W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Mar 23, 2024 – 09:32 PM EDT

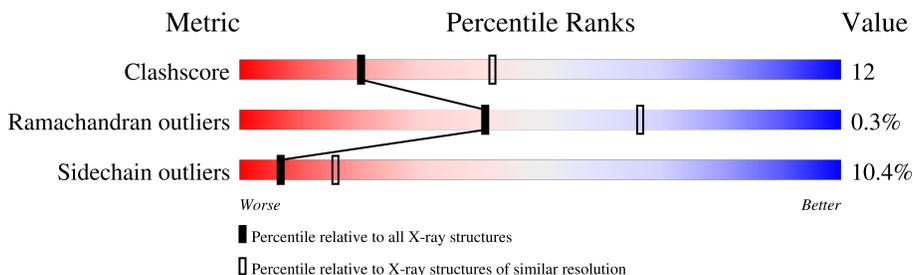|		
PDB ID	:	1OVW
Title	:	ENDOGLUCANASE I COMPLEXED WITH NON-HYDROLYSABLE SUBSTRATE ANALOGUE
Authors	:	Sulzenbacher, G.; Davies, G.J.; Schulein, M.
Deposited on	:	1996-10-17
Resolution	:	2.70 Å(reported)

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		0.3%
Sidechain outliers		10.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	398	69% 25% 5% ·
1	B	398	65% 27% 8% ·
1	C	398	70% 23% 6% ·
1	D	398	70% 25% 5% ·
2	E	3	100%
2	F	3	100%
2	G	3	33% 67%
2	H	3	33% 67%

WORLDWIDE PDB
PROTEIN DATA BANK

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.
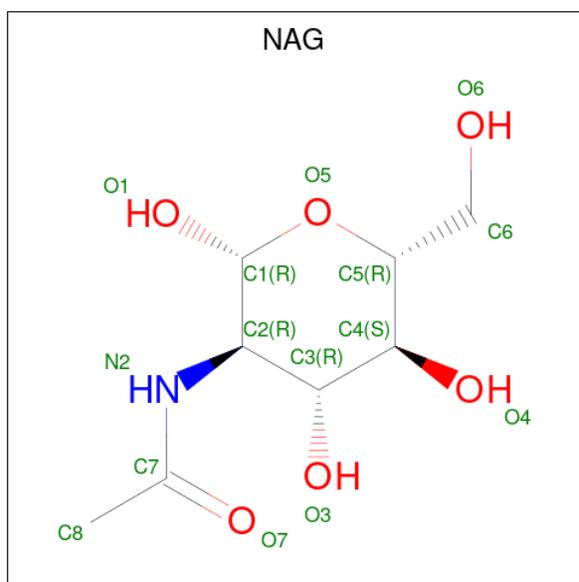
- Molecule 1 is a protein called ENDOGLUCANASE I.

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: $C_8H_{15}NO_6$).

NAG

O6
OH

O5
O1
HO O C6
C1(R) C5(R)
C2(R) C4(S)
N2 C3(R)
HN OH
O4
C7
OH
C8 O O3
O7

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

- Molecule 4 is water.

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

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: ENDOGLUCANASE I

Chain A:
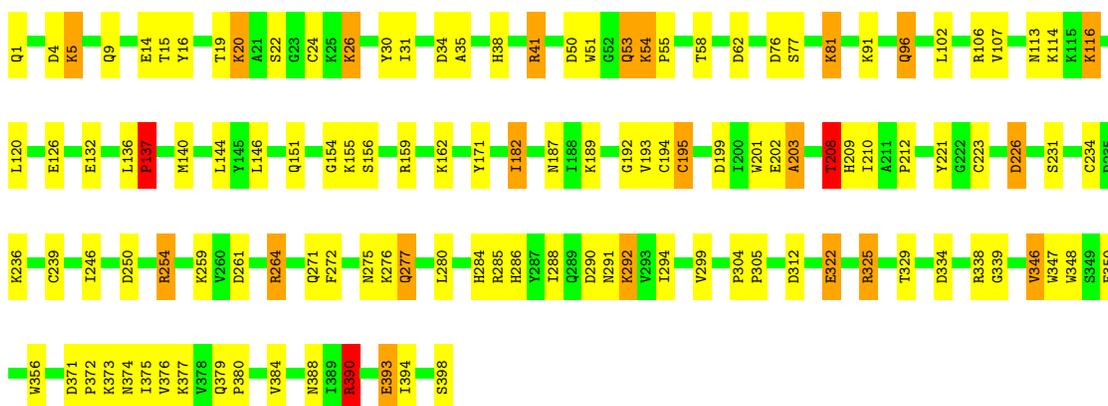
• Molecule 1: ENDOGLUCANASE I

Chain B:
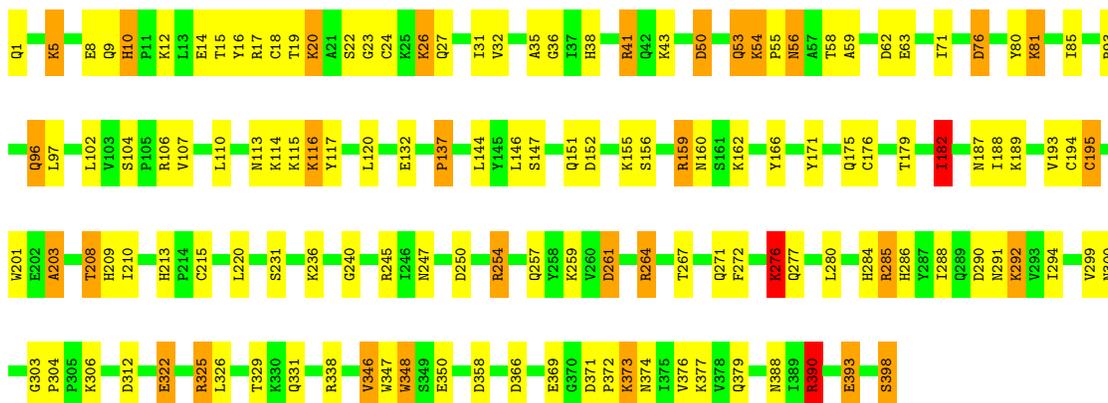
• Molecule 1: ENDOGLUCANASE I

Chain C:
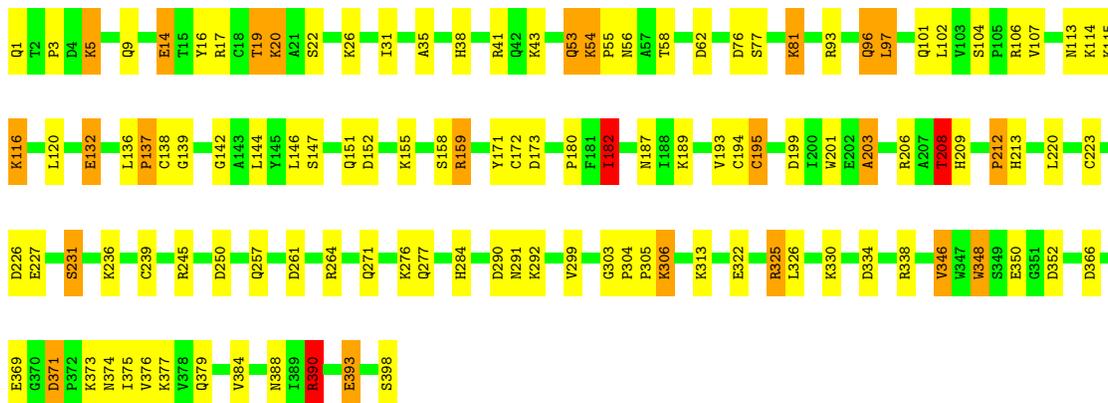
• Molecule 1: ENDOGLUCANASE I

Chain D:

70%   25%   5% ·
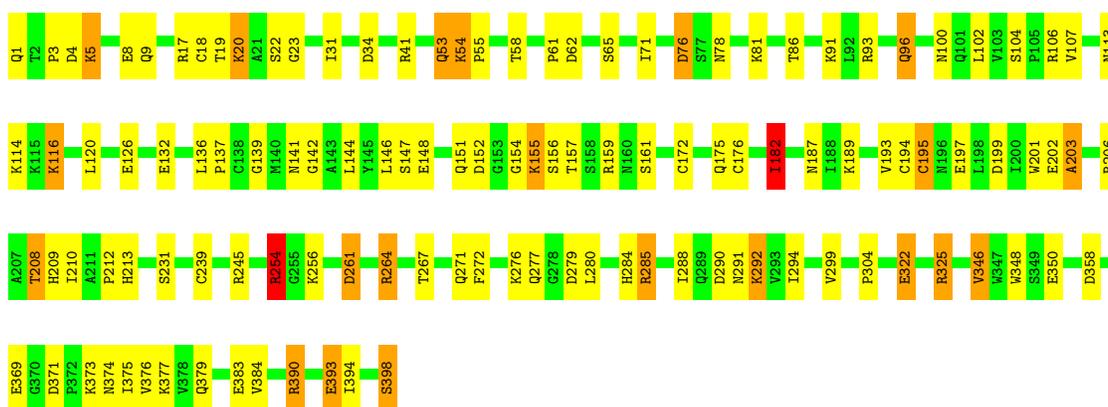
• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose

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%

SSG1 SGC2 SGC3

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

Chain H: 33%   67%

SSG1 SGC2 SGC3

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	68.16Å 78.28Å 142.46Å 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: SGC, NAG, PCA, SSG

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(^{o})	Ideal(^{o})
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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	396/398 (100%)	377 (95%)	18 (4%)	1 (0%)	41	66
1	B	396/398 (100%)	379 (96%)	16 (4%)	1 (0%)	41	66
1	C	396/398 (100%)	378 (96%)	17 (4%)	1 (0%)	41	66
1	D	396/398 (100%)	381 (96%)	14 (4%)	1 (0%)	41	66
All	All	1584/1592 (100%)	1515 (96%)	65 (4%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	195	CYS
1	A	195	CYS
1	B	195	CYS
1	C	195	CYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/323 (100%)	291 (90%)	32 (10%)	8	18
1	B	323/323 (100%)	285 (88%)	38 (12%)	5	12
1	C	323/323 (100%)	289 (90%)	34 (10%)	7	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	323/323 (100%)	292 (90%)	31 (10%)	8	19
All	All	1292/1292 (100%)	1157 (90%)	135 (10%)	7	16

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	116	LYS
1	D	156	SER
1	D	348	TRP
1	B	147	SER
1	B	137	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	GLN
1	C	96	GLN
1	D	96	GLN
1	C	286	HIS
1	A	331	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

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	B	1	1	7,8,9	1.29	0	9,10,12	1.87	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	PCA	D	1	1	7,8,9	1.18	0	9,10,12	1.80	3 (33%)
1	PCA	A	1	1	7,8,9	1.23	0	9,10,12	1.77	3 (33%)
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	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	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(^{o})	Ideal(^{o})
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%)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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(^{o})	Ideal(^{o})
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
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	H	2	SGC	4	0
2	E	2	SGC	2	0
2	G	1	SSG	4	0
2	F	3	SGC	1	0
2	F	1	SSG	5	0
2	G	2	SGC	3	0
2	H	1	SSG	5	0
2	E	1	SSG	5	0
2	F	2	SGC	3	0
2	E	3	SGC	1	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

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings
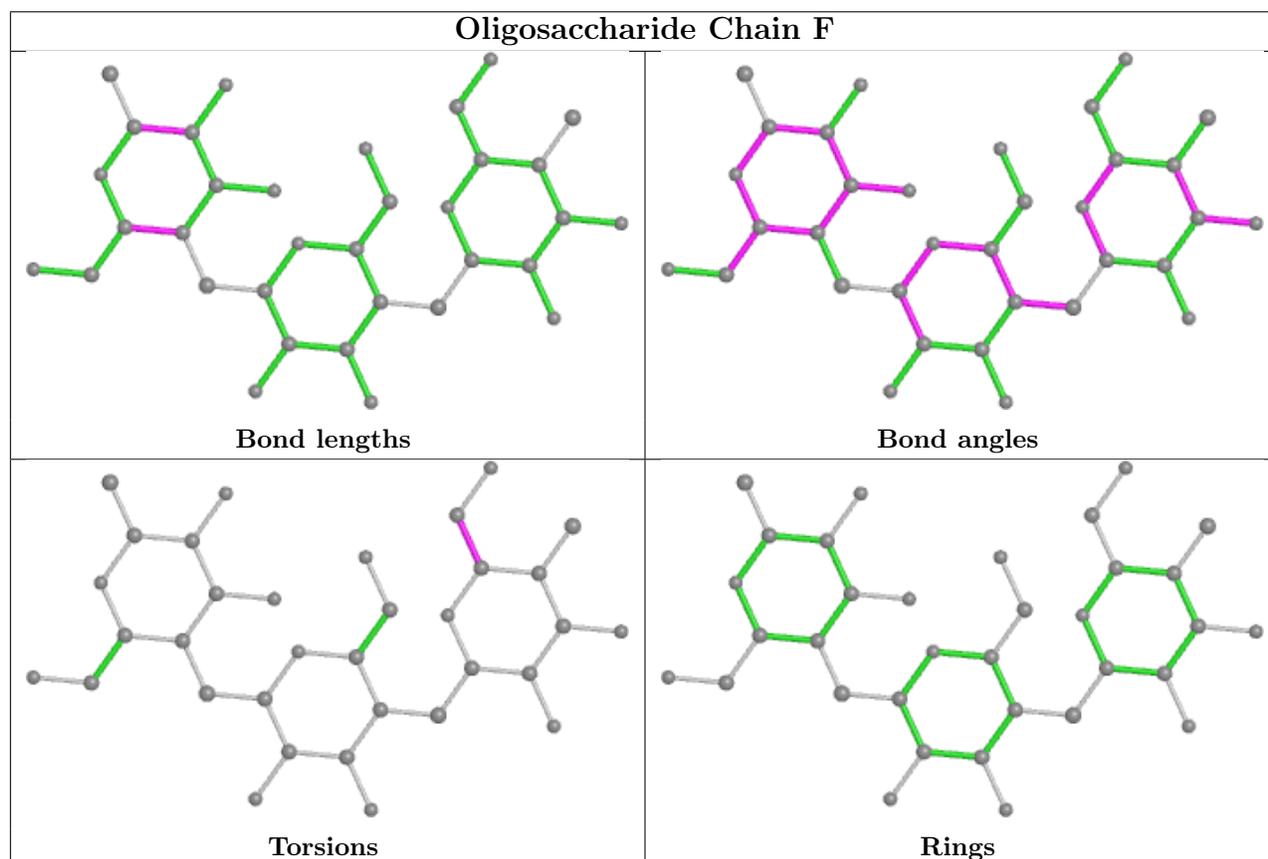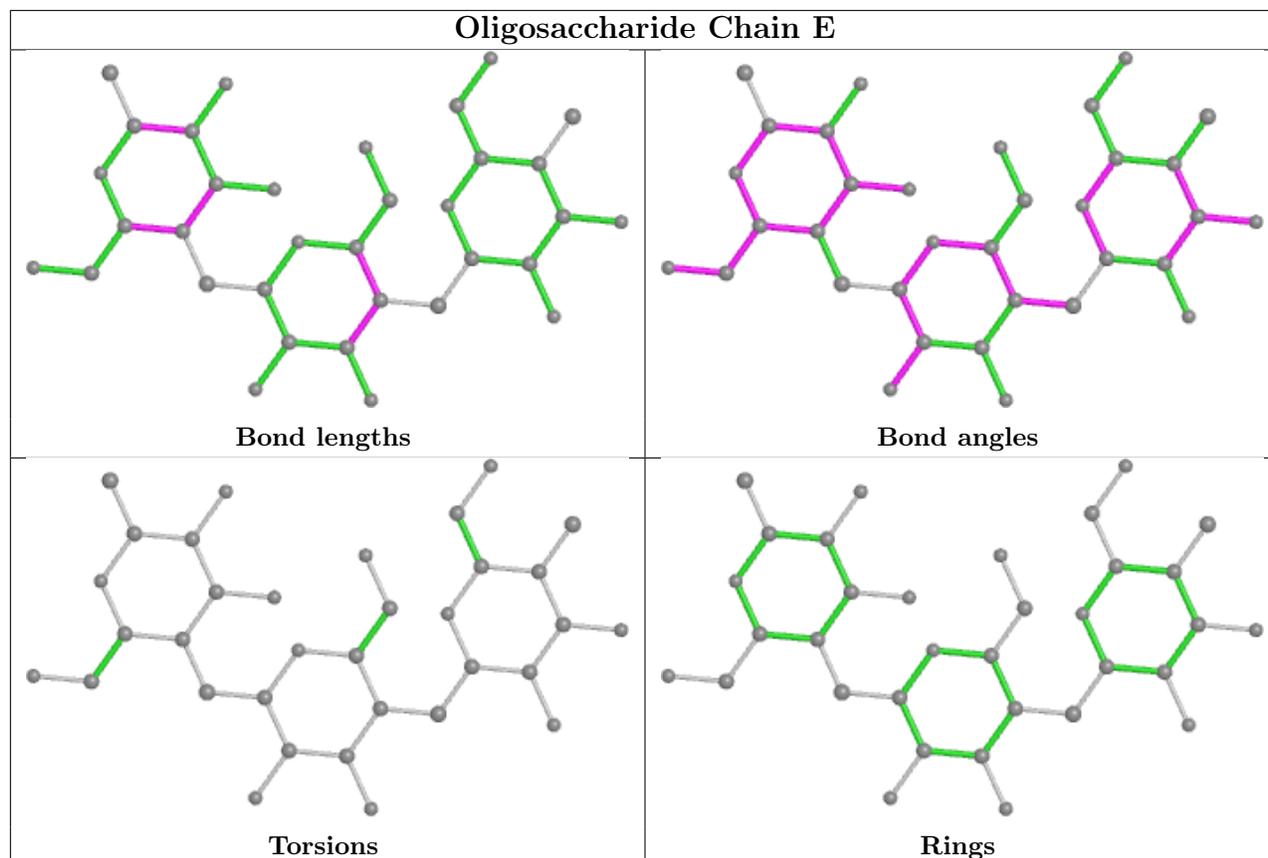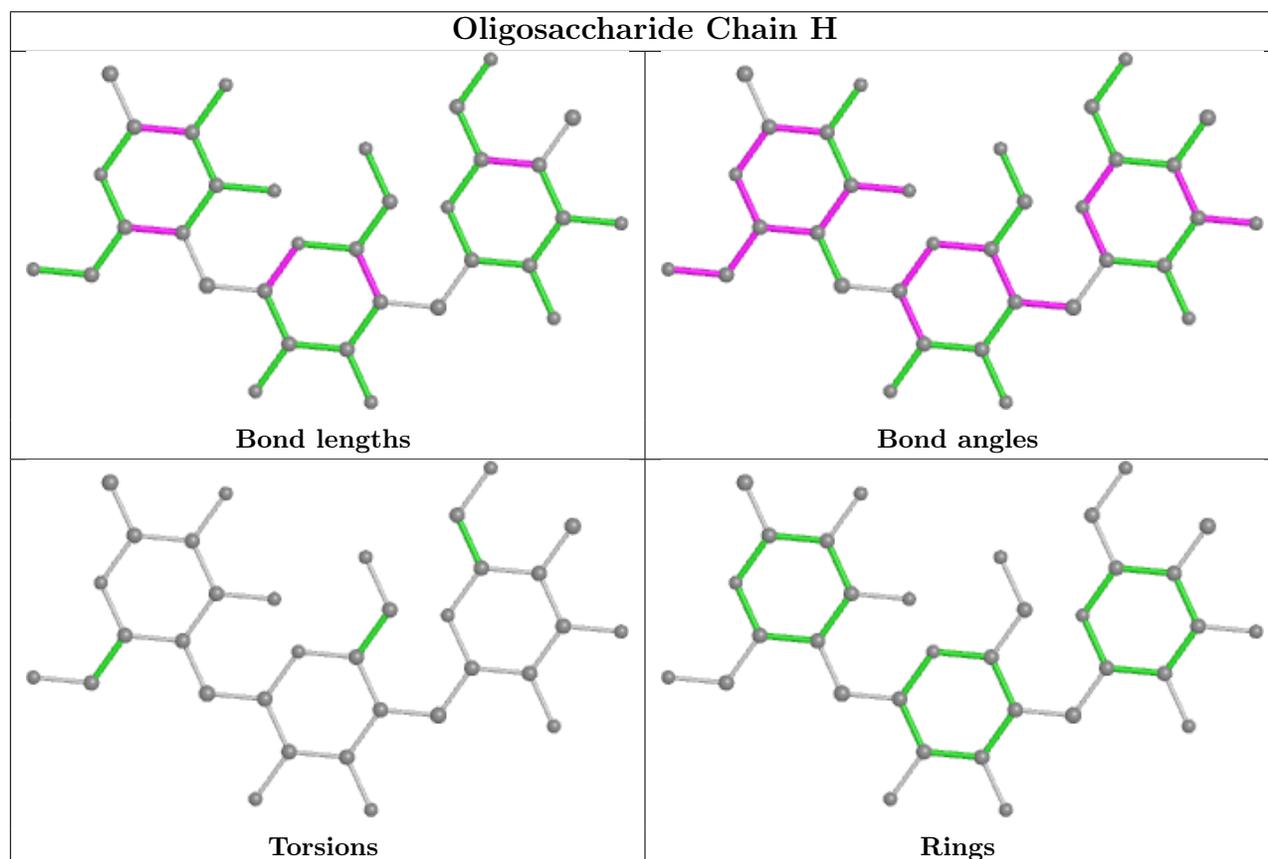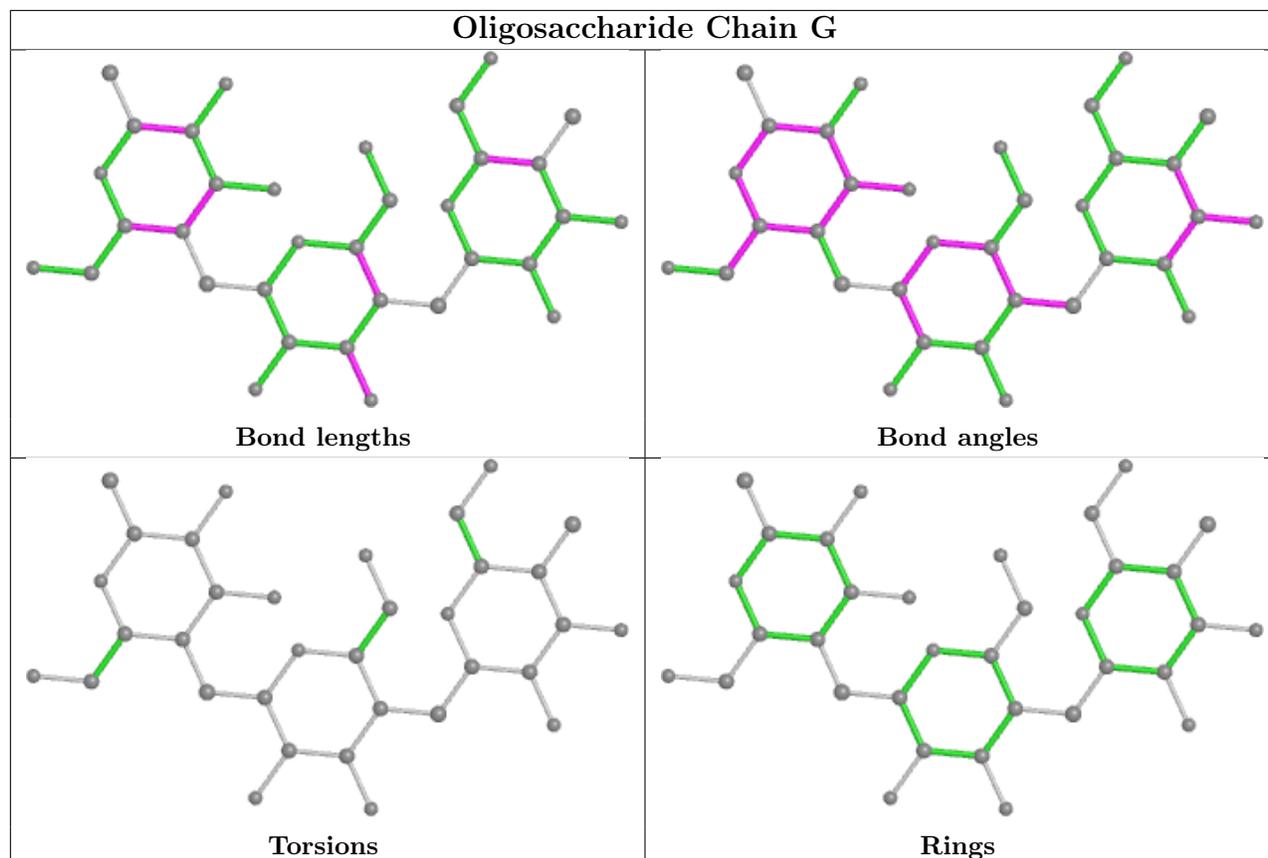
5.6 Ligand geometry ⓘ

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

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	B	400	1	-	2/6/23/26	0/1/1/1
3	NAG	C	400	1	-	2/6/23/26	0/1/1/1
3	NAG	A	399	1	-	0/6/23/26	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	D	400	1	-	2/6/23/26	0/1/1/1
3	NAG	A	400	1	-	2/6/23/26	0/1/1/1
3	NAG	C	399	1	-	0/6/23/26	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(^{o})	Ideal(^{o})
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	B	400	NAG	O5-C5-C6-O6
3	C	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.