



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 21, 2020 – 04:46 PM BST

PDB ID : 1OVW
Title : ENDOGLUCANASE I COMPLEXED WITH NON-HYDROLYSABLE SUB-
STRATE ANALOGUE
Authors : Sulzenbacher, G.; Davies, G.J.; Schulein, M.
Deposited on : 1996-10-17
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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)	:	2.14.6

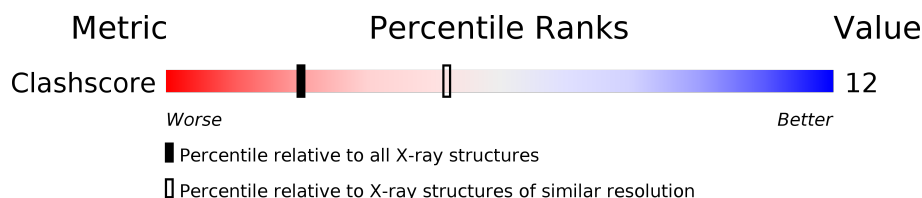
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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	3122 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	72% 26% .
1	B	398	69% 28% .
1	C	398	74% 23% .
1	D	398	73% 25% .
2	E	3	100%
2	F	3	100%
2	G	3	33% 67%
2	H	3	33% 67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13412 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ENDOGLUCANASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	B	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	C	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			
1	D	398	Total	C	N	O	S	0	0	0
			3023	1870	534	590	29			

- Molecule 2 is an oligosaccharide called 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	F	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	G	3	Total	C	O	S	0	0	0
			34	18	12	4			
2	H	3	Total	C	O	S	0	0	0
			34	18	12	4			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

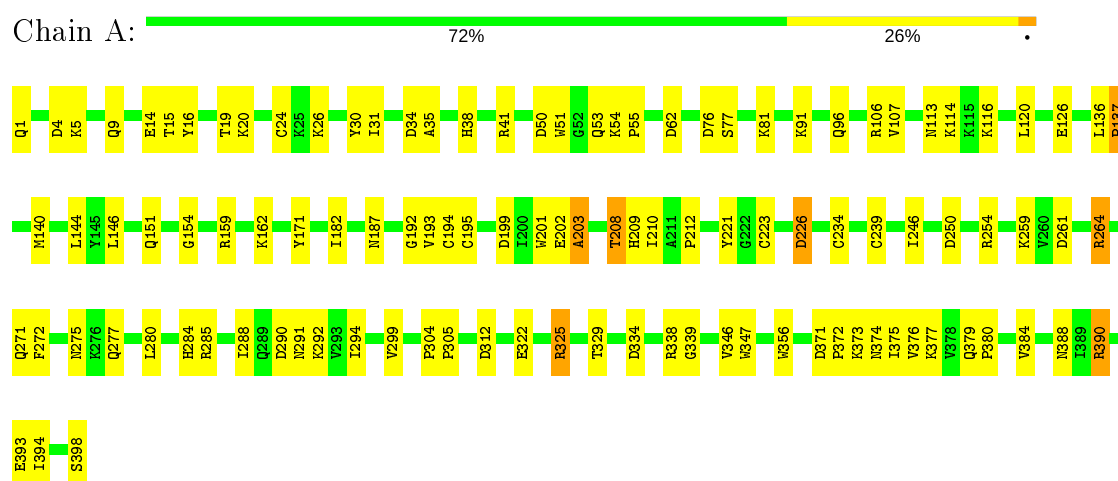
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	275	Total	O	0	0
			275	275		
4	B	267	Total	O	0	0
			267	267		
4	C	248	Total	O	0	0
			248	248		
4	D	282	Total	O	0	0
			282	282		

3 Residue-property plots

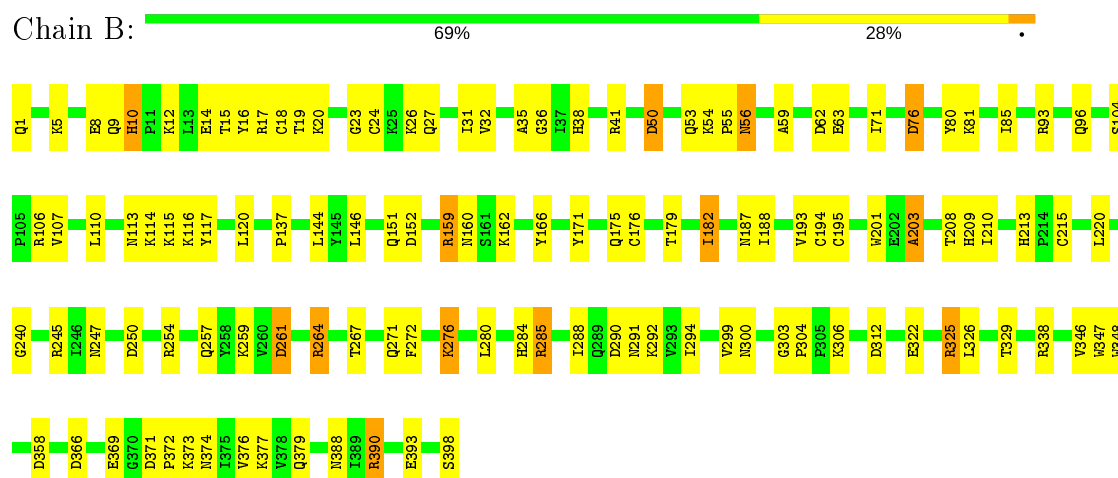
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: ENDOGLUCANASE I

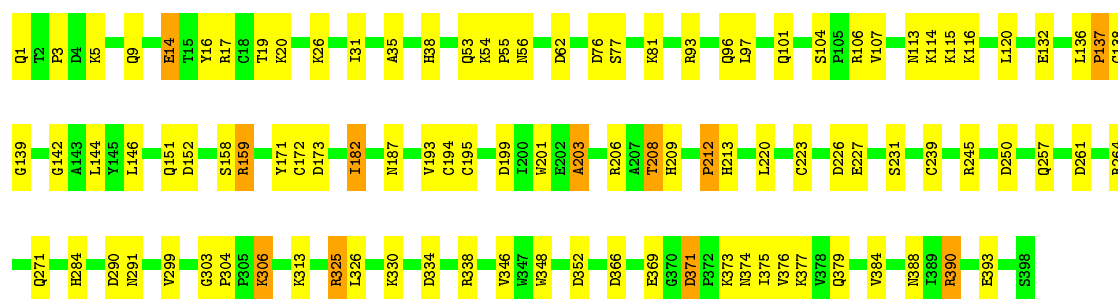


• Molecule 1: ENDOGLUCANASE I



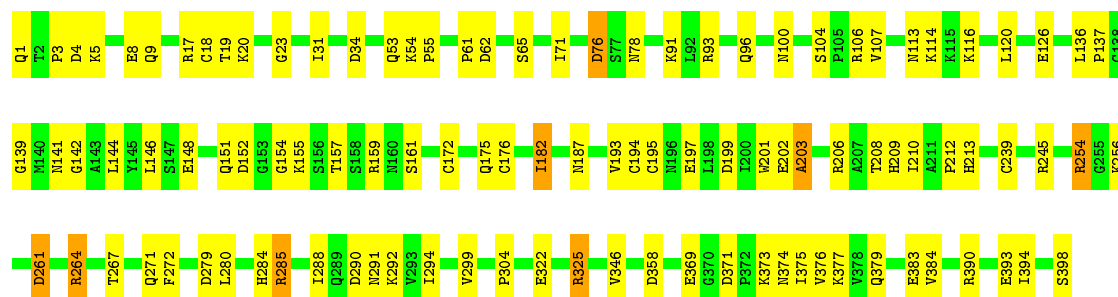
• Molecule 1: ENDOGLUCANASE I





• Molecule 1: ENDOGLUCANASE I

Chain D: 73% 25%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain E: 100%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain F: 100%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain G: 33% 67%



• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

Chain H: 33% 67%

SSCI
SSCI
SSCI

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.16 Å 78.28 Å 142.46 Å 90.00° 96.89° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70	Depositor
% Data completeness (in resolution range)	89.5 (15.00-2.70)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13412	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SSG, PCA, NAG, SGC

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	0/3077	1.54	31/4155 (0.7%)
1	B	0.67	0/3077	1.62	45/4155 (1.1%)
1	C	0.66	0/3077	1.61	49/4155 (1.2%)
1	D	0.67	0/3077	1.57	38/4155 (0.9%)
All	All	0.66	0/12308	1.58	163/16620 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	390	ARG	NE-CZ-NH1	21.63	131.11	120.30
1	D	390	ARG	NE-CZ-NH1	18.99	129.80	120.30
1	C	325	ARG	NE-CZ-NH1	17.52	129.06	120.30
1	C	390	ARG	NE-CZ-NH1	16.93	128.77	120.30
1	A	325	ARG	CD-NE-CZ	14.97	144.56	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	THR	Mainchain
1	B	15	THR	Mainchain

5.2 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	A	3023	0	2905	79	0
1	B	3023	0	2905	82	0
1	C	3023	0	2905	65	0
1	D	3023	0	2905	65	0
2	E	34	0	30	6	0
2	F	34	0	30	6	0
2	G	34	0	30	4	0
2	H	34	0	29	6	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	A	275	0	0	13	0
4	B	267	0	0	13	0
4	C	248	0	0	12	0
4	D	282	0	0	9	0
All	All	13412	0	11843	302	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 12.

The worst 5 of 302 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:D:182:ILE:HG21	4:D:940:HOH:O	1.64	0.95
1:A:203:ALA:HB2	1:A:208:THR:HG23	1.50	0.93
1:D:78:ASN:HB3	4:D:858:HOH:O	1.67	0.93
1:B:203:ALA:HB2	1:B:208:THR:HG23	1.52	0.88
1:D:203:ALA:HB2	1:D:208:THR:HG23	1.55	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	PCA	A	1	1	7,8,9	1.23	0	9,10,12	1.77	3 (33%)
1	PCA	D	1	1	7,8,9	1.18	0	9,10,12	1.80	3 (33%)
1	PCA	B	1	1	7,8,9	1.29	0	9,10,12	1.87	2 (22%)
1	PCA	C	1	1	7,8,9	1.41	0	9,10,12	2.28	2 (22%)

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	PCA	A	1	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PCA	OE-CD-CG	-4.61	118.73	126.76
1	B	1	PCA	OE-CD-CG	-4.17	119.48	126.76
1	A	1	PCA	OE-CD-CG	-3.64	120.40	126.76
1	C	1	PCA	O-C-CA	-3.32	116.08	124.78
1	D	1	PCA	OE-CD-CG	-2.99	121.54	126.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

12 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
2	SSG	E	1	2	10,12,12	1.91	3 (30%)	11,17,17	2.69	7 (63%)
2	SGC	E	2	2	10,11,12	1.95	2 (20%)	12,15,17	2.69	4 (33%)
2	SGC	E	3	2	10,11,12	0.90	0	12,15,17	1.61	3 (25%)
2	SSG	F	1	2	10,12,12	1.89	2 (20%)	11,17,17	2.19	5 (45%)
2	SGC	F	2	2	10,11,12	1.11	0	12,15,17	2.66	3 (25%)
2	SGC	F	3	2	10,11,12	0.86	0	12,15,17	1.37	2 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SSG	G	1	2	10,12,12	1.97	3 (30%)	11,17,17	2.65	5 (45%)
2	SGC	G	2	2	10,11,12	1.44	2 (20%)	12,15,17	2.61	3 (25%)
2	SGC	G	3	2	10,11,12	1.12	1 (10%)	12,15,17	1.52	2 (16%)
2	SSG	H	1	2	10,12,12	1.84	2 (20%)	11,17,17	2.50	5 (45%)
2	SGC	H	2	2	10,11,12	1.63	2 (20%)	12,15,17	2.74	3 (25%)
2	SGC	H	3	2	10,11,12	1.36	1 (10%)	12,15,17	1.44	2 (16%)

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
2	SSG	E	1	2	-	0/2/22/22	0/1/1/1
2	SGC	E	2	2	-	0/2/19/22	0/1/1/1
2	SGC	E	3	2	-	0/2/19/22	0/1/1/1
2	SSG	F	1	2	-	0/2/22/22	0/1/1/1
2	SGC	F	2	2	-	0/2/19/22	0/1/1/1
2	SGC	F	3	2	-	1/2/19/22	0/1/1/1
2	SSG	G	1	2	-	0/2/22/22	0/1/1/1
2	SGC	G	2	2	-	0/2/19/22	0/1/1/1
2	SGC	G	3	2	-	0/2/19/22	0/1/1/1
2	SSG	H	1	2	-	0/2/22/22	0/1/1/1
2	SGC	H	2	2	-	0/2/19/22	0/1/1/1
2	SGC	H	3	2	-	0/2/19/22	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	SGC	C3-C4	4.38	1.57	1.53
2	H	1	SSG	C1-C2	-4.17	1.46	1.53
2	E	1	SSG	C5-C4	-3.55	1.50	1.53
2	G	1	SSG	C5-C4	-3.47	1.50	1.53
2	F	1	SSG	C5-C4	-3.41	1.50	1.53

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	SGC	O5-C1-C2	6.61	120.98	110.77
2	H	2	SGC	O5-C1-C2	6.22	120.37	110.77
2	E	2	SGC	O5-C1-C2	6.15	120.26	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	SGC	O5-C1-C2	5.94	119.95	110.77
2	E	2	SGC	C1-O5-C5	5.20	119.24	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3	SGC	C4-C5-C6-O6

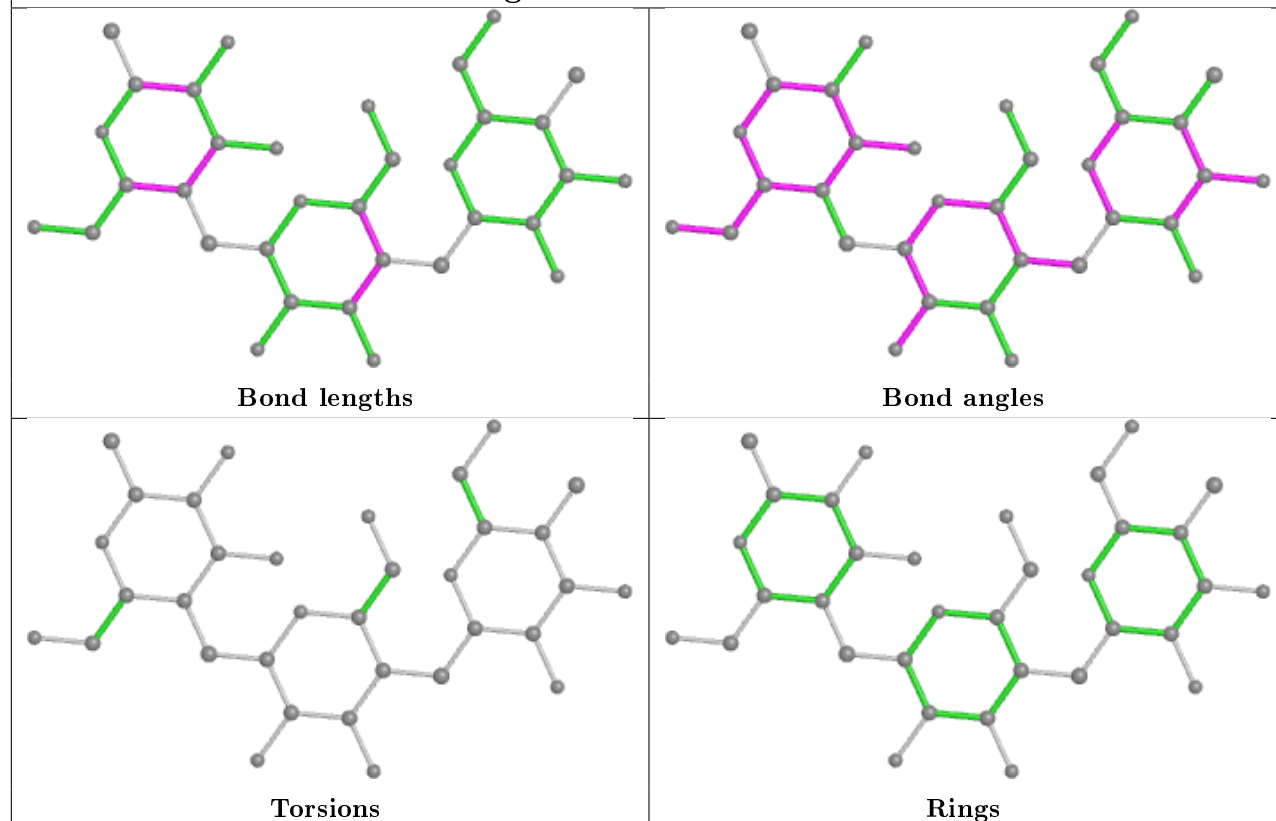
There are no ring outliers.

10 monomers are involved in 22 short contacts:

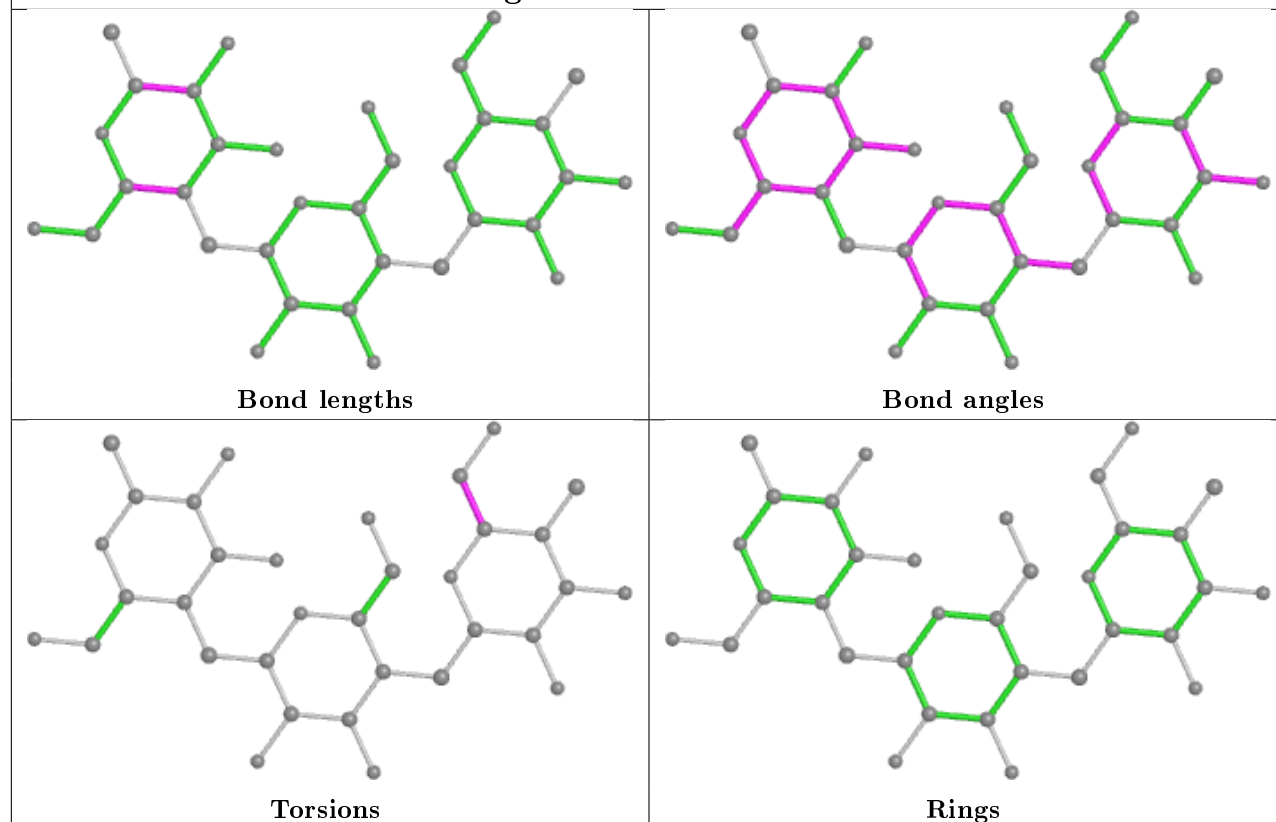
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	SSG	5	0
2	F	2	SGC	3	0
2	E	2	SGC	2	0
2	G	1	SSG	4	0
2	E	1	SSG	5	0
2	G	2	SGC	3	0
2	H	2	SGC	4	0
2	F	3	SGC	1	0
2	E	3	SGC	1	0
2	H	1	SSG	5	0

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

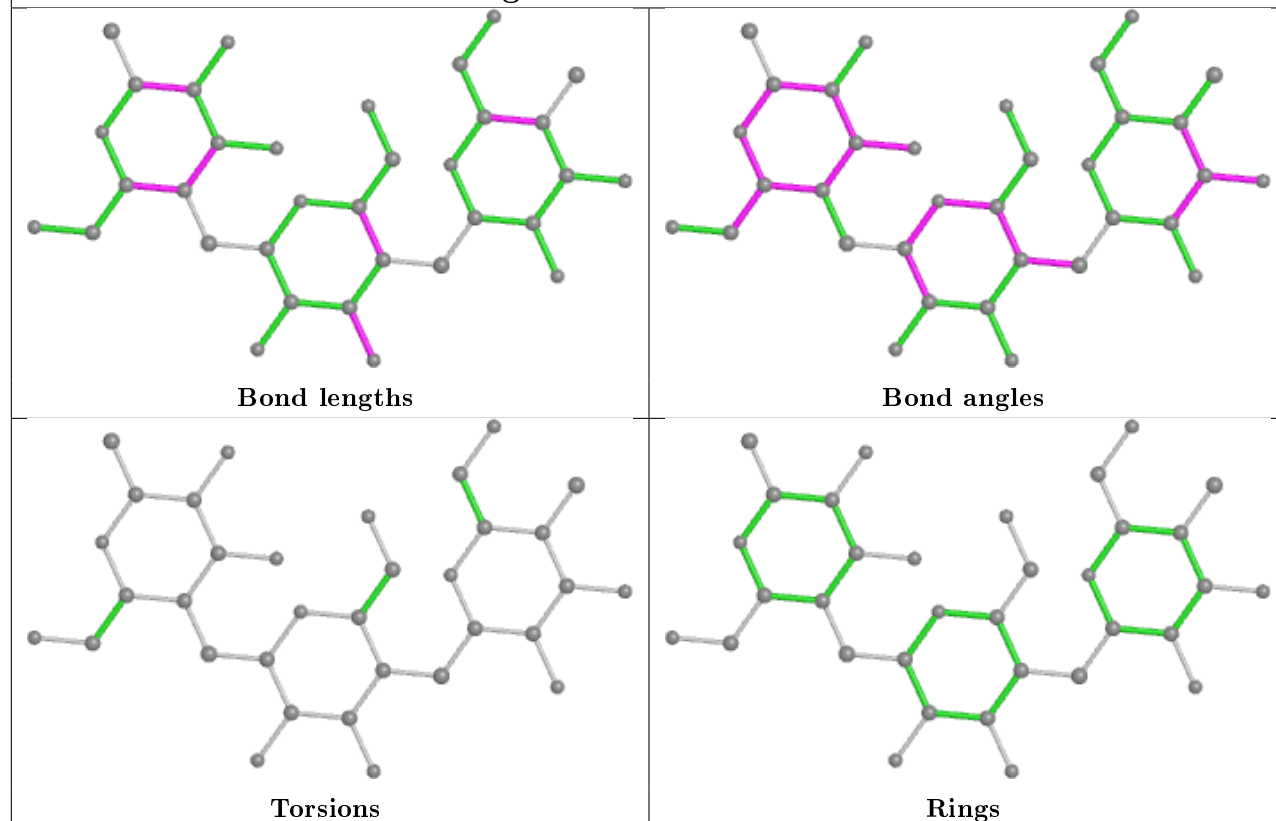
Oligosaccharide Chain E



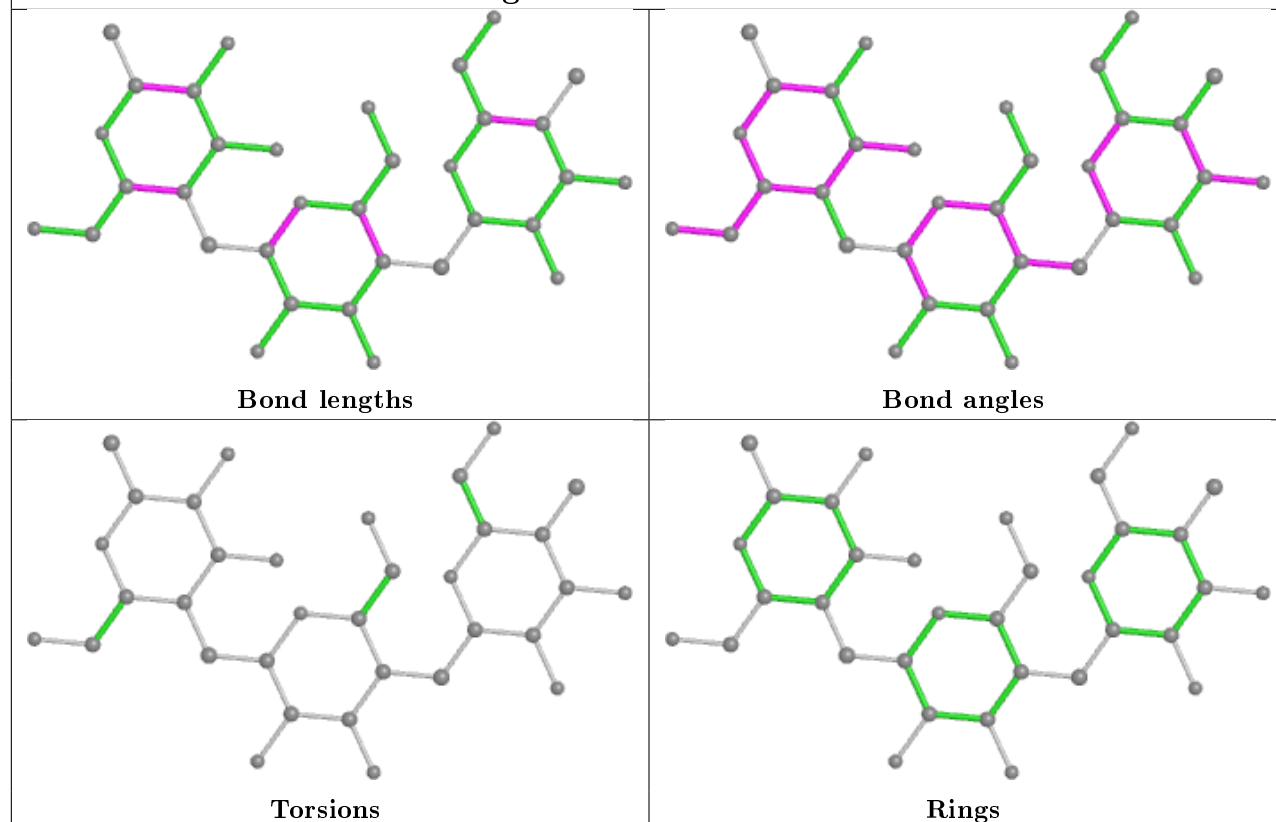
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry ⓘ

8 ligands 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
3	NAG	C	400	1	14,14,15	1.26	1 (7%)	17,19,21	1.51	3 (17%)
3	NAG	D	399	1	14,14,15	1.34	2 (14%)	17,19,21	2.20	5 (29%)
3	NAG	B	399	1	14,14,15	1.34	2 (14%)	17,19,21	1.75	3 (17%)
3	NAG	A	400	1	14,14,15	1.23	1 (7%)	17,19,21	1.50	3 (17%)
3	NAG	B	400	1	14,14,15	1.20	1 (7%)	17,19,21	1.54	4 (23%)
3	NAG	C	399	1	14,14,15	1.21	1 (7%)	17,19,21	2.10	5 (29%)
3	NAG	A	399	1	14,14,15	1.33	2 (14%)	17,19,21	1.18	1 (5%)
3	NAG	D	400	1	14,14,15	1.15	1 (7%)	17,19,21	1.31	2 (11%)

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
3	NAG	C	400	1	-	2/6/23/26	0/1/1/1
3	NAG	D	399	1	-	0/6/23/26	0/1/1/1
3	NAG	B	399	1	-	0/6/23/26	0/1/1/1
3	NAG	A	400	1	-	2/6/23/26	0/1/1/1
3	NAG	B	400	1	-	2/6/23/26	0/1/1/1
3	NAG	C	399	1	-	0/6/23/26	0/1/1/1
3	NAG	A	399	1	-	0/6/23/26	0/1/1/1
3	NAG	D	400	1	-	2/6/23/26	0/1/1/1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400	NAG	O7-C7	-3.69	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	399	NAG	O7-C7	-3.68	1.14	1.23
3	A	400	NAG	O7-C7	-3.66	1.15	1.23
3	A	399	NAG	O7-C7	-3.66	1.15	1.23
3	C	399	NAG	O7-C7	-3.51	1.15	1.23

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	399	NAG	O5-C1-C2	-5.29	102.94	111.29
3	D	399	NAG	C1-O5-C5	-5.01	105.41	112.19
3	B	399	NAG	C1-C2-N2	4.53	118.23	110.49
3	D	399	NAG	O5-C1-C2	-3.89	105.14	111.29
3	C	399	NAG	C1-O5-C5	-3.86	106.96	112.19

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	400	NAG	O5-C5-C6-O6
3	A	400	NAG	O5-C5-C6-O6
3	C	400	NAG	O5-C5-C6-O6
3	B	400	NAG	O5-C5-C6-O6
3	D	400	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.