

wwPDB X-ray Structure Validation Summary Report (i)

Sep 17, 2023 – 04:59 AM EDT

PDB ID	:	4TZ3
Title	:	Ensemble refinement of the E502A variant of sacteLam55A from Streptomyces
		sp. SirexAA-E in complex with laminarite traose
Authors	:	Bianchetti, C.M.; Takasuka, T.E.; Yik, E.J.; Bergeman, L.F.; Fox, B.G.
Deposited on	:	2014-07-09
Resolution	:	1.90 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 (i) symbol.

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.90 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	Similar resolution $(\#$ Entries, resolution range $(\mathring{A}))$		
D	(#Entries)	(# Entries, resolution range(A))		
R _{free}	130704	0207 (1.90-1.90)		
Ramachandran outliers	138981	6760 (1.90-1.90)		
Sidechain outliers	138945	6760 (1.90-1.90)		
RSRZ outliers	127900	6082 (1.90-1.90)		

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% 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	
			<u>6%</u>	
1	1-A	549	95%	5%
			6%	
1	10-A	549	95%	5%
			6%	
1	11-A	549	95%	5%•
			<u>6%</u>	
1	12-A	549	95%	5%•
			<u>6%</u>	
1	13-A	549	95%	••
			6%	
1	14-A	549	94%	5%•



2

14**-**B

4

5%•

		i previous	puye	
Mol	Chain	Length	Quality of chain	
1	15-A	549	94%	5%•
1	16-A	549	96%	•
1	17-A	549	94%	5%•
1	18-A	549	95%	5%•
1	19-A	549	95%	5%
1	2-A	549	95%	5%•
1	20-A	549	95%	5%•
1	21-A	549	95%	••
1	22-A	549	96%	•
1	23-A	549	95%	5%•
1	24-A	549	95%	•
1	25-A	549	94%	5%•
1	3-A	549	95%	5%
1	4-A	549	95%	•
1	5-A	549	94%	5%•
1	6-A	549	94%	5%•
1	7-A	549	95%	••
1	8-A	549	95%	5%
1	9-A	549	96%	•
2	1-B	4	100%	
2	10-B	4	100%	
2	11-B	4	100%	
2	12-B	4	100%	
2	13-B	4	100%	

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100%

Mol	Chain	Length	Quality of chain
2	15-B	4	100%
2	16-B	4	100%
2	17-B	4	100%
2	18-B	4	100%
2	19-B	4	100%
2	2-B	4	100%
2	20-B	4	100%
2	21-B	4	100%
2	22-B	4	100%
2	23-B	4	100%
2	24-B	4	100%
2	25-B	4	100%
2	3-B	4	100%
2	4-B	4	100%
2	5-B	4	100%
2	6-B	4	100%
2	7-B	4	100%
2	8-B	4	100%
2	9-B	4	100%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 210296 atoms, of which 98125 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace		
1	1 \	540	Total	С	Н	Ν	0	S	0	0	0	
1	1-A	549	8074	2629	3907	708	825	5	0	0	0	
1	2.4	540	Total	С	Н	Ν	0	S	0	0	0	
	2-A	549	8074	2629	3907	708	825	5	0	0	0	
1	2 1	540	Total	С	Н	Ν	Ο	S	0	0	0	
	<i></i> -А	549	8074	2629	3907	708	825	5	0	0	0	
1	4. A	540	Total	С	Н	Ν	0	S	0	0	0	
	4-A	549	8074	2629	3907	708	825	5	0	0	0	
1	۲ ۸	540	Total	С	Н	Ν	Ο	S	0	0	0	
1	0-A	549	8074	2629	3907	708	825	5	0	0	0	
1	6 1	540	Total	С	Н	Ν	0	S	0	0	0	
1	0-A	549	8074	2629	3907	708	825	5	0	0	0	
1	7 1	540	Total	С	Η	Ν	0	S	0	0	0	0
1	(-A	549	8074	2629	3907	708	825	5		0	0	
1	8 1	540	Total	С	Η	Ν	0	S	0	0	0	
1	0-A	549	8074	2629	3907	708	825	5	0	0	0	
1	ΟΔ	540	Total	С	Η	Ν	0	\mathbf{S}	0	0	0	
1	$J^-\Lambda$	049	8074	2629	3907	708	825	5		0	0	0
1	10 A	540	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	Ο	
1	10-7	049	8074	2629	3907	708	825	5		0	0	
1	11 Δ	540	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	Ο	
1	11-7	049	8074	2629	3907	708	825	5	0	0	0	
1	19 A	540	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	Ο	
1	12-11	045	8074	2629	3907	708	825	5	0	0	0	
1	13 <u>-</u> Δ	549	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0	
	10 11	045	8074	2629	3907	708	825	5	0	0	0	
1	14 - A	549	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0	
1	14-11	045	8074	2629	3907	708	825	5	0	0	0	
1	15-A	549	Total	\mathbf{C}	Η	Ν	Ο	\mathbf{S}	0	0	0	
	10-11	040	8074	2629	3907	708	825	5		0	0	
1	16-4	549	Total	\mathbf{C}	Н	Ν	0	\mathbf{S}	0	0	0	
	10-11	040	8074	2629	3907	708	825	5		0	0	

• Molecule 1 is a protein called Putative secreted protein.



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Mol	Chain	Residues			Atoms	5			ZeroOcc	AltConf	Trace		
1	17 Δ	540	Total	С	Н	Ν	0	S	0	0	0		
	17-A	549	8074	2629	3907	708	825	5	0	0	0		
1	18 /	540	Total	С	Η	Ν	0	\mathbf{S}	0	0	0		
	10-A	049	8074	2629	3907	708	825	5	0	0	0		
1	10 A	540	Total	С	Η	Ν	0	\mathbf{S}	0	0	0		
	19-A	049	8074	2629	3907	708	825	5	0	0	0		
1	20 1	540	Total	С	Η	Ν	0	\mathbf{S}	0	0	0	0	0
	20-A	049	8074	2629	3907	708	825	5		0	0		
1	91 A	540	Total	С	Η	Ν	0	\mathbf{S}	0	0	0		
	21-A	049	8074	2629	3907	708	825	5	0	0	0		
1	22 A	540	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0		
	22-7	049	8074	2629	3907	708	825	5	0	0	0		
1	23 A	540	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0		
	2 0 -A	049	8074	2629	3907	708	825	5	0	0	0		
1	24 4	540	Total	С	Η	Ν	0	\mathbf{S}	0	0	0		
	1 24-A	049	8074	2629	3907	708	825	5	0	0	0		
1	25 A	540	Total	С	Η	Ν	0	S	0	0	0		
	20-A	049	8074	2629	3907	708	825	5			U		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	502	ALA	GLU	engineered mutation	UNP G2NFJ9

• Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	1-B	4	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 45 & 24 & 21 \end{array}$	0	0	0
2	2-B	4	Total C O 45 24 21	0	0	0
2	3-B	4	Total C O 45 24 21	0	0	0
2	4-B	4	Total C O 45 24 21	0	0	0
2	5-B	4	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 45 & 24 & 21 \end{array}$	0	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	6-B	4	Total C O 45 24 21	0	0	0
2	7-B	4	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	0	0	0
2	8-B	4	Total C O 45 24 21	0	0	0
2	9-B	4	Total C O 45 24 21	0	0	0
2	10-B	4	Total C O 45 24 21	0	0	0
2	11-B	4	Total C O 45 24 21	0	0	0
2	12-B	4	Total C O 45 24 21	0	0	0
2	13-B	4	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 45 & 24 & 21 \end{array}$	0	0	0
2	14-B	4	Total C O 45 24 21	0	0	0
2	15-B	4	Total C O 45 24 21	0	0	0
2	16-B	4	Total C O 45 24 21	0	0	0
2	17-B	4	Total C O 45 24 21	0	0	0
2	18-B	4	Total C O 45 24 21	0	0	0
2	19-B	4	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 45 & 24 & 21 \end{array}$	0	0	0
2	20-B	4	Total C O 45 24 21	0	0	0
2	21-B	4	Total C O 45 24 21	0	0	0
2	22-B	4	Total C O 45 24 21	0	0	0
2	23-B	4	Total C O 45 24 21	0	0	0
2	24-B	4	Total C O 45 24 21	0	0	0
2	25-B	4	Total C O 45 24 21	0	0	0

• Molecule 3 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	1	Total C O 11 6 5	0	0
3	2-A	1	Total C O 11 6 5	0	0
3	3-A	1	Total C O 11 6 5	0	0
3	4-A	1	Total C O 11 6 5	0	0
3	5-A	1	Total C O 11 6 5	0	0
3	6-A	1	Total C O 11 6 5	0	0
3	7-A	1	Total C O 11 6 5	0	0
3	8-A	1	Total C O 11 6 5	0	0
3	9-A	1	Total C O 11 6 5	0	0
3	10-A	1	Total C O 11 6 5	0	0
3	11-A	1	Total C O 11 6 5	0	0
3	12-A	1	Total C O 11 6 5	0	0
3	13-A	1	Total C O 11 6 5	0	0
3	14-A	1	Total C O 11 6 5	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	15-A	1	Total C O 11 6 5	0	0
3	16-A	1	Total C O 11 6 5	0	0
3	17-A	1	Total C O 11 6 5	0	0
3	18-A	1	Total C O 11 6 5	0	0
3	19-A	1	Total C O 11 6 5	0	0
3	20-A	1	Total C O 11 6 5	0	0
3	21-A	1	Total C O 11 6 5	0	0
3	22-A	1	Total C O 11 6 5	0	0
3	23-A	1	Total C O 11 6 5	0	0
3	24-A	1	Total C O 11 6 5	0	0
3	25-A	1	Total C O 11 6 5	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
4	1 \	1	Total	С	Η	Ο	0	0
4	1-A	1	10	2	6	2	0	0
4		1	Total	С	Н	Ο	0	0
4	2-A	1	10	2	6	2	0	0
4		1	Total	С	Н	0	0	0
4	3-A	1	10	2	6	2	0	0
4		1	Total	С	Н	0	0	0
4	4-A	1	10	2	6	2	0	0
		1	Total	С	Н	0		0
4	b-A	1	10	2	6	2	0	0
			Total	С	Н	0		
4	6-A	1	10	2	6	2	0	0
			Total	С	Н	0		
4	7-A	1	10	2	6	2	0	0
			Total	С	Н	0		
4	8-A	1	10	2	6	2	0	0
			Total	С	H	0		
4	9-A	1	10	2	6	2	0	0
			Total	C	H	0		
4	10-A	1	10	2	6	2	0	0
			Total		H	0		
4	11-A	1	10	$\frac{0}{2}$	6	2	0	0
			Total		H	0		
4	12-A	1	10	2	6	2	0	0
			Total		H	0		
4	13-A	1	10	$\frac{0}{2}$	6	2	0	0
			Total		H	0		
4	14-A	1	10	$\frac{0}{2}$	6	2	0	0
			Total	$\overline{\mathbf{C}}$	H	0		
4	15-A	1	10	$\frac{0}{2}$	6	2	0	0
			Total	$\frac{2}{C}$	H	$\overline{0}$		
4	16-A	1	10	$\frac{0}{2}$	6	2	0	0
			Total	$\frac{2}{C}$	H	$\overline{0}$		
4	17-A	1	10	$\frac{0}{2}$	6	2	0	0
			Total	$\frac{2}{C}$	H	$\frac{2}{0}$		
4	18-A	1	10	$\frac{\circ}{2}$	6	2	0	0
			Total	$\frac{2}{C}$	H	$\frac{2}{0}$		
4	19-A	1	10	$\frac{1}{2}$	6	2	0	0
			Total	$\frac{2}{C}$	н Н	<u></u>		
4	20-A	1	100	$\frac{0}{2}$	6	$\frac{1}{2}$	0	0
			Total	$\frac{2}{C}$	н Н	<u></u>		
4	21-A	1	100	0 2	6	$\frac{1}{2}$	0	0
			Total	$\frac{2}{C}$	- Н	<u></u>		
4	22-A	1	100	0 2	6	0 9	0	0
1	1		10	4	0	4		



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Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
4	02 A	1	Total	С	Н	0	0	0	
4	23-A	1	10	2	6	2	0	0	
4	94 4	1	Total	С	Н	0	0	0	
4	24-A	1	10	2	6	2	0	0	
4	95 A	1	Total	С	Н	0	0	0	
4	20-A	L	10	2	6	2	0	0	
4	1 A	1	Total	С	Η	0	0	0	
4	1-A	L	10	2	6	2	0	0	
4	2.4	1	Total	С	Η	0	0	0	
4	2-A	L	10	2	6	2	0	0	
4	2Λ	1	Total	С	Н	0	0	0	
4	0-A	L	10	2	6	2	0	0	
4	4.4	1	Total	С	Η	0	0	0	
4	4-A	L	10	2	6	2	0	0	
4	5 1	1	Total	С	Н	0	0	0	
4	0-A	T	10	2	6	2	0	0	
4	6 4	1	Total	С	Н	0	0	0	
-1	0-A	T	10	2	6	2	0	0	
4	7Δ	1	Total	С	Η	0	0	0	
4	(-A	T	10	2	6	2	0	0	
4	1 8 4	1	Total	С	Η	0	0	0	
-1	0-A	T	10	2	6	2	0	0	
4	ο Δ	Ο_ Δ	1	Total	С	Η	0	0	0
т	5-11	I	10	2	6	2	0	0	
4	10-A	1	Total	С	Η	Ο	0	0	
т	10-11	I	10	2	6	2	0	0	
	11_A	1	Total	С	Η	Ο	0	0	
т	11-11	I	10	2	6	2	0	0	
	12-A	1	Total	С	Η	Ο	0	0	
	12 11	T	10	2	6	2	0	0	
4	13-A	1	Total	С	Н	Ο	0	0	
	10 11	1	10	2	6	2	0	0	
4	14-A	1	Total	С	Η	Ο	0	0	
	1111	T	10	2	6	2	Ŭ	0	
4	15-A	1	Total	С	Η	Ο	0	0	
	10 11	*	10	2	6	2			
4	16-A	1	Total	С	Η	Ο	0	0	
		*	10	2	6	2			
4	17-A	1	Total	С	Η	Ο	0	0	
	T 1 7 T	*	10	2	6	2			
4	18-A	1	Total	С	Η	Ο	0	0	
4 10-A		10	2	6	2				



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Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
4	10 1	1	Total	С	Н	0	0	0	
4	19-A	1	10	2	6	2	0	0	
4	20.1	1	Total	С	Н	0	0	0	
4	20-A	1	10	2	6	2	0	0	
4	01 A	1	Total	С	Η	0	0	0	
4	21-A	1	10	2	6	2	0	0	
4	-00 A	1	Total	С	Η	0	0	0	
4	22-A	1	10	2	6	2	0	0	
4	<u> </u>	1	Total	С	Η	0	0	0	
4	23-A	1	10	2	6	2	0	0	
4	94.4	1	Total	С	Η	0	0	0	
4	24-A	1	10	2	6	2	0	0	
4	25 1	1	Total	С	Η	0	0	0	
4	20-A	1	10	2	6	2	0	0	
4	1 A	1	Total	С	Н	0	0	0	
4	1-A	1	10	2	6	2	0	0	
4	2.4	1	Total	С	Н	0	0	0	
4	Z-A	1	10	2	6	2	0	0	
4	2 1	1	Total	С	Н	0	0	0	
4	3- А	1	10	2	6	2	0	0	
4	4 4	1	Total	С	Н	0	0	0	
4	4-A	1	10	2	6	2	0	0	
4	5 1	4 5 A	1	Total	С	Η	0	0	0
4	J-A	1	10	2	6	2	0	0	
4	6 1	1	Total	С	Η	0	0	0	
4	0-A	1	10	2	6	2	0	0	
4	7 1	1	Total	С	Η	0	0	0	
4	(-A	1	10	2	6	2	0	0	
4	ο Λ	1	Total	С	Η	0	0	0	
4	0-A	1	10	2	6	2	0	0	
4	0. 4	1	Total	С	Η	0	0	0	
4	9-A	1	10	2	6	2	0	0	
4	10 \	1	Total	С	Η	0	0	0	
4	10-A	1	10	2	6	2	0	0	
	11 A	1	Total	С	Η	0	0	Ο	
4	11-A		10	2	6	2	0	U	
1	12 A	1	Total	С	Η	0	0	0	
<u> </u>	12-17	T	10	2	6	2		U	
1	13 A	1	Total	С	Η	0	0	0	
<u>+</u>	10-A	1	10	2	6	2		U	
1	1/ A	1	Total	С	Η	0	0	Ο	
4	14-11		10	2	6	2			



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
4	15-A	1	Total C H	0	0	0	
		-	10 2 6	2			
4	16-A	1	Total C H	Ο	0	0	
	10 11	I	10 2 6	2	0	0	
4	17 Δ	1	Total C H	Ο	0	0	
4	11-7	1	$10 \ 2 \ 6$	2	0	0	
4	10 /	1	Total C H	0	0	0	
4	10-A	1	$10 \ 2 \ 6$	2	0	0	
4	10 1	1	Total C H	0	0	0	
4	19-A	1	10 2 6	2	0	0	
4	20 1	1	Total C H	0	0	0	
4	20-A	20-A	1	$10 \ 2 \ 6$	2	0	0
4	91 A	1	Total C H	0	0	0	
4	21-A	1	$10 \ 2 \ 6$	2	0	0	
4	- <u>-</u>	1	Total C H	0	0	0	
4	ZZ-A	1	10 2 6	2	0	0	
4	-02 A	1	Total C H	0	0	0	
4	20-A	1	10 2 6	2	0	0	
4	94.4	1	Total C H	Ο	0	0	
4	24-A	L	10 2 6	2	0	U	
4	25 1	1	Total C H	0	0	0	
4	20-A		$10 \ 2 \ 6$	2	U	U	

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• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	253	Total O 253 253	0	0
5	2-A	248	Total O 248 248	0	0
5	3-A	259	Total O 259 259	0	0
5	4-A	249	Total O 249 249	0	0
5	5-A	246	Total O 246 246	0	0
5	6-A	245	Total O 245 245	0	0
5	7-A	258	Total O 258 258	0	0
5	8-A	264	Total O 264 264	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	9-A	251	Total O 251 251	0	0
5	10-A	248	Total O 248 248	0	0
5	11-A	264	Total O 264 264	0	0
5	12-A	246	Total O 246 246	0	0
5	13-A	247	Total O 247 247	0	0
5	14-A	242	Total O 242 242	0	0
5	15-A	262	Total O 262 262	0	0
5	16-A	252	Total O 252 252	0	0
5	17-A	243	Total O 243 243	0	0
5	18-A	255	Total O 255 255	0	0
5	19-A	274	Total O 274 274	0	0
5	20-A	242	Total O 242 242	0	0
5	21-A	240	Total O 240 240	0	0
5	22-A	250	Total O 250 250	0	0
5	23-A	259	Total O 259 259	0	0
5	24-A	250	Total O 250 250	0	0
5	25-A	249	Total O 249 249	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 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: Putative secreted protein



• Molecule 1: Putative secreted protein 6% Chain 5-A: 94% 5%• • Molecule 1: Putative secreted protein 6% Chain 6-A: 94% 5%• • Molecule 1: Putative secreted protein 6%

Chain 7-A: 95% · ·

E3 17 B3 24 64 00 64 00 64 00 64 01 14 10 14 10 14 15 15

• Molecule 1: Putative secreted protein









D324 Q340 Q340 Q399 Q401 Q402 Q402 Q403 Q517 Q503 Q503

• Molecule 1: Putative secreted protein

Chain 19-A: 95% 5%

• Molecule 1: Putative secreted protein

V338 V338 V338 9345 P345 9345 P399 9401 P401 9 P401 9 P401 9 P502 9 P605 5529 S529 5529

• Molecule 1: Putative secreted protein

6%

Chain 21-A:

95%

. .

• Molecule 1: Putative secreted protein





• Molecule 1: Putative secreted protein



• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 1-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 2-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



Chain 3-B:	100%	•
BGC1 BGC2 BGC3 BGC3 BGC3 BGC4		
• Molecule 2: beta-D-glu-beta-D-glucopyranose	ucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-I	D-glucopyranose-(1-3)
Chain 4-B:	100%	-
BGC1 BGC2 BGC3 BGC4 BGC4		
• Molecule 2: beta-D-glu-beta-D-glucopyranose	ucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-I	D-glucopyranose-(1-3)
Chain 5-B:	100%	-
BGC1 BGC3 BGC3 BGC4		
• Molecule 2: beta-D-glu-beta-D-glucopyranose	ucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-I	D-glucopyranose-(1-3)
Chain 6-B:	100%	-
BGC1 BGC2 BGC3 BGC3 BGC3 BGC4		
• Molecule 2: beta-D-glu-beta-D-glucopyranose	ucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-I	D-glucopyranose-(1-3)
Chain 7-B:	100%	-
BGC1 BGC2 BGC3 BGC3 BGC3 BGC4		
• Molecule 2: beta-D-glu-beta-D-glucopyranose	ucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-I	D-glucopyranose-(1-3)
Chain 8-B:	100%	-
BGC 1 BGC 2 BGC 3 BGC 4		
• Moloculo 2: bota D al	ucopyranose (1-3) beta D-glucopyranose (1-3) beta I)-gluconvrance $(1, 3)$

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 9-B:

100%



• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 10-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 11-B: 100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 12-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 13-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 14-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 15-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 16-B:

100%



BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 17-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 18-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 19-B:	100%	
C @ 4		

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 20-B: 100%

BGC1 BGC2 BGC3 BGC3

BGC BGC BGC BGC

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 21-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 22-B:

100%

BGC1 BGC2 BGC3 BGC4



• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 23-B:

100%

BGC1 BGC2 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose

Chain 24-B:

100%

BGC1 BGC2 BGC3 BGC3 BGC4

• Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)-beta-D-glucopyranose-(1-3)

Chain 25-B:

100%

BGC1 BGC2 BGC3 BGC4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	51.28Å 100.21Å 54.22Å	Depositor
a, b, c, α , β , γ	90.00° 99.46° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	28.33 - 1.90	Depositor
Resolution (A)	28.33 - 1.90	EDS
% Data completeness	93.2 (28.33-1.90)	Depositor
(in resolution range)	90.3 (28.33-1.90)	EDS
R _{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.97 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.9_1692)	Depositor
D D.	0.113 , 0.151	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.143 , 0.178	DCC
R_{free} test set	1989 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	19.3	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35, 114.8	EDS
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	210296	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.90% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: BGC, EDO

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		
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	1-A	0.85	5/4280~(0.1%)	0.93	11/5848~(0.2%)	
1	2-A	0.85	4/4280~(0.1%)	0.91	7/5848~(0.1%)	
1	3-A	0.81	1/4280~(0.0%)	0.91	7/5848~(0.1%)	
1	4-A	0.83	3/4280~(0.1%)	0.91	7/5848~(0.1%)	
1	5-A	0.80	2/4280~(0.0%)	0.89	7/5848~(0.1%)	
1	6-A	0.86	5/4280~(0.1%)	0.91	7/5848~(0.1%)	
1	7-A	0.83	4/4280~(0.1%)	0.91	7/5848~(0.1%)	
1	8-A	0.83	4/4280~(0.1%)	0.86	4/5848~(0.1%)	
1	9-A	0.83	5/4280~(0.1%)	0.88	4/5848~(0.1%)	
1	10-A	0.85	4/4280~(0.1%)	0.91	6/5848~(0.1%)	
1	11-A	0.80	2/4280~(0.0%)	0.90	6/5848~(0.1%)	
1	12-A	0.83	2/4280~(0.0%)	0.92	8/5848~(0.1%)	
1	13-A	0.83	2/4280~(0.0%)	0.92	7/5848~(0.1%)	
1	14-A	0.84	6/4280~(0.1%)	0.92	6/5848~(0.1%)	
1	15-A	0.81	1/4280~(0.0%)	0.92	5/5848~(0.1%)	
1	16-A	0.82	2/4280~(0.0%)	0.90	5/5848~(0.1%)	
1	17-A	0.82	4/4280~(0.1%)	0.91	8/5848~(0.1%)	
1	18-A	0.82	4/4280~(0.1%)	0.94	13/5848~(0.2%)	
1	19-A	0.87	4/4280~(0.1%)	0.94	9/5848~(0.2%)	
1	20-A	0.85	5/4280~(0.1%)	0.92	9/5848~(0.2%)	
1	21-A	0.81	2/4280~(0.0%)	0.89	6/5848~(0.1%)	
1	22-A	0.82	3/4280~(0.1%)	0.89	3/5848~(0.1%)	
1	23-A	0.80	1/4280~(0.0%)	0.90	$12\overline{)5848}\ (0.2\%)$	
1	24-A	0.83	3/4280~(0.1%)	0.97	$15\overline{)5848}\ (0.3\%)$	
1	25-A	0.86	4/4280 (0.1%)	0.96	13/5848~(0.2%)	
All	All	0.83	82/107000~(0.1%)	0.91	$\overline{192/146200}~(0.1\%)$	

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	3-A	0	1
1	14-A	0	1
1	17-A	0	1
1	19-A	0	1
1	24-A	0	1
All	All	0	5

The worst 5 of 82 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-A	236	MET	CB-CG	8.44	1.78	1.51
1	10-A	198	SER	CB-OG	-8.39	1.31	1.42
1	19-A	404	ASP	CB-CG	8.26	1.69	1.51
1	4-A	404	ASP	CB-CG	8.12	1.68	1.51
1	1-A	236	MET	CG-SD	8.07	2.02	1.81

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	4-A	236	MET	CG-SD-CE	-14.71	76.66	100.20
1	18-A	236	MET	CG-SD-CE	-14.68	76.71	100.20
1	1-A	236	MET	CG-SD-CE	-14.32	77.28	100.20
1	24-A	87	ARG	NE-CZ-NH2	-13.75	113.42	120.30
1	14-A	236	MET	CG-SD-CE	-12.86	79.63	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	14-A	295	GLY	Peptide
1	17-A	62	GLY	Peptide
1	19-A	293	GLY	Peptide
1	24-A	251	GLU	Peptide
1	3-A	295	GLY	Peptide

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	1-A	4167	3907	3919	0	0
1	2-A	4167	3907	3919	0	0
1	3-A	4167	3907	3919	0	0
1	4-A	4167	3907	3919	0	0
1	5-A	4167	3907	3919	0	0
1	6-A	4167	3907	3919	0	0
1	7-A	4167	3907	3919	0	0
1	8-A	4167	3907	3919	0	0
1	9-A	4167	3907	3919	0	0
1	10-A	4167	3907	3919	0	0
1	11-A	4167	3907	3919	0	0
1	12-A	4167	3907	3919	0	0
1	13-A	4167	3907	3919	0	0
1	14-A	4167	3907	3919	0	0
1	15-A	4167	3907	3919	0	0
1	16-A	4167	3907	3919	0	0
1	17-A	4167	3907	3919	0	0
1	18-A	4167	3907	3919	0	0
1	19-A	4167	3907	3919	0	0
1	20-A	4167	3907	3919	0	0
1	21-A	4167	3907	3919	0	0
1	22-A	4167	3907	3919	0	0
1	23-A	4167	3907	3919	0	0
1	24-A	4167	3907	3919	0	0
1	25-A	4167	3907	3919	0	0
2	1-B	45	0	37	0	0
2	2-B	45	0	39	0	0
2	3-B	45	0	39	0	0
2	4-B	45	0	39	0	0
2	5-B	45	0	36	0	0
2	6-B	45	0	39	0	0
2	7-B	45	0	38	0	0
2	8-B	45	0	38	0	0
2	9-B	45	0	38	0	0
2	10-B	45	0	38	0	0
2	11-B	45	0	39	0	0
2	12-B	45	0	39	0	0
2	13-B	45	0	39	0	0
2	14-B	45	0	39	0	0
2	15-B	45	0	38	0	0
2	16-B	45	0	39	0	0
2	17-B	45	0	39	0	0
2	18-B	45	0	38	0	0



	Chain	Non-H	H(model)	H(addad)	Clashes	Symm-Clashes
2	10 P	45		$\frac{11(auueu)}{20}$		0
$\frac{2}{2}$	19-D 20 B	45	0	38	0	0
$\frac{2}{2}$	20-D 21 B	45	0	37	0	0
$\frac{2}{2}$	21-D 22 R	45	0	30	0	0
$\frac{2}{2}$	22-D 23 B	45	0	38	0	0
$\frac{2}{2}$	20-D 24 B	45	0	38	0	0
$\frac{2}{2}$	24-D 25 B	45	0	30	0	0
2	20-D 1_Δ	11	0	10	0	0
3	1-Λ 2-Δ	11	0	10	0	0
3	2-11 3-A	11	0	10	0	0
3	4-A	11	0	10	0	0
3	5-A	11	0	10	0	0
3	6-A	11	0	10	0	0
3	7-A	11	0	10	0	0
3	8-A	11	0	10	0	0
3	0_A	11	0	10	0	0
3	10-A	11	0	10	0	0
3	10 M	11	0	10	0	0
3	12-A	11	0	10	0	0
3	12-11 13-A	11	0	10	0	0
3	14-A	11	0	10	0	0
3	15-A	11	0	10	0	0
3	16-A	11	0	10	0	0
3	17-A	11	0	10	0	0
3	18-A	11	0	10	0	0
3	19-A	11	0	10	0	0
3	20-A	11	0	10	0	0
3	21-A	11	0	10	0	0
3	22-A	11	0	10	0	0
3	23-A	11	0	10	0	0
3	24-A	11	0	10	0	0
3	25-A	11	0	10	0	0
4	1-A	12	18	18	0	0
4	2-A	12	18	18	0	0
4	3-A	12	18	18	0	0
4	4-A	12	18	18	0	0
4	5-A	12	18	18	0	0
4	6-A	12	18	18	0	0
4	7-A	12	18	18	0	0
4	8-A	12	18	18	0	0
4	9-A	12	18	18	0	0
4	10-A	12	18	18	0	0



4T	CZ3

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	11-A	12	18	18	0	0
4	12-A	12	18	18	0	0
4	13-A	12	18	18	0	0
4	14-A	12	18	18	0	0
4	15-A	12	18	18	0	0
4	16-A	12	18	18	0	0
4	17-A	12	18	18	0	0
4	18-A	12	18	18	0	0
4	19-A	12	18	18	0	0
4	20-A	12	18	18	0	0
4	21-A	12	18	18	0	0
4	22-A	12	18	18	0	0
4	23-A	12	18	18	0	0
4	24-A	12	18	18	0	0
4	25-A	12	18	18	0	0
5	1-A	253	0	0	0	0
5	2-A	248	0	0	0	0
5	3-A	259	0	0	0	0
5	4-A	249	0	0	0	0
5	5-A	246	0	0	0	0
5	6-A	245	0	0	0	0
5	7-A	258	0	0	0	0
5	8-A	264	0	0	0	0
5	9-A	251	0	0	0	0
5	10-A	248	0	0	0	0
5	11-A	264	0	0	0	0
5	12-A	246	0	0	0	0
5	13-A	247	0	0	0	0
5	14-A	242	0	0	0	0
5	15-A	262	0	0	0	0
5	16-A	252	0	0	0	0
5	17-A	243	0	0	0	0
5	18-A	255	0	0	0	0
5	19-A	274	0	0	0	0
5	20-A	242	0	0	0	0
5	21-A	240	0	0	0	0
5	22-A	250	0	0	0	0
5	23-A	259	0	0	0	0
5	24-A	250	0	0	0	0
5	25-A	249	0	0	0	0
All	All	112171	98125	99634	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	Percer	ntiles
1	1-A	547/549~(100%)	508~(93%)	34 (6%)	5 (1%)	17	7
1	2-A	547/549~(100%)	503 (92%)	40 (7%)	4 (1%)	22	12
1	3-A	547/549~(100%)	508 (93%)	34 (6%)	5 (1%)	17	7
1	4-A	547/549~(100%)	512 (94%)	30 (6%)	5 (1%)	17	7
1	5-A	547/549~(100%)	510 (93%)	32 (6%)	5 (1%)	17	7
1	6-A	547/549~(100%)	503 (92%)	40 (7%)	4 (1%)	22	12
1	7-A	547/549~(100%)	506 (92%)	38 (7%)	3 (0%)	29	18
1	8-A	547/549~(100%)	509~(93%)	35 (6%)	3 (0%)	29	18
1	9-A	547/549~(100%)	502 (92%)	40 (7%)	5 (1%)	17	7
1	10-A	547/549~(100%)	501 (92%)	45 (8%)	1 (0%)	47	38
1	11-A	547/549~(100%)	511 (93%)	30 (6%)	6 (1%)	14	5
1	12-A	547/549~(100%)	511 (93%)	32 (6%)	4 (1%)	22	12
1	13-A	547/549~(100%)	505 (92%)	37 (7%)	5 (1%)	17	7
1	14-A	547/549~(100%)	509~(93%)	34 (6%)	4 (1%)	22	12
1	15-A	547/549~(100%)	511 (93%)	29~(5%)	7 (1%)	12	4
1	16-A	547/549~(100%)	499 (91%)	43 (8%)	5 (1%)	17	7
1	17-A	547/549~(100%)	502 (92%)	38 (7%)	7 (1%)	12	4
1	18-A	547/549~(100%)	510 (93%)	35 (6%)	2 (0%)	34	24
1	19-A	547/549~(100%)	503 (92%)	40 (7%)	4 (1%)	22	12
1	20-A	547/549~(100%)	505 (92%)	35~(6%)	7 (1%)	12	4



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	21-A	547/549~(100%)	513 (94%)	31~(6%)	3~(0%)	29	18
1	22-A	547/549~(100%)	507~(93%)	38~(7%)	2 (0%)	34	24
1	23-A	547/549~(100%)	506~(92%)	34~(6%)	7 (1%)	12	4
1	24-A	547/549~(100%)	501~(92%)	43 (8%)	3~(0%)	29	18
1	25-A	547/549~(100%)	501~(92%)	43 (8%)	3~(0%)	29	18
All	All	13675/13725~(100%)	12656 (92%)	910 (7%)	109 (1%)	19	9

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	509	ASP
1	3-A	314	ALA
1	4-A	297	PRO
1	6-A	77	ASP
1	6-A	319	ILE

5.3.2 Protein sidechains (i)

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed Rotameric Outliers		Outliers	Percer	ntiles
1	1-A	436/436~(100%)	419 (96%)	17~(4%)	32	23
1	2-A	436/436~(100%)	417 (96%)	19 (4%)	28	19
1	3-A	436/436~(100%)	416 (95%)	20~(5%)	27	17
1	4-A	436/436~(100%)	417 (96%)	19 (4%)	28	19
1	5-A	436/436~(100%)	413~(95%)	23~(5%)	22	13
1	6-A	436/436~(100%)	413 (95%)	23~(5%)	22	13
1	7-A	436/436~(100%)	418 (96%)	18 (4%)	30	21
1	8-A	436/436~(100%)	417 (96%)	19 (4%)	28	19
1	9-A	436/436~(100%)	422~(97%)	14 (3%)	39	30
1	10-A	$43\overline{6/436}~(100\%)$	419 (96%)	17 (4%)	32	23
1	11-A	436/436~(100%)	415 (95%)	21 (5%)	25	16





Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	12-A	436/436~(100%)	416~(95%)	20~(5%)	27	17	
1	13-A	436/436~(100%)	420~(96%)	16~(4%)	34	25	
1	14-A	436/436~(100%)	412 (94%)	24~(6%)	21	12	
1	15-A	436/436~(100%)	415~(95%)	21~(5%)	25	16	
1	16-A	436/436~(100%)	420 (96%)	16 (4%)	34	25	
1	17-A	436/436~(100%)	419 (96%)	17~(4%)	32	23	
1	18-A	436/436~(100%)	414 (95%)	22~(5%)	24	15	
1	19-A	436/436~(100%)	419 (96%)	17~(4%)	32	23	
1	20-A	436/436~(100%)	419 (96%)	17~(4%)	32	23	
1	21-A	436/436~(100%)	416 (95%)	20~(5%)	27	17	
1	22-A	436/436~(100%)	420 (96%)	16 (4%)	34	25	
1	23-A	436/436~(100%)	419 (96%)	17~(4%)	32	23	
1	24-A	436/436~(100%)	424 (97%)	12 (3%)	43	36	
1	25-A	436/436~(100%)	411 (94%)	25~(6%)	20	11	
All	All	10900/10900~(100%)	10430 (96%)	470 (4%)	29	19	

 $5~{\rm of}~470$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	13-A	75	THR
1	24-A	545	ASN
1	15-A	490	SER
1	24-A	340	GLN
1	21-A	570	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	22-A	306	GLN
1	23-A	466	HIS
1	25-A	150	GLN
1	10-A	217	GLN
1	10-A	127	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

100 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).

Mal	Tuno	Chain	Dog	Link	Bo	ond leng	ths	Bond angles		les
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BGC	1-B	1	2	$12,\!12,\!12$	2.49	4 (33%)	17,17,17	3.27	7 (41%)
2	BGC	1-B	2	2	$11,\!11,\!12$	2.76	4 (36%)	$15,\!15,\!17$	1.76	2 (13%)
2	BGC	1-B	3	2	$11,\!11,\!12$	3.07	5 (45%)	$15,\!15,\!17$	2.04	6 (40%)
2	BGC	1-B	4	2	11,11,12	2.86	5 (45%)	15,15,17	3.06	6 (40%)
2	BGC	10-B	1	2	12,12,12	2.26	5 (41%)	17,17,17	1.31	2 (11%)
2	BGC	10-B	2	2	11,11,12	2.97	5 (45%)	15,15,17	2.12	5 (33%)
2	BGC	10-B	3	2	11,11,12	3.25	6 (54%)	15,15,17	1.95	4 (26%)
2	BGC	10-B	4	2	11,11,12	2.66	5 (45%)	15,15,17	2.39	5 (33%)
2	BGC	11-B	1	2	12,12,12	2.33	5 (41%)	17,17,17	1.21	1 (5%)
2	BGC	11-B	2	2	11,11,12	2.89	4 (36%)	15,15,17	2.01	3 (20%)
2	BGC	11-B	3	2	11,11,12	2.94	5 (45%)	15,15,17	1.97	4 (26%)
2	BGC	11-B	4	2	11,11,12	2.68	5 (45%)	15,15,17	2.38	4 (26%)
2	BGC	12-B	1	2	12,12,12	2.44	6 (50%)	17,17,17	0.80	0
2	BGC	12-B	2	2	11,11,12	2.88	4 (36%)	15,15,17	1.60	1 (6%)
2	BGC	12-B	3	2	11,11,12	<mark>3.05</mark>	5 (45%)	15,15,17	1.97	4 (26%)
2	BGC	12-B	4	2	11,11,12	2.73	5 (45%)	15,15,17	1.92	5 (33%)
2	BGC	13-B	1	2	12,12,12	2.35	5 (41%)	17,17,17	1.23	2 (11%)
2	BGC	13-B	2	2	11,11,12	2.89	5 (45%)	15,15,17	1.55	2 (13%)



Mal	Tune	Chain	Dec	Tink	Bond lengths		Bond angles		
WIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ # Z > 2
2	BGC	13-B	3	2	11,11,12	3.07	6 (54%)	15,15,17	1.93 $4 (26\%)$
2	BGC	13-B	4	2	11,11,12	2.67	5 (45%)	15,15,17	2.27 4 (26%)
2	BGC	14-B	1	2	12,12,12	2.32	5 (41%)	$17,\!17,\!17$	0.97 1 (5%)
2	BGC	14-B	2	2	11,11,12	2.94	6 (54%)	$15,\!15,\!17$	1.84 4 (26%)
2	BGC	14-B	3	2	11,11,12	3.12	5(45%)	15,15,17	2.04 3 (20%)
2	BGC	14-B	4	2	11,11,12	2.70	5 (45%)	15,15,17	2.29 6 (40%)
2	BGC	15-B	1	2	12,12,12	2.25	5 (41%)	17,17,17	1.64 5 (29%)
2	BGC	15-B	2	2	11,11,12	2.97	5 (45%)	15,15,17	2.35 6 (40%)
2	BGC	15-B	3	2	11,11,12	2.89	6 (54%)	15,15,17	1.90 $3(20\%)$
2	BGC	15-B	4	2	11,11,12	2.63	4 (36%)	15,15,17	2.36 6 (40%)
2	BGC	16-B	1	2	12,12,12	2.21	4 (33%)	17,17,17	1.70 $2(11\%)$
2	BGC	16-B	2	2	11,11,12	2.96	6 (54%)	15,15,17	1.86 4 (26%)
2	BGC	16-B	3	2	11,11,12	3.17	6 (54%)	15,15,17	2.08 4 (26%)
2	BGC	16-B	4	2	11,11,12	2.80	5 (45%)	15,15,17	2.41 6 (40%)
2	BGC	17-B	1	2	12,12,12	2.48	5 (41%)	17,17,17	1.36 $3(17\%)$
2	BGC	17-B	2	2	11,11,12	3.10	6 (54%)	15,15,17	1.63 $3(20\%)$
2	BGC	17-B	3	2	11,11,12	2.97	6 (54%)	15,15,17	1.68 2 (13%)
2	BGC	17-B	4	2	11,11,12	2.64	5 (45%)	15,15,17	2.22 5 (33%)
2	BGC	18-B	1	2	12,12,12	2.35	5 (41%)	17,17,17	1.14 1 (5%)
2	BGC	18-B	2	2	11,11,12	2.97	4 (36%)	15,15,17	1.82 1 (6%)
2	BGC	18-B	3	2	11,11,12	2.89	5 (45%)	15,15,17	2.06 3 (20%)
2	BGC	18-B	4	2	11,11,12	2.70	5 (45%)	15,15,17	2.53 8 (53%)
2	BGC	19-B	1	2	12,12,12	2.27	5 (41%)	17,17,17	1.78 $4(23\%)$
2	BGC	19-B	2	2	11,11,12	2.96	4 (36%)	15,15,17	1.92 4 (26%)
2	BGC	19-B	3	2	11,11,12	3.10	6 (54%)	15,15,17	2.09 5 (33%)
2	BGC	19-B	4	2	11,11,12	2.76	4 (36%)	15,15,17	2.72 4 (26%)
2	BGC	2-B	1	2	12,12,12	2.36	5 (41%)	17,17,17	1.08 2 (11%)
2	BGC	2-B	2	2	11,11,12	3.08	6 (54%)	15,15,17	1.87 2 (13%)
2	BGC	2-B	3	2	11,11,12	3.14	5(45%)	15,15,17	1.77 $3(20\%)$
2	BGC	2-B	4	2	11,11,12	2.78	5 (45%)	15,15,17	2.42 6 (40%)
2	BGC	20-B	1	2	12,12,12	2.44	5 (41%)	17,17,17	1.10 0
2	BGC	20-B	2	2	11,11,12	3.02	5 (45%)	15,15,17	2.05 4 (26%)
2	BGC	20-B	3	2	11,11,12	2.99	6 (54%)	15,15,17	1.69 2 (13%)
2	BGC	20-B	4	2	11,11,12	2.82	5 (45%)	15,15,17	3.03 5 (33%)
2	BGC	21-B	1	2	12,12,12	2.32	5 (41%)	17,17,17	1.12 1 (5%)



Mal	Turne	Chain	Dec	Tink	Bond lengths		Bond angles			
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	BGC	21-B	2	2	11,11,12	<mark>3.04</mark>	5 (45%)	15,15,17	2.37	6 (40%)
2	BGC	21-B	3	2	11,11,12	3.04	6 (54%)	15,15,17	1.71	2 (13%)
2	BGC	21-B	4	2	11,11,12	2.77	5 (45%)	$15,\!15,\!17$	2.43	4 (26%)
2	BGC	22-B	1	2	12,12,12	2.34	5 (41%)	17,17,17	1.11	0
2	BGC	22-B	2	2	11,11,12	2.85	5 (45%)	$15,\!15,\!17$	2.28	3 (20%)
2	BGC	22-B	3	2	11,11,12	3.18	5 (45%)	15,15,17	1.35	2 (13%)
2	BGC	22-B	4	2	11,11,12	2.74	5 (45%)	15,15,17	2.48	5 (33%)
2	BGC	23-B	1	2	12,12,12	2.41	6 (50%)	17,17,17	1.86	6 (35%)
2	BGC	23-B	2	2	11,11,12	<mark>3.08</mark>	6 (54%)	15,15,17	2.06	5 (33%)
2	BGC	23-B	3	2	11,11,12	<mark>3.07</mark>	5 (45%)	15,15,17	2.29	5 (33%)
2	BGC	23-B	4	2	11,11,12	2.64	5 (45%)	15,15,17	2.48	6 (40%)
2	BGC	24-B	1	2	12,12,12	2.26	5 (41%)	17,17,17	1.50	2 (11%)
2	BGC	24-B	2	2	11,11,12	<mark>3.06</mark>	6 (54%)	15,15,17	1.69	2 (13%)
2	BGC	24-B	3	2	11,11,12	3.17	6 (54%)	15,15,17	1.57	2 (13%)
2	BGC	24-B	4	2	11,11,12	2.69	4 (36%)	15,15,17	2.45	4 (26%)
2	BGC	25-B	1	2	12,12,12	2.36	5 (41%)	17,17,17	1.38	3 (17%)
2	BGC	25-B	2	2	11,11,12	3.05	5 (45%)	15,15,17	2.02	6 (40%)
2	BGC	25-B	3	2	11,11,12	3.07	5 (45%)	15,15,17	1.89	3 (20%)
2	BGC	25-B	4	2	11,11,12	2.64	5 (45%)	15,15,17	2.12	4 (26%)
2	BGC	3-B	1	2	12,12,12	2.40	6 (50%)	17,17,17	1.12	1 (5%)
2	BGC	3-B	2	2	11,11,12	2.94	4 (36%)	15,15,17	1.70	3 (20%)
2	BGC	3-B	3	2	11,11,12	2.97	6 (54%)	15,15,17	1.74	2 (13%)
2	BGC	3-B	4	2	11,11,12	2.70	4 (36%)	15,15,17	2.26	6 (40%)
2	BGC	4-B	1	2	12,12,12	2.25	5 (41%)	17,17,17	1.58	4 (23%)
2	BGC	4-B	2	2	11,11,12	2.94	4 (36%)	15,15,17	2.00	3 (20%)
2	BGC	4-B	3	2	11,11,12	2.95	6 (54%)	15,15,17	1.77	2 (13%)
2	BGC	4-B	4	2	11,11,12	2.65	5 (45%)	15,15,17	2.12	4 (26%)
2	BGC	5-B	1	2	12,12,12	2.34	5 (41%)	17,17,17	1.41	3 (17%)
2	BGC	5-B	2	2	11,11,12	3.07	5(45%)	15,15,17	2.62	8 (53%)
2	BGC	5-B	3	2	11,11,12	<mark>3.23</mark>	5 (45%)	15,15,17	1.71	2 (13%)
2	BGC	5-B	4	2	11,11,12	2.75	6 (54%)	15,15,17	2.30	5 (33%)
2	BGC	6-B	1	2	12,12,12	2.33	5 (41%)	17,17,17	1.17	0
2	BGC	6-B	2	2	11,11,12	2.89	5 (45%)	15,15,17	1.55	2 (13%)
2	BGC	6-B	3	2	11,11,12	<mark>3.00</mark>	5 (45%)	15,15,17	1.63	3 (20%)
2	BGC	6-B	4	2	11,11,12	2.80	4 (36%)	15,15,17	2.93	7 (46%)



Mol	Type	Chain	Bos	Link	Bond lengths			ngths Bond angles		
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	BGC	7-B	1	2	12,12,12	2.49	5 (41%)	17,17,17	1.29	3 (17%)
2	BGC	7-B	2	2	$11,\!11,\!12$	2.89	4 (36%)	$15,\!15,\!17$	1.64	2 (13%)
2	BGC	7-B	3	2	$11,\!11,\!12$	3.13	6 (54%)	$15,\!15,\!17$	2.35	6 (40%)
2	BGC	7-B	4	2	11,11,12	2.80	5 (45%)	$15,\!15,\!17$	2.18	5 (33%)
2	BGC	8-B	1	2	12,12,12	2.33	5 (41%)	17,17,17	1.42	3 (17%)
2	BGC	8-B	2	2	11,11,12	2.99	6 (54%)	15,15,17	2.06	2 (13%)
2	BGC	8-B	3	2	11,11,12	3.00	6 (54%)	15,15,17	1.55	2 (13%)
2	BGC	8-B	4	2	11,11,12	2.66	5 (45%)	15,15,17	2.87	5 (33%)
2	BGC	9-B	1	2	12,12,12	2.50	5 (41%)	17,17,17	1.23	2 (11%)
2	BGC	9-B	2	2	$11,\!11,\!12$	3.13	4 (36%)	$15,\!15,\!17$	2.04	3 (20%)
2	BGC	9-B	3	2	11,11,12	3.17	5 (45%)	$15,\!15,\!17$	1.67	2 (13%)
2	BGC	9-B	4	2	$1\overline{1,11,12}$	2.91	5 (45%)	$15,\!15,\!17$	2.56	5 (33%)

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	BGC	1-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	1-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	1-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	1-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	10-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	10-B	2	2	-	1/2/19/22	0/1/1/1
2	BGC	10-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	10-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	11 - B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	11-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	11-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	11-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	12-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	12-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	12-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	12-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	13-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	13-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	13-B	3	2	-	1/2/19/22	0/1/1/1



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Iol	Type	Chain	Res	Link	Chirals	Torsions	Rings					
2	BGC	13-B	4	2	-	0/2/19/22	0/1/1/1					
2	BGC	14-B	1	2	-	0/2/22/22	0/1/1/1					
2	BGC	14-B	2	2	-	0/2/19/22	0/1/1/1					
2	BGC	14 - B	3	2	-	2/2/19/22	0/1/1/1					
2	BGC	14-B	4	2	-	0/2/19/22	0/1/1/1					
2	BGC	15-B	1	2	-	2/2/22/22	0/1/1/1					
2	BGC	15-B	2	2	-	2/2/19/22	0/1/1/1					
2	BGC	15-B	3	2	-	0/2/19/22	0/1/1/1					
2	BGC	15-B	4	2	-	2/2/19/22	0/1/1/1					
2	BGC	16-B	1	2	-	2/2/22/22	0/1/1/1					
2	BGC	16-B	2	2	-	0/2/19/22	0/1/1/1					
2	BGC	16-B	3	2	-	0/2/19/22	0/1/1/1					
2	BGC	16-B	4	2	-	1/2/19/22	0/1/1/1					
2	BGC	17-B	1	2	-	0/2/22/22	0/1/1/1					
2	BGC	17-B	2	2	-	0/2/19/22	0/1/1/1					
2	BGC	17-B	3	2	-	0/2/19/22	0/1/1/1					
2	BGC	17-B	4	2	-	0/2/19/22	0/1/1/1					
2	BGC	18-B	1	2	-	0/2/22/22	0/1/1/1					
2	BGC	18-B	2	2	-	0/2/19/22	0/1/1/1					
2	BGC	18-B	3	2	-	0/2/19/22	0/1/1/1					
2	BGC	18-B	4	2	-	2/2/19/22	0/1/1/1					
2	BGC	19-B	1	2	-	0/2/22/22	0/1/1/1					
2	BGC	19-B	2	2	-	2/2/19/22	0/1/1/1					
2	BGC	19-B	3	2	-	0/2/19/22	0/1/1/1					
2	BGC	19-B	4	2	-	0/2/19/22	0/1/1/1					
2	BGC	2-B	1	2	-	0/2/22/22	0/1/1/1					
2	BGC	2-B	2	2	-	0/2/19/22	0/1/1/1					
2	BGC	2-B	3	2	-	2/2/19/22	0/1/1/1					
2	BGC	2-B	4	2	-	0/2/19/22	0/1/1/1					
2	BGC	20-B	1	2	-	1/2/22/22	0/1/1/1					
2	BGC	20-B	2	2	-	2/2/19/22	0/1/1/1					
2	BGC	20-B	3	2	-	0/2/19/22	0/1/1/1					
2	BGC	20-B	4	2	-	0/2/19/22	0/1/1/1					
2	BGC	21-B	1	2	-	0/2/22/22	0/1/1/1					
2	BGC	21-B	2	2	-	2/2/19/22	0/1/1/1					
2	BGC	21-B	3	2	-	0/2/19/22	0/1/1/1					
2	BGC	21-B	4	2	-	0/2/19/22	0/1/1/1					
2	BGC	22-B	1	2	-	0/2/22/22	0/1/1/1					
2	BGC	22-B	2	2	-	0/2/19/22	0/1/1/1					
2	BGC	22-B	3	2	-	0/2/19/22	0/1/1/1					
	bnti lol 2 2 2 2 2 2 2 2	Bit in alea fro Iol Type 2 BGC 2 BG	Initiality of the previous Iol Type Chain 2 BGC 13-B 2 BGC 14-B 2 BGC 14-B 2 BGC 14-B 2 BGC 14-B 2 BGC 15-B 2 BGC 15-B 2 BGC 15-B 2 BGC 15-B 2 BGC 16-B 2 BGC 16-B 2 BGC 16-B 2 BGC 16-B 2 BGC 17-B 2 BGC 17-B 2 BGC 17-B 2 BGC 18-B 2 BGC 18-B 2 BGC 18-B 2 BGC 19-B 2 BGC 19-B 2 BGC 2-B 2 BGC 2-B 2	Initialized from previous page Iol Type Chain Res 2 BGC 13-B 4 2 BGC 14-B 1 2 BGC 14-B 2 2 BGC 14-B 3 2 BGC 15-B 1 2 BGC 15-B 3 2 BGC 15-B 3 2 BGC 15-B 3 2 BGC 16-B 1 2 BGC 16-B 3 2 BGC 17-B 1 2 BGC 17-B 1 2 BGC 17-B 3 2 BGC 18-B 1 2 BGC 18-B 1 2 BGC 18-B 1 2 BGC 19-B 3 2 BGC 19-B 3 2 BGC 2-B	Initialized from previous plage Iol Type Chain Res Link 2 BGC 13-B 4 2 2 BGC 14-B 1 2 2 BGC 14-B 3 2 2 BGC 14-B 3 2 2 BGC 14-B 4 2 2 BGC 15-B 1 2 2 BGC 15-B 3 2 2 BGC 16-B 1 2 2 BGC 16-B 3 2 2 BGC 16-B 4 2 2 BGC 17-B 1 2 2 BGC 17-B 3 2 2 BGC 18-B 1 2 2 BGC 18-B 3 2 2 BGC 19-B 2 2 2 BGC <td< td=""><td>Ion Type Chain Res Link Chirals 2 BGC 13-B 4 2 - 2 BGC 14-B 1 2 - 2 BGC 14-B 2 2 - 2 BGC 14-B 3 2 - 2 BGC 14-B 4 2 - 2 BGC 15-B 1 2 - 2 BGC 15-B 3 2 - 2 BGC 15-B 3 2 - 2 BGC 16-B 3 2 - 2 BGC 16-B 4 2 - 2 BGC 17-B 1 2 - 2 BGC 17-B 3 2 - - 2 BGC 18-B 3 2 - 2 BGC 18-B 3<td>Iol Type Chain Res Link Chirals Torsions 2 BGC 13-B 4 2 - 0/2/19/22 2 BGC 14-B 1 2 - 0/2/19/22 2 BGC 14-B 3 2 - 0/2/19/22 2 BGC 14-B 4 2 - 0/2/19/22 2 BGC 15-B 1 2 - 2/2/22/22 2 BGC 15-B 3 2 - 0/2/19/22 2 BGC 15-B 4 2 - 2/2/22/22 2 BGC 16-B 1 2 - 0/2/19/22 2 BGC 16-B 3 2 - 0/2/19/22 2 BGC 17-B 1 2 - 0/2/19/22 2 BGC 17-B 3 2 - 0/2/19/22 2 BGC <t< td=""></t<></td></td></td<>	Ion Type Chain Res Link Chirals 2 BGC 13-B 4 2 - 2 BGC 14-B 1 2 - 2 BGC 14-B 2 2 - 2 BGC 14-B 3 2 - 2 BGC 14-B 4 2 - 2 BGC 15-B 1 2 - 2 BGC 15-B 3 2 - 2 BGC 15-B 3 2 - 2 BGC 16-B 3 2 - 2 BGC 16-B 4 2 - 2 BGC 17-B 1 2 - 2 BGC 17-B 3 2 - - 2 BGC 18-B 3 2 - 2 BGC 18-B 3 <td>Iol Type Chain Res Link Chirals Torsions 2 BGC 13-B 4 2 - 0/2/19/22 2 BGC 14-B 1 2 - 0/2/19/22 2 BGC 14-B 3 2 - 0/2/19/22 2 BGC 14-B 4 2 - 0/2/19/22 2 BGC 15-B 1 2 - 2/2/22/22 2 BGC 15-B 3 2 - 0/2/19/22 2 BGC 15-B 4 2 - 2/2/22/22 2 BGC 16-B 1 2 - 0/2/19/22 2 BGC 16-B 3 2 - 0/2/19/22 2 BGC 17-B 1 2 - 0/2/19/22 2 BGC 17-B 3 2 - 0/2/19/22 2 BGC <t< td=""></t<></td>	Iol Type Chain Res Link Chirals Torsions 2 BGC 13-B 4 2 - 0/2/19/22 2 BGC 14-B 1 2 - 0/2/19/22 2 BGC 14-B 3 2 - 0/2/19/22 2 BGC 14-B 4 2 - 0/2/19/22 2 BGC 15-B 1 2 - 2/2/22/22 2 BGC 15-B 3 2 - 0/2/19/22 2 BGC 15-B 4 2 - 2/2/22/22 2 BGC 16-B 1 2 - 0/2/19/22 2 BGC 16-B 3 2 - 0/2/19/22 2 BGC 17-B 1 2 - 0/2/19/22 2 BGC 17-B 3 2 - 0/2/19/22 2 BGC <t< td=""></t<>					

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	22-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	23-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	23-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	23-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	23-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	24-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	24-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	24-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	24-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	25-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	25-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	25-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	25-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	3-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	3-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	3-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	3-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	4-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	4-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	4-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	4-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	5-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	5-B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	5-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	5-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	6-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	6-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	6-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	6-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	7-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	7-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	7-B	3	2	-	2/2/19/22	0/1/1/1
2	BGC	7-B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	8-B	1	2	-	2/2/22/22	0/1/1/1
2	BGC	8-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	8-B	3	2	-	0/2/19/22	0/1/1/1
2	BGC	8-B	4	2	-	2/2/19/22	0/1/1/1
2	BGC	9-B	1	2	-	0/2/22/22	0/1/1/1
2	BGC	9-B	2	2	-	0/2/19/22	0/1/1/1
2	BGC	9-B	3	2	-	0/2/19/22	0/1/1/1



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	9-B	4	2	-	0/2/19/22	0/1/1/1

The worst 5 of 508 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	10-B	3	BGC	C2-C3	-7.25	1.41	1.52
2	23-B	2	BGC	C2-C3	-7.09	1.42	1.52
2	22-B	3	BGC	C2-C3	-7.03	1.42	1.52
2	9-B	2	BGC	C2-C3	-6.97	1.42	1.52
2	2-B	2	BGC	C2-C3	-6.95	1.42	1.52

The worst 5 of 354 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
2	1-B	4	BGC	C1-O5-C5	8.51	123.72	112.19
2	1-B	1	BGC	C3-C4-C5	8.05	124.61	110.24
2	1-B	1	BGC	O4-C4-C5	-7.75	90.05	109.30
2	20-B	4	BGC	C1-C2-C3	7.68	119.11	109.67
2	19-B	4	BGC	C1-O5-C5	7.28	122.05	112.19

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	23-B	3	BGC	C4-C5-C6-O6
2	1-B	4	BGC	O5-C5-C6-O6
2	23-B	3	BGC	O5-C5-C6-O6
2	8-B	4	BGC	C4-C5-C6-O6
2	8-B	4	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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)

100 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).

Mal	Type	Chain	Dog	Link	Bo	ond leng	ths	B	ond ang	gles
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	EDO	14-A	702	-	3, 3, 3	0.43	0	2,2,2	0.29	0
4	EDO	25-A	703	-	3,3,3	0.43	0	2,2,2	0.31	0
4	EDO	9-A	704	-	3,3,3	0.62	0	2,2,2	0.35	0
4	EDO	15-A	704	-	3, 3, 3	0.55	0	$2,\!2,\!2$	0.17	0
3	BGC	5-A	701	-	11,11,12	0.79	0	$15,\!15,\!17$	1.77	3 (20%)
3	BGC	21-A	701	-	11,11,12	0.86	0	$15,\!15,\!17$	2.57	4 (26%)
4	EDO	4-A	702	-	3,3,3	0.41	0	2,2,2	0.16	0
4	EDO	6-A	704	-	3,3,3	0.68	0	2,2,2	0.19	0
4	EDO	16-A	704	-	3,3,3	0.61	0	2,2,2	0.17	0
4	EDO	23-A	703	-	$3,\!3,\!3$	0.48	0	2,2,2	0.24	0
4	EDO	18-A	704	-	3,3,3	0.63	0	2,2,2	0.19	0
4	EDO	1-A	703	-	$3,\!3,\!3$	0.38	0	2,2,2	0.24	0
4	EDO	13-A	704	-	3,3,3	0.60	0	2,2,2	0.34	0
4	EDO	25-A	702	-	3,3,3	0.46	0	2,2,2	0.19	0
4	EDO	24-A	703	-	3,3,3	0.52	0	2,2,2	0.11	0
4	EDO	15-A	703	-	$3,\!3,\!3$	0.51	0	2,2,2	0.10	0



	T a	Chain	Dag	T : 1-	Bo	ond leng	ths	B	ond ang	gles
IVIOI	Tybe	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
4	EDO	3-A	703	-	3, 3, 3	0.49	0	2,2,2	0.09	0
3	BGC	1-A	701	-	11,11,12	0.74	0	$15,\!15,\!17$	1.27	1 (6%)
4	EDO	5-A	702	-	3,3,3	0.51	0	2,2,2	0.23	0
4	EDO	21-A	702	-	3,3,3	0.44	0	2,2,2	0.68	0
4	EDO	5-A	704	-	3,3,3	0.63	0	2,2,2	0.15	0
4	EDO	21-A	703	-	3, 3, 3	0.55	0	2,2,2	0.11	0
3	BGC	8-A	701	-	$11,\!11,\!12$	1.07	1 (9%)	15,15,17	1.99	<mark>5 (33%)</mark>
3	BGC	14-A	701	-	$11,\!11,\!12$	0.89	0	$15,\!15,\!17$	3.01	7 (46%)
4	EDO	1-A	702	-	3,3,3	0.47	0	2,2,2	0.32	0
4	EDO	10-A	704	-	3, 3, 3	0.60	0	2,2,2	0.12	0
4	EDO	14-A	703	-	3,3,3	0.52	0	2,2,2	0.03	0
4	EDO	8-A	702	-	3,3,3	0.46	0	2,2,2	0.09	0
4	EDO	8-A	704	-	3,3,3	0.61	0	2,2,2	0.33	0
4	EDO	17-A	704	-	3,3,3	0.64	0	2,2,2	0.34	0
3	BGC	19-A	701	-	11, 11, 12	0.77	0	$15,\!15,\!17$	1.95	<mark>5 (33%)</mark>
4	EDO	12-A	703	-	3,3,3	0.56	0	2,2,2	0.02	0
3	BGC	24-A	701	-	$11,\!11,\!12$	1.20	1 (9%)	$15,\!15,\!17$	1.75	3 (20%)
4	EDO	19-A	703	-	3, 3, 3	0.36	0	2,2,2	0.40	0
4	EDO	4-A	704	-	3, 3, 3	0.65	0	2,2,2	0.19	0
4	EDO	9-A	702	-	3,3,3	0.62	0	2,2,2	0.16	0
3	BGC	12-A	701	-	11,11,12	0.87	0	$15,\!15,\!17$	2.31	<mark>6 (40%)</mark>
4	EDO	23-A	704	-	3,3,3	0.40	0	2,2,2	0.30	0
4	EDO	3-A	702	-	3, 3, 3	0.40	0	2,2,2	0.17	0
4	EDO	20-A	702	-	3,3,3	0.41	0	2,2,2	0.22	0
4	EDO	22-A	702	-	3,3,3	0.37	0	2,2,2	0.32	0
3	BGC	23-A	701	-	11,11,12	0.75	0	$15,\!15,\!17$	1.78	4 (26%)
4	EDO	8-A	703	-	3,3,3	0.50	0	2,2,2	0.35	0
4	EDO	12-A	702	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	12-A	704	-	3,3,3	0.57	0	2,2,2	0.47	0
4	EDO	19-A	702	-	3,3,3	0.41	0	2,2,2	0.28	0
4	EDO	6-A	703	-	3,3,3	0.54	0	2,2,2	0.05	0
3	BGC	10-A	701	-	11,11,12	1.23	1 (9%)	15,15,17	2.27	7 (46%)
4	EDO	24-A	704	-	3,3,3	0.63	0	2,2,2	0.18	0
4	EDO	2-A	704	-	3,3,3	0.65	0	2,2,2	0.16	0
4	EDO	10-A	703	-	3,3,3	0.49	0	2,2,2	0.08	0
4	EDO	18-A	703	-	3,3,3	0.48	0	2,2,2	0.18	0
4	EDO	10-A	702	-	3,3,3	0.41	0	2,2,2	0.17	0
3	BGC	15-A	701	-	11,11,12	1.06	1 (9%)	15,15,17	2.72	4 (26%)
4	EDO	21-A	704	-	3,3,3	0.57	0	2,2,2	0.18	0
4	EDO	20-A	703	-	3,3,3	0.41	0	2,2,2	0.21	0
4	EDO	11-A	704	-	3,3,3	0.53	0	2,2,2	0.49	0



	T a	Chain	Dag	T : 1-	Bo	ond leng	ths	B	ond ang	gles
IVI01	Type	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	BGC	4-A	701	-	11,11,12	0.68	0	15,15,17	0.92	0
4	EDO	18-A	702	-	3,3,3	0.47	0	2,2,2	0.28	0
3	BGC	6-A	701	-	$11,\!11,\!12$	0.79	0	$15,\!15,\!17$	1.39	3 (20%)
3	BGC	16-A	701	-	$11,\!11,\!12$	0.93	0	$15,\!15,\!17$	2.90	7 (46%)
3	BGC	18-A	701	-	$11,\!11,\!12$	0.70	0	$15,\!15,\!17$	1.51	4 (26%)
4	EDO	5-A	703	-	3,3,3	0.48	0	2,2,2	0.13	0
3	BGC	25-A	701	-	11,11,12	0.59	0	15,15,17	2.12	4 (26%)
3	BGC	2-A	701	-	11,11,12	0.91	1 (9%)	15,15,17	<mark>3.37</mark>	8 (53%)
3	BGC	13-A	701	-	11,11,12	0.77	0	15,15,17	1.80	4 (26%)
4	EDO	2-A	703	-	3,3,3	0.50	0	2,2,2	0.08	0
4	EDO	2-A	702	-	3,3,3	0.39	0	2,2,2	0.38	0
4	EDO	15-A	702	-	3,3,3	0.42	0	2,2,2	0.42	0
4	EDO	11-A	703	-	3,3,3	0.56	0	2,2,2	0.09	0
4	EDO	16-A	702	-	3,3,3	0.40	0	2,2,2	0.42	0
3	BGC	22-A	701	-	11,11,12	1.07	0	15,15,17	3.70	10 (66%)
4	EDO	11-A	702	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	13-A	702	-	3,3,3	0.41	0	2,2,2	0.54	0
4	EDO	1-A	704	-	3,3,3	0.41	0	2,2,2	0.17	0
4	EDO	14-A	704	-	3,3,3	0.54	0	2,2,2	0.51	0
4	EDO	25-A	704	-	3,3,3	0.31	0	2,2,2	0.30	0
4	EDO	24-A	702	-	3,3,3	0.43	0	2,2,2	0.16	0
4	EDO	22-A	704	-	3,3,3	0.62	0	2,2,2	0.25	0
3	BGC	3-A	701	-	11,11,12	1.20	1 (9%)	15,15,17	3.01	6 (40%)
4	EDO	19-A	704	-	3,3,3	0.64	0	2,2,2	0.28	0
3	BGC	20-A	701	-	11,11,12	0.79	0	15,15,17	2.35	6 (40%)
3	BGC	7-A	701	-	11,11,12	0.84	0	15,15,17	1.84	3 (20%)
3	BGC	17-A	701	-	11,11,12	0.80	0	15,15,17	2.30	4 (26%)
4	EDO	13-A	703	-	3,3,3	0.61	0	2,2,2	0.03	0
4	EDO	22-A	703	-	3,3,3	0.52	0	2,2,2	0.19	0
4	EDO	7-A	702	-	3,3,3	0.62	0	2,2,2	0.26	0
4	EDO	17-A	702	-	3,3,3	0.49	0	2,2,2	0.37	0
4	EDO	7-A	704	-	3,3,3	0.53	0	2,2,2	0.13	0
3	BGC	9-A	701	-	11,11,12	0.69	0	15,15,17	1.82	3 (20%)
4	EDO	4-A	703	-	3,3,3	0.51	0	2,2,2	0.11	0
4	EDO	9-A	703	-	3,3,3	0.54	0	2,2,2	0.27	0
4	EDO	3-A	704	-	$3,\!3,\!3$	0.60	0	2,2,2	0.23	0
4	EDO	20-A	704	-	3,3,3	0.34	0	2,2,2	0.53	0
4	EDO	16-A	703	-	3,3,3	0.52	0	2,2,2	0.10	0
3	BGC	11-A	701	-	11,11,12	1.10	1 (9%)	15,15,17	2.33	6 (40%)
4	EDO	23-A	702	_	3,3,3	0.50	0	2,2,2	0.21	0



Mol T	Turne	Chain	in Res	LinkBond lengths		$_{\rm ths}$	Bond angles			
IVIOI	туре	Unain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
4	EDO	7-A	703	-	3,3,3	0.37	0	2,2,2	0.26	0
4	EDO	17-A	703	-	3,3,3	0.66	0	2,2,2	0.03	0
4	EDO	6-A	702	-	3,3,3	0.44	0	2,2,2	0.36	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
4	EDO	14-A	702	-	-	0/1/1/1	-
4	EDO	25-A	703	-	-	0/1/1/1	-
4	EDO	9-A	704	-	-	0/1/1/1	-
4	EDO	15-A	704	-	-	0/1/1/1	-
3	BGC	5-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	21-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	4-A	702	-	-	0/1/1/1	-
4	EDO	6-A	704	-	-	0/1/1/1	-
4	EDO	16-A	704	-	-	0/1/1/1	-
4	EDO	23-A	703	-	-	0/1/1/1	-
4	EDO	18-A	704	-	-	0/1/1/1	-
4	EDO	1-A	703	-	-	0/1/1/1	-
4	EDO	13-A	704	-	-	1/1/1/1	-
4	EDO	25-A	702	-	-	1/1/1/1	-
4	EDO	24-A	703	-	-	0/1/1/1	-
4	EDO	15-A	703	-	-	0/1/1/1	-
4	EDO	3-A	703	-	-	0/1/1/1	-
3	BGC	1-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	5-A	702	-	-	1/1/1/1	-
4	EDO	21-A	702	-	-	0/1/1/1	-
4	EDO	5-A	704	-	-	0/1/1/1	-
4	EDO	21-A	703	-	-	0/1/1/1	-
3	BGC	8-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	14-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	1-A	702	-	-	0/1/1/1	-
4	EDO	10-A	704	-	-	1/1/1/1	-
4	EDO	14-A	703	-	-	0/1/1/1	-
4	EDO	8-A	702	-	-	1/1/1/1	-
4	EDO	8-A	704	-	-	0/1/1/1	-
4	EDO	17-A	704	-	-	0/1/1/1	-
3	BGC	19-A	701	-	-	$1/2/\overline{19/22}$	0/1/1/1
4	EDO	12-A	703	-	-	0/1/1/1	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	24-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	19-A	703	-	-	0/1/1/1	-
4	EDO	4-A	704	-	-	0/1/1/1	-
4	EDO	9-A	702	-	-	1/1/1/1	-
3	BGC	12-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	23-A	704	-	-	1/1/1/1	-
4	EDO	3-A	702	-	-	0/1/1/1	-
4	EDO	20-A	702	-	-	0/1/1/1	-
4	EDO	22-A	702	-	-	0/1/1/1	-
3	BGC	23-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	8-A	703	-	-	0/1/1/1	-
4	EDO	12-A	702	-	-	0/1/1/1	-
4	EDO	12-A	704	-	-	0/1/1/1	-
4	EDO	19-A	702	-	-	0/1/1/1	-
4	EDO	6-A	703	-	-	0/1/1/1	-
3	BGC	10-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	24-A	704	-	-	0/1/1/1	-
4	EDO	2-A	704	-	-	0/1/1/1	-
4	EDO	10-A	703	-	-	0/1/1/1	-
4	EDO	18-A	703	-	-	0/1/1/1	-
4	EDO	10-A	702	-	-	0/1/1/1	-
3	BGC	15-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	21-A	704	-	-	0/1/1/1	-
4	EDO	20-A	703	-	-	0/1/1/1	-
4	EDO	11-A	704	-	-	1/1/1/1	-
3	BGC	4-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	18-A	702	-	-	0/1/1/1	-
3	BGC	6-A	701	-	-	1/2/19/22	0/1/1/1
3	BGC	16-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	18-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	5-A	703	-	-	0/1/1/1	-
3	BGC	25-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	2-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	13-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	2-A	703	-	-	1/1/1/1	-
4	EDO	2-A	702	-	-	0/1/1/1	-
4	EDO	15-A	702	-	-	0/1/1/1	-
4	EDO	11-A	703	-	-	0/1/1/1	-
4	EDO	16-A	702	-	-	$\frac{0/1/1/1}{1/2}$	-
	BGC	22-A	701	-	-	$\frac{1/2}{19/22}$	0/1/1/1
4	EDO	11-A	702	-	-	$\frac{0/1/1/1}{0/1/1/1}$	-
4	EDO	13-A	702	-	-	0/1/1/1	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	1-A	704	-	-	0/1/1/1	-
4	EDO	14-A	704	-	-	0/1/1/1	-
4	EDO	25-A	704	-	-	0/1/1/1	-
4	EDO	24-A	702	-	-	1/1/1/1	-
4	EDO	22-A	704	-	-	0/1/1/1	-
3	BGC	3-A	701	-	-	1/2/19/22	0/1/1/1
4	EDO	19-A	704	-	-	0/1/1/1	-
3	BGC	20-A	701	-	-	1/2/19/22	0/1/1/1
3	BGC	7-A	701	-	-	0/2/19/22	0/1/1/1
3	BGC	17-A	701	-	-	0/2/19/22	0/1/1/1
4	EDO	13-A	703	-	-	0/1/1/1	-
4	EDO	22-A	703	-	-	1/1/1/1	-
4	EDO	7-A	702	-	-	1/1/1/1	-
4	EDO	17-A	702	-	-	0/1/1/1	-
4	EDO	7-A	704	-	-	0/1/1/1	-
3	BGC	9-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	4-A	703	-	-	0/1/1/1	-
4	EDO	9-A	703	-	-	0/1/1/1	-
4	EDO	3-A	704	-	-	0/1/1/1	-
4	EDO	20-A	704	-	-	1/1/1/1	-
4	EDO	16-A	703	-	-	0/1/1/1	-
3	BGC	11-A	701	-	-	2/2/19/22	0/1/1/1
4	EDO	23-A	702	-	-	1/1/1/1	-
4	EDO	7-A	703	-	-	0/1/1/1	-
4	EDO	17-A	703	-	-	1/1/1/1	-
4	EDO	6-A	702	-	-	0/1/1/1	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-A	701	BGC	O5-C1	-3.65	1.37	1.43
3	3-A	701	BGC	O5-C1	-2.77	1.39	1.43
3	24-A	701	BGC	O2-C2	-2.27	1.38	1.43
3	15-A	701	BGC	C2-C3	2.27	1.55	1.52
3	11-A	701	BGC	O5-C1	-2.22	1.40	1.43

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	22-A	701	BGC	C1-O5-C5	9.00	124.39	112.19
3	14-A	701	BGC	C1-O5-C5	8.06	123.11	112.19
3	2-A	701	BGC	C1-C2-C3	8.01	119.52	109.67



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	3-A	701	BGC	O5-C5-C6	6.60	117.55	107.20
3	22-A	701	BGC	C1-C2-C3	6.58	117.76	109.67

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	21-A	701	BGC	O5-C5-C6-O6
3	15-A	701	BGC	O5-C5-C6-O6
3	23-A	701	BGC	O5-C5-C6-O6
3	9-A	701	BGC	O5-C5-C6-O6
3	9-A	701	BGC	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 (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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2		$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$	
1	1-A	549/549~(100%)	0.06	34~(6%)	20	23	17, 18, 20, 22	549 (100%)
1	2-A	549/549~(100%)	0.06	34~(6%)	20	23	17, 18, 20, 22	549~(100%)
1	3-A	549/549~(100%)	0.06	34~(6%)	20	23	17, 18, 20, 22	549 (100%)
1	4-A	549/549~(100%)	0.06	34~(6%)	20	23	17, 18, 20, 22	549 (100%)
1	5-A	549/549~(100%)	0.06	34~(6%)	20	23	17, 18, 20, 22	549 (100%)
1	6-A	549/549~(100%)	0.06	34~(6%)	20	23	17, 18, 20, 22	549 (100%)
1	7-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	8-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	9-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	10-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	11-A	549/549~(100%)	0.06	34~(6%)	20	23	17, 18, 20, 22	549 (100%)
1	12-A	549/549~(100%)	0.06	34~(6%)	20	23	17, 18, 20, 22	549 (100%)
1	13-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	14-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	15-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	16-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	17-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	18-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	19-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	20-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	21-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	22-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	23-A	549/549~(100%)	0.06	34 (6%)	20	23	17, 18, 20, 22	549 (100%)
1	24-A	$54\overline{9/549}~(100\%)$	0.06	34~(6%)	20	23	17, 18, 20, 22	549~(100%)



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Mol	Chain	Analysed	< RSRZ >	$\#RSRZ{>}2$		$OWAB(Å^2)$	$Q{<}0.9$			
1	25-A	549/549~(100%)	0.06	34 (6%) 2	20 23	17, 18, 20, 22	549 (100%)			
All	All	13725/13725~(100%)	0.06	850 (6%)	23 23	17, 18, 20, 22	13725 (100%)			

The worst 5 of 850 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	293	GLY	8.6
1	2-A	293	GLY	8.6
1	3-A	293	GLY	8.6
1	4-A	293	GLY	8.6
1	5-A	293	GLY	8.6

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^{th} 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	$B-factors(Å^2)$	Q<0.9
2	BGC	1-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	2-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	3-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	4-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	5-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	6-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	7-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	8-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	9-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	10-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	11 - B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	12-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	13-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	14 - B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	15-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	16-B	1	12/12	0.96	0.15	18,21,31,34	12



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Mol 2	Type	Chain	Res	Atoms	BSCC	BSR	R_tactors(A ²)	
2	Daa		-	120112	10000		D-lactors(A)	Q<0.9
4	BGC	17-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	18-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	19-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	20-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	21-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	22-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	23-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	24-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	25-B	1	12/12	0.96	0.15	18,21,31,34	12
2	BGC	1-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	2-B	2	11/12	0.96	0.06	$16,\!20,\!21,\!23$	11
2	BGC	3-B	2	11/12	0.96	0.06	$16,\!20,\!21,\!23$	11
2	BGC	4-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	5-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	6-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	7-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	8-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	9-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	10-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	11-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	12-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	13-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	14-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	15-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	16-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	17-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	18-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	19-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	20-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	21-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	22-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	23-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	24-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	25-B	2	11/12	0.96	0.06	16,20,21,23	11
2	BGC	1-B	3	11/12	0.97	0.07	15,17,22,23	11
2	BGC	2-B	3	11/12	0.97	0.07	15.17.22.23	11
2	BGC	3-B	3	11/12	0.97	0.07	15,17,22.23	11
2	BGC	4-B	3	11/12	0.97	0.07	15.17.22.23	11
2	BGC	5-B	3	11/12	0.97	0.07	15.17.22.23	11
2	BGC	6-B	3	11/12	0.97	0.07	15.17.22.23	11
2	BGC	7-R	3	11/12	0.97	0.07	15,17,22,23	11
2	BGC	8-B	3	11/12	0.97	0.07	15.17.22.23	11
$ \begin{array}{c} 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ 2 \\$	BGC	24-B 25-B 1-B 2-B 3-B 4-B 5-B 6-B 7-B 8-B 9-B 10-B 11-B 12-B 13-B 14-B 13-B 14-B 13-B 14-B 15-B 16-B 17-B 18-B 19-B 20-B 21-B 20-B 21-B 22-B 23-B 23-B 24-B 22-B 23-B 23-B 23-B 24-B 25-B 3-B 24-B 25-B 3-B 24-B 25-B 3-B 24-B 25-B 3-B 24-B 25-B 3-B 24-B 25-B 25-B 24-B 25-B 23-B 24-B 25-B 23-B 24-B 25-B 24-B 25-B 23-B 24-B 25-B 24-B 24-B 25-B 24-B 24-B 25-B 24-B 25-B 24-B 24-B 25-B 24-B 25-B 24-B 24-B 25-B 25-B 25-B 24-B 25-B 25-B 25-B 25-B 25-B 25-B 25-B 25	$ \begin{array}{r} 1 \\ 2 \\ 3 \\ $	$\begin{array}{c} 12/12 \\ 12/12 \\ 11/12 \\$	$\begin{array}{c} 0.96\\$	0.15 0.06 0.07 0.07 0.07 0.07 0.07 0.07 0.07 0.07 0.07 0.07 0.07	$\begin{array}{c} 10,21,31,34\\ 18,21,31,34\\ 16,20,21,23\\ 15,17,22,23$	12 12 12 11 11 11 11 11 11 11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q < 0.9	
2	BGC	9-B	3	11/12	0.97	0.07	$15,\!17,\!22,\!23$	11	
2	BGC	10-B	3	11/12	0.97	0.07	$15,\!17,\!22,\!23$	11	
2	BGC	11-B	3	11/12	0.97	0.07	$15,\!17,\!22,\!23$	11	
2	BGC	12-B	3	11/12	0.97	0.07	$15,\!17,\!22,\!23$	11	
2	BGC	13-B	3	11/12	0.97	0.07	$15,\!17,\!22,\!23$	11	
2	BGC	14-B	3	11/12	0.97	0.07	$15,\!17,\!22,\!23$	11	
2	BGC	15-B	3	11/12	0.97	0.07	$15,\!17,\!22,\!23$	11	
2	BGC	16-B	3	11/12	0.97	0.07	$15,\!17,\!22,\!23$	11	
2	BGC	17-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	18-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	19-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	20-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	21-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	22-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	23-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	24-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	25-B	3	11/12	0.97	0.07	15,17,22,23	11	
2	BGC	1-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	2-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	3-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	4-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	5-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	6-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	7-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	8-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	9-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	10-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	11-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	12-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	13-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	14-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	15-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	16-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	17-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	18-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	19-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	20-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	21-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	22-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	23-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	24-B	4	11/12	0.97	0.10	14,17,18,18	11	
2	BGC	25-B	4	11/12	0.97	0.10	14,17,18,18	11	

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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.

















































6.4 Ligands (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^{th} 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	$B-factors(A^2)$	Q<0.9
3	BGC	1-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	2-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	3-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	4-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	5-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	6-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	7-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	8-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	9-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	10-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	11-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	12-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	13-A	701	11/12	0.89	0.29	21,26,31,34	11
3	BGC	14-A	701	11/12	0.89	0.29	21,26,31,34	11



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors (A^2)	$Q{<}0.9$	
3	BGC	15-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	16-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	17-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	18-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	19-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	20-A	701	11/12	0.89	0.29	$21,\!26,\!31,\!34$	11	
3	BGC	21-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	22-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	23-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	24-A	701	11/12	0.89	0.29	21,26,31,34	11	
3	BGC	25-A	701	11/12	0.89	0.29	21,26,31,34	11	
4	EDO	1-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	2-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	3-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	4-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	5-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	6-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	7-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	8-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	9-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	10-A	704	$\frac{4}{4}$	0.92	0.30	30,32,35,35	10	
4	EDO	11-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	12-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	13-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	14-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	15-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	16-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	17-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	18-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	19-A	704	4/4	0.92	0.30	30,32,35,35	10	
4	EDO	20-A	704	4/4	0.92	0.30	30.32.35.35	10	
4	EDO	21-A	704	4/4	0.92	0.30	30.32.35.35	10	
4	EDO	22-A	704	4/4	0.92	0.30	30.32.35.35	10	
4	EDO	23-A	704	4/4	0.92	0.30	30.32.35.35	10	
4	EDO	24-A	704	4/4	0.92	0.30	30.32.35.35	10	
4	EDO	25-A	704	4/4	0.92	0.30	30 32 35 35	10	
4	EDO	1-A	703	4/4	0.97	0.07	17.17.22.22	10	
4	EDO	2-A	703	4/4	0.97	0.07	17.17.22.22	10	
4	EDO	3-A	703	4/4	0.97	0.07	17.17.22.22	10	
4	EDO	4-A	703	4/4	0.97	0.07	17.17.22.22	10	
	EDO	5-A	703	4/4	0.97	0.07	17 17 22 22	10	
<u> </u>	EDO	6-A	703	4/4	0.97	0.07	17 17 22 22	10	
4	EDO EDO	5-A 6-A	703 703	$\frac{4/4}{4/4}$	0.97 0.97	$\begin{array}{c} 0.07 \\ 0.07 \end{array}$	$\frac{17,17,22,22}{17,17,22,22}$	10 10	

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors (A^2)	$Q{<}0.9$	
4	EDO	7-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	8-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	9-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	10-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	11-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	12-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	13-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	14-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	15-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	16-A	703	4/4	0.97	0.07	$17,\!17,\!22,\!22$	10	
4	EDO	17-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	18-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	19-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	20-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	21-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	22-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	23-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	24-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	25-A	703	4/4	0.97	0.07	17,17,22,22	10	
4	EDO	1-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	2-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	3-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	4-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	5-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	6-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	7-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	8-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	9-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	10-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	11-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	12-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	13-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	14-A	702	$\frac{1}{4/4}$	0.98	0.11	15,17,21,21	10	
4	EDO	15-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	16-A	702	4/4	0.98	0.11	15,17,21,21	10	
4	EDO	17-A	702	4/4	0.98	0.11	15,17.21.21	10	
4	EDO	18-A	702	4/4	0.98	0.11	15,17.21.21	10	
4	EDO	19-A	702	4/4	0.98	0.11	15.17.21.21	10	
4	EDO	20-A	702	4/4	0.98	0.11	15.17.21.21	10	
4	EDO	21-A	702	4/4	0.98	0.11	15.17.21.21	10	
4	EDO	22-A	702	4/4	0.98	0.11	15.17.21.21	10	
4	EDO	23-A	702	4/4	0.98	0.11	15.17.21.21	10	
$ \begin{array}{r} 4 \\ 4 $	EDO EDO EDO EDO EDO EDO EDO EDO EDO EDO	2-A 3-A 4-A 5-A 6-A 7-A 8-A 9-A 10-A 11-A 12-A 13-A 14-A 15-A 16-A 17-A 18-A 19-A 20-A 21-A 22-A 23-A	702 7	$\begin{array}{r} 4/4 \\$	0.98 0.98	$\begin{array}{c} 0.11\\$	$\begin{array}{r} 15,17,21,21\\ 15,17,21\\ 15,$	$\begin{array}{c} 10\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10\\ 10\\$	

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q<0.9
4	EDO	24-A	702	4/4	0.98	0.11	$15,\!17,\!21,\!21$	10
4	EDO	25-A	702	4/4	0.98	0.11	15,17,21,21	10

6.5 Other polymers (i)

There are no such residues in this entry.

