1	4-A	30	IDS	O5-C1	-2.15	1.40	1.43
1	12-A	16	IDS	O5-C1	-2.15	1.40	1.43
1	5-A	5	SGN	O5-C1	-2.15	1.40	1.43
1	10-A	22	IDS	O5-C1	-2.15	1.40	1.43
1	5-A	11	SGN	O5-C1	-2.14	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-A	11	SGN	O5-C1	-2.14	1.40	1.43
1	5-A	3	SGN	O5-C1	-2.14	1.40	1.43
1	7-A	5	SGN	O5-C1	-2.14	1.40	1.43
1	6-A	5	SGN	O5-C1	-2.14	1.40	1.43
1	11-A	5	SGN	O5-C1	-2.14	1.40	1.43
1	2-A	11	SGN	O5-C1	-2.14	1.40	1.43
1	11-A	11	SGN	O5-C1	-2.14	1.40	1.43
1	14-A	16	IDS	O5-C1	-2.14	1.40	1.43
1	8-A	22	IDS	O5-C1	-2.14	1.40	1.43
1	7-A	28	IDS	O5-C1	-2.14	1.40	1.43
1	12-A	20	IDS	O5-C1	-2.14	1.40	1.43
1	1-A	11	SGN	O5-C1	-2.13	1.40	1.43
1	14-A	5	SGN	O5-C1	-2.13	1.40	1.43
1	10-A	30	IDS	O5-C1	-2.13	1.40	1.43
1	12-A	3	SGN	O5-C1	-2.13	1.40	1.43
1	2-A	22	IDS	O5-C1	-2.13	1.40	1.43
1	7-A	23	SGN	O5-C1	-2.13	1.40	1.43
1	11-A	26	IDS	O5-C1	-2.13	1.40	1.43
1	1-A	8	IDS	O5-C1	-2.13	1.40	1.43
1	7-A	15	SGN	O5-C1	-2.13	1.40	1.43
1	3-A	20	IDS	O5-C1	-2.13	1.40	1.43
1	12-A	5	SGN	O5-C1	-2.13	1.40	1.43
1	13-A	22	IDS	O5-C1	-2.13	1.40	1.43
1	4-A	2	IDS	O5-C1	-2.13	1.40	1.43
1	13-A	5	SGN	O5-C1	-2.13	1.40	1.43
1	8-A	8	IDS	O5-C1	-2.13	1.40	1.43
1	3-A	15	SGN	O5-C1	-2.13	1.40	1.43
1	4-A	22	IDS	O5-C1	-2.13	1.40	1.43
1	11-A	12	IDS	O5-C1	-2.12	1.40	1.43
1	9-A	8	IDS	O5-C1	-2.12	1.40	1.43
1	5-A	9	SGN	O5-C1	-2.12	1.40	1.43
1	2-A	15	SGN	O5-C1	-2.12	1.40	1.43
1	8-A	15	SGN	O5-C1	-2.12	1.40	1.43
1	14-A	15	SGN	O5-C1	-2.12	1.40	1.43
1	12-A	22	IDS	O5-C1	-2.12	1.40	1.43
1	4-A	8	IDS	O5-C1	-2.12	1.40	1.43
1	8-A	20	IDS	O5-C1	-2.12	1.40	1.43
1	11-A	15	SGN	O5-C1	-2.12	1.40	1.43
1	4-A	5	SGN	O5-C1	-2.12	1.40	1.43
1	6-A	8	IDS	O5-C1	-2.12	1.40	1.43
1	5-A	20	IDS	O5-C1	-2.12	1.40	1.43
1	8-A	6	IDS	O5-C1	-2.12	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	15	SGN	O5-C1	-2.12	1.40	1.43
1	14-A	12	IDS	O5-C1	-2.12	1.40	1.43
1	13-A	14	IDS	O5-C1	-2.12	1.40	1.43
1	5-A	15	SGN	O5-C1	-2.12	1.40	1.43
1	1-A	12	IDS	O5-C1	-2.11	1.40	1.43
1	7-A	16	IDS	O5-C1	-2.11	1.40	1.43
1	3-A	12	IDS	O5-C1	-2.11	1.40	1.43
1	5-A	30	IDS	O5-C1	-2.11	1.40	1.43
1	11-A	2	IDS	O5-C1	-2.11	1.40	1.43
1	2-A	30	IDS	O5-C1	-2.11	1.40	1.43
1	5-A	18	IDS	O5-C1	-2.11	1.40	1.43
1	1-A	14	IDS	O5-C1	-2.11	1.40	1.43
1	6-A	14	IDS	O5-C1	-2.11	1.40	1.43
1	9-A	15	SGN	O5-C1	-2.11	1.40	1.43
1	14-A	30	IDS	O5-C1	-2.11	1.40	1.43
1	2-A	2	IDS	O5-C1	-2.11	1.40	1.43
1	8-A	10	IDS	O5-C1	-2.11	1.40	1.43
1	10-A	26	IDS	O5-C1	-2.11	1.40	1.43
1	12-A	15	SGN	O5-C1	-2.10	1.40	1.43
1	13-A	30	IDS	O5-C1	-2.10	1.40	1.43
1	8-A	5	SGN	O5-C1	-2.10	1.40	1.43
1	2-A	12	IDS	O5-C1	-2.10	1.40	1.43
1	6-A	16	IDS	O5-C1	-2.10	1.40	1.43
1	12-A	28	IDS	O5-C1	-2.10	1.40	1.43
1	2-A	5	SGN	O5-C1	-2.10	1.40	1.43
1	12-A	26	IDS	O5-C1	-2.10	1.40	1.43
1	9-A	16	IDS	O5-C1	-2.10	1.40	1.43
1	6-A	26	IDS	O5-C1	-2.10	1.40	1.43
1	7-A	30	IDS	O5-C1	-2.10	1.40	1.43
1	1-A	4	IDS	O5-C1	-2.10	1.40	1.43
1	14-A	26	IDS	O5-C1	-2.10	1.40	1.43
1	3-A	5	SGN	O5-C1	-2.10	1.40	1.43
1	14-A	23	SGN	O5-C1	-2.10	1.40	1.43
1	10-A	2	IDS	O5-C1	-2.10	1.40	1.43
1	2-A	18	IDS	O5-C1	-2.10	1.40	1.43
1	11-A	18	IDS	O5-C1	-2.10	1.40	1.43
1	1-A	20	IDS	O5-C1	-2.10	1.40	1.43
1	5-A	22	IDS	O5-C1	-2.10	1.40	1.43
1	9-A	24	IDS	O5-C1	-2.10	1.40	1.43
1	3-A	24	IDS	O5-C1	-2.10	1.40	1.43
1	11-A	28	IDS	O5-C1	-2.10	1.40	1.43
1	9-A	5	SGN	O5-C1	-2.10	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-A	14	IDS	O5-C1	-2.10	1.40	1.43
1	11-A	16	IDS	O5-C1	-2.09	1.40	1.43
1	10-A	18	IDS	O5-C1	-2.09	1.40	1.43
1	4-A	12	IDS	O5-C1	-2.09	1.40	1.43
1	6-A	28	IDS	O5-C1	-2.09	1.40	1.43
1	8-A	28	IDS	O5-C1	-2.09	1.40	1.43
1	9-A	20	IDS	O5-C1	-2.09	1.40	1.43
1	5-A	12	IDS	O5-C1	-2.09	1.40	1.43
1	1-A	2	IDS	O5-C1	-2.09	1.40	1.43
1	10-A	8	IDS	O5-C1	-2.09	1.40	1.43
1	7-A	6	IDS	O5-C1	-2.09	1.40	1.43
1	10-A	14	IDS	O5-C1	-2.09	1.40	1.43
1	14-A	20	IDS	O5-C1	-2.09	1.40	1.43
1	10-A	12	IDS	O5-C1	-2.09	1.40	1.43
1	3-A	8	IDS	O5-C1	-2.09	1.40	1.43
1	12-A	8	IDS	O5-C1	-2.09	1.40	1.43
1	2-A	16	IDS	O5-C1	-2.09	1.40	1.43
1	9-A	28	IDS	O5-C1	-2.09	1.40	1.43
1	11-A	14	IDS	O5-C1	-2.08	1.40	1.43
1	4-A	6	IDS	O5-C1	-2.08	1.40	1.43
1	2-A	20	IDS	O5-C1	-2.08	1.40	1.43
1	3-A	4	IDS	O5-C1	-2.08	1.40	1.43
1	7-A	4	IDS	O5-C1	-2.08	1.40	1.43
1	3-A	30	IDS	O5-C1	-2.08	1.40	1.43
1	6-A	4	IDS	O5-C1	-2.08	1.40	1.43
1	14-A	28	IDS	O5-C1	-2.08	1.40	1.43
1	5-A	10	IDS	O5-C1	-2.08	1.40	1.43
1	3-A	28	IDS	O5-C1	-2.08	1.40	1.43
1	10-A	16	IDS	O5-C1	-2.08	1.40	1.43
1	1-A	26	IDS	O5-C1	-2.08	1.40	1.43
1	13-A	26	IDS	O5-C1	-2.08	1.40	1.43
1	14-A	8	IDS	O5-C1	-2.07	1.40	1.43
1	14-A	6	IDS	O5-C1	-2.07	1.40	1.43
1	4-A	28	IDS	O5-C1	-2.07	1.40	1.43
1	8-A	14	IDS	O5-C1	-2.07	1.40	1.43
1	3-A	16	IDS	O5-C1	-2.07	1.40	1.43
1	12-A	18	IDS	O5-C1	-2.07	1.40	1.43
1	10-A	20	IDS	O5-C1	-2.07	1.40	1.43
1	12-A	24	IDS	O5-C1	-2.07	1.40	1.43
1	4-A	4	IDS	O5-C1	-2.07	1.40	1.43
1	13-A	16	IDS	O5-C1	-2.07	1.40	1.43
1	1-A	24	IDS	O5-C1	-2.07	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	12	IDS	O5-C1	-2.07	1.40	1.43
1	4-A	26	IDS	O5-C1	-2.07	1.40	1.43
1	2-A	4	IDS	O5-C1	-2.07	1.40	1.43
1	7-A	8	IDS	O5-C1	-2.07	1.40	1.43
1	6-A	18	IDS	O5-C1	-2.07	1.40	1.43
1	13-A	10	IDS	O5-C1	-2.07	1.40	1.43
1	13-A	12	IDS	O5-C1	-2.06	1.40	1.43
1	14-A	10	IDS	O5-C1	-2.06	1.40	1.43
1	13-A	6	IDS	O5-C1	-2.06	1.40	1.43
1	13-A	8	IDS	O5-C1	-2.06	1.40	1.43
1	12-A	10	IDS	O5-C1	-2.06	1.40	1.43
1	9-A	26	IDS	O5-C1	-2.06	1.40	1.43
1	5-A	6	IDS	O5-C1	-2.06	1.40	1.43
1	2-A	8	IDS	O5-C1	-2.06	1.40	1.43
1	5-A	16	IDS	O5-C1	-2.06	1.40	1.43
1	1-A	18	IDS	O5-C1	-2.06	1.40	1.43
1	5-A	24	IDS	O5-C1	-2.06	1.40	1.43
1	1-A	28	IDS	O5-C1	-2.06	1.40	1.43
1	8-A	30	IDS	O5-C1	-2.06	1.40	1.43
1	6-A	6	IDS	O5-C1	-2.06	1.40	1.43
1	7-A	10	IDS	O5-C1	-2.06	1.40	1.43
1	11-A	8	IDS	O5-C1	-2.06	1.40	1.43
1	14-A	14	IDS	O5-C1	-2.06	1.40	1.43
1	6-A	30	IDS	O5-C1	-2.06	1.40	1.43
1	4-A	16	IDS	O5-C1	-2.06	1.40	1.43
1	9-A	6	IDS	O5-C1	-2.06	1.40	1.43
1	1-A	10	IDS	O5-C1	-2.05	1.40	1.43
1	1-A	6	IDS	O5-C1	-2.05	1.40	1.43
1	10-A	28	IDS	O5-C1	-2.05	1.40	1.43
1	8-A	16	IDS	O5-C1	-2.05	1.40	1.43
1	5-A	14	IDS	O5-C1	-2.05	1.40	1.43
1	2-A	26	IDS	O5-C1	-2.05	1.40	1.43
1	4-A	10	IDS	O5-C1	-2.05	1.40	1.43
1	11-A	30	IDS	O5-C1	-2.05	1.40	1.43
1	10-A	6	IDS	O5-C1	-2.05	1.40	1.43
1	2-A	24	IDS	O5-C1	-2.05	1.40	1.43
1	2-A	28	IDS	O5-C1	-2.05	1.40	1.43
1	1-A	16	IDS	O5-C1	-2.05	1.40	1.43
1	9-A	18	IDS	O5-C1	-2.05	1.40	1.43
1	1-A	30	IDS	O5-C1	-2.05	1.40	1.43
1	12-A	4	IDS	O5-C1	-2.05	1.40	1.43
1	10-A	10	IDS	O5-C1	-2.05	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	20	IDS	O5-C1	-2.05	1.40	1.43
1	11-A	6	IDS	O5-C1	-2.05	1.40	1.43
1	14-A	18	IDS	O5-C1	-2.04	1.40	1.43
1	8-A	18	IDS	O5-C1	-2.04	1.40	1.43
1	11-A	10	IDS	O5-C1	-2.04	1.40	1.43
1	3-A	14	IDS	O5-C1	-2.04	1.40	1.43
1	2-A	6	IDS	O5-C1	-2.04	1.40	1.43
1	9-A	30	IDS	O5-C1	-2.04	1.40	1.43
1	12-A	12	IDS	O5-C1	-2.04	1.40	1.43
1	3-A	26	IDS	O5-C1	-2.04	1.40	1.43
1	3-A	10	IDS	O5-C1	-2.04	1.40	1.43
1	4-A	18	IDS	O5-C1	-2.04	1.40	1.43
1	11-A	20	IDS	O5-C1	-2.04	1.40	1.43
1	3-A	6	IDS	O5-C1	-2.03	1.40	1.43
1	2-A	10	IDS	O5-C1	-2.03	1.40	1.43
1	7-A	20	IDS	O5-C1	-2.03	1.40	1.43
1	6-A	10	IDS	O5-C1	-2.03	1.40	1.43
1	13-A	4	IDS	O5-C1	-2.03	1.40	1.43
1	12-A	14	IDS	O5-C1	-2.03	1.40	1.43
1	5-A	4	IDS	O5-C1	-2.03	1.40	1.43
1	9-A	14	IDS	O5-C1	-2.03	1.40	1.43
1	7-A	14	IDS	O5-C1	-2.03	1.40	1.43
1	10-A	24	IDS	O5-C1	-2.03	1.40	1.43
1	13-A	18	IDS	O5-C1	-2.03	1.40	1.43
1	11-A	4	IDS	O5-C1	-2.02	1.40	1.43
1	2-A	14	IDS	O5-C1	-2.02	1.40	1.43
1	7-A	26	IDS	O5-C1	-2.02	1.40	1.43
1	9-A	10	IDS	O5-C1	-2.02	1.40	1.43
1	12-A	30	IDS	O5-C1	-2.02	1.40	1.43
1	3-A	18	IDS	O5-C1	-2.02	1.40	1.43
1	5-A	8	IDS	O5-C1	-2.02	1.40	1.43
1	13-A	24	IDS	O5-C1	-2.02	1.40	1.43
1	6-A	24	IDS	O5-C1	-2.01	1.40	1.43
1	12-A	6	IDS	O5-C1	-2.01	1.40	1.43
1	7-A	18	IDS	O5-C1	-2.00	1.40	1.43

All (840) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	12	IDS	C2-O2-S	8.05	128.41	117.91
1	12-A	12	IDS	C2-O2-S	8.03	128.38	117.91
1	13-A	12	IDS	C2-O2-S	8.03	128.38	117.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	16	IDS	C2-O2-S	8.02	128.37	117.91
1	10-A	16	IDS	C2-O2-S	8.01	128.36	117.91
1	11-A	12	IDS	C2-O2-S	8.01	128.36	117.91
1	4-A	26	IDS	C2-O2-S	8.01	128.35	117.91
1	7-A	30	IDS	C2-O2-S	8.00	128.35	117.91
1	6-A	12	IDS	C2-O2-S	8.00	128.35	117.91
1	14-A	22	IDS	C2-O2-S	8.00	128.35	117.91
1	8-A	2	IDS	C2-O2-S	8.00	128.34	117.91
1	8-A	12	IDS	C2-O2-S	8.00	128.34	117.91
1	5-A	30	IDS	C2-O2-S	8.00	128.34	117.91
1	9-A	30	IDS	C2-O2-S	8.00	128.34	117.91
1	3-A	12	IDS	C2-O2-S	7.99	128.34	117.91
1	10-A	12	IDS	C2-O2-S	7.99	128.34	117.91
1	5-A	12	IDS	C2-O2-S	7.99	128.33	117.91
1	6-A	24	IDS	C2-O2-S	7.99	128.33	117.91
1	5-A	28	IDS	C2-O2-S	7.99	128.33	117.91
1	5-A	2	IDS	C2-O2-S	7.99	128.33	117.91
1	8-A	30	IDS	C2-O2-S	7.99	128.33	117.91
1	3-A	10	IDS	C2-O2-S	7.99	128.33	117.91
1	7-A	12	IDS	C2-O2-S	7.99	128.33	117.91
1	2-A	12	IDS	C2-O2-S	7.99	128.33	117.91
1	4-A	12	IDS	C2-O2-S	7.99	128.33	117.91
1	2-A	8	IDS	C2-O2-S	7.98	128.32	117.91
1	10-A	30	IDS	C2-O2-S	7.98	128.32	117.91
1	11-A	16	IDS	C2-O2-S	7.98	128.32	117.91
1	14-A	28	IDS	C2-O2-S	7.98	128.32	117.91
1	14-A	8	IDS	C2-O2-S	7.98	128.31	117.91
1	1-A	28	IDS	C2-O2-S	7.98	128.31	117.91
1	3-A	22	IDS	C2-O2-S	7.98	128.31	117.91
1	12-A	28	IDS	C2-O2-S	7.98	128.31	117.91
1	1-A	12	IDS	C2-O2-S	7.98	128.31	117.91
1	1-A	22	IDS	C2-O2-S	7.98	128.31	117.91
1	13-A	30	IDS	C2-O2-S	7.98	128.31	117.91
1	10-A	2	IDS	C2-O2-S	7.97	128.31	117.91
1	6-A	8	IDS	C2-O2-S	7.97	128.31	117.91
1	9-A	4	IDS	C2-O2-S	7.97	128.31	117.91
1	2-A	28	IDS	C2-O2-S	7.97	128.30	117.91
1	2-A	2	IDS	C2-O2-S	7.97	128.30	117.91
1	2-A	16	IDS	C2-O2-S	7.97	128.30	117.91
1	2-A	22	IDS	C2-O2-S	7.97	128.30	117.91
1	3-A	28	IDS	C2-O2-S	7.97	128.30	117.91
1	5-A	24	IDS	C2-O2-S	7.97	128.30	117.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	2	IDS	C2-O2-S	7.96	128.30	117.91
1	7-A	26	IDS	C2-O2-S	7.96	128.30	117.91
1	6-A	22	IDS	C2-O2-S	7.96	128.30	117.91
1	12-A	30	IDS	C2-O2-S	7.96	128.30	117.91
1	3-A	24	IDS	C2-O2-S	7.96	128.29	117.91
1	14-A	16	IDS	C2-O2-S	7.96	128.29	117.91
1	10-A	14	IDS	C2-O2-S	7.96	128.29	117.91
1	8-A	26	IDS	C2-O2-S	7.96	128.29	117.91
1	14-A	4	IDS	C2-O2-S	7.96	128.29	117.91
1	13-A	8	IDS	C2-O2-S	7.96	128.29	117.91
1	9-A	14	IDS	C2-O2-S	7.96	128.29	117.91
1	7-A	16	IDS	C2-O2-S	7.96	128.29	117.91
1	9-A	16	IDS	C2-O2-S	7.96	128.29	117.91
1	7-A	22	IDS	C2-O2-S	7.96	128.29	117.91
1	3-A	4	IDS	C2-O2-S	7.95	128.28	117.91
1	13-A	16	IDS	C2-O2-S	7.95	128.28	117.91
1	6-A	16	IDS	C2-O2-S	7.95	128.28	117.91
1	3-A	2	IDS	C2-O2-S	7.95	128.28	117.91
1	10-A	26	IDS	C2-O2-S	7.95	128.28	117.91
1	4-A	30	IDS	C2-O2-S	7.95	128.28	117.91
1	6-A	2	IDS	C2-O2-S	7.95	128.28	117.91
1	13-A	2	IDS	C2-O2-S	7.95	128.28	117.91
1	10-A	24	IDS	C2-O2-S	7.95	128.28	117.91
1	8-A	28	IDS	C2-O2-S	7.95	128.28	117.91
1	7-A	10	IDS	C2-O2-S	7.95	128.28	117.91
1	1-A	18	IDS	C2-O2-S	7.95	128.28	117.91
1	4-A	22	IDS	C2-O2-S	7.95	128.28	117.91
1	6-A	4	IDS	C2-O2-S	7.95	128.28	117.91
1	7-A	20	IDS	C2-O2-S	7.95	128.28	117.91
1	5-A	26	IDS	C2-O2-S	7.95	128.28	117.91
1	5-A	10	IDS	C2-O2-S	7.95	128.27	117.91
1	12-A	16	IDS	C2-O2-S	7.95	128.27	117.91
1	13-A	22	IDS	C2-O2-S	7.95	128.27	117.91
1	14-A	2	IDS	C2-O2-S	7.95	128.27	117.91
1	1-A	4	IDS	C2-O2-S	7.95	128.27	117.91
1	12-A	4	IDS	C2-O2-S	7.95	128.27	117.91
1	4-A	14	IDS	C2-O2-S	7.95	128.27	117.91
1	8-A	4	IDS	C2-O2-S	7.94	128.27	117.91
1	5-A	14	IDS	C2-O2-S	7.94	128.27	117.91
1	8-A	16	IDS	C2-O2-S	7.94	128.27	117.91
1	4-A	28	IDS	C2-O2-S	7.94	128.27	117.91
1	1-A	24	IDS	C2-O2-S	7.94	128.27	117.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	8	IDS	C2-O2-S	7.94	128.27	117.91
1	12-A	22	IDS	C2-O2-S	7.94	128.27	117.91
1	7-A	8	IDS	C2-O2-S	7.94	128.27	117.91
1	9-A	10	IDS	C2-O2-S	7.94	128.27	117.91
1	1-A	2	IDS	C2-O2-S	7.94	128.26	117.91
1	6-A	28	IDS	C2-O2-S	7.94	128.26	117.91
1	13-A	28	IDS	C2-O2-S	7.94	128.26	117.91
1	11-A	30	IDS	C2-O2-S	7.94	128.26	117.91
1	7-A	2	IDS	C2-O2-S	7.94	128.26	117.91
1	12-A	14	IDS	C2-O2-S	7.94	128.26	117.91
1	3-A	16	IDS	C2-O2-S	7.94	128.26	117.91
1	10-A	20	IDS	C2-O2-S	7.94	128.26	117.91
1	7-A	28	IDS	C2-O2-S	7.94	128.26	117.91
1	5-A	6	IDS	C2-O2-S	7.94	128.26	117.91
1	6-A	14	IDS	C2-O2-S	7.94	128.26	117.91
1	10-A	22	IDS	C2-O2-S	7.94	128.26	117.91
1	4-A	24	IDS	C2-O2-S	7.94	128.26	117.91
1	3-A	8	IDS	C2-O2-S	7.93	128.26	117.91
1	14-A	12	IDS	C2-O2-S	7.93	128.26	117.91
1	11-A	22	IDS	C2-O2-S	7.93	128.26	117.91
1	2-A	30	IDS	C2-O2-S	7.93	128.26	117.91
1	5-A	4	IDS	C2-O2-S	7.93	128.26	117.91
1	10-A	10	IDS	C2-O2-S	7.93	128.26	117.91
1	13-A	14	IDS	C2-O2-S	7.93	128.26	117.91
1	8-A	18	IDS	C2-O2-S	7.93	128.26	117.91
1	8-A	22	IDS	C2-O2-S	7.93	128.26	117.91
1	14-A	30	IDS	C2-O2-S	7.93	128.26	117.91
1	4-A	4	IDS	C2-O2-S	7.93	128.25	117.91
1	7-A	6	IDS	C2-O2-S	7.93	128.25	117.91
1	4-A	16	IDS	C2-O2-S	7.93	128.25	117.91
1	1-A	10	IDS	C2-O2-S	7.93	128.25	117.91
1	13-A	18	IDS	C2-O2-S	7.93	128.25	117.91
1	11-A	24	IDS	C2-O2-S	7.93	128.25	117.91
1	12-A	26	IDS	C2-O2-S	7.93	128.25	117.91
1	11-A	4	IDS	C2-O2-S	7.93	128.25	117.91
1	8-A	6	IDS	C2-O2-S	7.93	128.25	117.91
1	3-A	14	IDS	C2-O2-S	7.93	128.25	117.91
1	4-A	2	IDS	C2-O2-S	7.93	128.25	117.91
1	12-A	20	IDS	C2-O2-S	7.93	128.25	117.91
1	9-A	8	IDS	C2-O2-S	7.93	128.25	117.91
1	7-A	24	IDS	C2-O2-S	7.93	128.25	117.91
1	10-A	28	IDS	C2-O2-S	7.93	128.25	117.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	30	IDS	C2-O2-S	7.93	128.25	117.91
1	8-A	24	IDS	C2-O2-S	7.93	128.25	117.91
1	12-A	24	IDS	C2-O2-S	7.93	128.25	117.91
1	9-A	6	IDS	C2-O2-S	7.93	128.25	117.91
1	9-A	2	IDS	C2-O2-S	7.93	128.25	117.91
1	2-A	4	IDS	C2-O2-S	7.93	128.25	117.91
1	8-A	20	IDS	C2-O2-S	7.93	128.25	117.91
1	5-A	16	IDS	C2-O2-S	7.92	128.25	117.91
1	14-A	6	IDS	C2-O2-S	7.92	128.24	117.91
1	11-A	14	IDS	C2-O2-S	7.92	128.24	117.91
1	3-A	20	IDS	C2-O2-S	7.92	128.24	117.91
1	13-A	20	IDS	C2-O2-S	7.92	128.24	117.91
1	8-A	10	IDS	C2-O2-S	7.92	128.24	117.91
1	12-A	18	IDS	C2-O2-S	7.92	128.24	117.91
1	9-A	22	IDS	C2-O2-S	7.92	128.24	117.91
1	6-A	6	IDS	C2-O2-S	7.92	128.24	117.91
1	1-A	30	IDS	C2-O2-S	7.92	128.24	117.91
1	4-A	6	IDS	C2-O2-S	7.92	128.24	117.91
1	2-A	20	IDS	C2-O2-S	7.92	128.24	117.91
1	12-A	6	IDS	C2-O2-S	7.92	128.24	117.91
1	10-A	8	IDS	C2-O2-S	7.92	128.24	117.91
1	2-A	24	IDS	C2-O2-S	7.92	128.24	117.91
1	13-A	26	IDS	C2-O2-S	7.92	128.24	117.91
1	3-A	30	IDS	C2-O2-S	7.92	128.24	117.91
1	12-A	2	IDS	C2-O2-S	7.92	128.24	117.91
1	6-A	18	IDS	C2-O2-S	7.92	128.24	117.91
1	5-A	22	IDS	C2-O2-S	7.92	128.24	117.91
1	13-A	10	IDS	C2-O2-S	7.92	128.23	117.91
1	3-A	18	IDS	C2-O2-S	7.92	128.23	117.91
1	9-A	18	IDS	C2-O2-S	7.92	128.23	117.91
1	11-A	18	IDS	C2-O2-S	7.91	128.23	117.91
1	12-A	8	IDS	C2-O2-S	7.91	128.23	117.91
1	11-A	8	IDS	C2-O2-S	7.91	128.23	117.91
1	2-A	18	IDS	C2-O2-S	7.91	128.23	117.91
1	9-A	28	IDS	C2-O2-S	7.91	128.23	117.91
1	13-A	24	IDS	C2-O2-S	7.91	128.23	117.91
1	6-A	20	IDS	C2-O2-S	7.91	128.23	117.91
1	11-A	28	IDS	C2-O2-S	7.91	128.23	117.91
1	4-A	8	IDS	C2-O2-S	7.91	128.23	117.91
1	8-A	8	IDS	C2-O2-S	7.91	128.23	117.91
1	14-A	20	IDS	C2-O2-S	7.91	128.23	117.91
1	9-A	24	IDS	C2-O2-S	7.91	128.23	117.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	6	IDS	C2-O2-S	7.91	128.22	117.91
1	9-A	26	IDS	C2-O2-S	7.91	128.22	117.91
1	7-A	4	IDS	C2-O2-S	7.91	128.22	117.91
1	5-A	8	IDS	C2-O2-S	7.91	128.22	117.91
1	1-A	20	IDS	C2-O2-S	7.91	128.22	117.91
1	4-A	20	IDS	C2-O2-S	7.90	128.22	117.91
1	13-A	4	IDS	C2-O2-S	7.90	128.22	117.91
1	10-A	6	IDS	C2-O2-S	7.90	128.22	117.91
1	2-A	10	IDS	C2-O2-S	7.90	128.22	117.91
1	6-A	26	IDS	C2-O2-S	7.90	128.22	117.91
1	12-A	10	IDS	C2-O2-S	7.90	128.22	117.91
1	5-A	18	IDS	C2-O2-S	7.90	128.22	117.91
1	4-A	10	IDS	C2-O2-S	7.90	128.21	117.91
1	3-A	26	IDS	C2-O2-S	7.90	128.21	117.91
1	10-A	18	IDS	C2-O2-S	7.90	128.21	117.91
1	2-A	14	IDS	C2-O2-S	7.90	128.21	117.91
1	5-A	20	IDS	C2-O2-S	7.90	128.21	117.91
1	9-A	20	IDS	C2-O2-S	7.90	128.21	117.91
1	14-A	26	IDS	C2-O2-S	7.90	128.21	117.91
1	11-A	10	IDS	C2-O2-S	7.89	128.21	117.91
1	7-A	14	IDS	C2-O2-S	7.89	128.21	117.91
1	14-A	24	IDS	C2-O2-S	7.89	128.21	117.91
1	2-A	6	IDS	C2-O2-S	7.89	128.20	117.91
1	13-A	6	IDS	C2-O2-S	7.89	128.20	117.91
1	6-A	10	IDS	C2-O2-S	7.89	128.20	117.91
1	1-A	14	IDS	C2-O2-S	7.89	128.20	117.91
1	14-A	18	IDS	C2-O2-S	7.89	128.20	117.91
1	2-A	26	IDS	C2-O2-S	7.89	128.20	117.91
1	10-A	4	IDS	C2-O2-S	7.89	128.20	117.91
1	14-A	14	IDS	C2-O2-S	7.89	128.20	117.91
1	7-A	18	IDS	C2-O2-S	7.88	128.18	117.91
1	11-A	20	IDS	C2-O2-S	7.88	128.18	117.91
1	11-A	26	IDS	C2-O2-S	7.87	128.18	117.91
1	8-A	14	IDS	C2-O2-S	7.87	128.18	117.91
1	4-A	18	IDS	C2-O2-S	7.87	128.17	117.91
1	11-A	6	IDS	C2-O2-S	7.87	128.17	117.91
1	14-A	10	IDS	C2-O2-S	7.86	128.16	117.91
1	1-A	26	IDS	C2-O2-S	7.85	128.15	117.91
1	1-A	6	IDS	C2-O2-S	7.84	128.14	117.91
1	5-A	30	IDS	O6B-C6-C5	3.04	121.70	113.03
1	11-A	30	IDS	O6B-C6-C5	3.03	121.69	113.03
1	13-A	30	IDS	O6B-C6-C5	3.02	121.66	113.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	30	IDS	O6B-C6-C5	3.02	121.65	113.03
1	10-A	30	IDS	O6B-C6-C5	3.02	121.65	113.03
1	8-A	30	IDS	O6B-C6-C5	3.02	121.64	113.03
1	1-A	30	IDS	O6B-C6-C5	3.02	121.64	113.03
1	4-A	30	IDS	O6B-C6-C5	3.02	121.64	113.03
1	14-A	30	IDS	O6B-C6-C5	3.01	121.64	113.03
1	9-A	30	IDS	O6B-C6-C5	3.01	121.62	113.03
1	12-A	30	IDS	O6B-C6-C5	3.01	121.61	113.03
1	3-A	30	IDS	O6B-C6-C5	3.00	121.60	113.03
1	7-A	30	IDS	O6B-C6-C5	3.00	121.60	113.03
1	2-A	30	IDS	O6B-C6-C5	2.99	121.57	113.03
1	8-A	9	SGN	O1S-S1-O2S	-2.92	113.26	120.16
1	9-A	27	SGN	O1S-S1-O2S	-2.92	113.27	120.16
1	3-A	9	SGN	O1S-S1-O2S	-2.92	113.27	120.16
1	2-A	19	SGN	O1S-S1-O2S	-2.91	113.28	120.16
1	5-A	17	SGN	O1S-S1-O2S	-2.91	113.29	120.16
1	9-A	9	SGN	O1S-S1-O2S	-2.91	113.29	120.16
1	6-A	27	SGN	O1S-S1-O2S	-2.90	113.30	120.16
1	14-A	19	SGN	O1S-S1-O2S	-2.90	113.30	120.16
1	11-A	7	SGN	O1S-S1-O2S	-2.90	113.30	120.16
1	10-A	9	SGN	O1S-S1-O2S	-2.90	113.30	120.16
1	1-A	9	SGN	O1S-S1-O2S	-2.90	113.30	120.16
1	5-A	27	SGN	O1S-S1-O2S	-2.90	113.30	120.16
1	5-A	9	SGN	O1S-S1-O2S	-2.90	113.31	120.16
1	5-A	19	SGN	O1S-S1-O2S	-2.90	113.31	120.16
1	8-A	27	SGN	O1S-S1-O2S	-2.90	113.31	120.16
1	11-A	27	SGN	O1S-S1-O2S	-2.90	113.31	120.16
1	7-A	9	SGN	O1S-S1-O2S	-2.90	113.31	120.16
1	11-A	9	SGN	O1S-S1-O2S	-2.89	113.32	120.16
1	12-A	19	SGN	O1S-S1-O2S	-2.89	113.32	120.16
1	13-A	19	SGN	O1S-S1-O2S	-2.89	113.32	120.16
1	3-A	23	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	6-A	19	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	1-A	3	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	2-A	17	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	7-A	19	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	9-A	3	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	1-A	15	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	9-A	7	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	1-A	19	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	4-A	29	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	3-A	19	SGN	O1S-S1-O2S	-2.89	113.33	120.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	27	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	13-A	27	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	14-A	9	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	4-A	19	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	10-A	27	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	5-A	29	SGN	O1S-S1-O2S	-2.89	113.33	120.16
1	11-A	21	SGN	O1S-S1-O2S	-2.89	113.34	120.16
1	3-A	7	SGN	O1S-S1-O2S	-2.89	113.34	120.16
1	1-A	1	SGN	O1S-S1-O2S	-2.89	113.34	120.16
1	12-A	9	SGN	O1S-S1-O2S	-2.88	113.34	120.16
1	10-A	23	SGN	O1S-S1-O2S	-2.88	113.34	120.16
1	14-A	27	SGN	O1S-S1-O2S	-2.88	113.34	120.16
1	2-A	27	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	4-A	7	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	2-A	13	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	5-A	23	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	9-A	29	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	11-A	3	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	13-A	13	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	14-A	7	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	12-A	21	SGN	O1S-S1-O2S	-2.88	113.35	120.16
1	7-A	13	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	9-A	13	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	10-A	17	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	4-A	9	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	7-A	7	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	6-A	7	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	9-A	19	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	7-A	27	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	6-A	21	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	6-A	15	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	10-A	29	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	12-A	7	SGN	O1S-S1-O2S	-2.88	113.36	120.16
1	12-A	13	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	14-A	15	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	9-A	17	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	11-A	29	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	1-A	27	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	8-A	7	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	8-A	19	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	6-A	23	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	10-A	7	SGN	O1S-S1-O2S	-2.87	113.37	120.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	21	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	8-A	5	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	7-A	5	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	13-A	23	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	4-A	27	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	12-A	27	SGN	O1S-S1-O2S	-2.87	113.37	120.16
1	6-A	3	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	13-A	9	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	4-A	5	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	2-A	11	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	7-A	21	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	2-A	9	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	6-A	29	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	6-A	13	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	9-A	15	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	6-A	17	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	10-A	1	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	4-A	13	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	14-A	29	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	4-A	3	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	7-A	15	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	1-A	23	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	5-A	3	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	12-A	11	SGN	O1S-S1-O2S	-2.87	113.38	120.16
1	12-A	25	SGN	O1S-S1-O2S	-2.87	113.39	120.16
1	5-A	7	SGN	O1S-S1-O2S	-2.87	113.39	120.16
1	8-A	15	SGN	O1S-S1-O2S	-2.87	113.39	120.16
1	12-A	23	SGN	O1S-S1-O2S	-2.87	113.39	120.16
1	5-A	13	SGN	O1S-S1-O2S	-2.87	113.39	120.16
1	5-A	11	SGN	O1S-S1-O2S	-2.86	113.39	120.16
1	5-A	1	SGN	O1S-S1-O2S	-2.86	113.39	120.16
1	12-A	15	SGN	O1S-S1-O2S	-2.86	113.39	120.16
1	5-A	25	SGN	O1S-S1-O2S	-2.86	113.39	120.16
1	11-A	17	SGN	O1S-S1-O2S	-2.86	113.39	120.16
1	8-A	23	SGN	O1S-S1-O2S	-2.86	113.39	120.16
1	12-A	1	SGN	O1S-S1-O2S	-2.86	113.40	120.16
1	9-A	23	SGN	O1S-S1-O2S	-2.86	113.40	120.16
1	5-A	15	SGN	O1S-S1-O2S	-2.86	113.40	120.16
1	14-A	21	SGN	O1S-S1-O2S	-2.86	113.40	120.16
1	7-A	3	SGN	O1S-S1-O2S	-2.86	113.40	120.16
1	11-A	13	SGN	O1S-S1-O2S	-2.86	113.40	120.16
1	4-A	17	SGN	O1S-S1-O2S	-2.86	113.40	120.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	29	SGN	O1S-S1-O2S	-2.86	113.40	120.16
1	4-A	21	SGN	O1S-S1-O2S	-2.86	113.40	120.16
1	6-A	9	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	1-A	11	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	11-A	5	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	10-A	19	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	2-A	23	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	10-A	5	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	1-A	21	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	9-A	21	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	13-A	21	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	13-A	11	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	3-A	25	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	11-A	25	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	3-A	3	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	11-A	15	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	1-A	29	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	4-A	1	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	13-A	3	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	2-A	21	SGN	O1S-S1-O2S	-2.86	113.41	120.16
1	13-A	1	SGN	O1S-S1-O2S	-2.85	113.41	120.16
1	8-A	11	SGN	O1S-S1-O2S	-2.85	113.41	120.16
1	3-A	17	SGN	O1S-S1-O2S	-2.85	113.41	120.16
1	12-A	17	SGN	O1S-S1-O2S	-2.85	113.41	120.16
1	13-A	29	SGN	O1S-S1-O2S	-2.85	113.41	120.16
1	9-A	11	SGN	O1S-S1-O2S	-2.85	113.41	120.16
1	2-A	15	SGN	O1S-S1-O2S	-2.85	113.41	120.16
1	2-A	29	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	8-A	1	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	12-A	29	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	3-A	5	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	12-A	3	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	8-A	17	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	3-A	21	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	11-A	23	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	9-A	1	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	10-A	13	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	7-A	17	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	7-A	29	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	2-A	7	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	11-A	11	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	11-A	19	SGN	O1S-S1-O2S	-2.85	113.42	120.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	29	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	6-A	1	SGN	O1S-S1-O2S	-2.85	113.42	120.16
1	8-A	3	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	6-A	11	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	4-A	23	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	2-A	1	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	13-A	15	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	13-A	7	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	14-A	11	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	6-A	25	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	14-A	17	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	1-A	17	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	14-A	13	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	4-A	15	SGN	O1S-S1-O2S	-2.85	113.43	120.16
1	7-A	11	SGN	O1S-S1-O2S	-2.85	113.44	120.16
1	3-A	1	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	3-A	13	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	8-A	13	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	13-A	17	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	14-A	23	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	14-A	25	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	5-A	5	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	4-A	11	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	10-A	21	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	14-A	1	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	10-A	15	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	1-A	25	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	5-A	21	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	9-A	5	SGN	O1S-S1-O2S	-2.84	113.44	120.16
1	13-A	5	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	10-A	11	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	3-A	15	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	11-A	1	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	7-A	23	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	2-A	25	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	14-A	3	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	1-A	7	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	10-A	25	SGN	O1S-S1-O2S	-2.84	113.45	120.16
1	3-A	11	SGN	O1S-S1-O2S	-2.84	113.46	120.16
1	14-A	20	IDS	O6B-C6-O6A	-2.84	117.65	124.09
1	14-A	5	SGN	O1S-S1-O2S	-2.84	113.46	120.16
1	9-A	25	SGN	O1S-S1-O2S	-2.84	113.46	120.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	16	IDS	O6B-C6-O6A	-2.84	117.65	124.09
1	4-A	6	IDS	O6B-C6-O6A	-2.83	117.65	124.09
1	1-A	13	SGN	O1S-S1-O2S	-2.83	113.47	120.16
1	6-A	5	SGN	O1S-S1-O2S	-2.83	113.47	120.16
1	2-A	6	IDS	O6B-C6-O6A	-2.83	117.66	124.09
1	3-A	6	IDS	O6B-C6-O6A	-2.83	117.66	124.09
1	7-A	6	IDS	O6B-C6-O6A	-2.83	117.66	124.09
1	9-A	16	IDS	O6B-C6-O6A	-2.83	117.66	124.09
1	2-A	5	SGN	O1S-S1-O2S	-2.83	113.47	120.16
1	12-A	5	SGN	O1S-S1-O2S	-2.83	113.47	120.16
1	14-A	16	IDS	O6B-C6-O6A	-2.83	117.67	124.09
1	13-A	20	IDS	O6B-C6-O6A	-2.83	117.67	124.09
1	4-A	26	IDS	O6B-C6-O6A	-2.83	117.67	124.09
1	1-A	5	SGN	O1S-S1-O2S	-2.83	113.48	120.16
1	7-A	1	SGN	O1S-S1-O2S	-2.83	113.48	120.16
1	6-A	10	IDS	O6B-C6-O6A	-2.83	117.67	124.09
1	8-A	25	SGN	O1S-S1-O2S	-2.83	113.48	120.16
1	2-A	3	SGN	O1S-S1-O2S	-2.83	113.48	120.16
1	6-A	26	IDS	O6B-C6-O6A	-2.82	117.68	124.09
1	1-A	6	IDS	O6B-C6-O6A	-2.82	117.68	124.09
1	9-A	20	IDS	O6B-C6-O6A	-2.82	117.68	124.09
1	1-A	20	IDS	O6B-C6-O6A	-2.82	117.69	124.09
1	13-A	25	SGN	O1S-S1-O2S	-2.82	113.50	120.16
1	12-A	10	IDS	O6B-C6-O6A	-2.82	117.69	124.09
1	4-A	25	SGN	O1S-S1-O2S	-2.82	113.50	120.16
1	10-A	6	IDS	O6B-C6-O6A	-2.82	117.69	124.09
1	1-A	26	IDS	O6B-C6-O6A	-2.82	117.69	124.09
1	11-A	10	IDS	O6B-C6-O6A	-2.82	117.69	124.09
1	7-A	16	IDS	O6B-C6-O6A	-2.82	117.69	124.09
1	7-A	25	SGN	O1S-S1-O2S	-2.82	113.50	120.16
1	1-A	10	IDS	O6B-C6-O6A	-2.82	117.69	124.09
1	10-A	3	SGN	O1S-S1-O2S	-2.82	113.51	120.16
1	1-A	16	IDS	O6B-C6-O6A	-2.82	117.70	124.09
1	3-A	26	IDS	O6B-C6-O6A	-2.82	117.70	124.09
1	13-A	6	IDS	O6B-C6-O6A	-2.82	117.70	124.09
1	6-A	16	IDS	O6B-C6-O6A	-2.82	117.70	124.09
1	9-A	6	IDS	O6B-C6-O6A	-2.81	117.70	124.09
1	8-A	14	IDS	O6B-C6-O6A	-2.81	117.70	124.09
1	2-A	26	IDS	O6B-C6-O6A	-2.81	117.70	124.09
1	13-A	4	IDS	O6B-C6-O6A	-2.81	117.70	124.09
1	3-A	8	IDS	O6B-C6-O6A	-2.81	117.70	124.09
1	11-A	12	IDS	O6B-C6-O6A	-2.81	117.70	124.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	12-A	26	IDS	O6B-C6-O6A	-2.81	117.70	124.09
1	5-A	30	IDS	O6B-C6-O6A	-2.81	117.70	124.09
1	6-A	6	IDS	O6B-C6-O6A	-2.81	117.70	124.09
1	11-A	6	IDS	O6B-C6-O6A	-2.81	117.71	124.09
1	14-A	6	IDS	O6B-C6-O6A	-2.81	117.71	124.09
1	14-A	26	IDS	O6B-C6-O6A	-2.81	117.71	124.09
1	10-A	16	IDS	O6B-C6-O6A	-2.81	117.71	124.09
1	13-A	16	IDS	O6B-C6-O6A	-2.81	117.71	124.09
1	11-A	16	IDS	O6B-C6-O6A	-2.81	117.71	124.09
1	9-A	26	IDS	O6B-C6-O6A	-2.81	117.71	124.09
1	10-A	20	IDS	O6B-C6-O6A	-2.81	117.72	124.09
1	5-A	4	IDS	O6B-C6-O6A	-2.81	117.72	124.09
1	7-A	26	IDS	O6B-C6-O6A	-2.81	117.72	124.09
1	13-A	26	IDS	O6B-C6-O6A	-2.81	117.72	124.09
1	8-A	4	IDS	O6B-C6-O6A	-2.81	117.72	124.09
1	8-A	16	IDS	O6B-C6-O6A	-2.80	117.72	124.09
1	4-A	10	IDS	O6B-C6-O6A	-2.80	117.72	124.09
1	2-A	10	IDS	O6B-C6-O6A	-2.80	117.72	124.09
1	3-A	16	IDS	O6B-C6-O6A	-2.80	117.72	124.09
1	11-A	26	IDS	O6B-C6-O6A	-2.80	117.72	124.09
1	8-A	6	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	12-A	16	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	4-A	4	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	8-A	26	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	8-A	30	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	5-A	16	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	10-A	26	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	7-A	4	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	4-A	20	IDS	O6B-C6-O6A	-2.80	117.73	124.09
1	6-A	12	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	4-A	16	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	13-A	18	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	12-A	2	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	3-A	10	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	11-A	28	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	6-A	20	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	12-A	30	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	10-A	10	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	1-A	30	IDS	O6B-C6-O6A	-2.80	117.74	124.09
1	9-A	10	IDS	O6B-C6-O6A	-2.79	117.74	124.09
1	13-A	10	IDS	O6B-C6-O6A	-2.79	117.74	124.09
1	7-A	10	IDS	O6B-C6-O6A	-2.79	117.75	124.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-A	2	IDS	O6B-C6-O6A	-2.79	117.75	124.09
1	8-A	20	IDS	O6B-C6-O6A	-2.79	117.75	124.09
1	9-A	4	IDS	O6B-C6-O6A	-2.79	117.75	124.09
1	12-A	4	IDS	O6B-C6-O6A	-2.79	117.75	124.09
1	12-A	6	IDS	O6B-C6-O6A	-2.79	117.76	124.09
1	11-A	8	IDS	O6B-C6-O6A	-2.79	117.76	124.09
1	5-A	6	IDS	O6B-C6-O6A	-2.79	117.76	124.09
1	2-A	30	IDS	O6B-C6-O6A	-2.79	117.76	124.09
1	3-A	30	IDS	O6B-C6-O6A	-2.79	117.76	124.09
1	2-A	12	IDS	O6B-C6-O6A	-2.79	117.77	124.09
1	14-A	28	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	2-A	20	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	7-A	20	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	14-A	30	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	13-A	28	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	11-A	30	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	2-A	4	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	8-A	18	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	7-A	28	IDS	O6B-C6-O6A	-2.78	117.77	124.09
1	14-A	10	IDS	O6B-C6-O6A	-2.78	117.78	124.09
1	4-A	30	IDS	O6B-C6-O6A	-2.78	117.78	124.09
1	5-A	10	IDS	O6B-C6-O6A	-2.78	117.78	124.09
1	10-A	12	IDS	O6B-C6-O6A	-2.78	117.78	124.09
1	5-A	14	IDS	O6B-C6-O6A	-2.78	117.78	124.09
1	10-A	30	IDS	O6B-C6-O6A	-2.78	117.78	124.09
1	14-A	4	IDS	O6B-C6-O6A	-2.78	117.78	124.09
1	8-A	10	IDS	O6B-C6-O6A	-2.78	117.78	124.09
1	6-A	24	IDS	O6B-C6-O6A	-2.78	117.79	124.09
1	7-A	12	IDS	O6B-C6-O6A	-2.77	117.79	124.09
1	9-A	12	IDS	O6B-C6-O6A	-2.77	117.79	124.09
1	10-A	18	IDS	O6B-C6-O6A	-2.77	117.79	124.09
1	11-A	18	IDS	O6B-C6-O6A	-2.77	117.79	124.09
1	6-A	14	IDS	O6B-C6-O6A	-2.77	117.79	124.09
1	2-A	18	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	12-A	20	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	6-A	30	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	6-A	4	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	3-A	20	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	5-A	26	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	14-A	24	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	3-A	4	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	3-A	14	IDS	O6B-C6-O6A	-2.77	117.80	124.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	22	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	2-A	24	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	11-A	4	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	4-A	12	IDS	O6B-C6-O6A	-2.77	117.80	124.09
1	12-A	12	IDS	O6B-C6-O6A	-2.77	117.81	124.09
1	5-A	20	IDS	O6B-C6-O6A	-2.77	117.81	124.09
1	5-A	2	IDS	O6B-C6-O6A	-2.77	117.81	124.09
1	7-A	14	IDS	O6B-C6-O6A	-2.77	117.81	124.09
1	7-A	22	IDS	O6B-C6-O6A	-2.77	117.81	124.09
1	13-A	12	IDS	O6B-C6-O6A	-2.77	117.81	124.09
1	1-A	8	IDS	O6B-C6-O6A	-2.77	117.81	124.09
1	12-A	14	IDS	O6B-C6-O6A	-2.77	117.81	124.09
1	9-A	28	IDS	O6B-C6-O6A	-2.76	117.81	124.09
1	8-A	2	IDS	O6B-C6-O6A	-2.76	117.82	124.09
1	10-A	4	IDS	O6B-C6-O6A	-2.76	117.82	124.09
1	12-A	8	IDS	O6B-C6-O6A	-2.76	117.82	124.09
1	8-A	8	IDS	O6B-C6-O6A	-2.76	117.82	124.09
1	4-A	28	IDS	O6B-C6-O6A	-2.76	117.82	124.09
1	1-A	14	IDS	O6B-C6-O6A	-2.76	117.82	124.09
1	5-A	22	IDS	O6B-C6-O6A	-2.76	117.82	124.09
1	4-A	18	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	11-A	20	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	14-A	2	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	5-A	18	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	5-A	28	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	6-A	18	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	1-A	24	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	7-A	18	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	9-A	22	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	12-A	28	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	13-A	14	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	3-A	28	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	6-A	28	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	7-A	8	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	1-A	18	IDS	O6B-C6-O6A	-2.76	117.83	124.09
1	10-A	22	IDS	O6B-C6-O6A	-2.75	117.83	124.09
1	5-A	8	IDS	O6B-C6-O6A	-2.75	117.83	124.09
1	8-A	28	IDS	O6B-C6-O6A	-2.75	117.83	124.09
1	1-A	4	IDS	O6B-C6-O6A	-2.75	117.84	124.09
1	1-A	12	IDS	O6B-C6-O6A	-2.75	117.84	124.09
1	6-A	22	IDS	O6B-C6-O6A	-2.75	117.84	124.09
1	2-A	28	IDS	O6B-C6-O6A	-2.75	117.84	124.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	11-A	2	IDS	O6B-C6-O6A	-2.75	117.84	124.09
1	14-A	14	IDS	O6B-C6-O6A	-2.75	117.84	124.09
1	14-A	12	IDS	O6B-C6-O6A	-2.75	117.84	124.09
1	10-A	2	IDS	O6B-C6-O6A	-2.75	117.84	124.09
1	3-A	12	IDS	O6B-C6-O6A	-2.75	117.84	124.09
1	13-A	8	IDS	O6B-C6-O6A	-2.75	117.85	124.09
1	9-A	18	IDS	O6B-C6-O6A	-2.75	117.85	124.09
1	10-A	24	IDS	O6B-C6-O6A	-2.75	117.86	124.09
1	11-A	24	IDS	O6B-C6-O6A	-2.75	117.86	124.09
1	9-A	30	IDS	O6B-C6-O6A	-2.75	117.86	124.09
1	10-A	8	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	8-A	24	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	13-A	30	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	4-A	14	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	6-A	8	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	12-A	22	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	1-A	28	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	4-A	24	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	4-A	8	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	11-A	14	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	9-A	2	IDS	O6B-C6-O6A	-2.74	117.86	124.09
1	7-A	2	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	13-A	22	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	9-A	14	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	8-A	12	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	9-A	24	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	12-A	24	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	3-A	2	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	4-A	2	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	9-A	8	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	4-A	22	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	3-A	24	IDS	O6B-C6-O6A	-2.74	117.87	124.09
1	10-A	28	IDS	O6B-C6-O6A	-2.74	117.88	124.09
1	14-A	8	IDS	O6B-C6-O6A	-2.74	117.88	124.09
1	14-A	22	IDS	O6B-C6-O6A	-2.73	117.88	124.09
1	12-A	18	IDS	O6B-C6-O6A	-2.73	117.88	124.09
1	2-A	14	IDS	O6B-C6-O6A	-2.73	117.89	124.09
1	7-A	30	IDS	O6B-C6-O6A	-2.73	117.89	124.09
1	1-A	2	IDS	O6B-C6-O6A	-2.73	117.89	124.09
1	2-A	2	IDS	O6B-C6-O6A	-2.73	117.90	124.09
1	14-A	18	IDS	O6B-C6-O6A	-2.73	117.90	124.09
1	5-A	12	IDS	O6B-C6-O6A	-2.73	117.90	124.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13-A	24	IDS	O6B-C6-O6A	-2.73	117.90	124.09
1	2-A	22	IDS	O6B-C6-O6A	-2.72	117.91	124.09
1	10-A	14	IDS	O6B-C6-O6A	-2.72	117.91	124.09
1	7-A	24	IDS	O6B-C6-O6A	-2.72	117.91	124.09
1	6-A	2	IDS	O6B-C6-O6A	-2.72	117.91	124.09
1	2-A	8	IDS	O6B-C6-O6A	-2.72	117.92	124.09
1	3-A	18	IDS	O6B-C6-O6A	-2.71	117.92	124.09
1	8-A	22	IDS	O6B-C6-O6A	-2.71	117.93	124.09
1	3-A	22	IDS	O6B-C6-O6A	-2.71	117.94	124.09
1	5-A	24	IDS	O6B-C6-O6A	-2.71	117.94	124.09
1	1-A	22	IDS	O6B-C6-O6A	-2.71	117.95	124.09
1	12-A	26	IDS	O6B-C6-C5	2.22	121.78	113.65
1	11-A	26	IDS	O6B-C6-C5	2.22	121.77	113.65
1	10-A	6	IDS	O6B-C6-C5	2.22	121.76	113.65
1	7-A	26	IDS	O6B-C6-C5	2.22	121.76	113.65
1	13-A	26	IDS	O6B-C6-C5	2.22	121.76	113.65
1	2-A	16	IDS	O6B-C6-C5	2.21	121.76	113.65
1	12-A	6	IDS	O6B-C6-C5	2.21	121.76	113.65
1	7-A	16	IDS	O6B-C6-C5	2.21	121.75	113.65
1	9-A	26	IDS	O6B-C6-C5	2.21	121.75	113.65
1	14-A	6	IDS	O6B-C6-C5	2.21	121.75	113.65
1	3-A	6	IDS	O6B-C6-C5	2.21	121.74	113.65
1	14-A	16	IDS	O6B-C6-C5	2.21	121.74	113.65
1	1-A	6	IDS	O6B-C6-C5	2.21	121.74	113.65
1	4-A	6	IDS	O6B-C6-C5	2.21	121.74	113.65
1	3-A	16	IDS	O6B-C6-C5	2.21	121.74	113.65
1	3-A	8	IDS	O6B-C6-C5	2.21	121.74	113.65
1	2-A	6	IDS	O6B-C6-C5	2.21	121.73	113.65
1	1-A	16	IDS	O6B-C6-C5	2.21	121.73	113.65
1	6-A	6	IDS	O6B-C6-C5	2.21	121.73	113.65
1	4-A	26	IDS	O6B-C6-C5	2.21	121.73	113.65
1	13-A	6	IDS	O6B-C6-C5	2.21	121.72	113.65
1	10-A	16	IDS	O6B-C6-C5	2.21	121.72	113.65
1	10-A	26	IDS	O6B-C6-C5	2.21	121.72	113.65
1	2-A	26	IDS	O6B-C6-C5	2.21	121.72	113.65
1	5-A	16	IDS	O6B-C6-C5	2.20	121.72	113.65
1	9-A	6	IDS	O6B-C6-C5	2.20	121.72	113.65
1	11-A	16	IDS	O6B-C6-C5	2.20	121.72	113.65
1	1-A	10	IDS	O6B-C6-C5	2.20	121.71	113.65
1	6-A	26	IDS	O6B-C6-C5	2.20	121.71	113.65
1	7-A	6	IDS	O6B-C6-C5	2.20	121.71	113.65
1	8-A	8	IDS	O6B-C6-C5	2.20	121.71	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	26	IDS	O6B-C6-C5	2.20	121.71	113.65
1	5-A	26	IDS	O6B-C6-C5	2.20	121.71	113.65
1	6-A	10	IDS	O6B-C6-C5	2.20	121.70	113.65
1	5-A	6	IDS	O6B-C6-C5	2.20	121.70	113.65
1	8-A	26	IDS	O6B-C6-C5	2.20	121.70	113.65
1	6-A	8	IDS	O6B-C6-C5	2.20	121.70	113.65
1	11-A	8	IDS	O6B-C6-C5	2.20	121.69	113.65
1	13-A	16	IDS	O6B-C6-C5	2.20	121.69	113.65
1	14-A	28	IDS	O6B-C6-C5	2.20	121.69	113.65
1	8-A	16	IDS	O6B-C6-C5	2.20	121.69	113.65
1	3-A	26	IDS	O6B-C6-C5	2.20	121.69	113.65
1	12-A	16	IDS	O6B-C6-C5	2.20	121.69	113.65
1	11-A	10	IDS	O6B-C6-C5	2.20	121.69	113.65
1	11-A	6	IDS	O6B-C6-C5	2.19	121.69	113.65
1	14-A	20	IDS	O6B-C6-C5	2.19	121.68	113.65
1	4-A	16	IDS	O6B-C6-C5	2.19	121.68	113.65
1	1-A	20	IDS	O6B-C6-C5	2.19	121.68	113.65
1	9-A	16	IDS	O6B-C6-C5	2.19	121.68	113.65
1	12-A	2	IDS	O6B-C6-C5	2.19	121.68	113.65
1	1-A	8	IDS	O6B-C6-C5	2.19	121.67	113.65
1	5-A	8	IDS	O6B-C6-C5	2.19	121.67	113.65
1	9-A	12	IDS	O6B-C6-C5	2.19	121.67	113.65
1	11-A	12	IDS	O6B-C6-C5	2.19	121.67	113.65
1	14-A	26	IDS	O6B-C6-C5	2.19	121.67	113.65
1	8-A	6	IDS	O6B-C6-C5	2.19	121.67	113.65
1	5-A	10	IDS	O6B-C6-C5	2.19	121.67	113.65
1	3-A	10	IDS	O6B-C6-C5	2.19	121.67	113.65
1	10-A	20	IDS	O6B-C6-C5	2.19	121.67	113.65
1	7-A	4	IDS	O6B-C6-C5	2.19	121.67	113.65
1	13-A	10	IDS	O6B-C6-C5	2.19	121.66	113.65
1	12-A	10	IDS	O6B-C6-C5	2.19	121.66	113.65
1	8-A	2	IDS	O6B-C6-C5	2.19	121.65	113.65
1	3-A	12	IDS	O6B-C6-C5	2.19	121.65	113.65
1	6-A	16	IDS	O6B-C6-C5	2.19	121.65	113.65
1	3-A	20	IDS	O6B-C6-C5	2.19	121.65	113.65
1	13-A	8	IDS	O6B-C6-C5	2.19	121.65	113.65
1	2-A	10	IDS	O6B-C6-C5	2.19	121.65	113.65
1	11-A	2	IDS	O6B-C6-C5	2.19	121.65	113.65
1	4-A	12	IDS	O6B-C6-C5	2.18	121.65	113.65
1	7-A	8	IDS	O6B-C6-C5	2.18	121.65	113.65
1	2-A	28	IDS	O6B-C6-C5	2.18	121.65	113.65
1	4-A	4	IDS	O6B-C6-C5	2.18	121.64	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	28	IDS	O6B-C6-C5	2.18	121.64	113.65
1	11-A	28	IDS	O6B-C6-C5	2.18	121.64	113.65
1	4-A	10	IDS	O6B-C6-C5	2.18	121.64	113.65
1	7-A	12	IDS	O6B-C6-C5	2.18	121.64	113.65
1	5-A	2	IDS	O6B-C6-C5	2.18	121.64	113.65
1	9-A	22	IDS	O6B-C6-C5	2.18	121.64	113.65
1	10-A	12	IDS	O6B-C6-C5	2.18	121.64	113.65
1	8-A	14	IDS	O6B-C6-C5	2.18	121.64	113.65
1	2-A	4	IDS	O6B-C6-C5	2.18	121.63	113.65
1	1-A	24	IDS	O6B-C6-C5	2.18	121.63	113.65
1	10-A	10	IDS	O6B-C6-C5	2.18	121.63	113.65
1	13-A	28	IDS	O6B-C6-C5	2.18	121.63	113.65
1	4-A	18	IDS	O6B-C6-C5	2.18	121.63	113.65
1	13-A	20	IDS	O6B-C6-C5	2.18	121.63	113.65
1	7-A	2	IDS	O6B-C6-C5	2.18	121.63	113.65
1	14-A	2	IDS	O6B-C6-C5	2.18	121.62	113.65
1	14-A	4	IDS	O6B-C6-C5	2.18	121.62	113.65
1	7-A	10	IDS	O6B-C6-C5	2.18	121.62	113.65
1	13-A	4	IDS	O6B-C6-C5	2.18	121.62	113.65
1	14-A	8	IDS	O6B-C6-C5	2.18	121.62	113.65
1	2-A	8	IDS	O6B-C6-C5	2.18	121.62	113.65
1	1-A	18	IDS	O6B-C6-C5	2.18	121.62	113.65
1	6-A	20	IDS	O6B-C6-C5	2.18	121.62	113.65
1	11-A	20	IDS	O6B-C6-C5	2.18	121.62	113.65
1	13-A	12	IDS	O6B-C6-C5	2.18	121.62	113.65
1	7-A	28	IDS	O6B-C6-C5	2.18	121.62	113.65
1	14-A	12	IDS	O6B-C6-C5	2.18	121.61	113.65
1	2-A	18	IDS	O6B-C6-C5	2.18	121.61	113.65
1	5-A	28	IDS	O6B-C6-C5	2.18	121.61	113.65
1	10-A	8	IDS	O6B-C6-C5	2.17	121.61	113.65
1	8-A	18	IDS	O6B-C6-C5	2.17	121.61	113.65
1	12-A	8	IDS	O6B-C6-C5	2.17	121.61	113.65
1	9-A	10	IDS	O6B-C6-C5	2.17	121.61	113.65
1	2-A	12	IDS	O6B-C6-C5	2.17	121.61	113.65
1	3-A	28	IDS	O6B-C6-C5	2.17	121.61	113.65
1	9-A	8	IDS	O6B-C6-C5	2.17	121.61	113.65
1	8-A	10	IDS	O6B-C6-C5	2.17	121.61	113.65
1	7-A	22	IDS	O6B-C6-C5	2.17	121.61	113.65
1	8-A	4	IDS	O6B-C6-C5	2.17	121.61	113.65
1	6-A	12	IDS	O6B-C6-C5	2.17	121.61	113.65
1	11-A	24	IDS	O6B-C6-C5	2.17	121.61	113.65
1	2-A	2	IDS	O6B-C6-C5	2.17	121.60	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	18	IDS	O6B-C6-C5	2.17	121.60	113.65
1	10-A	18	IDS	O6B-C6-C5	2.17	121.60	113.65
1	12-A	12	IDS	O6B-C6-C5	2.17	121.60	113.65
1	8-A	20	IDS	O6B-C6-C5	2.17	121.60	113.65
1	3-A	4	IDS	O6B-C6-C5	2.17	121.60	113.65
1	9-A	2	IDS	O6B-C6-C5	2.17	121.60	113.65
1	12-A	4	IDS	O6B-C6-C5	2.17	121.60	113.65
1	13-A	2	IDS	O6B-C6-C5	2.17	121.60	113.65
1	14-A	10	IDS	O6B-C6-C5	2.17	121.60	113.65
1	8-A	12	IDS	O6B-C6-C5	2.17	121.60	113.65
1	6-A	14	IDS	O6B-C6-C5	2.17	121.60	113.65
1	12-A	20	IDS	O6B-C6-C5	2.17	121.60	113.65
1	10-A	22	IDS	O6B-C6-C5	2.17	121.60	113.65
1	5-A	22	IDS	O6B-C6-C5	2.17	121.60	113.65
1	13-A	18	IDS	O6B-C6-C5	2.17	121.59	113.65
1	4-A	24	IDS	O6B-C6-C5	2.17	121.59	113.65
1	4-A	8	IDS	O6B-C6-C5	2.17	121.59	113.65
1	5-A	14	IDS	O6B-C6-C5	2.17	121.59	113.65
1	6-A	28	IDS	O6B-C6-C5	2.17	121.59	113.65
1	9-A	4	IDS	O6B-C6-C5	2.17	121.59	113.65
1	1-A	28	IDS	O6B-C6-C5	2.17	121.59	113.65
1	6-A	24	IDS	O6B-C6-C5	2.17	121.59	113.65
1	1-A	12	IDS	O6B-C6-C5	2.17	121.58	113.65
1	4-A	28	IDS	O6B-C6-C5	2.17	121.58	113.65
1	11-A	18	IDS	O6B-C6-C5	2.17	121.58	113.65
1	14-A	24	IDS	O6B-C6-C5	2.17	121.58	113.65
1	9-A	24	IDS	O6B-C6-C5	2.17	121.58	113.65
1	5-A	12	IDS	O6B-C6-C5	2.17	121.58	113.65
1	2-A	20	IDS	O6B-C6-C5	2.17	121.58	113.65
1	9-A	20	IDS	O6B-C6-C5	2.16	121.58	113.65
1	4-A	20	IDS	O6B-C6-C5	2.16	121.57	113.65
1	14-A	14	IDS	O6B-C6-C5	2.16	121.57	113.65
1	9-A	28	IDS	O6B-C6-C5	2.16	121.57	113.65
1	10-A	28	IDS	O6B-C6-C5	2.16	121.57	113.65
1	6-A	18	IDS	O6B-C6-C5	2.16	121.57	113.65
1	2-A	24	IDS	O6B-C6-C5	2.16	121.57	113.65
1	7-A	20	IDS	O6B-C6-C5	2.16	121.57	113.65
1	14-A	22	IDS	O6B-C6-C5	2.16	121.57	113.65
1	1-A	2	IDS	O6B-C6-C5	2.16	121.57	113.65
1	3-A	18	IDS	O6B-C6-C5	2.16	121.57	113.65
1	7-A	18	IDS	O6B-C6-C5	2.16	121.57	113.65
1	13-A	22	IDS	O6B-C6-C5	2.16	121.57	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	14	IDS	O6B-C6-C5	2.16	121.56	113.65
1	3-A	22	IDS	O6B-C6-C5	2.16	121.56	113.65
1	1-A	14	IDS	O6B-C6-C5	2.16	121.56	113.65
1	14-A	18	IDS	O6B-C6-C5	2.16	121.56	113.65
1	5-A	4	IDS	O6B-C6-C5	2.16	121.56	113.65
1	4-A	14	IDS	O6B-C6-C5	2.16	121.56	113.65
1	10-A	4	IDS	O6B-C6-C5	2.16	121.55	113.65
1	12-A	28	IDS	O6B-C6-C5	2.16	121.55	113.65
1	4-A	2	IDS	O6B-C6-C5	2.16	121.55	113.65
1	6-A	2	IDS	O6B-C6-C5	2.16	121.55	113.65
1	12-A	14	IDS	O6B-C6-C5	2.16	121.55	113.65
1	6-A	22	IDS	O6B-C6-C5	2.16	121.55	113.65
1	3-A	2	IDS	O6B-C6-C5	2.16	121.55	113.65
1	5-A	18	IDS	O6B-C6-C5	2.16	121.54	113.65
1	8-A	24	IDS	O6B-C6-C5	2.16	121.54	113.65
1	7-A	14	IDS	O6B-C6-C5	2.16	121.54	113.65
1	11-A	4	IDS	O6B-C6-C5	2.16	121.54	113.65
1	3-A	24	IDS	O6B-C6-C5	2.15	121.54	113.65
1	2-A	22	IDS	O6B-C6-C5	2.15	121.54	113.65
1	11-A	22	IDS	O6B-C6-C5	2.15	121.54	113.65
1	8-A	22	IDS	O6B-C6-C5	2.15	121.53	113.65
1	5-A	24	IDS	O6B-C6-C5	2.15	121.53	113.65
1	5-A	20	IDS	O6B-C6-C5	2.15	121.53	113.65
1	12-A	18	IDS	O6B-C6-C5	2.15	121.53	113.65
1	7-A	24	IDS	O6B-C6-C5	2.15	121.53	113.65
1	10-A	2	IDS	O6B-C6-C5	2.15	121.53	113.65
1	1-A	4	IDS	O6B-C6-C5	2.15	121.52	113.65
1	10-A	24	IDS	O6B-C6-C5	2.15	121.52	113.65
1	12-A	24	IDS	O6B-C6-C5	2.15	121.52	113.65
1	3-A	14	IDS	O6B-C6-C5	2.15	121.51	113.65
1	4-A	22	IDS	O6B-C6-C5	2.15	121.51	113.65
1	13-A	24	IDS	O6B-C6-C5	2.15	121.51	113.65
1	6-A	4	IDS	O6B-C6-C5	2.15	121.51	113.65
1	1-A	22	IDS	O6B-C6-C5	2.15	121.50	113.65
1	12-A	22	IDS	O6B-C6-C5	2.14	121.50	113.65
1	11-A	14	IDS	O6B-C6-C5	2.14	121.50	113.65
1	2-A	14	IDS	O6B-C6-C5	2.14	121.49	113.65
1	13-A	14	IDS	O6B-C6-C5	2.14	121.49	113.65
1	10-A	14	IDS	O6B-C6-C5	2.14	121.49	113.65

There are no chirality outliers.

All (1405) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1-A	1	SGN	C4-C5-C6-O6
1	1-A	1	SGN	O5-C5-C6-O6
1	1-A	1	SGN	C2-N2-S1-O2S
1	1-A	1	SGN	C2-N2-S1-O3S
1	2-A	1	SGN	C2-N2-S1-O1S
1	3-A	1	SGN	C4-C5-C6-O6
1	3-A	1	SGN	C6-O6-S2-O6S
1	4-A	1	SGN	O5-C5-C6-O6
1	4-A	1	SGN	C2-N2-S1-O2S
1	4-A	1	SGN	C2-N2-S1-O3S
1	5-A	1	SGN	C4-C5-C6-O6
1	5-A	1	SGN	O5-C5-C6-O6
1	5-A	1	SGN	C2-N2-S1-O2S
1	5-A	1	SGN	C2-N2-S1-O3S
1	6-A	1	SGN	O5-C5-C6-O6
1	6-A	1	SGN	C2-N2-S1-O1S
1	7-A	1	SGN	C1-C2-N2-S1
1	7-A	1	SGN	C3-C2-N2-S1
1	7-A	1	SGN	C4-C5-C6-O6
1	7-A	1	SGN	O5-C5-C6-O6
1	7-A	1	SGN	C2-N2-S1-O2S
1	7-A	1	SGN	C2-N2-S1-O3S
1	8-A	1	SGN	C2-N2-S1-O1S
1	13-A	1	SGN	C1-C2-N2-S1
1	13-A	1	SGN	C3-C2-N2-S1
1	13-A	1	SGN	C2-N2-S1-O2S
1	13-A	1	SGN	C2-N2-S1-O3S
1	14-A	1	SGN	C4-C5-C6-O6
1	14-A	1	SGN	O5-C5-C6-O6
1	1-A	2	IDS	C1-C2-O2-S
1	1-A	2	IDS	C3-C2-O2-S
1	4-A	2	IDS	C4-C5-C6-O6A
1	4-A	2	IDS	C4-C5-C6-O6B
1	5-A	2	IDS	C1-C2-O2-S
1	5-A	2	IDS	C3-C2-O2-S
1	6-A	2	IDS	C1-C2-O2-S
1	6-A	2	IDS	C3-C2-O2-S
1	9-A	2	IDS	C2-O2-S-O3S
1	10-A	2	IDS	C2-O2-S-O2S
1	1-A	3	SGN	C4-C5-C6-O6
1	1-A	3	SGN	O5-C5-C6-O6
1	1-A	3	SGN	C2-N2-S1-O2S
1	2-A	3	SGN	C2-N2-S1-O2S

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	12-A	5	SGN	C2-N2-S1-O2S
1	12-A	5	SGN	C2-N2-S1-O3S
1	14-A	5	SGN	O5-C5-C6-O6
1	14-A	5	SGN	C2-N2-S1-O2S
1	3-A	6	IDS	C2-O2-S-O3S
1	6-A	6	IDS	C1-C2-O2-S
1	6-A	6	IDS	C3-C2-O2-S
1	7-A	6	IDS	C1-C2-O2-S
1	7-A	6	IDS	C3-C2-O2-S
1	7-A	6	IDS	C2-O2-S-O3S
1	8-A	6	IDS	C1-C2-O2-S
1	8-A	6	IDS	C3-C2-O2-S
1	8-A	6	IDS	C2-O2-S-O2S
1	9-A	6	IDS	C2-O2-S-O3S
1	13-A	6	IDS	C1-C2-O2-S
1	13-A	6	IDS	C3-C2-O2-S
1	14-A	6	IDS	C1-C2-O2-S
1	14-A	6	IDS	C2-O2-S-O1S
1	14-A	6	IDS	C2-O2-S-O2S
1	14-A	6	IDS	C2-O2-S-O3S
1	2-A	7	SGN	C2-N2-S1-O1S
1	3-A	7	SGN	C2-N2-S1-O2S
1	3-A	7	SGN	C2-N2-S1-O3S
1	5-A	7	SGN	C2-N2-S1-O2S
1	5-A	7	SGN	C2-N2-S1-O3S
1	8-A	7	SGN	C2-N2-S1-O1S
1	9-A	7	SGN	O5-C5-C6-O6
1	9-A	7	SGN	C2-N2-S1-O1S
1	10-A	7	SGN	O5-C5-C6-O6
1	10-A	7	SGN	C2-N2-S1-O2S
1	13-A	7	SGN	C4-C5-C6-O6
1	13-A	7	SGN	O5-C5-C6-O6
1	14-A	7	SGN	C4-C5-C6-O6
1	14-A	7	SGN	O5-C5-C6-O6
1	1-A	8	IDS	C2-O2-S-O3S
1	2-A	8	IDS	C2-O2-S-O2S
1	3-A	8	IDS	C4-C5-C6-O6A
1	3-A	8	IDS	C4-C5-C6-O6B
1	5-A	8	IDS	C1-C2-O2-S
1	5-A	8	IDS	C3-C2-O2-S
1	5-A	8	IDS	C4-C5-C6-O6A
1	5-A	8	IDS	C4-C5-C6-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	7-A	8	IDS	C1-C2-O2-S
1	7-A	8	IDS	C3-C2-O2-S
1	8-A	8	IDS	C4-C5-C6-O6A
1	11-A	8	IDS	C2-O2-S-O3S
1	14-A	8	IDS	C1-C2-O2-S
1	14-A	8	IDS	C3-C2-O2-S
1	14-A	8	IDS	C4-C5-C6-O6A
1	14-A	8	IDS	C4-C5-C6-O6B
1	14-A	8	IDS	C2-O2-S-O1S
1	14-A	8	IDS	C2-O2-S-O2S
1	14-A	8	IDS	C2-O2-S-O3S
1	2-A	9	SGN	C2-N2-S1-O2S
1	3-A	9	SGN	O5-C5-C6-O6
1	3-A	9	SGN	C2-N2-S1-O2S
1	3-A	9	SGN	C2-N2-S1-O3S
1	4-A	9	SGN	C2-N2-S1-O1S
1	5-A	9	SGN	C4-C5-C6-O6
1	5-A	9	SGN	O5-C5-C6-O6
1	6-A	9	SGN	C4-C5-C6-O6
1	6-A	9	SGN	O5-C5-C6-O6
1	8-A	9	SGN	C4-C5-C6-O6
1	8-A	9	SGN	O5-C5-C6-O6
1	10-A	9	SGN	C4-C5-C6-O6
1	10-A	9	SGN	O5-C5-C6-O6
1	11-A	9	SGN	O5-C5-C6-O6
1	11-A	9	SGN	C2-N2-S1-O2S
1	12-A	9	SGN	C4-C5-C6-O6
1	12-A	9	SGN	C2-N2-S1-O2S
1	12-A	9	SGN	C2-N2-S1-O3S
1	13-A	9	SGN	O5-C5-C6-O6
1	13-A	9	SGN	C2-N2-S1-O2S
1	13-A	9	SGN	C2-N2-S1-O3S
1	14-A	9	SGN	C4-C5-C6-O6
1	14-A	9	SGN	O5-C5-C6-O6
1	1-A	10	IDS	C1-C2-O2-S
1	1-A	10	IDS	C3-C2-O2-S
1	2-A	10	IDS	C4-C5-C6-O6A
1	2-A	10	IDS	C4-C5-C6-O6B
1	2-A	10	IDS	C2-O2-S-O3S
1	3-A	10	IDS	C1-C2-O2-S
1	3-A	10	IDS	C3-C2-O2-S
1	5-A	10	IDS	C1-C2-O2-S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	5-A	10	IDS	C3-C2-O2-S
1	5-A	10	IDS	C4-C5-C6-O6A
1	5-A	10	IDS	C4-C5-C6-O6B
1	5-A	10	IDS	C2-O2-S-O1S
1	5-A	10	IDS	C2-O2-S-O2S
1	5-A	10	IDS	C2-O2-S-O3S
1	7-A	10	IDS	C1-C2-O2-S
1	7-A	10	IDS	C3-C2-O2-S
1	8-A	10	IDS	C1-C2-O2-S
1	8-A	10	IDS	C3-C2-O2-S
1	8-A	10	IDS	C2-O2-S-O3S
1	9-A	10	IDS	C4-C5-C6-O6A
1	9-A	10	IDS	C2-O2-S-O3S
1	11-A	10	IDS	C1-C2-O2-S
1	11-A	10	IDS	C3-C2-O2-S
1	11-A	10	IDS	C2-O2-S-O3S
1	12-A	10	IDS	C2-O2-S-O3S
1	13-A	10	IDS	C2-O2-S-O3S
1	14-A	10	IDS	C2-O2-S-O3S
1	2-A	11	SGN	C4-C5-C6-O6
1	3-A	11	SGN	C4-C5-C6-O6
1	3-A	11	SGN	C2-N2-S1-O2S
1	3-A	11	SGN	C2-N2-S1-O3S
1	4-A	11	SGN	C2-N2-S1-O1S
1	4-A	11	SGN	C6-O6-S2-O4S
1	5-A	11	SGN	C4-C5-C6-O6
1	5-A	11	SGN	O5-C5-C6-O6
1	6-A	11	SGN	C2-N2-S1-O2S
1	7-A	11	SGN	C4-C5-C6-O6
1	7-A	11	SGN	O5-C5-C6-O6
1	7-A	11	SGN	C2-N2-S1-O1S
1	8-A	11	SGN	C2-N2-S1-O1S
1	9-A	11	SGN	C2-N2-S1-O2S
1	11-A	11	SGN	O5-C5-C6-O6
1	12-A	11	SGN	C2-N2-S1-O1S
1	14-A	11	SGN	C4-C5-C6-O6
1	14-A	11	SGN	O5-C5-C6-O6
1	14-A	11	SGN	C2-N2-S1-O2S
1	14-A	11	SGN	C2-N2-S1-O3S
1	2-A	12	IDS	C4-C5-C6-O6A
1	2-A	12	IDS	C4-C5-C6-O6B
1	5-A	12	IDS	C4-C5-C6-O6A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	5-A	12	IDS	C4-C5-C6-O6B
1	7-A	12	IDS	C1-C2-O2-S
1	7-A	12	IDS	C3-C2-O2-S
1	7-A	12	IDS	C2-O2-S-O1S
1	7-A	12	IDS	C2-O2-S-O2S
1	7-A	12	IDS	C2-O2-S-O3S
1	11-A	12	IDS	C4-C5-C6-O6A
1	11-A	12	IDS	C4-C5-C6-O6B
1	11-A	12	IDS	C2-O2-S-O3S
1	12-A	12	IDS	C1-C2-O2-S
1	12-A	12	IDS	C3-C2-O2-S
1	12-A	12	IDS	C4-C5-C6-O6A
1	12-A	12	IDS	C4-C5-C6-O6B
1	13-A	12	IDS	C1-C2-O2-S
1	13-A	12	IDS	C3-C2-O2-S
1	2-A	13	SGN	C2-N2-S1-O2S
1	2-A	13	SGN	C6-O6-S2-O6S
1	3-A	13	SGN	C4-C5-C6-O6
1	3-A	13	SGN	O5-C5-C6-O6
1	4-A	13	SGN	C4-C5-C6-O6
1	4-A	13	SGN	O5-C5-C6-O6
1	4-A	13	SGN	C2-N2-S1-O2S
1	4-A	13	SGN	C2-N2-S1-O3S
1	5-A	13	SGN	C4-C5-C6-O6
1	5-A	13	SGN	O5-C5-C6-O6
1	5-A	13	SGN	C2-N2-S1-O2S
1	7-A	13	SGN	O5-C5-C6-O6
1	7-A	13	SGN	C2-N2-S1-O2S
1	8-A	13	SGN	C2-N2-S1-O2S
1	9-A	13	SGN	C4-C5-C6-O6
1	9-A	13	SGN	O5-C5-C6-O6
1	10-A	13	SGN	C2-N2-S1-O1S
1	11-A	13	SGN	C2-N2-S1-O2S
1	12-A	13	SGN	C6-O6-S2-O4S
1	14-A	13	SGN	C2-N2-S1-O2S
1	2-A	14	IDS	C4-C5-C6-O6A
1	2-A	14	IDS	C4-C5-C6-O6B
1	2-A	14	IDS	C2-O2-S-O3S
1	6-A	14	IDS	C2-O2-S-O3S
1	7-A	14	IDS	C1-C2-O2-S
1	7-A	14	IDS	C3-C2-O2-S
1	7-A	14	IDS	C2-O2-S-O3S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	8-A	14	IDS	C1-C2-O2-S
1	8-A	14	IDS	C3-C2-O2-S
1	9-A	14	IDS	C2-O2-S-O3S
1	10-A	14	IDS	C2-O2-S-O2S
1	13-A	14	IDS	C4-C5-C6-O6A
1	13-A	14	IDS	C4-C5-C6-O6B
1	13-A	14	IDS	C2-O2-S-O1S
1	13-A	14	IDS	C2-O2-S-O3S
1	1-A	15	SGN	C4-C5-C6-O6
1	1-A	15	SGN	O5-C5-C6-O6
1	1-A	15	SGN	C2-N2-S1-O2S
1	2-A	15	SGN	C4-C5-C6-O6
1	2-A	15	SGN	O5-C5-C6-O6
1	2-A	15	SGN	C2-N2-S1-O2S
1	3-A	15	SGN	C4-C5-C6-O6
1	3-A	15	SGN	O5-C5-C6-O6
1	5-A	15	SGN	C4-C5-C6-O6
1	5-A	15	SGN	O5-C5-C6-O6
1	5-A	15	SGN	C2-N2-S1-O2S
1	7-A	15	SGN	C4-C5-C6-O6
1	7-A	15	SGN	C2-N2-S1-O1S
1	8-A	15	SGN	O5-C5-C6-O6
1	8-A	15	SGN	C2-N2-S1-O2S
1	8-A	15	SGN	C2-N2-S1-O3S
1	9-A	15	SGN	C4-C5-C6-O6
1	9-A	15	SGN	O5-C5-C6-O6
1	10-A	15	SGN	C2-N2-S1-O2S
1	10-A	15	SGN	C2-N2-S1-O3S
1	12-A	15	SGN	C2-N2-S1-O2S
1	12-A	15	SGN	C2-N2-S1-O3S
1	12-A	15	SGN	C6-O6-S2-O4S
1	14-A	15	SGN	O5-C5-C6-O6
1	14-A	15	SGN	C2-N2-S1-O1S
1	1-A	16	IDS	C4-C5-C6-O6A
1	1-A	16	IDS	C4-C5-C6-O6B
1	2-A	16	IDS	C4-C5-C6-O6A
1	2-A	16	IDS	C4-C5-C6-O6B
1	4-A	16	IDS	C1-C2-O2-S
1	4-A	16	IDS	C3-C2-O2-S
1	4-A	16	IDS	C4-C5-C6-O6A
1	4-A	16	IDS	C4-C5-C6-O6B
1	6-A	16	IDS	C4-C5-C6-O6A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	6-A	16	IDS	C4-C5-C6-O6B
1	7-A	16	IDS	C2-O2-S-O3S
1	8-A	16	IDS	C1-C2-O2-S
1	8-A	16	IDS	C2-O2-S-O1S
1	8-A	16	IDS	C2-O2-S-O2S
1	8-A	16	IDS	C2-O2-S-O3S
1	9-A	16	IDS	C4-C5-C6-O6A
1	9-A	16	IDS	C4-C5-C6-O6B
1	11-A	16	IDS	C1-C2-O2-S
1	11-A	16	IDS	C3-C2-O2-S
1	12-A	16	IDS	C2-O2-S-O1S
1	12-A	16	IDS	C2-O2-S-O3S
1	13-A	16	IDS	C2-O2-S-O3S
1	1-A	17	SGN	C4-C5-C6-O6
1	1-A	17	SGN	O5-C5-C6-O6
1	1-A	17	SGN	C2-N2-S1-O1S
1	2-A	17	SGN	C2-N2-S1-O1S
1	3-A	17	SGN	O5-C5-C6-O6
1	3-A	17	SGN	C2-N2-S1-O1S
1	4-A	17	SGN	C4-C5-C6-O6
1	4-A	17	SGN	O5-C5-C6-O6
1	4-A	17	SGN	C6-O6-S2-O6S
1	5-A	17	SGN	C4-C5-C6-O6
1	5-A	17	SGN	O5-C5-C6-O6
1	5-A	17	SGN	C2-N2-S1-O1S
1	7-A	17	SGN	C2-N2-S1-O2S
1	8-A	17	SGN	C2-N2-S1-O1S
1	9-A	17	SGN	C2-N2-S1-O1S
1	10-A	17	SGN	O5-C5-C6-O6
1	11-A	17	SGN	C4-C5-C6-O6
1	11-A	17	SGN	O5-C5-C6-O6
1	11-A	17	SGN	C2-N2-S1-O1S
1	12-A	17	SGN	C2-N2-S1-O2S
1	13-A	17	SGN	O5-C5-C6-O6
1	13-A	17	SGN	C2-N2-S1-O2S
1	13-A	17	SGN	C2-N2-S1-O3S
1	14-A	17	SGN	C4-C5-C6-O6
1	14-A	17	SGN	O5-C5-C6-O6
1	4-A	18	IDS	C2-O2-S-O3S
1	5-A	18	IDS	C1-C2-O2-S
1	5-A	18	IDS	C3-C2-O2-S
1	5-A	18	IDS	C2-O2-S-O1S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	5-A	18	IDS	C2-O2-S-O3S
1	6-A	18	IDS	C2-O2-S-O3S
1	7-A	18	IDS	C1-C2-O2-S
1	7-A	18	IDS	C3-C2-O2-S
1	7-A	18	IDS	C2-O2-S-O2S
1	8-A	18	IDS	C1-C2-O2-S
1	8-A	18	IDS	C3-C2-O2-S
1	9-A	18	IDS	C1-C2-O2-S
1	9-A	18	IDS	C3-C2-O2-S
1	9-A	18	IDS	C4-C5-C6-O6A
1	9-A	18	IDS	C4-C5-C6-O6B
1	10-A	18	IDS	C1-C2-O2-S
1	10-A	18	IDS	C3-C2-O2-S
1	10-A	18	IDS	C4-C5-C6-O6A
1	10-A	18	IDS	C4-C5-C6-O6B
1	13-A	18	IDS	C2-O2-S-O3S
1	1-A	19	SGN	C2-N2-S1-O1S
1	2-A	19	SGN	C2-N2-S1-O2S
1	3-A	19	SGN	C2-N2-S1-O1S
1	4-A	19	SGN	C4-C5-C6-O6
1	4-A	19	SGN	O5-C5-C6-O6
1	4-A	19	SGN	C2-N2-S1-O2S
1	4-A	19	SGN	C2-N2-S1-O3S
1	5-A	19	SGN	C2-N2-S1-O2S
1	6-A	19	SGN	C4-C5-C6-O6
1	6-A	19	SGN	O5-C5-C6-O6
1	6-A	19	SGN	C2-N2-S1-O2S
1	6-A	19	SGN	C2-N2-S1-O3S
1	7-A	19	SGN	C4-C5-C6-O6
1	7-A	19	SGN	O5-C5-C6-O6
1	8-A	19	SGN	C4-C5-C6-O6
1	8-A	19	SGN	O5-C5-C6-O6
1	8-A	19	SGN	C2-N2-S1-O1S
1	11-A	19	SGN	C2-N2-S1-O1S
1	12-A	19	SGN	C2-N2-S1-O2S
1	2-A	20	IDS	C1-C2-O2-S
1	2-A	20	IDS	C3-C2-O2-S
1	2-A	20	IDS	C2-O2-S-O3S
1	4-A	20	IDS	C2-O2-S-O1S
1	4-A	20	IDS	C2-O2-S-O2S
1	4-A	20	IDS	C2-O2-S-O3S
1	6-A	20	IDS	C2-O2-S-O3S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	12-A	20	IDS	C2-O2-S-O1S
1	12-A	20	IDS	C2-O2-S-O2S
1	12-A	20	IDS	C2-O2-S-O3S
1	14-A	20	IDS	C1-C2-O2-S
1	14-A	20	IDS	C3-C2-O2-S
1	1-A	21	SGN	C2-N2-S1-O2S
1	3-A	21	SGN	C4-C5-C6-O6
1	3-A	21	SGN	O5-C5-C6-O6
1	3-A	21	SGN	C2-N2-S1-O2S
1	4-A	21	SGN	C4-C5-C6-O6
1	4-A	21	SGN	C2-N2-S1-O2S
1	4-A	21	SGN	C2-N2-S1-O3S
1	5-A	21	SGN	O5-C5-C6-O6
1	5-A	21	SGN	C2-N2-S1-O2S
1	5-A	21	SGN	C2-N2-S1-O3S
1	6-A	21	SGN	C4-C5-C6-O6
1	6-A	21	SGN	O5-C5-C6-O6
1	6-A	21	SGN	C2-N2-S1-O2S
1	7-A	21	SGN	C4-C5-C6-O6
1	7-A	21	SGN	O5-C5-C6-O6
1	7-A	21	SGN	C2-N2-S1-O2S
1	7-A	21	SGN	C2-N2-S1-O3S
1	7-A	21	SGN	C6-O6-S2-O6S
1	8-A	21	SGN	C4-C5-C6-O6
1	8-A	21	SGN	O5-C5-C6-O6
1	9-A	21	SGN	C2-N2-S1-O2S
1	10-A	21	SGN	C2-N2-S1-O1S
1	11-A	21	SGN	C4-C5-C6-O6
1	11-A	21	SGN	O5-C5-C6-O6
1	12-A	21	SGN	C4-C5-C6-O6
1	12-A	21	SGN	O5-C5-C6-O6
1	12-A	21	SGN	C2-N2-S1-O1S
1	13-A	21	SGN	C4-C5-C6-O6
1	13-A	21	SGN	O5-C5-C6-O6
1	13-A	21	SGN	C2-N2-S1-O2S
1	14-A	21	SGN	C4-C5-C6-O6
1	14-A	21	SGN	O5-C5-C6-O6
1	14-A	21	SGN	C2-N2-S1-O2S
1	14-A	21	SGN	C2-N2-S1-O3S
1	1-A	22	IDS	C1-C2-O2-S
1	1-A	22	IDS	C3-C2-O2-S
1	2-A	22	IDS	C1-C2-O2-S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	2-A	22	IDS	C3-C2-O2-S
1	2-A	22	IDS	C2-O2-S-O3S
1	3-A	22	IDS	C2-O2-S-O1S
1	3-A	22	IDS	C2-O2-S-O2S
1	3-A	22	IDS	C2-O2-S-O3S
1	4-A	22	IDS	C4-C5-C6-O6A
1	4-A	22	IDS	C4-C5-C6-O6B
1	4-A	22	IDS	C2-O2-S-O1S
1	4-A	22	IDS	C2-O2-S-O3S
1	7-A	22	IDS	C4-C5-C6-O6A
1	7-A	22	IDS	C2-O2-S-O1S
1	7-A	22	IDS	C2-O2-S-O3S
1	8-A	22	IDS	C1-C2-O2-S
1	8-A	22	IDS	C3-C2-O2-S
1	10-A	22	IDS	C4-C5-C6-O6A
1	10-A	22	IDS	C4-C5-C6-O6B
1	11-A	22	IDS	C4-C5-C6-O6A
1	12-A	22	IDS	C1-C2-O2-S
1	12-A	22	IDS	C3-C2-O2-S
1	12-A	22	IDS	C2-O2-S-O1S
1	12-A	22	IDS	C2-O2-S-O2S
1	12-A	22	IDS	C2-O2-S-O3S
1	13-A	22	IDS	C1-C2-O2-S
1	13-A	22	IDS	C3-C2-O2-S
1	13-A	22	IDS	C4-C5-C6-O6A
1	13-A	22	IDS	C4-C5-C6-O6B
1	13-A	22	IDS	C2-O2-S-O3S
1	14-A	22	IDS	C1-C2-O2-S
1	14-A	22	IDS	C3-C2-O2-S
1	14-A	22	IDS	C4-C5-C6-O6A
1	14-A	22	IDS	C4-C5-C6-O6B
1	2-A	23	SGN	C4-C5-C6-O6
1	2-A	23	SGN	O5-C5-C6-O6
1	2-A	23	SGN	C2-N2-S1-O2S
1	3-A	23	SGN	O5-C5-C6-O6
1	3-A	23	SGN	C2-N2-S1-O2S
1	3-A	23	SGN	C2-N2-S1-O3S
1	4-A	23	SGN	C2-N2-S1-O1S
1	7-A	23	SGN	C2-N2-S1-O2S
1	7-A	23	SGN	C2-N2-S1-O3S
1	8-A	23	SGN	O5-C5-C6-O6
1	10-A	23	SGN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	10-A	23	SGN	O5-C5-C6-O6
1	10-A	23	SGN	C2-N2-S1-O1S
1	12-A	23	SGN	C2-N2-S1-O2S
1	12-A	23	SGN	C2-N2-S1-O3S
1	13-A	23	SGN	C2-N2-S1-O1S
1	14-A	23	SGN	C4-C5-C6-O6
1	14-A	23	SGN	O5-C5-C6-O6
1	14-A	23	SGN	C2-N2-S1-O2S
1	2-A	24	IDS	C2-O2-S-O3S
1	5-A	24	IDS	C1-C2-O2-S
1	5-A	24	IDS	C3-C2-O2-S
1	7-A	24	IDS	C2-O2-S-O3S
1	9-A	24	IDS	C1-C2-O2-S
1	9-A	24	IDS	C3-C2-O2-S
1	10-A	24	IDS	C1-C2-O2-S
1	10-A	24	IDS	C3-C2-O2-S
1	11-A	24	IDS	C2-O2-S-O1S
1	11-A	24	IDS	C2-O2-S-O3S
1	12-A	24	IDS	C4-C5-C6-O6A
1	3-A	25	SGN	C4-C5-C6-O6
1	3-A	25	SGN	O5-C5-C6-O6
1	4-A	25	SGN	C4-C5-C6-O6
1	4-A	25	SGN	O5-C5-C6-O6
1	4-A	25	SGN	C2-N2-S1-O1S
1	5-A	25	SGN	O5-C5-C6-O6
1	5-A	25	SGN	C2-N2-S1-O2S
1	5-A	25	SGN	C2-N2-S1-O3S
1	6-A	25	SGN	C4-C5-C6-O6
1	6-A	25	SGN	O5-C5-C6-O6
1	7-A	25	SGN	O5-C5-C6-O6
1	7-A	25	SGN	C2-N2-S1-O2S
1	7-A	25	SGN	C2-N2-S1-O3S
1	8-A	25	SGN	C2-N2-S1-O2S
1	9-A	25	SGN	C4-C5-C6-O6
1	9-A	25	SGN	O5-C5-C6-O6
1	10-A	25	SGN	C4-C5-C6-O6
1	10-A	25	SGN	O5-C5-C6-O6
1	11-A	25	SGN	C2-N2-S1-O2S
1	11-A	25	SGN	C2-N2-S1-O3S
1	12-A	25	SGN	C4-C5-C6-O6
1	12-A	25	SGN	O5-C5-C6-O6
1	12-A	25	SGN	C2-N2-S1-O1S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	14-A	25	SGN	C4-C5-C6-O6
1	14-A	25	SGN	O5-C5-C6-O6
1	14-A	25	SGN	C2-N2-S1-O2S
1	14-A	25	SGN	C2-N2-S1-O3S
1	2-A	26	IDS	C2-O2-S-O3S
1	4-A	26	IDS	C2-O2-S-O1S
1	4-A	26	IDS	C2-O2-S-O2S
1	4-A	26	IDS	C2-O2-S-O3S
1	7-A	26	IDS	C4-C5-C6-O6A
1	7-A	26	IDS	C4-C5-C6-O6B
1	9-A	26	IDS	C1-C2-O2-S
1	9-A	26	IDS	C3-C2-O2-S
1	10-A	26	IDS	C1-C2-O2-S
1	10-A	26	IDS	C3-C2-O2-S
1	11-A	26	IDS	C2-O2-S-O3S
1	13-A	26	IDS	C1-C2-O2-S
1	13-A	26	IDS	C3-C2-O2-S
1	1-A	27	SGN	C4-C5-C6-O6
1	1-A	27	SGN	O5-C5-C6-O6
1	1-A	27	SGN	C2-N2-S1-O1S
1	2-A	27	SGN	C2-N2-S1-O2S
1	2-A	27	SGN	C2-N2-S1-O3S
1	3-A	27	SGN	C4-C5-C6-O6
1	3-A	27	SGN	O5-C5-C6-O6
1	4-A	27	SGN	C4-C5-C6-O6
1	4-A	27	SGN	O5-C5-C6-O6
1	5-A	27	SGN	C4-C5-C6-O6
1	5-A	27	SGN	O5-C5-C6-O6
1	5-A	27	SGN	C2-N2-S1-O2S
1	6-A	27	SGN	O5-C5-C6-O6
1	7-A	27	SGN	C4-C5-C6-O6
1	7-A	27	SGN	O5-C5-C6-O6
1	7-A	27	SGN	C2-N2-S1-O2S
1	10-A	27	SGN	O5-C5-C6-O6
1	11-A	27	SGN	C2-N2-S1-O2S
1	11-A	27	SGN	C2-N2-S1-O3S
1	12-A	27	SGN	C2-N2-S1-O2S
1	13-A	27	SGN	C2-N2-S1-O2S
1	1-A	28	IDS	C4-C5-C6-O6A
1	1-A	28	IDS	C4-C5-C6-O6B
1	2-A	28	IDS	C1-C2-O2-S
1	2-A	28	IDS	C3-C2-O2-S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	3-A	28	IDS	C2-O2-S-O3S
1	4-A	28	IDS	C2-O2-S-O1S
1	4-A	28	IDS	C2-O2-S-O2S
1	4-A	28	IDS	C2-O2-S-O3S
1	6-A	28	IDS	C2-O2-S-O3S
1	7-A	28	IDS	C4-C5-C6-O6A
1	7-A	28	IDS	C4-C5-C6-O6B
1	7-A	28	IDS	C2-O2-S-O3S
1	9-A	28	IDS	C4-C5-C6-O6A
1	9-A	28	IDS	C4-C5-C6-O6B
1	12-A	28	IDS	C1-C2-O2-S
1	12-A	28	IDS	C3-C2-O2-S
1	12-A	28	IDS	C2-O2-S-O1S
1	12-A	28	IDS	C2-O2-S-O2S
1	12-A	28	IDS	C2-O2-S-O3S
1	13-A	28	IDS	C2-O2-S-O3S
1	1-A	29	SGN	C4-C5-C6-O6
1	1-A	29	SGN	O5-C5-C6-O6
1	2-A	29	SGN	C4-C5-C6-O6
1	2-A	29	SGN	O5-C5-C6-O6
1	3-A	29	SGN	C4-C5-C6-O6
1	3-A	29	SGN	O5-C5-C6-O6
1	3-A	29	SGN	C2-N2-S1-O2S
1	4-A	29	SGN	C2-N2-S1-O2S
1	4-A	29	SGN	C2-N2-S1-O3S
1	5-A	29	SGN	C4-C5-C6-O6
1	5-A	29	SGN	O5-C5-C6-O6
1	6-A	29	SGN	C4-C5-C6-O6
1	6-A	29	SGN	O5-C5-C6-O6
1	7-A	29	SGN	C2-N2-S1-O2S
1	7-A	29	SGN	C2-N2-S1-O3S
1	7-A	29	SGN	C6-O6-S2-O6S
1	9-A	29	SGN	C4-C5-C6-O6
1	9-A	29	SGN	O5-C5-C6-O6
1	9-A	29	SGN	C2-N2-S1-O2S
1	10-A	29	SGN	C2-N2-S1-O1S
1	11-A	29	SGN	C6-O6-S2-O4S
1	12-A	29	SGN	C4-C5-C6-O6
1	12-A	29	SGN	O5-C5-C6-O6
1	12-A	29	SGN	C2-N2-S1-O2S
1	12-A	29	SGN	C2-N2-S1-O3S
1	13-A	29	SGN	C2-N2-S1-O2S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	13-A	29	SGN	C2-N2-S1-O3S
1	2-A	30	IDS	C1-C2-O2-S
1	2-A	30	IDS	C3-C2-O2-S
1	8-A	30	IDS	C1-C2-O2-S
1	8-A	30	IDS	C3-C2-O2-S
1	12-A	30	IDS	C1-C2-O2-S
1	12-A	30	IDS	C3-C2-O2-S
1	9-A	1	SGN	C6-O6-S2-O4S
1	10-A	1	SGN	C6-O6-S2-O5S
1	11-A	1	SGN	C6-O6-S2-O4S
1	5-A	5	SGN	C6-O6-S2-O4S
1	5-A	5	SGN	C6-O6-S2-O5S
1	12-A	5	SGN	C6-O6-S2-O5S
1	4-A	7	SGN	C6-O6-S2-O4S
1	5-A	7	SGN	C6-O6-S2-O4S
1	3-A	9	SGN	C6-O6-S2-O4S
1	6-A	9	SGN	C6-O6-S2-O4S
1	13-A	9	SGN	C6-O6-S2-O5S
1	12-A	11	SGN	C6-O6-S2-O4S
1	1-A	13	SGN	C6-O6-S2-O5S
1	1-A	15	SGN	C6-O6-S2-O4S
1	4-A	15	SGN	C6-O6-S2-O4S
1	5-A	15	SGN	C6-O6-S2-O4S
1	2-A	17	SGN	C6-O6-S2-O4S
1	3-A	17	SGN	C6-O6-S2-O4S
1	8-A	17	SGN	C6-O6-S2-O4S
1	14-A	17	SGN	C6-O6-S2-O4S
1	2-A	21	SGN	C6-O6-S2-O4S
1	1-A	23	SGN	C6-O6-S2-O4S
1	6-A	25	SGN	C6-O6-S2-O5S
1	4-A	27	SGN	C6-O6-S2-O4S
1	11-A	27	SGN	C6-O6-S2-O4S
1	13-A	29	SGN	C6-O6-S2-O4S
1	6-A	1	SGN	C6-O6-S2-O4S
1	10-A	1	SGN	C6-O6-S2-O4S
1	11-A	3	SGN	C6-O6-S2-O4S
1	12-A	3	SGN	C6-O6-S2-O5S
1	6-A	5	SGN	C6-O6-S2-O4S
1	7-A	5	SGN	C6-O6-S2-O4S
1	12-A	5	SGN	C6-O6-S2-O4S
1	6-A	7	SGN	C6-O6-S2-O4S
1	7-A	7	SGN	C6-O6-S2-O4S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	11-A	7	SGN	C6-O6-S2-O4S
1	14-A	7	SGN	C6-O6-S2-O4S
1	9-A	9	SGN	C6-O6-S2-O4S
1	13-A	9	SGN	C6-O6-S2-O4S
1	7-A	11	SGN	C6-O6-S2-O4S
1	8-A	11	SGN	C6-O6-S2-O4S
1	1-A	13	SGN	C6-O6-S2-O4S
1	5-A	13	SGN	C6-O6-S2-O4S
1	2-A	15	SGN	C6-O6-S2-O4S
1	5-A	17	SGN	C6-O6-S2-O4S
1	6-A	17	SGN	C6-O6-S2-O5S
1	13-A	17	SGN	C6-O6-S2-O4S
1	9-A	23	SGN	C6-O6-S2-O4S
1	3-A	25	SGN	C6-O6-S2-O4S
1	4-A	25	SGN	C6-O6-S2-O4S
1	5-A	25	SGN	C6-O6-S2-O5S
1	6-A	25	SGN	C6-O6-S2-O4S
1	11-A	25	SGN	C6-O6-S2-O4S
1	10-A	27	SGN	C6-O6-S2-O4S
1	12-A	27	SGN	C6-O6-S2-O4S
1	1-A	29	SGN	C6-O6-S2-O4S
1	6-A	29	SGN	C6-O6-S2-O4S
1	8-A	29	SGN	C6-O6-S2-O4S
1	3-A	1	SGN	O5-C5-C6-O6
1	12-A	3	SGN	O5-C5-C6-O6
1	4-A	5	SGN	O5-C5-C6-O6
1	2-A	7	SGN	C1-C2-N2-S1
1	5-A	7	SGN	O5-C5-C6-O6
1	7-A	7	SGN	O5-C5-C6-O6
1	6-A	9	SGN	C1-C2-N2-S1
1	12-A	9	SGN	O5-C5-C6-O6
1	13-A	9	SGN	C1-C2-N2-S1
1	1-A	11	SGN	O5-C5-C6-O6
1	4-A	11	SGN	O5-C5-C6-O6
1	9-A	11	SGN	O5-C5-C6-O6
1	1-A	13	SGN	O5-C5-C6-O6
1	8-A	13	SGN	C1-C2-N2-S1
1	10-A	13	SGN	C1-C2-N2-S1
1	6-A	15	SGN	C1-C2-N2-S1
1	7-A	15	SGN	O5-C5-C6-O6
1	2-A	19	SGN	O5-C5-C6-O6
1	9-A	21	SGN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	12-A	21	SGN	C1-C2-N2-S1
1	11-A	23	SGN	C1-C2-N2-S1
1	11-A	23	SGN	O5-C5-C6-O6
1	4-A	29	SGN	C1-C2-N2-S1
1	11-A	29	SGN	O5-C5-C6-O6
1	9-A	5	SGN	C4-C5-C6-O6
1	14-A	5	SGN	C4-C5-C6-O6
1	7-A	7	SGN	C4-C5-C6-O6
1	11-A	9	SGN	C4-C5-C6-O6
1	1-A	13	SGN	C4-C5-C6-O6
1	9-A	19	SGN	C4-C5-C6-O6
1	8-A	23	SGN	C4-C5-C6-O6
1	10-A	27	SGN	C4-C5-C6-O6
1	7-A	1	SGN	C6-O6-S2-O6S
1	9-A	1	SGN	C6-O6-S2-O6S
1	10-A	1	SGN	C6-O6-S2-O6S
1	11-A	1	SGN	C6-O6-S2-O6S
1	8-A	3	SGN	C6-O6-S2-O6S
1	9-A	3	SGN	C6-O6-S2-O6S
1	11-A	3	SGN	C6-O6-S2-O6S
1	12-A	3	SGN	C6-O6-S2-O6S
1	3-A	5	SGN	C6-O6-S2-O6S
1	5-A	5	SGN	C6-O6-S2-O6S
1	6-A	5	SGN	C6-O6-S2-O6S
1	12-A	5	SGN	C6-O6-S2-O6S
1	4-A	7	SGN	C6-O6-S2-O6S
1	5-A	7	SGN	C6-O6-S2-O6S
1	7-A	7	SGN	C6-O6-S2-O6S
1	11-A	7	SGN	C6-O6-S2-O6S
1	3-A	9	SGN	C6-O6-S2-O6S
1	6-A	9	SGN	C6-O6-S2-O6S
1	13-A	9	SGN	C6-O6-S2-O6S
1	4-A	11	SGN	C6-O6-S2-O6S
1	5-A	11	SGN	C6-O6-S2-O6S
1	7-A	11	SGN	C6-O6-S2-O6S
1	8-A	11	SGN	C6-O6-S2-O6S
1	12-A	11	SGN	C6-O6-S2-O6S
1	14-A	11	SGN	C6-O6-S2-O6S
1	1-A	13	SGN	C6-O6-S2-O6S
1	5-A	13	SGN	C6-O6-S2-O6S
1	12-A	13	SGN	C6-O6-S2-O6S
1	13-A	13	SGN	C6-O6-S2-O6S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1-A	15	SGN	C6-O6-S2-O6S
1	4-A	15	SGN	C6-O6-S2-O6S
1	5-A	15	SGN	C6-O6-S2-O6S
1	12-A	15	SGN	C6-O6-S2-O6S
1	2-A	17	SGN	C6-O6-S2-O6S
1	3-A	17	SGN	C6-O6-S2-O6S
1	6-A	17	SGN	C6-O6-S2-O6S
1	8-A	17	SGN	C6-O6-S2-O6S
1	10-A	17	SGN	C6-O6-S2-O6S
1	13-A	17	SGN	C6-O6-S2-O6S
1	14-A	17	SGN	C6-O6-S2-O6S
1	4-A	19	SGN	C6-O6-S2-O6S
1	8-A	19	SGN	C6-O6-S2-O6S
1	2-A	21	SGN	C6-O6-S2-O6S
1	5-A	21	SGN	C6-O6-S2-O6S
1	1-A	23	SGN	C6-O6-S2-O6S
1	7-A	23	SGN	C6-O6-S2-O6S
1	8-A	23	SGN	C6-O6-S2-O6S
1	5-A	25	SGN	C6-O6-S2-O6S
1	6-A	25	SGN	C6-O6-S2-O6S
1	13-A	25	SGN	C6-O6-S2-O6S
1	2-A	27	SGN	C6-O6-S2-O6S
1	4-A	27	SGN	C6-O6-S2-O6S
1	5-A	27	SGN	C6-O6-S2-O6S
1	11-A	27	SGN	C6-O6-S2-O6S
1	12-A	27	SGN	C6-O6-S2-O6S
1	11-A	29	SGN	C6-O6-S2-O6S
1	13-A	29	SGN	C6-O6-S2-O6S
1	5-A	2	IDS	C2-O2-S-O1S
1	5-A	2	IDS	C2-O2-S-O2S
1	9-A	2	IDS	C2-O2-S-O1S
1	10-A	2	IDS	C2-O2-S-O1S
1	14-A	2	IDS	C2-O2-S-O1S
1	9-A	4	IDS	C2-O2-S-O1S
1	13-A	4	IDS	C2-O2-S-O1S
1	13-A	4	IDS	C2-O2-S-O2S
1	7-A	6	IDS	C2-O2-S-O1S
1	8-A	6	IDS	C2-O2-S-O1S
1	9-A	6	IDS	C2-O2-S-O1S
1	1-A	8	IDS	C2-O2-S-O1S
1	2-A	8	IDS	C2-O2-S-O1S
1	4-A	8	IDS	C2-O2-S-O1S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	4-A	8	IDS	C2-O2-S-O2S
1	11-A	8	IDS	C2-O2-S-O1S
1	4-A	10	IDS	C2-O2-S-O1S
1	4-A	10	IDS	C2-O2-S-O2S
1	9-A	10	IDS	C2-O2-S-O1S
1	11-A	10	IDS	C2-O2-S-O1S
1	11-A	10	IDS	C2-O2-S-O2S
1	12-A	10	IDS	C2-O2-S-O1S
1	13-A	10	IDS	C2-O2-S-O1S
1	14-A	10	IDS	C2-O2-S-O1S
1	2-A	12	IDS	C2-O2-S-O1S
1	2-A	12	IDS	C2-O2-S-O2S
1	8-A	12	IDS	C2-O2-S-O1S
1	8-A	12	IDS	C2-O2-S-O2S
1	2-A	14	IDS	C2-O2-S-O1S
1	2-A	14	IDS	C2-O2-S-O2S
1	6-A	14	IDS	C2-O2-S-O1S
1	7-A	14	IDS	C2-O2-S-O1S
1	9-A	14	IDS	C2-O2-S-O1S
1	10-A	14	IDS	C2-O2-S-O1S
1	13-A	14	IDS	C2-O2-S-O2S
1	14-A	14	IDS	C2-O2-S-O1S
1	14-A	14	IDS	C2-O2-S-O2S
1	3-A	16	IDS	C2-O2-S-O1S
1	3-A	16	IDS	C2-O2-S-O2S
1	6-A	16	IDS	C2-O2-S-O1S
1	6-A	16	IDS	C2-O2-S-O2S
1	7-A	16	IDS	C2-O2-S-O1S
1	10-A	16	IDS	C2-O2-S-O1S
1	11-A	16	IDS	C2-O2-S-O1S
1	11-A	16	IDS	C2-O2-S-O2S
1	12-A	16	IDS	C2-O2-S-O2S
1	1-A	18	IDS	C2-O2-S-O1S
1	1-A	18	IDS	C2-O2-S-O2S
1	3-A	18	IDS	C2-O2-S-O1S
1	3-A	18	IDS	C2-O2-S-O2S
1	4-A	18	IDS	C2-O2-S-O1S
1	5-A	18	IDS	C2-O2-S-O2S
1	7-A	18	IDS	C2-O2-S-O1S
1	10-A	18	IDS	C2-O2-S-O1S
1	12-A	18	IDS	C2-O2-S-O1S
1	12-A	18	IDS	C2-O2-S-O2S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	13-A	18	IDS	C2-O2-S-O1S
1	1-A	20	IDS	C2-O2-S-O1S
1	1-A	20	IDS	C2-O2-S-O2S
1	2-A	20	IDS	C2-O2-S-O1S
1	6-A	20	IDS	C2-O2-S-O1S
1	4-A	22	IDS	C2-O2-S-O2S
1	7-A	22	IDS	C2-O2-S-O2S
1	13-A	22	IDS	C2-O2-S-O1S
1	7-A	24	IDS	C2-O2-S-O1S
1	8-A	24	IDS	C2-O2-S-O1S
1	8-A	24	IDS	C2-O2-S-O2S
1	11-A	24	IDS	C2-O2-S-O2S
1	13-A	24	IDS	C2-O2-S-O1S
1	13-A	24	IDS	C2-O2-S-O2S
1	8-A	26	IDS	C2-O2-S-O1S
1	8-A	26	IDS	C2-O2-S-O2S
1	9-A	26	IDS	C2-O2-S-O1S
1	9-A	26	IDS	C2-O2-S-O2S
1	11-A	26	IDS	C2-O2-S-O1S
1	14-A	26	IDS	C2-O2-S-O1S
1	14-A	26	IDS	C2-O2-S-O2S
1	13-A	28	IDS	C2-O2-S-O1S
1	3-A	30	IDS	C2-O2-S-O1S
1	3-A	30	IDS	C2-O2-S-O2S
1	4-A	30	IDS	C2-O2-S-O1S
1	4-A	30	IDS	C2-O2-S-O2S
1	7-A	7	SGN	C3-C2-N2-S1
1	6-A	9	SGN	C3-C2-N2-S1
1	6-A	11	SGN	C3-C2-N2-S1
1	12-A	11	SGN	C3-C2-N2-S1
1	10-A	13	SGN	C3-C2-N2-S1
1	6-A	15	SGN	C3-C2-N2-S1
1	3-A	17	SGN	C3-C2-N2-S1
1	10-A	17	SGN	C3-C2-N2-S1
1	3-A	19	SGN	C3-C2-N2-S1
1	1-A	1	SGN	C6-O6-S2-O5S
1	9-A	1	SGN	C6-O6-S2-O5S
1	13-A	1	SGN	C6-O6-S2-O5S
1	11-A	3	SGN	C6-O6-S2-O5S
1	6-A	5	SGN	C6-O6-S2-O5S
1	7-A	5	SGN	C6-O6-S2-O5S
1	6-A	7	SGN	C6-O6-S2-O5S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	7-A	7	SGN	C6-O6-S2-O5S
1	11-A	7	SGN	C6-O6-S2-O5S
1	3-A	9	SGN	C6-O6-S2-O5S
1	9-A	9	SGN	C6-O6-S2-O5S
1	2-A	11	SGN	C6-O6-S2-O5S
1	7-A	11	SGN	C6-O6-S2-O5S
1	8-A	11	SGN	C6-O6-S2-O5S
1	9-A	11	SGN	C6-O6-S2-O5S
1	12-A	11	SGN	C6-O6-S2-O5S
1	14-A	11	SGN	C6-O6-S2-O5S
1	4-A	13	SGN	C6-O6-S2-O5S
1	5-A	13	SGN	C6-O6-S2-O5S
1	8-A	13	SGN	C6-O6-S2-O5S
1	13-A	13	SGN	C6-O6-S2-O4S
1	13-A	13	SGN	C6-O6-S2-O5S
1	1-A	15	SGN	C6-O6-S2-O5S
1	2-A	15	SGN	C6-O6-S2-O5S
1	5-A	15	SGN	C6-O6-S2-O5S
1	11-A	15	SGN	C6-O6-S2-O5S
1	3-A	17	SGN	C6-O6-S2-O5S
1	5-A	17	SGN	C6-O6-S2-O5S
1	8-A	17	SGN	C6-O6-S2-O5S
1	13-A	17	SGN	C6-O6-S2-O5S
1	14-A	17	SGN	C6-O6-S2-O5S
1	4-A	19	SGN	C6-O6-S2-O4S
1	4-A	19	SGN	C6-O6-S2-O5S
1	8-A	19	SGN	C6-O6-S2-O4S
1	8-A	19	SGN	C6-O6-S2-O5S
1	9-A	19	SGN	C6-O6-S2-O5S
1	5-A	21	SGN	C6-O6-S2-O4S
1	5-A	21	SGN	C6-O6-S2-O5S
1	7-A	23	SGN	C6-O6-S2-O4S
1	7-A	23	SGN	C6-O6-S2-O5S
1	8-A	23	SGN	C6-O6-S2-O4S
1	8-A	23	SGN	C6-O6-S2-O5S
1	9-A	23	SGN	C6-O6-S2-O5S
1	4-A	25	SGN	C6-O6-S2-O5S
1	11-A	25	SGN	C6-O6-S2-O5S
1	13-A	25	SGN	C6-O6-S2-O5S
1	2-A	27	SGN	C6-O6-S2-O5S
1	4-A	27	SGN	C6-O6-S2-O5S
1	5-A	27	SGN	C6-O6-S2-O4S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	5-A	27	SGN	C6-O6-S2-O5S
1	9-A	27	SGN	C6-O6-S2-O5S
1	10-A	27	SGN	C6-O6-S2-O5S
1	12-A	27	SGN	C6-O6-S2-O5S
1	14-A	27	SGN	C6-O6-S2-O5S
1	6-A	29	SGN	C6-O6-S2-O5S
1	8-A	29	SGN	C6-O6-S2-O5S
1	10-A	29	SGN	C6-O6-S2-O5S
1	13-A	29	SGN	C6-O6-S2-O5S
1	4-A	30	IDS	O5-C5-C6-O6A
1	3-A	1	SGN	C2-N2-S1-O1S
1	4-A	1	SGN	C2-N2-S1-O1S
1	5-A	1	SGN	C2-N2-S1-O1S
1	9-A	1	SGN	C2-N2-S1-O1S
1	5-A	3	SGN	C2-N2-S1-O2S
1	8-A	3	SGN	C2-N2-S1-O1S
1	9-A	5	SGN	C2-N2-S1-O2S
1	11-A	5	SGN	C2-N2-S1-O2S
1	13-A	5	SGN	C2-N2-S1-O1S
1	3-A	7	SGN	C2-N2-S1-O1S
1	4-A	7	SGN	C2-N2-S1-O2S
1	12-A	9	SGN	C2-N2-S1-O1S
1	3-A	11	SGN	C2-N2-S1-O1S
1	1-A	13	SGN	C2-N2-S1-O1S
1	3-A	13	SGN	C2-N2-S1-O1S
1	12-A	13	SGN	C2-N2-S1-O2S
1	13-A	13	SGN	C2-N2-S1-O2S
1	11-A	15	SGN	C2-N2-S1-O1S
1	12-A	15	SGN	C2-N2-S1-O1S
1	5-A	23	SGN	C2-N2-S1-O1S
1	5-A	25	SGN	C2-N2-S1-O1S
1	6-A	25	SGN	C2-N2-S1-O1S
1	9-A	25	SGN	C2-N2-S1-O2S
1	10-A	25	SGN	C2-N2-S1-O1S
1	14-A	25	SGN	C2-N2-S1-O1S
1	6-A	29	SGN	C2-N2-S1-O2S
1	14-A	29	SGN	C2-N2-S1-O1S
1	1-A	1	SGN	C6-O6-S2-O4S
1	6-A	1	SGN	C6-O6-S2-O5S
1	8-A	1	SGN	C6-O6-S2-O4S
1	8-A	1	SGN	C6-O6-S2-O5S
1	11-A	1	SGN	C6-O6-S2-O5S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	13-A	1	SGN	C6-O6-S2-O4S
1	4-A	3	SGN	C6-O6-S2-O4S
1	4-A	3	SGN	C6-O6-S2-O5S
1	8-A	3	SGN	C6-O6-S2-O5S
1	9-A	3	SGN	C6-O6-S2-O4S
1	12-A	3	SGN	C6-O6-S2-O4S
1	3-A	5	SGN	C6-O6-S2-O5S
1	4-A	7	SGN	C6-O6-S2-O5S
1	5-A	7	SGN	C6-O6-S2-O5S
1	10-A	7	SGN	C6-O6-S2-O5S
1	12-A	7	SGN	C6-O6-S2-O4S
1	12-A	7	SGN	C6-O6-S2-O5S
1	14-A	7	SGN	C6-O6-S2-O5S
1	6-A	9	SGN	C6-O6-S2-O5S
1	2-A	11	SGN	C6-O6-S2-O4S
1	4-A	11	SGN	C6-O6-S2-O5S
1	9-A	11	SGN	C6-O6-S2-O4S
1	14-A	11	SGN	C6-O6-S2-O4S
1	2-A	13	SGN	C6-O6-S2-O4S
1	3-A	13	SGN	C6-O6-S2-O5S
1	8-A	13	SGN	C6-O6-S2-O4S
1	12-A	13	SGN	C6-O6-S2-O5S
1	4-A	15	SGN	C6-O6-S2-O5S
1	11-A	15	SGN	C6-O6-S2-O4S
1	12-A	15	SGN	C6-O6-S2-O5S
1	2-A	17	SGN	C6-O6-S2-O5S
1	6-A	17	SGN	C6-O6-S2-O4S
1	10-A	17	SGN	C6-O6-S2-O4S
1	2-A	21	SGN	C6-O6-S2-O5S
1	1-A	23	SGN	C6-O6-S2-O5S
1	2-A	23	SGN	C6-O6-S2-O4S
1	2-A	23	SGN	C6-O6-S2-O5S
1	3-A	23	SGN	C6-O6-S2-O4S
1	3-A	23	SGN	C6-O6-S2-O5S
1	6-A	23	SGN	C6-O6-S2-O5S
1	3-A	25	SGN	C6-O6-S2-O5S
1	5-A	25	SGN	C6-O6-S2-O4S
1	13-A	25	SGN	C6-O6-S2-O4S
1	1-A	27	SGN	C6-O6-S2-O5S
1	2-A	27	SGN	C6-O6-S2-O4S
1	9-A	27	SGN	C6-O6-S2-O4S
1	11-A	27	SGN	C6-O6-S2-O5S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	14-A	27	SGN	C6-O6-S2-O4S
1	1-A	29	SGN	C6-O6-S2-O5S
1	3-A	29	SGN	C6-O6-S2-O4S
1	3-A	29	SGN	C6-O6-S2-O5S
1	10-A	29	SGN	C6-O6-S2-O4S
1	11-A	29	SGN	C6-O6-S2-O5S
1	10-A	5	SGN	O5-C5-C6-O6
1	1-A	7	SGN	C1-C2-N2-S1
1	7-A	7	SGN	C1-C2-N2-S1
1	13-A	7	SGN	C1-C2-N2-S1
1	3-A	9	SGN	C1-C2-N2-S1
1	2-A	11	SGN	O5-C5-C6-O6
1	3-A	11	SGN	O5-C5-C6-O6
1	6-A	11	SGN	C1-C2-N2-S1
1	3-A	17	SGN	C1-C2-N2-S1
1	10-A	17	SGN	C1-C2-N2-S1
1	3-A	19	SGN	C1-C2-N2-S1
1	9-A	19	SGN	O5-C5-C6-O6
1	4-A	21	SGN	O5-C5-C6-O6
1	4-A	1	SGN	C4-C5-C6-O6
1	6-A	1	SGN	C4-C5-C6-O6
1	12-A	3	SGN	C4-C5-C6-O6
1	4-A	5	SGN	C4-C5-C6-O6
1	12-A	5	SGN	C4-C5-C6-O6
1	9-A	7	SGN	C4-C5-C6-O6
1	10-A	7	SGN	C4-C5-C6-O6
1	3-A	9	SGN	C4-C5-C6-O6
1	13-A	9	SGN	C4-C5-C6-O6
1	1-A	11	SGN	C4-C5-C6-O6
1	11-A	11	SGN	C4-C5-C6-O6
1	7-A	13	SGN	C4-C5-C6-O6
1	8-A	15	SGN	C4-C5-C6-O6
1	14-A	15	SGN	C4-C5-C6-O6
1	3-A	17	SGN	C4-C5-C6-O6
1	10-A	17	SGN	C4-C5-C6-O6
1	13-A	17	SGN	C4-C5-C6-O6
1	5-A	21	SGN	C4-C5-C6-O6
1	3-A	23	SGN	C4-C5-C6-O6
1	11-A	23	SGN	C4-C5-C6-O6
1	5-A	25	SGN	C4-C5-C6-O6
1	7-A	25	SGN	C4-C5-C6-O6
1	13-A	25	SGN	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	6-A	27	SGN	C4-C5-C6-O6
1	14-A	6	IDS	C3-C2-O2-S
1	1-A	1	SGN	C6-O6-S2-O6S
1	13-A	1	SGN	C6-O6-S2-O6S
1	6-A	7	SGN	C6-O6-S2-O6S
1	2-A	11	SGN	C6-O6-S2-O6S
1	9-A	11	SGN	C6-O6-S2-O6S
1	4-A	13	SGN	C6-O6-S2-O6S
1	8-A	13	SGN	C6-O6-S2-O6S
1	2-A	15	SGN	C6-O6-S2-O6S
1	11-A	15	SGN	C6-O6-S2-O6S
1	9-A	23	SGN	C6-O6-S2-O6S
1	4-A	25	SGN	C6-O6-S2-O6S
1	9-A	27	SGN	C6-O6-S2-O6S
1	10-A	27	SGN	C6-O6-S2-O6S
1	14-A	27	SGN	C6-O6-S2-O6S
1	6-A	29	SGN	C6-O6-S2-O6S
1	10-A	7	SGN	C6-O6-S2-O4S
1	10-A	17	SGN	C6-O6-S2-O5S
1	7-A	29	SGN	C6-O6-S2-O4S
1	5-A	2	IDS	C2-O2-S-O3S
1	10-A	2	IDS	C2-O2-S-O3S
1	14-A	2	IDS	C2-O2-S-O3S
1	13-A	4	IDS	C2-O2-S-O3S
1	8-A	6	IDS	C2-O2-S-O3S
1	2-A	8	IDS	C2-O2-S-O3S
1	4-A	8	IDS	C2-O2-S-O3S
1	7-A	8	IDS	C2-O2-S-O1S
1	4-A	10	IDS	C2-O2-S-O3S
1	2-A	12	IDS	C2-O2-S-O3S
1	8-A	12	IDS	C2-O2-S-O3S
1	10-A	14	IDS	C2-O2-S-O3S
1	14-A	14	IDS	C2-O2-S-O3S
1	3-A	16	IDS	C2-O2-S-O3S
1	6-A	16	IDS	C2-O2-S-O3S
1	10-A	16	IDS	C2-O2-S-O3S
1	11-A	16	IDS	C2-O2-S-O3S
1	1-A	18	IDS	C2-O2-S-O3S
1	3-A	18	IDS	C2-O2-S-O3S
1	7-A	18	IDS	C2-O2-S-O3S
1	12-A	18	IDS	C2-O2-S-O3S
1	1-A	20	IDS	C2-O2-S-O3S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	7-A	24	IDS	C2-O2-S-O2S
1	8-A	24	IDS	C2-O2-S-O3S
1	13-A	24	IDS	C2-O2-S-O3S
1	8-A	26	IDS	C2-O2-S-O3S
1	9-A	26	IDS	C2-O2-S-O3S
1	14-A	26	IDS	C2-O2-S-O3S
1	3-A	30	IDS	C2-O2-S-O3S
1	4-A	30	IDS	C2-O2-S-O3S
1	13-A	3	SGN	C3-C2-N2-S1
1	1-A	7	SGN	C3-C2-N2-S1
1	2-A	7	SGN	C3-C2-N2-S1
1	1-A	9	SGN	C3-C2-N2-S1
1	3-A	9	SGN	C3-C2-N2-S1
1	9-A	9	SGN	C3-C2-N2-S1
1	13-A	9	SGN	C3-C2-N2-S1
1	10-A	11	SGN	C3-C2-N2-S1
1	8-A	13	SGN	C3-C2-N2-S1
1	12-A	21	SGN	C3-C2-N2-S1
1	11-A	23	SGN	C3-C2-N2-S1
1	8-A	25	SGN	C3-C2-N2-S1
1	11-A	25	SGN	C3-C2-N2-S1
1	4-A	29	SGN	C3-C2-N2-S1
1	9-A	30	IDS	C4-C5-C6-O6A
1	3-A	1	SGN	C6-O6-S2-O4S
1	5-A	1	SGN	C6-O6-S2-O5S
1	2-A	2	IDS	C4-C5-C6-O6A
1	2-A	2	IDS	C4-C5-C6-O6B
1	6-A	2	IDS	C4-C5-C6-O6A
1	6-A	2	IDS	C4-C5-C6-O6B
1	13-A	2	IDS	C4-C5-C6-O6A
1	13-A	2	IDS	C4-C5-C6-O6B
1	9-A	3	SGN	C6-O6-S2-O5S
1	10-A	4	IDS	C4-C5-C6-O6A
1	10-A	4	IDS	C4-C5-C6-O6B
1	11-A	6	IDS	C4-C5-C6-O6A
1	8-A	8	IDS	C4-C5-C6-O6B
1	3-A	10	IDS	C4-C5-C6-O6A
1	9-A	10	IDS	C4-C5-C6-O6B
1	12-A	10	IDS	C4-C5-C6-O6B
1	13-A	12	IDS	C4-C5-C6-O6A
1	4-A	13	SGN	C6-O6-S2-O4S
1	10-A	15	SGN	C6-O6-S2-O5S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	11-A	16	IDS	C4-C5-C6-O6B
1	4-A	17	SGN	C6-O6-S2-O4S
1	7-A	21	SGN	C6-O6-S2-O4S
1	9-A	21	SGN	C6-O6-S2-O5S
1	7-A	22	IDS	C4-C5-C6-O6B
1	8-A	22	IDS	C4-C5-C6-O6A
1	8-A	22	IDS	C4-C5-C6-O6B
1	11-A	22	IDS	C4-C5-C6-O6B
1	12-A	24	IDS	C4-C5-C6-O6B
1	2-A	28	IDS	C4-C5-C6-O6A
1	4-A	28	IDS	C4-C5-C6-O6A
1	4-A	28	IDS	C4-C5-C6-O6B
1	13-A	3	SGN	C1-C2-N2-S1
1	1-A	9	SGN	C1-C2-N2-S1
1	9-A	9	SGN	C1-C2-N2-S1
1	10-A	11	SGN	C1-C2-N2-S1
1	12-A	11	SGN	C1-C2-N2-S1
1	13-A	13	SGN	O5-C5-C6-O6
1	8-A	25	SGN	C1-C2-N2-S1
1	11-A	25	SGN	C1-C2-N2-S1
1	13-A	25	SGN	O5-C5-C6-O6
1	6-A	16	IDS	C1-C2-O2-S
1	10-A	16	IDS	C1-C2-O2-S
1	14-A	26	IDS	C1-C2-O2-S
1	4-A	11	SGN	C4-C5-C6-O6
1	13-A	13	SGN	C4-C5-C6-O6
1	9-A	21	SGN	C4-C5-C6-O6
1	9-A	27	SGN	C4-C5-C6-O6
1	10-A	29	SGN	C4-C5-C6-O6
1	11-A	29	SGN	C4-C5-C6-O6
1	13-A	5	SGN	C6-O6-S2-O5S
1	2-A	13	SGN	C6-O6-S2-O5S
1	6-A	15	SGN	C6-O6-S2-O5S
1	13-A	15	SGN	C6-O6-S2-O5S
1	9-A	19	SGN	C6-O6-S2-O4S
1	10-A	25	SGN	C6-O6-S2-O5S
1	12-A	25	SGN	C6-O6-S2-O5S
1	7-A	29	SGN	C6-O6-S2-O5S
1	9-A	29	SGN	C6-O6-S2-O5S
1	6-A	1	SGN	C6-O6-S2-O6S
1	8-A	1	SGN	C6-O6-S2-O6S
1	4-A	3	SGN	C6-O6-S2-O6S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	7-A	5	SGN	C6-O6-S2-O6S
1	10-A	7	SGN	C6-O6-S2-O6S
1	12-A	7	SGN	C6-O6-S2-O6S
1	14-A	7	SGN	C6-O6-S2-O6S
1	9-A	9	SGN	C6-O6-S2-O6S
1	5-A	17	SGN	C6-O6-S2-O6S
1	2-A	23	SGN	C6-O6-S2-O6S
1	3-A	23	SGN	C6-O6-S2-O6S
1	3-A	25	SGN	C6-O6-S2-O6S
1	11-A	25	SGN	C6-O6-S2-O6S
1	1-A	29	SGN	C6-O6-S2-O6S
1	3-A	29	SGN	C6-O6-S2-O6S
1	8-A	29	SGN	C6-O6-S2-O6S
1	10-A	29	SGN	C6-O6-S2-O6S
1	1-A	30	IDS	O5-C5-C6-O6A
1	9-A	30	IDS	O5-C5-C6-O6A
1	1-A	1	SGN	C2-N2-S1-O1S
1	7-A	1	SGN	C2-N2-S1-O1S
1	10-A	1	SGN	C2-N2-S1-O1S
1	9-A	2	IDS	C2-O2-S-O2S
1	7-A	3	SGN	C2-N2-S1-O2S
1	11-A	3	SGN	C2-N2-S1-O1S
1	14-A	3	SGN	C2-N2-S1-O1S
1	2-A	4	IDS	C2-O2-S-O1S
1	8-A	4	IDS	C2-O2-S-O1S
1	14-A	4	IDS	C2-O2-S-O1S
1	2-A	5	SGN	C2-N2-S1-O2S
1	4-A	5	SGN	C2-N2-S1-O1S
1	7-A	5	SGN	C2-N2-S1-O1S
1	8-A	5	SGN	C2-N2-S1-O1S
1	12-A	5	SGN	C2-N2-S1-O1S
1	7-A	6	IDS	C2-O2-S-O2S
1	9-A	6	IDS	C2-O2-S-O2S
1	1-A	7	SGN	C2-N2-S1-O1S
1	6-A	7	SGN	C2-N2-S1-O1S
1	7-A	7	SGN	C2-N2-S1-O1S
1	13-A	7	SGN	C2-N2-S1-O1S
1	14-A	7	SGN	C2-N2-S1-O1S
1	1-A	8	IDS	C2-O2-S-O2S
1	11-A	8	IDS	C2-O2-S-O2S
1	1-A	9	SGN	C2-N2-S1-O1S
1	3-A	9	SGN	C2-N2-S1-O1S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	6-A	9	SGN	C2-N2-S1-O2S
1	8-A	9	SGN	C2-N2-S1-O2S
1	14-A	9	SGN	C2-N2-S1-O1S
1	12-A	10	IDS	C2-O2-S-O2S
1	13-A	10	IDS	C2-O2-S-O2S
1	5-A	11	SGN	C2-N2-S1-O2S
1	9-A	12	IDS	C2-O2-S-O1S
1	12-A	12	IDS	C2-O2-S-O1S
1	4-A	13	SGN	C2-N2-S1-O1S
1	9-A	13	SGN	C2-N2-S1-O2S
1	7-A	14	IDS	C2-O2-S-O2S
1	9-A	14	IDS	C2-O2-S-O2S
1	4-A	15	SGN	C2-N2-S1-O1S
1	6-A	15	SGN	C2-N2-S1-O1S
1	8-A	15	SGN	C2-N2-S1-O1S
1	10-A	15	SGN	C2-N2-S1-O1S
1	7-A	16	IDS	C2-O2-S-O2S
1	4-A	17	SGN	C2-N2-S1-O1S
1	10-A	17	SGN	C2-N2-S1-O1S
1	13-A	17	SGN	C2-N2-S1-O1S
1	6-A	18	IDS	C2-O2-S-O1S
1	13-A	18	IDS	C2-O2-S-O2S
1	6-A	19	SGN	C2-N2-S1-O1S
1	13-A	19	SGN	C2-N2-S1-O1S
1	2-A	20	IDS	C2-O2-S-O2S
1	4-A	21	SGN	C2-N2-S1-O1S
1	5-A	21	SGN	C2-N2-S1-O1S
1	7-A	21	SGN	C2-N2-S1-O1S
1	8-A	21	SGN	C2-N2-S1-O2S
1	11-A	21	SGN	C2-N2-S1-O2S
1	14-A	21	SGN	C2-N2-S1-O1S
1	2-A	22	IDS	C2-O2-S-O1S
1	13-A	22	IDS	C2-O2-S-O2S
1	1-A	23	SGN	C2-N2-S1-O2S
1	3-A	23	SGN	C2-N2-S1-O1S
1	6-A	23	SGN	C2-N2-S1-O2S
1	8-A	23	SGN	C2-N2-S1-O2S
1	9-A	23	SGN	C2-N2-S1-O1S
1	2-A	24	IDS	C2-O2-S-O1S
1	2-A	25	SGN	C2-N2-S1-O1S
1	3-A	25	SGN	C2-N2-S1-O2S
1	7-A	25	SGN	C2-N2-S1-O1S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	11-A	25	SGN	C2-N2-S1-O1S
1	2-A	26	IDS	C2-O2-S-O1S
1	11-A	26	IDS	C2-O2-S-O2S
1	2-A	27	SGN	C2-N2-S1-O1S
1	9-A	27	SGN	C2-N2-S1-O1S
1	10-A	27	SGN	C2-N2-S1-O1S
1	1-A	28	IDS	C2-O2-S-O1S
1	3-A	28	IDS	C2-O2-S-O1S
1	6-A	28	IDS	C2-O2-S-O1S
1	7-A	28	IDS	C2-O2-S-O1S
1	13-A	28	IDS	C2-O2-S-O2S
1	2-A	29	SGN	C2-N2-S1-O1S
1	7-A	29	SGN	C2-N2-S1-O1S
1	11-A	29	SGN	C2-N2-S1-O1S
1	12-A	29	SGN	C2-N2-S1-O1S
1	13-A	29	SGN	C2-N2-S1-O1S
1	6-A	30	IDS	C2-O2-S-O1S
1	3-A	1	SGN	C6-O6-S2-O5S
1	7-A	3	SGN	C6-O6-S2-O5S
1	4-A	17	SGN	C6-O6-S2-O5S
1	7-A	21	SGN	C6-O6-S2-O5S
1	6-A	23	SGN	C6-O6-S2-O4S
1	1-A	27	SGN	C6-O6-S2-O4S
1	2-A	1	SGN	O5-C5-C6-O6
1	2-A	11	SGN	C1-C2-N2-S1
1	13-A	19	SGN	O5-C5-C6-O6
1	3-A	21	SGN	C1-C2-N2-S1
1	9-A	21	SGN	C1-C2-N2-S1
1	1-A	25	SGN	C1-C2-N2-S1
1	9-A	27	SGN	O5-C5-C6-O6
1	14-A	27	SGN	C1-C2-N2-S1
1	10-A	29	SGN	O5-C5-C6-O6
1	13-A	7	SGN	C3-C2-N2-S1
1	2-A	11	SGN	C3-C2-N2-S1
1	9-A	21	SGN	C3-C2-N2-S1
1	14-A	27	SGN	C3-C2-N2-S1
1	5-A	7	SGN	C4-C5-C6-O6
1	9-A	11	SGN	C4-C5-C6-O6
1	2-A	19	SGN	C4-C5-C6-O6
1	13-A	19	SGN	C4-C5-C6-O6
1	5-A	1	SGN	C6-O6-S2-O4S
1	7-A	1	SGN	C6-O6-S2-O4S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	3-A	13	SGN	C6-O6-S2-O4S
1	9-A	21	SGN	C6-O6-S2-O4S
1	6-A	4	IDS	C3-C2-O2-S
1	8-A	16	IDS	C3-C2-O2-S
1	9-A	19	SGN	C6-O6-S2-O6S
1	6-A	23	SGN	C6-O6-S2-O6S
1	1-A	27	SGN	C6-O6-S2-O6S
1	12-A	30	IDS	O5-C5-C6-O6B
1	7-A	1	SGN	C6-O6-S2-O5S
1	5-A	11	SGN	C6-O6-S2-O4S
1	14-A	19	SGN	O5-C5-C6-O6
1	7-A	2	IDS	C2-O2-S-O3S
1	14-A	2	IDS	C2-O2-S-O2S
1	8-A	4	IDS	C2-O2-S-O2S
1	9-A	4	IDS	C2-O2-S-O2S
1	4-A	6	IDS	C2-O2-S-O3S
1	12-A	6	IDS	C2-O2-S-O3S
1	7-A	8	IDS	C2-O2-S-O3S
1	9-A	10	IDS	C2-O2-S-O2S
1	14-A	10	IDS	C2-O2-S-O2S
1	1-A	12	IDS	C2-O2-S-O3S
1	1-A	14	IDS	C2-O2-S-O3S
1	6-A	14	IDS	C2-O2-S-O2S
1	10-A	16	IDS	C2-O2-S-O2S
1	4-A	18	IDS	C2-O2-S-O2S
1	10-A	18	IDS	C2-O2-S-O3S
1	11-A	18	IDS	C2-O2-S-O3S
1	14-A	18	IDS	C2-O2-S-O3S
1	6-A	20	IDS	C2-O2-S-O2S
1	2-A	24	IDS	C2-O2-S-O2S
1	2-A	26	IDS	C2-O2-S-O2S
1	10-A	26	IDS	C2-O2-S-O3S
1	3-A	28	IDS	C2-O2-S-O2S
1	6-A	28	IDS	C2-O2-S-O2S
1	7-A	28	IDS	C2-O2-S-O2S
1	9-A	30	IDS	C2-O2-S-O3S
1	2-A	1	SGN	C4-C5-C6-O6
1	13-A	3	SGN	C4-C5-C6-O6
1	14-A	15	SGN	C3-C2-N2-S1
1	3-A	21	SGN	C3-C2-N2-S1
1	9-A	25	SGN	C3-C2-N2-S1
1	6-A	29	SGN	C3-C2-N2-S1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	5-A	30	IDS	O5-C5-C6-O6A
1	7-A	30	IDS	O5-C5-C6-O6A
1	10-A	30	IDS	O5-C5-C6-O6A
1	5-A	11	SGN	C6-O6-S2-O5S
1	6-A	13	SGN	C6-O6-S2-O5S
1	10-A	15	SGN	C6-O6-S2-O4S
1	10-A	21	SGN	C6-O6-S2-O5S
1	13-A	21	SGN	C6-O6-S2-O5S
1	3-A	1	SGN	C3-C2-N2-S1
1	8-A	2	IDS	O5-C5-C6-O6B
1	9-A	2	IDS	O5-C5-C6-O6B
1	10-A	2	IDS	O5-C5-C6-O6B
1	2-A	4	IDS	O5-C5-C6-O6B
1	4-A	4	IDS	O5-C5-C6-O6B
1	8-A	4	IDS	O5-C5-C6-O6A
1	8-A	4	IDS	O5-C5-C6-O6B
1	9-A	4	IDS	O5-C5-C6-O6A
1	9-A	4	IDS	O5-C5-C6-O6B
1	2-A	6	IDS	O5-C5-C6-O6B
1	12-A	6	IDS	O5-C5-C6-O6B
1	1-A	8	IDS	O5-C5-C6-O6B
1	6-A	8	IDS	O5-C5-C6-O6B
1	12-A	8	IDS	O5-C5-C6-O6B
1	11-A	10	IDS	O5-C5-C6-O6A
1	11-A	10	IDS	O5-C5-C6-O6B
1	4-A	12	IDS	O5-C5-C6-O6B
1	9-A	12	IDS	O5-C5-C6-O6B
1	1-A	14	IDS	O5-C5-C6-O6B
1	7-A	14	IDS	O5-C5-C6-O6B
1	14-A	16	IDS	O5-C5-C6-O6B
1	5-A	20	IDS	O5-C5-C6-O6B
1	8-A	20	IDS	O5-C5-C6-O6B
1	12-A	20	IDS	O5-C5-C6-O6B
1	6-A	22	IDS	O5-C5-C6-O6A
1	6-A	22	IDS	O5-C5-C6-O6B
1	1-A	24	IDS	O5-C5-C6-O6B
1	6-A	24	IDS	O5-C5-C6-O6A
1	6-A	24	IDS	O5-C5-C6-O6B
1	7-A	24	IDS	O5-C5-C6-O6B
1	8-A	24	IDS	O5-C5-C6-O6B
1	14-A	24	IDS	O5-C5-C6-O6B
1	2-A	26	IDS	O5-C5-C6-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	10-A	26	IDS	O5-C5-C6-O6B
1	6-A	28	IDS	O5-C5-C6-O6B
1	10-A	28	IDS	O5-C5-C6-O6B
1	11-A	1	SGN	C2-N2-S1-O1S
1	13-A	1	SGN	C2-N2-S1-O1S
1	14-A	1	SGN	C2-N2-S1-O2S
1	12-A	3	SGN	C2-N2-S1-O2S
1	6-A	5	SGN	C2-N2-S1-O1S
1	10-A	5	SGN	C2-N2-S1-O1S
1	12-A	7	SGN	C2-N2-S1-O1S
1	5-A	9	SGN	C2-N2-S1-O1S
1	9-A	9	SGN	C2-N2-S1-O1S
1	13-A	9	SGN	C2-N2-S1-O1S
1	1-A	11	SGN	C2-N2-S1-O2S
1	2-A	11	SGN	C2-N2-S1-O1S
1	11-A	11	SGN	C2-N2-S1-O1S
1	9-A	15	SGN	C2-N2-S1-O2S
1	14-A	17	SGN	C2-N2-S1-O2S
1	7-A	19	SGN	C2-N2-S1-O1S
1	10-A	19	SGN	C2-N2-S1-O1S
1	14-A	19	SGN	C2-N2-S1-O2S
1	2-A	21	SGN	C2-N2-S1-O1S
1	11-A	23	SGN	C2-N2-S1-O2S
1	1-A	25	SGN	C2-N2-S1-O2S
1	13-A	25	SGN	C2-N2-S1-O2S
1	3-A	27	SGN	C2-N2-S1-O2S
1	4-A	27	SGN	C2-N2-S1-O1S
1	8-A	27	SGN	C2-N2-S1-O1S
1	11-A	27	SGN	C2-N2-S1-O1S
1	14-A	27	SGN	C2-N2-S1-O2S
1	4-A	29	SGN	C2-N2-S1-O1S
1	8-A	29	SGN	C2-N2-S1-O1S
1	11-A	13	SGN	C6-O6-S2-O6S
1	1-A	30	IDS	C4-C5-C6-O6A
1	1-A	30	IDS	C4-C5-C6-O6B
1	12-A	30	IDS	C4-C5-C6-O6B
1	7-A	2	IDS	C4-C5-C6-O6B
1	10-A	2	IDS	C4-C5-C6-O6B
1	12-A	2	IDS	C4-C5-C6-O6B
1	1-A	6	IDS	C4-C5-C6-O6B
1	4-A	6	IDS	C4-C5-C6-O6B
1	9-A	6	IDS	C4-C5-C6-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	12-A	8	IDS	C4-C5-C6-O6B
1	3-A	10	IDS	C4-C5-C6-O6B
1	13-A	12	IDS	C4-C5-C6-O6B
1	11-A	13	SGN	C6-O6-S2-O4S
1	11-A	13	SGN	C6-O6-S2-O5S
1	10-A	14	IDS	C4-C5-C6-O6B
1	12-A	14	IDS	C4-C5-C6-O6B
1	14-A	16	IDS	C4-C5-C6-O6B
1	1-A	20	IDS	C4-C5-C6-O6B
1	6-A	21	SGN	C6-O6-S2-O5S
1	8-A	24	IDS	C4-C5-C6-O6B
1	13-A	24	IDS	C4-C5-C6-O6B
1	5-A	28	IDS	C4-C5-C6-O6B
1	6-A	3	SGN	O5-C5-C6-O6
1	13-A	3	SGN	O5-C5-C6-O6
1	9-A	23	SGN	O5-C5-C6-O6
1	9-A	25	SGN	C1-C2-N2-S1
1	6-A	29	SGN	C1-C2-N2-S1

There are no ring outliers.

378 monomers are involved in 922 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	10-A	18	IDS	4	0
1	8-A	19	SGN	5	0
1	9-A	6	IDS	6	0
1	9-A	23	SGN	9	0
1	13-A	18	IDS	6	0
1	14-A	16	IDS	5	0
1	14-A	15	SGN	3	0
1	11-A	5	SGN	7	0
1	10-A	30	IDS	2	0
1	8-A	5	SGN	3	0
1	14-A	21	SGN	2	0
1	2-A	26	IDS	10	0
1	6-A	20	IDS	1	0
1	3-A	27	SGN	1	0
1	4-A	12	IDS	12	0
1	1-A	20	IDS	2	0
1	14-A	2	IDS	3	0
1	1-A	17	SGN	3	0
1	9-A	21	SGN	8	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	11-A	25	SGN	2	0
1	7-A	21	SGN	6	0
1	9-A	1	SGN	2	0
1	5-A	1	SGN	5	0
1	13-A	9	SGN	6	0
1	4-A	13	SGN	13	0
1	7-A	6	IDS	1	0
1	8-A	24	IDS	12	0
1	2-A	18	IDS	3	0
1	11-A	10	IDS	2	0
1	14-A	26	IDS	1	0
1	3-A	9	SGN	1	0
1	5-A	22	IDS	8	0
1	1-A	8	IDS	4	0
1	5-A	11	SGN	1	0
1	4-A	23	SGN	9	0
1	10-A	15	SGN	4	0
1	12-A	18	IDS	1	0
1	11-A	21	SGN	6	0
1	12-A	10	IDS	5	0
1	11-A	16	IDS	7	0
1	1-A	9	SGN	4	0
1	9-A	18	IDS	12	0
1	9-A	20	IDS	15	0
1	8-A	7	SGN	1	0
1	2-A	23	SGN	9	0
1	13-A	23	SGN	1	0
1	7-A	3	SGN	9	0
1	5-A	27	SGN	4	0
1	1-A	3	SGN	2	0
1	6-A	21	SGN	3	0
1	12-A	29	SGN	1	0
1	14-A	25	SGN	6	0
1	6-A	18	IDS	6	0
1	3-A	22	IDS	10	0
1	5-A	24	IDS	1	0
1	10-A	24	IDS	3	0
1	10-A	29	SGN	5	0
1	4-A	6	IDS	12	0
1	12-A	11	SGN	6	0
1	11-A	20	IDS	8	0
1	11-A	28	IDS	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	6-A	29	SGN	6	0
1	3-A	15	SGN	2	0
1	14-A	14	IDS	5	0
1	1-A	6	IDS	3	0
1	11-A	26	IDS	1	0
1	10-A	3	SGN	5	0
1	8-A	15	SGN	3	0
1	5-A	9	SGN	1	0
1	6-A	11	SGN	5	0
1	3-A	16	IDS	6	0
1	2-A	27	SGN	10	0
1	13-A	6	IDS	5	0
1	13-A	30	IDS	1	0
1	13-A	3	SGN	2	0
1	4-A	20	IDS	15	0
1	14-A	18	IDS	1	0
1	10-A	22	IDS	2	0
1	7-A	23	SGN	6	0
1	6-A	2	IDS	2	0
1	1-A	16	IDS	2	0
1	6-A	7	SGN	2	0
1	9-A	25	SGN	19	0
1	7-A	29	SGN	2	0
1	13-A	15	SGN	7	0
1	2-A	1	SGN	1	0
1	11-A	9	SGN	2	0
1	5-A	23	SGN	5	0
1	13-A	2	IDS	3	0
1	6-A	30	IDS	6	0
1	8-A	14	IDS	3	0
1	2-A	25	SGN	3	0
1	12-A	20	IDS	4	0
1	3-A	18	IDS	1	0
1	12-A	14	IDS	4	0
1	4-A	5	SGN	1	0
1	7-A	18	IDS	2	0
1	10-A	14	IDS	4	0
1	14-A	4	IDS	5	0
1	6-A	14	IDS	4	0
1	1-A	7	SGN	6	0
1	12-A	23	SGN	1	0
1	5-A	13	SGN	3	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1-A	23	SGN	7	0
1	12-A	17	SGN	1	0
1	14-A	20	IDS	6	0
1	9-A	17	SGN	12	0
1	5-A	14	IDS	9	0
1	12-A	5	SGN	1	0
1	2-A	20	IDS	4	0
1	9-A	27	SGN	2	0
1	11-A	23	SGN	9	0
1	3-A	3	SGN	6	0
1	9-A	5	SGN	2	0
1	2-A	15	SGN	2	0
1	10-A	16	IDS	2	0
1	5-A	4	IDS	2	0
1	5-A	25	SGN	9	0
1	2-A	17	SGN	2	0
1	3-A	30	IDS	11	0
1	5-A	29	SGN	3	0
1	6-A	27	SGN	1	0
1	10-A	21	SGN	1	0
1	6-A	12	IDS	10	0
1	13-A	16	IDS	7	0
1	11-A	15	SGN	7	0
1	3-A	14	IDS	6	0
1	14-A	23	SGN	8	0
1	9-A	19	SGN	17	0
1	7-A	2	IDS	6	0
1	1-A	4	IDS	3	0
1	10-A	7	SGN	2	0
1	9-A	11	SGN	3	0
1	13-A	4	IDS	7	0
1	2-A	4	IDS	2	0
1	5-A	28	IDS	6	0
1	3-A	20	IDS	13	0
1	14-A	24	IDS	10	0
1	6-A	17	SGN	6	0
1	8-A	10	IDS	11	0
1	4-A	7	SGN	11	0
1	5-A	16	IDS	1	0
1	11-A	18	IDS	6	0
1	4-A	21	SGN	5	0
1	2-A	19	SGN	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2-A	28	IDS	5	0
1	10-A	2	IDS	3	0
1	8-A	20	IDS	1	0
1	8-A	1	SGN	1	0
1	12-A	24	IDS	7	0
1	9-A	13	SGN	10	0
1	12-A	27	SGN	13	0
1	8-A	23	SGN	7	0
1	14-A	6	IDS	6	0
1	4-A	25	SGN	8	0
1	12-A	22	IDS	2	0
1	3-A	19	SGN	5	0
1	12-A	19	SGN	3	0
1	13-A	13	SGN	12	0
1	12-A	8	IDS	4	0
1	14-A	17	SGN	4	0
1	7-A	14	IDS	2	0
1	4-A	11	SGN	7	0
1	3-A	17	SGN	5	0
1	4-A	26	IDS	3	0
1	9-A	28	IDS	2	0
1	10-A	19	SGN	4	0
1	2-A	13	SGN	1	0
1	1-A	22	IDS	5	0
1	5-A	10	IDS	1	0
1	8-A	18	IDS	7	0
1	6-A	19	SGN	2	0
1	9-A	12	IDS	7	0
1	7-A	25	SGN	4	0
1	13-A	26	IDS	2	0
1	12-A	13	SGN	5	0
1	2-A	9	SGN	1	0
1	9-A	16	IDS	11	0
1	11-A	4	IDS	4	0
1	12-A	30	IDS	1	0
1	7-A	26	IDS	8	0
1	11-A	8	IDS	2	0
1	6-A	13	SGN	7	0
1	14-A	19	SGN	5	0
1	11-A	17	SGN	7	0
1	12-A	6	IDS	7	0
1	7-A	17	SGN	8	0

Continued on next page...

Continued from previous page...

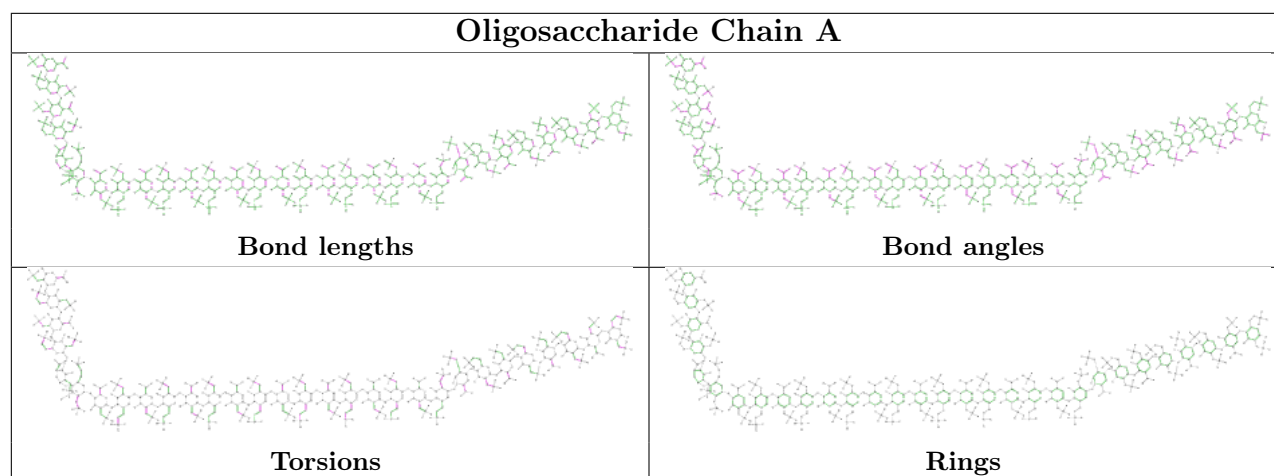
Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	4-A	14	IDS	3	0
1	7-A	7	SGN	3	0
1	8-A	9	SGN	9	0
1	10-A	26	IDS	2	0
1	14-A	5	SGN	2	0
1	10-A	6	IDS	3	0
1	4-A	10	IDS	15	0
1	9-A	26	IDS	13	0
1	6-A	6	IDS	2	0
1	13-A	24	IDS	1	0
1	7-A	5	SGN	2	0
1	11-A	13	SGN	7	0
1	12-A	16	IDS	6	0
1	5-A	12	IDS	1	0
1	14-A	13	SGN	6	0
1	9-A	7	SGN	4	0
1	2-A	11	SGN	3	0
1	1-A	27	SGN	2	0
1	11-A	22	IDS	3	0
1	4-A	18	IDS	7	0
1	14-A	22	IDS	5	0
1	13-A	20	IDS	3	0
1	14-A	11	SGN	4	0
1	6-A	8	IDS	5	0
1	4-A	15	SGN	6	0
1	3-A	8	IDS	1	0
1	1-A	24	IDS	6	0
1	5-A	26	IDS	9	0
1	2-A	21	SGN	5	0
1	2-A	29	SGN	5	0
1	5-A	30	IDS	1	0
1	9-A	2	IDS	5	0
1	2-A	7	SGN	4	0
1	11-A	11	SGN	1	0
1	12-A	15	SGN	6	0
1	3-A	12	IDS	2	0
1	6-A	9	SGN	6	0
1	8-A	11	SGN	2	0
1	14-A	1	SGN	3	0
1	1-A	2	IDS	5	0
1	8-A	12	IDS	2	0
1	10-A	10	IDS	4	0

Continued on next page...

Continued from previous page...

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

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



4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.