



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2025 – 06:14 PM JST

PDB ID : 9JU0 / pdb\_00009ju0  
Title : C-terminally truncated dextran dextrinase bound with acarbose  
Authors : Tagami, T.; Matsugaki, N.; Saburi, W.; Okuyama, M.; Mori, H.  
Deposited on : 2024-10-07  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

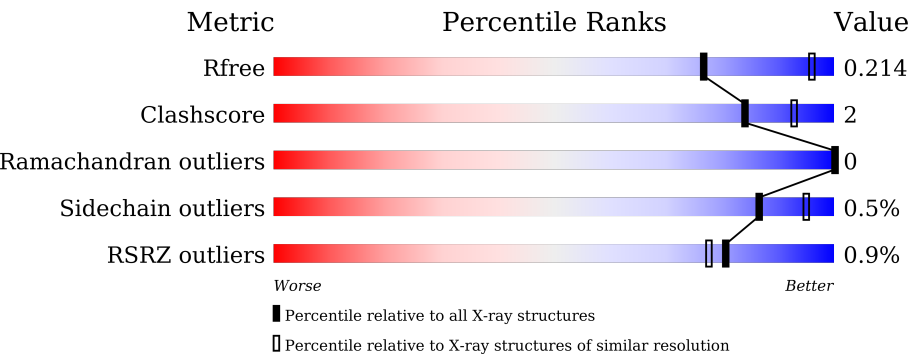
MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

# 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 2.50 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.



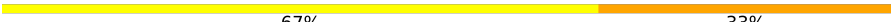

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	923	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%</div> <div>92%</div> <div>6%</div> <div>.</div>
1	BBB	923	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%</div> <div>91%</div> <div>6%</div> <div>.</div>
1	CCC	923	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%</div> <div>91%</div> <div>5%</div> <div>.</div>
1	DDD	923	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%</div> <div>91%</div> <div>6%</div> <div>.</div>
2	AaA	3	<div><div></div><div></div><div></div></div> <div>33%</div> <div>33%</div> <div>33%</div>
2	BaB	3	<div><div></div><div></div><div></div></div> <div>33%</div> <div>33%</div> <div>33%</div>

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Mol	Chain	Length	Quality of chain	
2	CaC	3		
2	DaD	3		

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28457 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 Dextran dextrinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	897	Total	C	N	O	S	0	0	0
			6686	4121	1104	1444	17			
1	BBB	894	Total	C	N	O	S	0	1	0
			6682	4119	1108	1438	17			
1	CCC	893	Total	C	N	O	S	0	1	0
			6669	4112	1102	1438	17			
1	DDD	893	Total	C	N	O	S	0	0	0
			6660	4107	1100	1436	17			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-18	MET	-	initiating methionine	UNP A0A0M5MSC0
AAA	-17	ASN	-	expression tag	UNP A0A0M5MSC0
AAA	-16	HIS	-	expression tag	UNP A0A0M5MSC0
AAA	-15	LYS	-	expression tag	UNP A0A0M5MSC0
AAA	-14	VAL	-	expression tag	UNP A0A0M5MSC0
AAA	-13	HIS	-	expression tag	UNP A0A0M5MSC0
AAA	-12	HIS	-	expression tag	UNP A0A0M5MSC0
AAA	-11	HIS	-	expression tag	UNP A0A0M5MSC0
AAA	-10	HIS	-	expression tag	UNP A0A0M5MSC0
AAA	-9	HIS	-	expression tag	UNP A0A0M5MSC0
AAA	-8	HIS	-	expression tag	UNP A0A0M5MSC0
AAA	-7	ILE	-	expression tag	UNP A0A0M5MSC0
AAA	-6	GLU	-	expression tag	UNP A0A0M5MSC0
AAA	-5	GLY	-	expression tag	UNP A0A0M5MSC0
AAA	-4	ARG	-	expression tag	UNP A0A0M5MSC0
AAA	-3	HIS	-	expression tag	UNP A0A0M5MSC0
AAA	-2	MET	-	expression tag	UNP A0A0M5MSC0
AAA	-1	GLU	-	expression tag	UNP A0A0M5MSC0
AAA	0	LEU	-	expression tag	UNP A0A0M5MSC0
AAA	743	GLN	PRO	conflict	UNP A0A0M5MSC0
AAA	903	SER	-	expression tag	UNP A0A0M5MSC0

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	904	ARG	-	expression tag	UNP A0A0M5MSC0
BBB	-18	MET	-	initiating methionine	UNP A0A0M5MSC0
BBB	-17	ASN	-	expression tag	UNP A0A0M5MSC0
BBB	-16	HIS	-	expression tag	UNP A0A0M5MSC0
BBB	-15	LYS	-	expression tag	UNP A0A0M5MSC0
BBB	-14	VAL	-	expression tag	UNP A0A0M5MSC0
BBB	-13	HIS	-	expression tag	UNP A0A0M5MSC0
BBB	-12	HIS	-	expression tag	UNP A0A0M5MSC0
BBB	-11	HIS	-	expression tag	UNP A0A0M5MSC0
BBB	-10	HIS	-	expression tag	UNP A0A0M5MSC0
BBB	-9	HIS	-	expression tag	UNP A0A0M5MSC0
BBB	-8	HIS	-	expression tag	UNP A0A0M5MSC0
BBB	-7	ILE	-	expression tag	UNP A0A0M5MSC0
BBB	-6	GLU	-	expression tag	UNP A0A0M5MSC0
BBB	-5	GLY	-	expression tag	UNP A0A0M5MSC0
BBB	-4	ARG	-	expression tag	UNP A0A0M5MSC0
BBB	-3	HIS	-	expression tag	UNP A0A0M5MSC0
BBB	-2	MET	-	expression tag	UNP A0A0M5MSC0
BBB	-1	GLU	-	expression tag	UNP A0A0M5MSC0
BBB	0	LEU	-	expression tag	UNP A0A0M5MSC0
BBB	743	GLN	PRO	conflict	UNP A0A0M5MSC0
BBB	903	SER	-	expression tag	UNP A0A0M5MSC0
BBB	904	ARG	-	expression tag	UNP A0A0M5MSC0
CCC	-18	MET	-	initiating methionine	UNP A0A0M5MSC0
CCC	-17	ASN	-	expression tag	UNP A0A0M5MSC0
CCC	-16	HIS	-	expression tag	UNP A0A0M5MSC0
CCC	-15	LYS	-	expression tag	UNP A0A0M5MSC0
CCC	-14	VAL	-	expression tag	UNP A0A0M5MSC0
CCC	-13	HIS	-	expression tag	UNP A0A0M5MSC0
CCC	-12	HIS	-	expression tag	UNP A0A0M5MSC0
CCC	-11	HIS	-	expression tag	UNP A0A0M5MSC0
CCC	-10	HIS	-	expression tag	UNP A0A0M5MSC0
CCC	-9	HIS	-	expression tag	UNP A0A0M5MSC0
CCC	-8	HIS	-	expression tag	UNP A0A0M5MSC0
CCC	-7	ILE	-	expression tag	UNP A0A0M5MSC0
CCC	-6	GLU	-	expression tag	UNP A0A0M5MSC0
CCC	-5	GLY	-	expression tag	UNP A0A0M5MSC0
CCC	-4	ARG	-	expression tag	UNP A0A0M5MSC0
CCC	-3	HIS	-	expression tag	UNP A0A0M5MSC0
CCC	-2	MET	-	expression tag	UNP A0A0M5MSC0
CCC	-1	GLU	-	expression tag	UNP A0A0M5MSC0
CCC	0	LEU	-	expression tag	UNP A0A0M5MSC0

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	743	GLN	PRO	conflict	UNP A0A0M5MSC0
CCC	903	SER	-	expression tag	UNP A0A0M5MSC0
CCC	904	ARG	-	expression tag	UNP A0A0M5MSC0
DDD	-18	MET	-	initiating methionine	UNP A0A0M5MSC0
DDD	-17	ASN	-	expression tag	UNP A0A0M5MSC0
DDD	-16	HIS	-	expression tag	UNP A0A0M5MSC0
DDD	-15	LYS	-	expression tag	UNP A0A0M5MSC0
DDD	-14	VAL	-	expression tag	UNP A0A0M5MSC0
DDD	-13	HIS	-	expression tag	UNP A0A0M5MSC0
DDD	-12	HIS	-	expression tag	UNP A0A0M5MSC0
DDD	-11	HIS	-	expression tag	UNP A0A0M5MSC0
DDD	-10	HIS	-	expression tag	UNP A0A0M5MSC0
DDD	-9	HIS	-	expression tag	UNP A0A0M5MSC0
DDD	-8	HIS	-	expression tag	UNP A0A0M5MSC0
DDD	-7	ILE	-	expression tag	UNP A0A0M5MSC0
DDD	-6	GLU	-	expression tag	UNP A0A0M5MSC0
DDD	-5	GLY	-	expression tag	UNP A0A0M5MSC0
DDD	-4	ARG	-	expression tag	UNP A0A0M5MSC0
DDD	-3	HIS	-	expression tag	UNP A0A0M5MSC0
DDD	-2	MET	-	expression tag	UNP A0A0M5MSC0
DDD	-1	GLU	-	expression tag	UNP A0A0M5MSC0
DDD	0	LEU	-	expression tag	UNP A0A0M5MSC0
DDD	743	GLN	PRO	conflict	UNP A0A0M5MSC0
DDD	903	SER	-	expression tag	UNP A0A0M5MSC0
DDD	904	ARG	-	expression tag	UNP A0A0M5MSC0

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[[[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AaA	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	BaB	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	CaC	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	DaD	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		

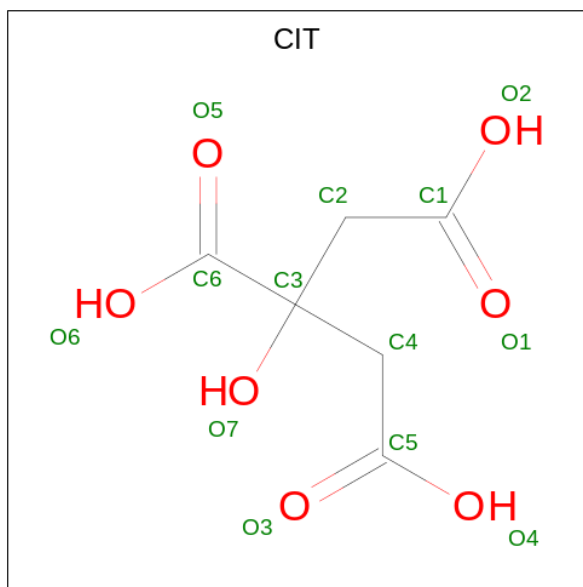
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	CCC	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula:  $C_6H_8O_7$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	BBB	1	Total	C	O	0	0
			13	6	7		
4	DDD	1	Total	C	O	0	0
			13	6	7		

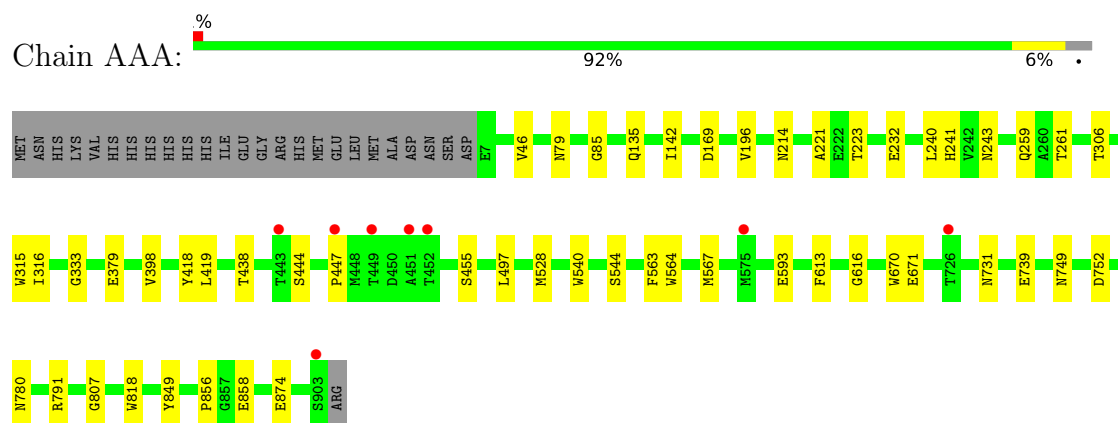
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	437	Total	O	0	0
			437	437		
5	BBB	375	Total	O	0	0
			375	375		
5	CCC	371	Total	O	0	0
			371	371		
5	DDD	267	Total	O	0	0
			267	267		

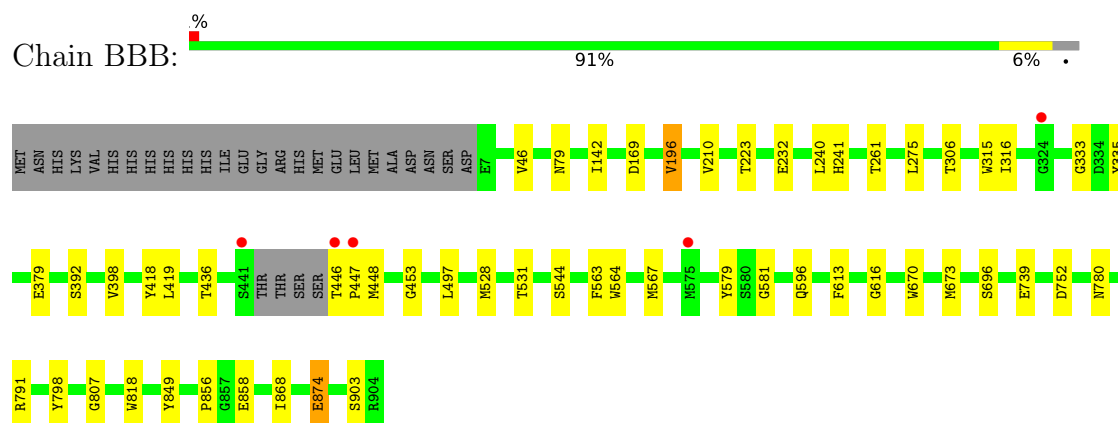
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

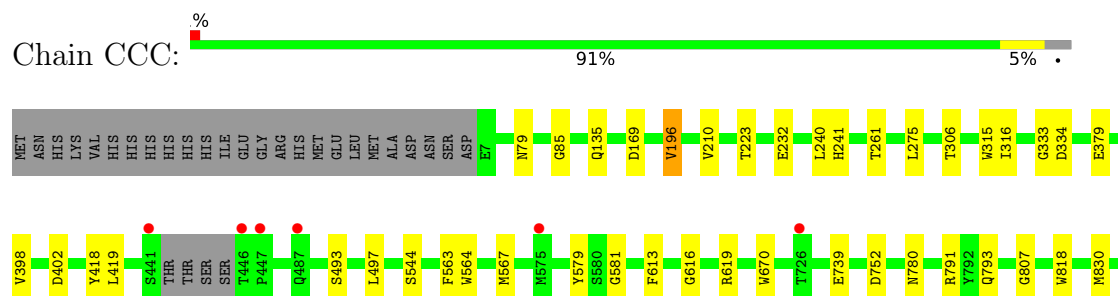
#### • Molecule 1: Dextran dextrinase

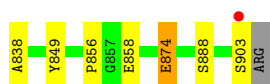


#### • Molecule 1: Dextran dextrinase



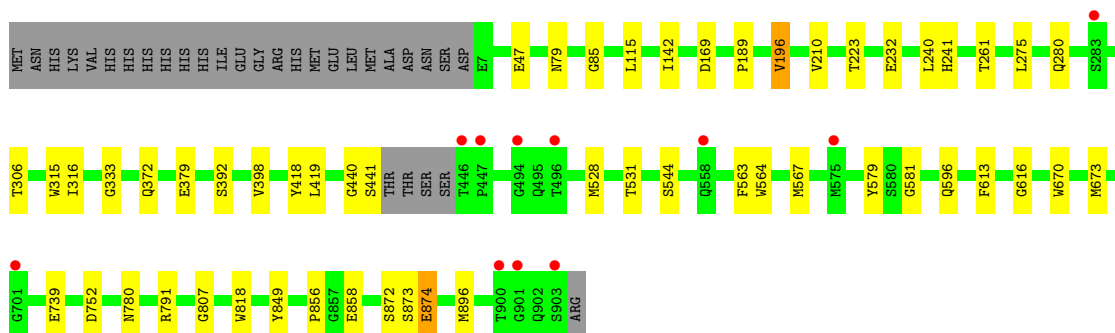
#### • Molecule 1: Dextran dextrinase





- Molecule 1: Dextran dextrinase

Chain DDD: 91% 6% .



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain AaA: 33% 33% 33%



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain BaB: 33% 33% 33%



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain CaC: 67% 33%



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl}]\text{amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain DaD: 67% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.26Å 138.97Å 264.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 2.50 49.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.11-2.50) 99.9 (49.11-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.24	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX v1.19.1	Depositor
R, $R_{free}$	0.182 , 0.211 0.186 , 0.214	Depositor DCC
$R_{free}$ test set	2000 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 26.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: EDO, AC1, CIT, GLC

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	AAA	0.96	0/6837	1.35	4/9372 (0.0%)
1	BBB	0.97	0/6832	1.35	4/9361 (0.0%)
1	CCC	0.98	0/6819	1.35	4/9345 (0.0%)
1	DDD	0.98	0/6810	1.35	4/9333 (0.0%)
All	All	0.97	0/27298	1.35	16/37411 (0.0%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	874	GLU	CB-CA-C	5.98	118.11	110.34
1	CCC	807	GLY	CA-C-O	-5.80	118.45	122.22
1	AAA	807	GLY	CA-C-O	-5.79	118.46	122.22
1	BBB	874	GLU	CB-CA-C	5.75	117.81	110.34
1	CCC	874	GLU	CB-CA-C	5.74	117.80	110.34

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	6686	0	6139	29	0
1	BBB	6682	0	6139	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	6669	0	6121	28	0
1	DDD	6660	0	6114	30	0
2	AaA	44	0	30	2	0
2	BaB	44	0	30	1	0
2	CaC	44	0	30	1	0
2	DaD	44	0	30	1	0
3	AAA	56	0	84	1	0
3	BBB	20	0	30	1	0
3	CCC	24	0	36	1	0
3	DDD	8	0	12	2	0
4	BBB	13	0	5	0	0
4	DDD	13	0	5	0	0
5	AAA	437	0	0	0	0
5	BBB	375	0	0	1	0
5	CCC	371	0	0	1	0
5	DDD	267	0	0	0	0
All	All	28457	0	24805	112	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 2.

The worst 5 of 112 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:AAA:731:ASN:HD22	1:AAA:749:ASN:HD21	1.23	0.81
1:CCC:830:MET:HE3	1:CCC:888:SER:HB2	1.71	0.71
1:DDD:85:GLY:H	3:DDD:1002:EDO:H11	1.59	0.68
1:DDD:896:MET:HA	1:DDD:896:MET:HE2	1.77	0.65
1:BBB:528:MET:CE	1:BBB:531:THR:HA	2.29	0.63

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	AAA	895/923 (97%)	873 (98%)	22 (2%)	0	100	100
1	BBB	891/923 (96%)	870 (98%)	21 (2%)	0	100	100
1	CCC	890/923 (96%)	870 (98%)	20 (2%)	0	100	100
1	DDD	889/923 (96%)	868 (98%)	21 (2%)	0	100	100
All	All	3565/3692 (97%)	3481 (98%)	84 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	718/742 (97%)	716 (100%)	2 (0%)	91	97
1	BBB	716/742 (96%)	711 (99%)	5 (1%)	81	93
1	CCC	715/742 (96%)	712 (100%)	3 (0%)	89	96
1	DDD	714/742 (96%)	709 (99%)	5 (1%)	81	93
All	All	2863/2968 (96%)	2848 (100%)	15 (0%)	86	95

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	419	LEU
1	DDD	419	LEU
1	CCC	493	SER
1	DDD	596	GLN
1	DDD	372	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 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	GLC	AaA	1	2	12,12,12	0.71	0	17,17,17	0.94	0
2	GLC	AaA	2	2	11,11,12	0.38	0	15,15,17	1.33	2 (13%)
2	AC1	AaA	3	2	21,22,23	0.60	0	22,32,34	1.16	3 (13%)
2	GLC	BaB	1	2	12,12,12	0.55	0	17,17,17	0.82	0
2	GLC	BaB	2	2	11,11,12	0.63	0	15,15,17	1.35	1 (6%)
2	AC1	BaB	3	2	21,22,23	0.84	0	22,32,34	1.30	2 (9%)
2	GLC	CaC	1	2	12,12,12	0.62	0	17,17,17	1.97	5 (29%)
2	GLC	CaC	2	2	11,11,12	0.50	0	15,15,17	1.41	1 (6%)
2	AC1	CaC	3	2	21,22,23	0.53	0	22,32,34	0.98	1 (4%)
2	GLC	DaD	1	2	12,12,12	0.74	0	17,17,17	0.80	1 (5%)
2	GLC	DaD	2	2	11,11,12	0.34	0	15,15,17	1.52	2 (13%)
2	AC1	DaD	3	2	21,22,23	0.71	0	22,32,34	1.06	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
2	GLC	AaA	1	2	-	2/2/22/22	0/1/1/1
2	GLC	AaA	2	2	-	0/2/19/22	0/1/1/1
2	AC1	AaA	3	2	-	2/6/43/46	0/2/2/2
2	GLC	BaB	1	2	-	0/2/22/22	0/1/1/1
2	GLC	BaB	2	2	-	0/2/19/22	0/1/1/1
2	AC1	BaB	3	2	-	1/6/43/46	0/2/2/2
2	GLC	CaC	1	2	-	2/2/22/22	0/1/1/1
2	GLC	CaC	2	2	-	0/2/19/22	0/1/1/1
2	AC1	CaC	3	2	-	3/6/43/46	0/2/2/2
2	GLC	DaD	1	2	-	0/2/22/22	0/1/1/1
2	GLC	DaD	2	2	-	2/2/19/22	0/1/1/1
2	AC1	DaD	3	2	-	1/6/43/46	0/2/2/2

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DaD	2	GLC	C1-O5-C5	4.36	118.09	112.19
2	CaC	1	GLC	C1-O5-C5	4.35	121.88	113.66
2	CaC	1	GLC	O5-C5-C4	4.24	117.40	109.69
2	CaC	2	GLC	C1-O5-C5	4.23	117.93	112.19
2	BaB	2	GLC	C1-O5-C5	3.95	117.54	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

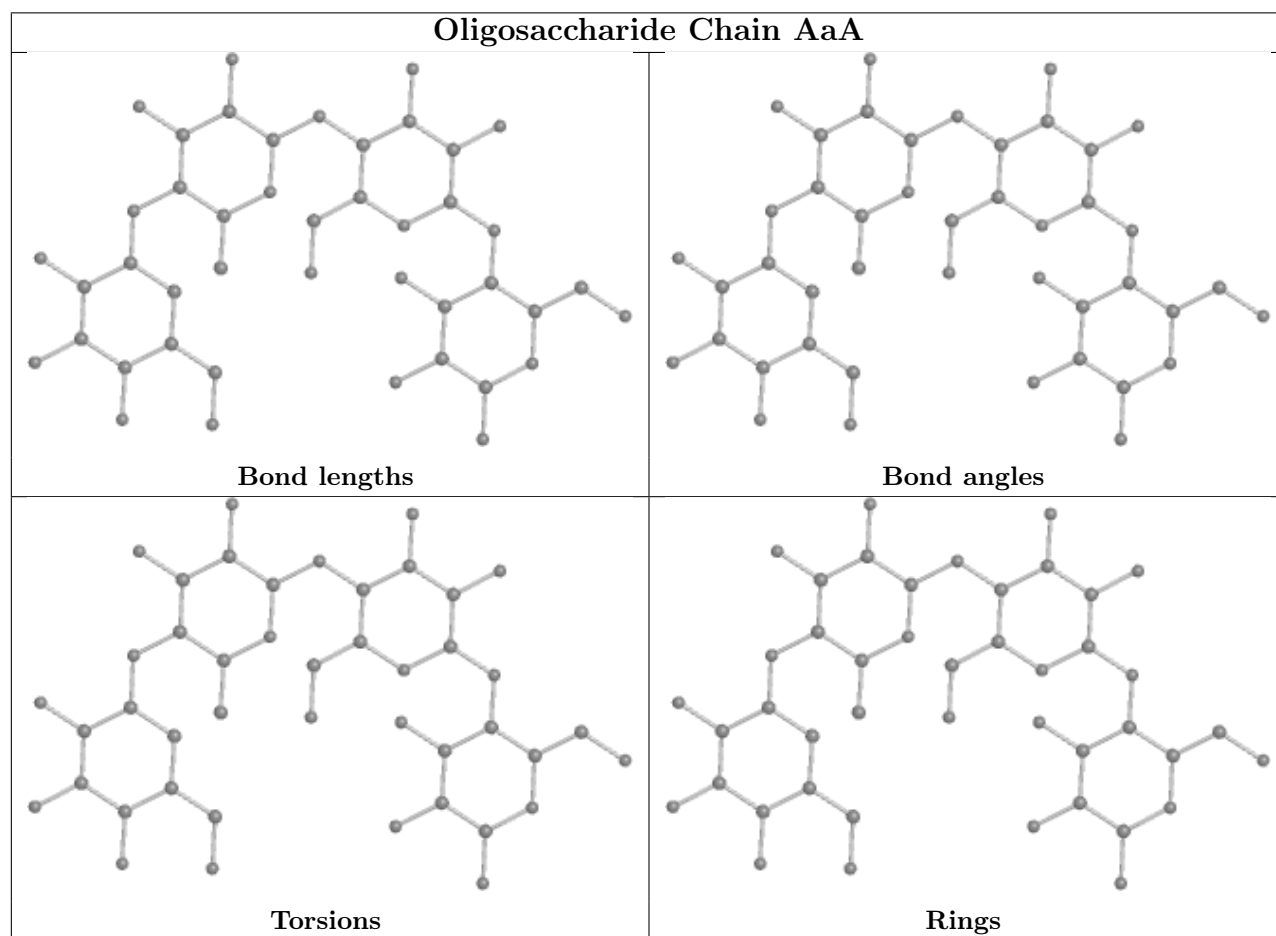
Mol	Chain	Res	Type	Atoms
2	AaA	1	GLC	C4-C5-C6-O6
2	AaA	1	GLC	O5-C5-C6-O6
2	DaD	2	GLC	C4-C5-C6-O6
2	CaC	1	GLC	O5-C5-C6-O6
2	DaD	2	GLC	O5-C5-C6-O6

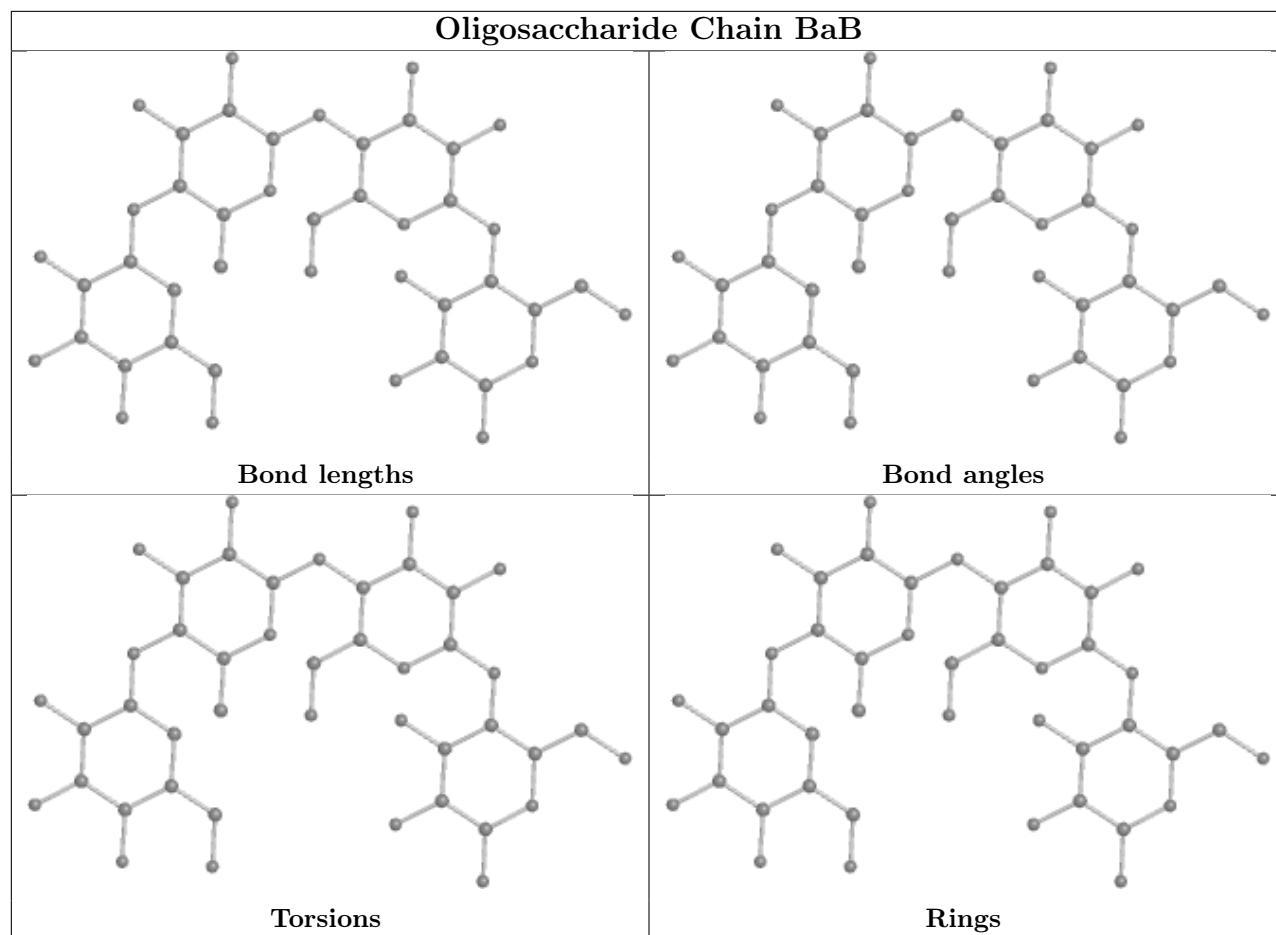
There are no ring outliers.

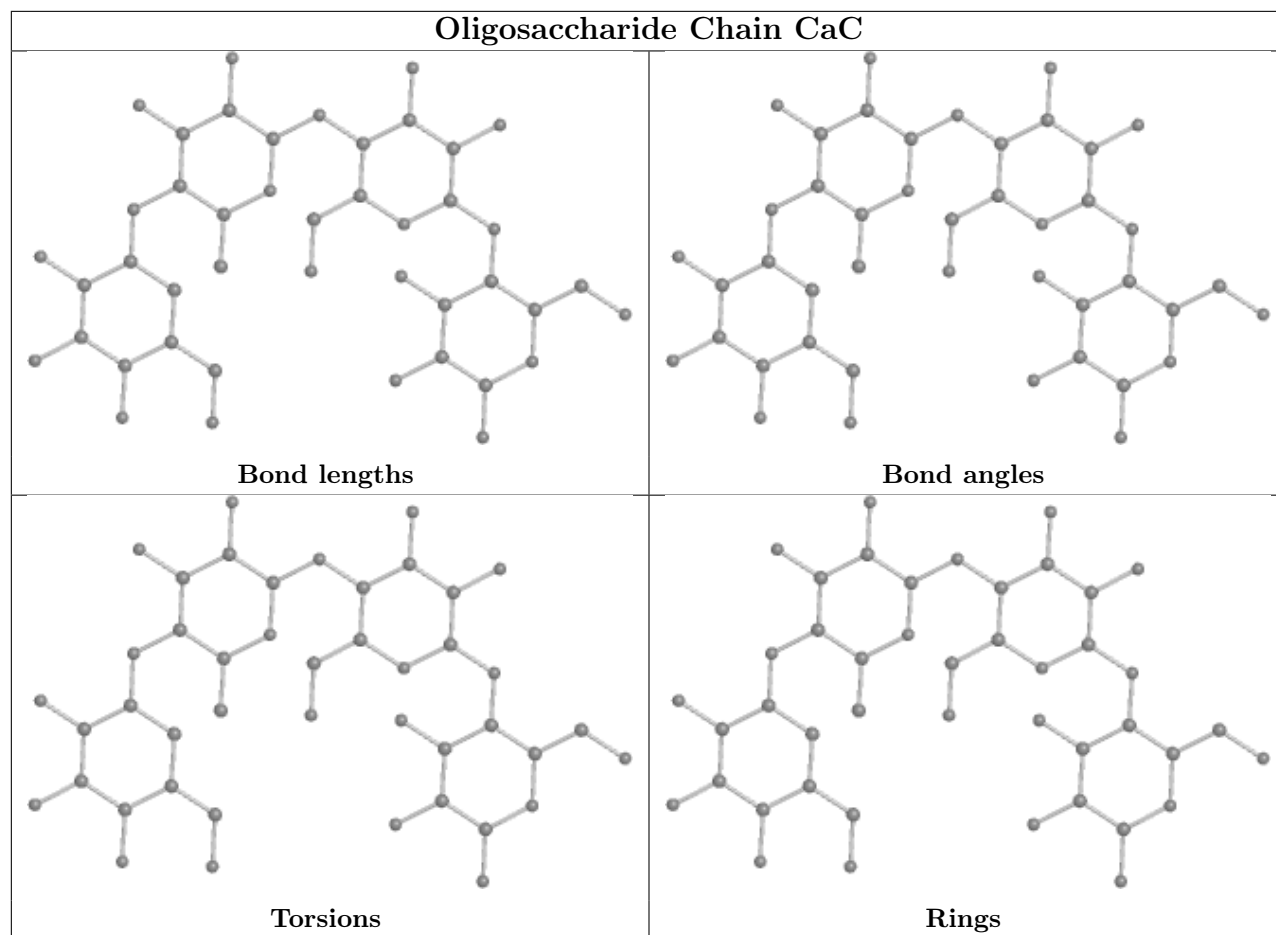
4 monomers are involved in 5 short contacts:

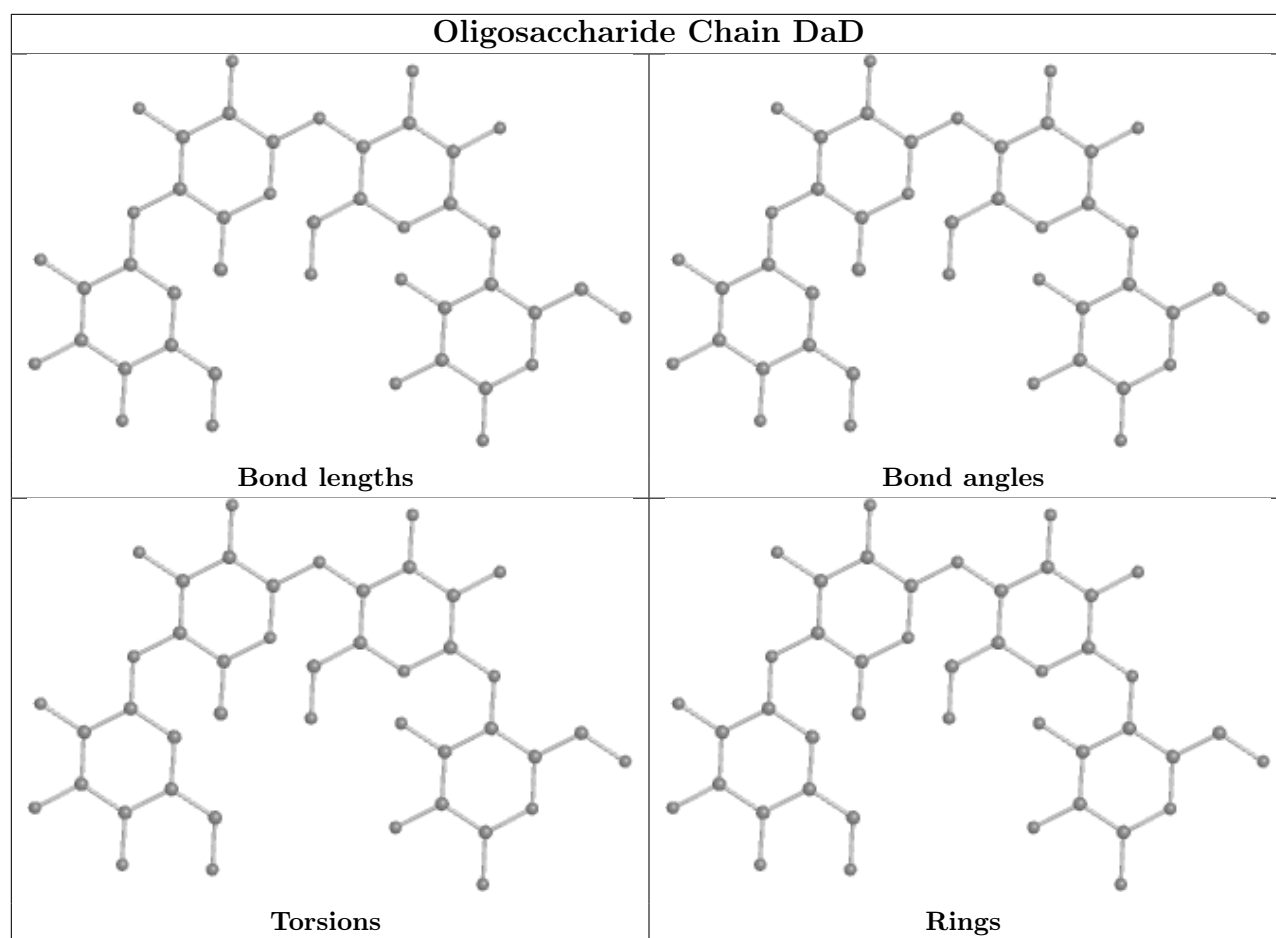
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AaA	3	AC1	2	0
2	BaB	3	AC1	1	0
2	DaD	3	AC1	1	0
2	CaC	3	AC1	1	0

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









## 5.6 Ligand geometry [i](#)

29 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	EDO	AAA	1006	-	3,3,3	0.29	0	2,2,2	0.27	0
3	EDO	AAA	1008	-	3,3,3	0.17	0	2,2,2	0.29	0
3	EDO	BBB	1005	-	3,3,3	0.31	0	2,2,2	0.40	0
3	EDO	AAA	1003	-	3,3,3	0.22	0	2,2,2	0.12	0
3	EDO	BBB	1006	-	3,3,3	0.36	0	2,2,2	0.62	0
3	EDO	DDD	1003	-	3,3,3	0.14	0	2,2,2	0.11	0
3	EDO	CCC	1005	-	3,3,3	0.30	0	2,2,2	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	BBB	1001	-	3,3,3	0.18	0	2,2,2	0.10	0
3	EDO	AAA	1011	-	3,3,3	0.07	0	2,2,2	0.09	0
3	EDO	AAA	1007	-	3,3,3	0.42	0	2,2,2	0.47	0
4	CIT	DDD	1001	-	12,12,12	1.32	1 (8%)	17,17,17	1.43	3 (17%)
3	EDO	CCC	1006	-	3,3,3	0.43	0	2,2,2	0.52	0
3	EDO	BBB	1002	-	3,3,3	0.21	0	2,2,2	0.37	0
3	EDO	AAA	1009	-	3,3,3	0.21	0	2,2,2	0.26	0
3	EDO	CCC	1001	-	3,3,3	0.23	0	2,2,2	0.18	0
3	EDO	BBB	1003	-	3,3,3	0.17	0	2,2,2	0.38	0
3	EDO	AAA	1001	-	3,3,3	0.16	0	2,2,2	0.31	0
3	EDO	AAA	1004	-	3,3,3	0.08	0	2,2,2	0.18	0
3	EDO	CCC	1002	-	3,3,3	0.31	0	2,2,2	0.56	0
3	EDO	CCC	1003	-	3,3,3	0.04	0	2,2,2	0.03	0
3	EDO	AAA	1010	-	3,3,3	0.15	0	2,2,2	0.24	0
3	EDO	DDD	1002	-	3,3,3	0.25	0	2,2,2	0.50	0
3	EDO	AAA	1002	-	3,3,3	0.03	0	2,2,2	0.29	0
4	CIT	BBB	1004	-	12,12,12	1.18	1 (8%)	17,17,17	1.46	2 (11%)
3	EDO	AAA	1012	-	3,3,3	0.17	0	2,2,2	0.41	0
3	EDO	AAA	1014	-	3,3,3	0.52	0	2,2,2	0.63	0
3	EDO	CCC	1004	-	3,3,3	0.15	0	2,2,2	0.04	0
3	EDO	AAA	1013	-	3,3,3	0.14	0	2,2,2	0.19	0
3	EDO	AAA	1005	-	3,3,3	0.13	0	2,2,2	0.06	0

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	EDO	AAA	1006	-	-	1/1/1/1	-
3	EDO	AAA	1008	-	-	1/1/1/1	-
3	EDO	BBB	1005	-	-	0/1/1/1	-
3	EDO	AAA	1003	-	-	1/1/1/1	-
3	EDO	BBB	1006	-	-	1/1/1/1	-
3	EDO	DDD	1003	-	-	1/1/1/1	-
3	EDO	CCC	1005	-	-	1/1/1/1	-
3	EDO	BBB	1001	-	-	1/1/1/1	-
3	EDO	AAA	1011	-	-	1/1/1/1	-
3	EDO	AAA	1007	-	-	0/1/1/1	-
4	CIT	DDD	1001	-	-	2/16/16/16	-
3	EDO	CCC	1006	-	-	0/1/1/1	-
3	EDO	BBB	1002	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	AAA	1009	-	-	1/1/1/1	-
3	EDO	CCC	1001	-	-	0/1/1/1	-
3	EDO	BBB	1003	-	-	1/1/1/1	-
3	EDO	AAA	1001	-	-	1/1/1/1	-
3	EDO	AAA	1004	-	-	0/1/1/1	-
3	EDO	CCC	1002	-	-	0/1/1/1	-
3	EDO	CCC	1003	-	-	1/1/1/1	-
3	EDO	AAA	1010	-	-	0/1/1/1	-
3	EDO	DDD	1002	-	-	1/1/1/1	-
3	EDO	AAA	1002	-	-	1/1/1/1	-
4	CIT	BBB	1004	-	-	2/16/16/16	-
3	EDO	AAA	1012	-	-	0/1/1/1	-
3	EDO	AAA	1014	-	-	0/1/1/1	-
3	EDO	CCC	1004	-	-	0/1/1/1	-
3	EDO	AAA	1013	-	-	1/1/1/1	-
3	EDO	AAA	1005	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	DDD	1001	CIT	C3-C6	2.99	1.56	1.53
4	BBB	1004	CIT	C3-C6	2.45	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BBB	1004	CIT	O5-C6-C3	-4.02	116.56	122.25
4	DDD	1001	CIT	O5-C6-C3	-3.24	117.66	122.25
4	BBB	1004	CIT	O6-C6-C3	2.91	118.10	113.05
4	DDD	1001	CIT	O6-C6-C3	2.61	117.58	113.05
4	DDD	1001	CIT	O3-C5-C4	-2.01	117.08	122.94

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	1009	EDO	O1-C1-C2-O2
3	AAA	1002	EDO	O1-C1-C2-O2
3	AAA	1003	EDO	O1-C1-C2-O2
3	AAA	1006	EDO	O1-C1-C2-O2
3	AAA	1008	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	1006	EDO	1	0
3	BBB	1006	EDO	1	0
3	CCC	1005	EDO	1	0
3	DDD	1002	EDO	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AAA	897/923 (97%)	-0.48	8 (0%) 81 78	22, 30, 47, 80	0
1	BBB	894/923 (96%)	-0.35	5 (0%) 85 83	14, 34, 54, 100	1 (0%)
1	CCC	893/923 (96%)	-0.29	7 (0%) 82 79	18, 36, 53, 89	1 (0%)
1	DDD	893/923 (96%)	-0.11	11 (1%) 76 73	26, 43, 64, 96	0
All	All	3577/3692 (96%)	-0.31	31 (0%) 81 78	14, 36, 57, 100	2 (0%)

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	446	THR	4.8
1	CCC	446	THR	4.4
1	BBB	447	PRO	3.9
1	AAA	447	PRO	3.4
1	BBB	446	THR	3.4

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

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	AaA	1	12/12	-	-	38,44,47,47	0
2	GLC	AaA	2	11/12	-	-	26,31,33,34	0

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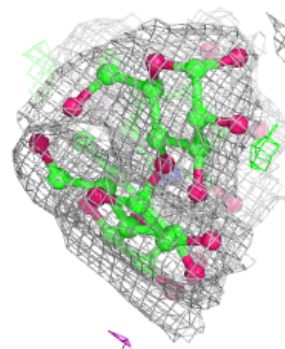
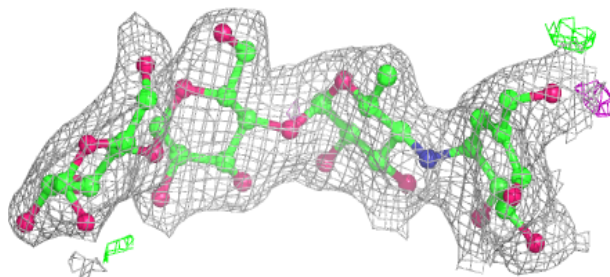
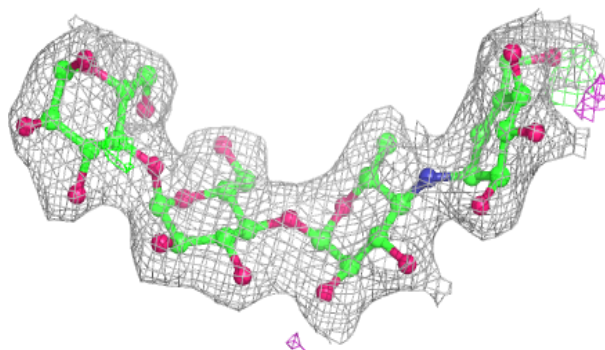
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AC1	AaA	3	21/22	-	-	20,22,24,25	0
2	GLC	BaB	1	12/12	-	-	44,51,55,55	0
2	GLC	BaB	2	11/12	-	-	30,32,36,37	0
2	AC1	BaB	3	21/22	-	-	21,23,28,29	0
2	GLC	CaC	1	12/12	-	-	52,61,62,64	0
2	GLC	CaC	2	11/12	-	-	35,38,43,44	0
2	AC1	CaC	3	21/22	-	-	28,32,35,36	0
2	GLC	DaD	1	12/12	-	-	50,60,62,63	0
2	GLC	DaD	2	11/12	-	-	32,37,41,42	0
2	AC1	DaD	3	21/22	-	-	30,32,33,34	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

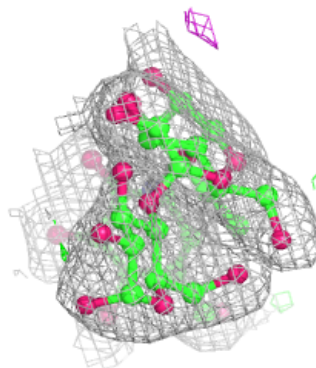
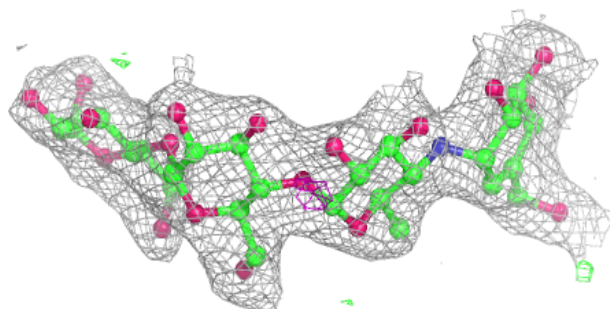
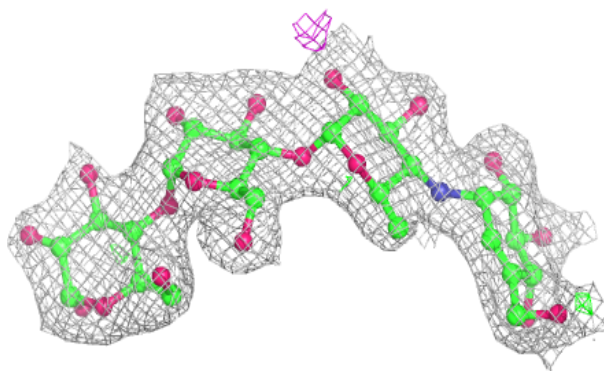
#### Electron density around Chain AaA:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

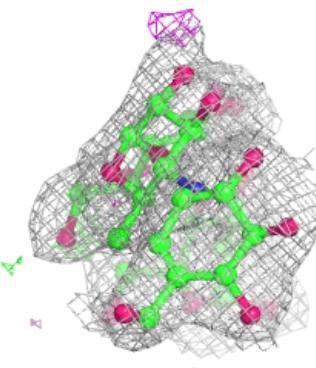
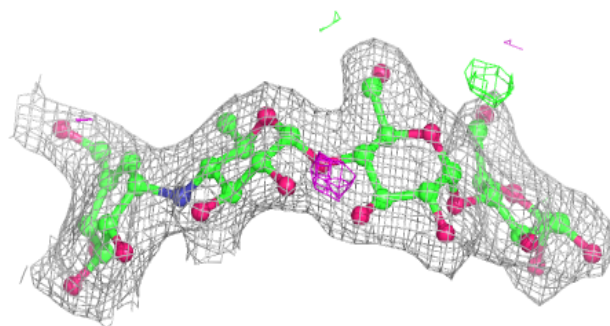
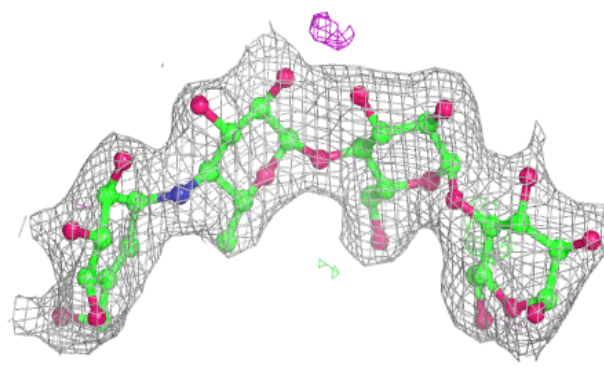


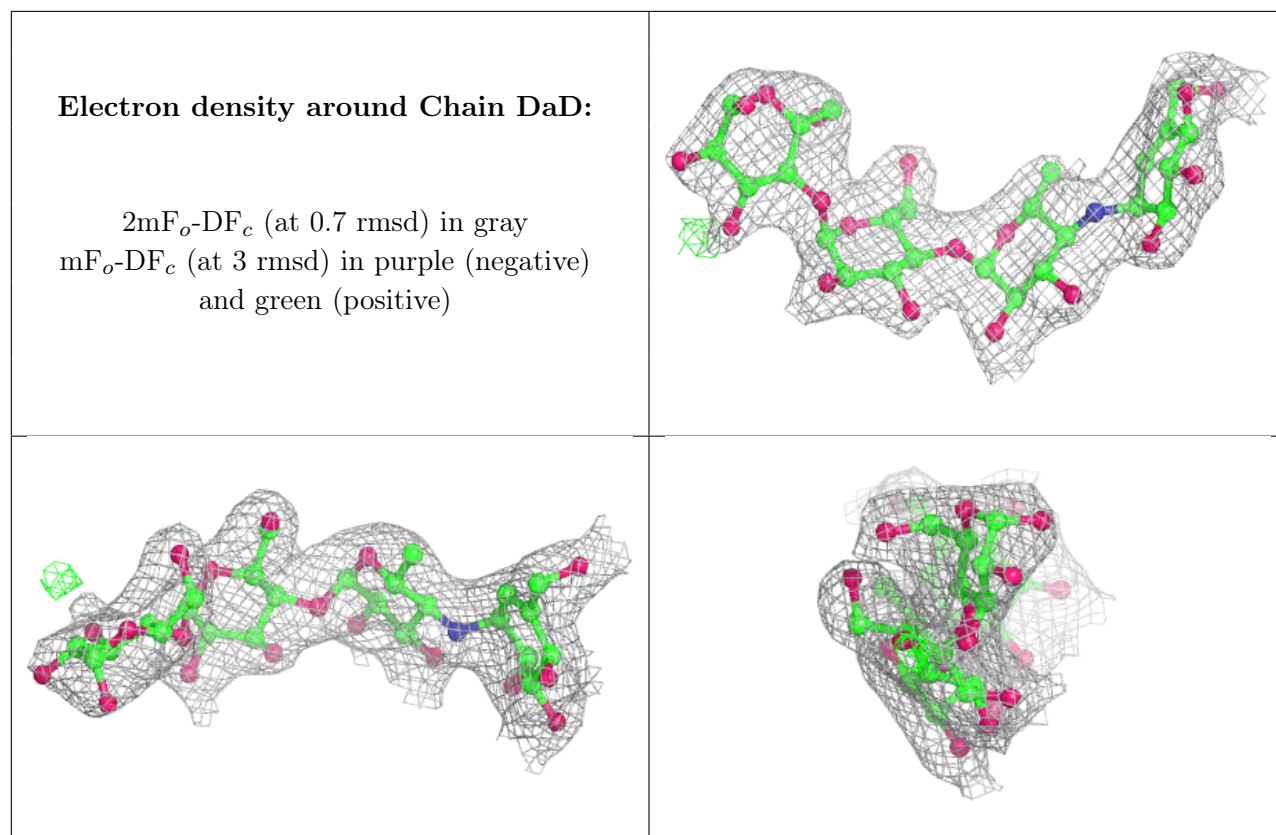
**Electron density around Chain BaB:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain CaC:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	DDD	1002	4/4	0.78	0.23	47,50,50,52	0
3	EDO	AAA	1006	4/4	0.79	0.17	44,45,45,46	0
3	EDO	CCC	1004	4/4	0.81	0.19	51,55,58,59	0
3	EDO	BBB	1002	4/4	0.81	0.19	48,49,52,54	0
3	EDO	CCC	1005	4/4	0.82	0.21	46,46,47,47	0
3	EDO	CCC	1006	4/4	0.82	0.17	38,41,43,43	0
3	EDO	AAA	1005	4/4	0.82	0.21	48,51,51,52	0
3	EDO	BBB	1006	4/4	0.83	0.17	39,40,41,41	0
3	EDO	DDD	1003	4/4	0.83	0.16	50,51,53,55	0
3	EDO	AAA	1003	4/4	0.84	0.17	47,49,50,51	0
3	EDO	AAA	1013	4/4	0.85	0.16	41,49,50,51	0
3	EDO	AAA	1002	4/4	0.86	0.12	38,39,39,39	0
3	EDO	AAA	1008	4/4	0.86	0.21	54,56,56,60	0
3	EDO	AAA	1009	4/4	0.87	0.15	44,48,48,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	CCC	1002	4/4	0.88	0.12	34,37,38,39	0
3	EDO	AAA	1011	4/4	0.88	0.15	49,52,53,55	0
4	CIT	DDD	1001	13/13	0.88	0.12	56,62,70,73	0
3	EDO	BBB	1005	4/4	0.89	0.11	31,34,35,38	0
3	EDO	AAA	1014	4/4	0.89	0.16	31,32,33,33	0
3	EDO	AAA	1012	4/4	0.89	0.12	40,41,42,44	0
4	CIT	BBB	1004	13/13	0.90	0.10	47,60,63,66	0
3	EDO	BBB	1003	4/4	0.90	0.17	42,44,46,46	0
3	EDO	AAA	1007	4/4	0.91	0.11	31,35,35,35	0
3	EDO	AAA	1010	4/4	0.91	0.23	53,55,55,57	0
3	EDO	BBB	1001	4/4	0.91	0.17	39,39,39,39	0
3	EDO	CCC	1003	4/4	0.92	0.16	46,49,51,51	0
3	EDO	CCC	1001	4/4	0.95	0.09	39,41,41,43	0
3	EDO	AAA	1004	4/4	0.95	0.10	40,43,44,44	0
3	EDO	AAA	1001	4/4	0.98	0.05	28,28,28,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.