



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 10:56 am GMT

PDB ID : 3ZMR  
Title : Bacteroides ovatus GH5 xyloglucanase in complex with a XXXG heptasaccharide  
Authors : Larsbrink, J.; Rogers, T.E.; Hemsworth, G.R.; McKee, L.S.; Spadiut, O.; Klintner, S.; Pudlo, N.A.; Urs, K.; Kelly, A.G.; Cederholm, S.N.; Davies, G.J.; Martens, E.C.; Brumer, H.  
Deposited on : 2013-02-12  
Resolution : 1.43 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

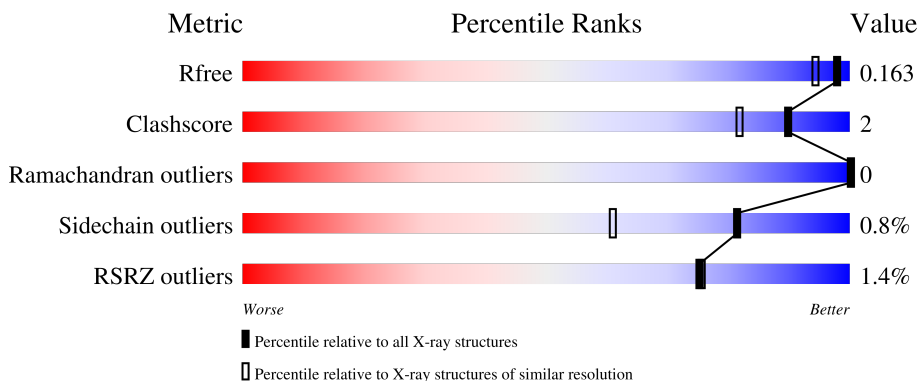
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

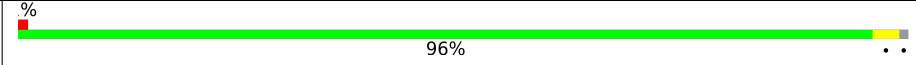
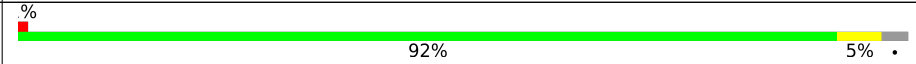
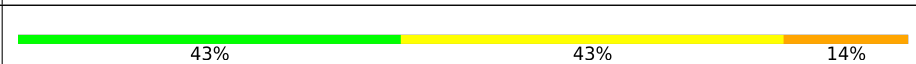
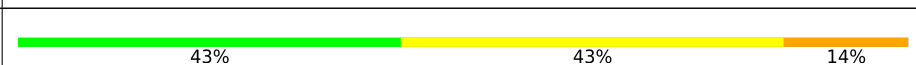
The reported resolution of this entry is 1.43 Å.

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))
$R_{free}$	130704	2021 (1.46-1.42)
Clashscore	141614	2086 (1.46-1.42)
Ramachandran outliers	138981	2047 (1.46-1.42)
Sidechain outliers	138945	2047 (1.46-1.42)
RSRZ outliers	127900	1993 (1.46-1.42)

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	A	475	 96%
1	B	475	 92% 5%
2	C	7	 43% 43% 14%
3	D	7	 43% 43% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLO	D	1	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8939 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.

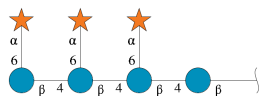
- Molecule 1 is a protein called CELLULASE (GLYCOSYL HYDROLASE FAMILY 5).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	469	3697	2325	638	720	14	0	7	0
1	B	462	3677	2324	622	716	15	0	14	0

There are 18 discrepancies between the modelled and reference sequences:

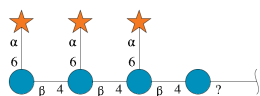
Chain	Residue	Modelled	Actual	Comment	Reference
A	36	MET	-	expression tag	UNP A7LXT7
A	503	LEU	-	expression tag	UNP A7LXT7
A	504	GLU	-	expression tag	UNP A7LXT7
A	505	HIS	-	expression tag	UNP A7LXT7
A	506	HIS	-	expression tag	UNP A7LXT7
A	507	HIS	-	expression tag	UNP A7LXT7
A	508	HIS	-	expression tag	UNP A7LXT7
A	509	HIS	-	expression tag	UNP A7LXT7
A	510	HIS	-	expression tag	UNP A7LXT7
B	36	MET	-	expression tag	UNP A7LXT7
B	503	LEU	-	expression tag	UNP A7LXT7
B	504	GLU	-	expression tag	UNP A7LXT7
B	505	HIS	-	expression tag	UNP A7LXT7
B	506	HIS	-	expression tag	UNP A7LXT7
B	507	HIS	-	expression tag	UNP A7LXT7
B	508	HIS	-	expression tag	UNP A7LXT7
B	509	HIS	-	expression tag	UNP A7LXT7
B	510	HIS	-	expression tag	UNP A7LXT7

- Molecule 2 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose.



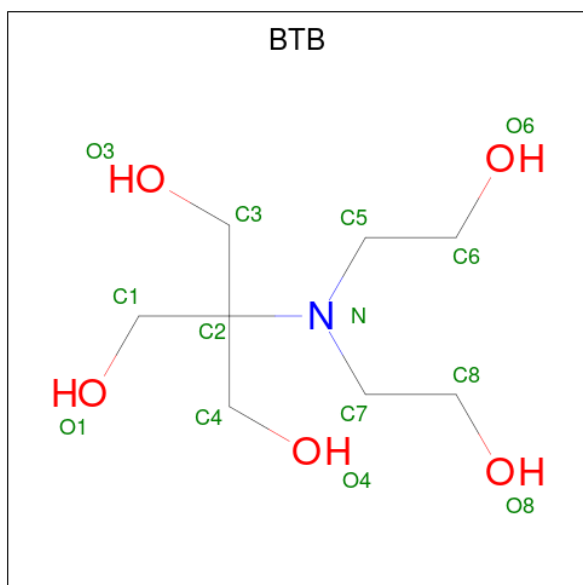
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	7	Total	C	O	0	1	0
			71	39	32			

- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-D-glucose.



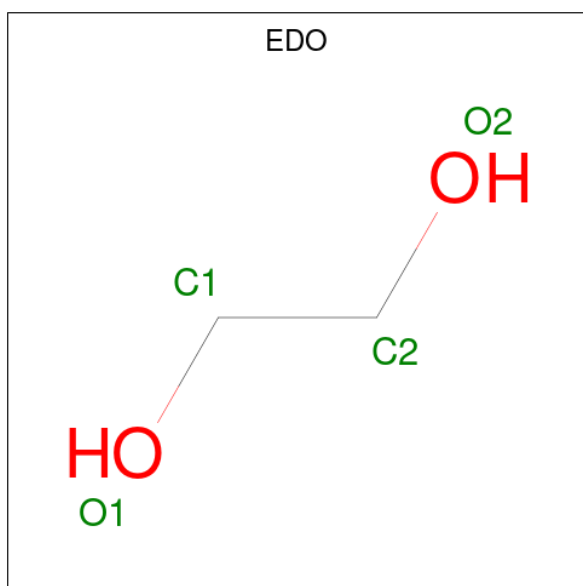
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	7	Total	C	O	0	0	0
			72	39	33			

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



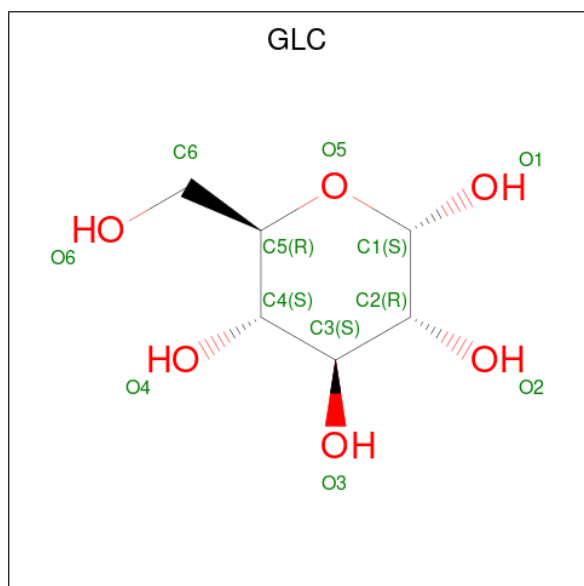
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			11	6	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	724	Total	O	0	0
			724	724		
7	B	617	Total	O	0	0
			617	617		

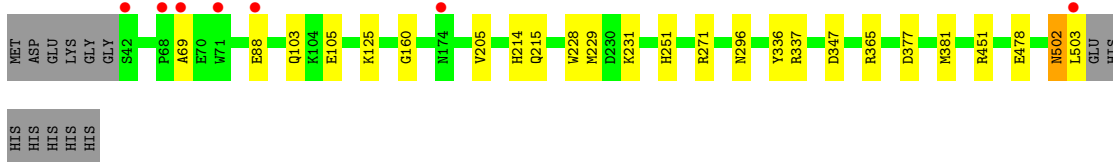
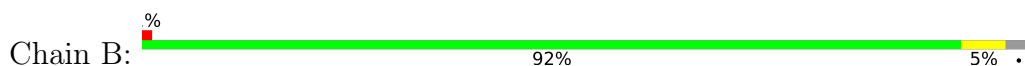
### 3 Residue-property plots [i](#)

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: CELLULASE (GLYCOSYL HYDROLASE FAMILY 5)



- Molecule 1: CELLULASE (GLYCOSYL HYDROLASE FAMILY 5)



- Molecule 2: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-[alpha-D-xylopyranose-(1-6)]beta-D-glucopyranose-(1-4)-D-glucose





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.83Å 147.24Å 84.14Å 90.00° 92.84° 90.00°	Depositor
Resolution (Å)	72.99 – 1.43 72.99 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.5 (72.99-1.43) 99.5 (72.99-1.43)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 1.43Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.122 , 0.157 0.130 , 0.163	Depositor DCC
$R_{free}$ test set	10458 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.3	Xtrriage
Anisotropy	0.256	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	8939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: BTB, XYS, BGC, GLC, EDO, GLO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.56	0/3801	0.74	2/5173 (0.0%)
1	B	0.56	0/3800	0.74	3/5174 (0.1%)
All	All	0.56	0/7601	0.74	5/10347 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	451	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	337	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	292	PHE	CB-CG-CD1	5.19	124.44	120.80
1	A	333	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	503	LEU	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	502	ASN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3697	0	3534	6	0
1	B	3677	0	3550	18	0
2	C	71	0	53	1	0
3	D	72	0	60	3	0
4	A	14	0	19	2	0
5	A	28	0	42	0	0
5	B	28	0	42	8	0
6	A	11	0	3	0	0
7	A	724	0	0	1	0
7	B	617	0	0	3	0
All	All	8939	0	7303	27	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.

All (27) 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:B:347[B]:ASP:OD1	5:B:1505:EDO:H12	1.51	1.09
1:B:347[B]:ASP:OD1	5:B:1505:EDO:C1	2.13	0.96
1:B:271:ARG:NH1	5:B:1510:EDO:O1	2.12	0.82
4:A:1511:BTB:H31	4:A:1511:BTB:O8	1.81	0.80
1:B:365[B]:ARG:NH1	7:B:2431:HOH:O	2.20	0.73
1:B:69:ALA:O	1:B:88:GLU:HG2	1.89	0.72
1:A:289:ARG:NH1	7:A:2416:HOH:O	2.25	0.69
1:A:297:GLU:OE2	2:C:1[B]:BGC:C1	2.41	0.68
1:B:336:TYR:CD1	5:B:1507:EDO:H21	2.30	0.66
1:B:229[A]:MET:HE3	1:B:229[A]:MET:HA	1.81	0.62
1:B:105:GLU:OE1	5:B:1509:EDO:H21	2.01	0.59
1:B:251:HIS:CE1	3:D:1:GLO:H1	2.38	0.59
1:A:159:ALA:HB2	1:A:501:LEU:HD21	1.87	0.55
1:B:502:ASN:OD1	1:B:502:ASN:O	2.28	0.52
1:B:231:LYS:HE2	7:B:2235:HOH:O	2.10	0.50
1:B:160:GLY:HA3	1:B:205[B]:VAL:HG13	1.96	0.47
1:A:357[B]:MET:SD	1:A:358:PRO:HD2	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347[B]:ASP:OD1	5:B:1505:EDO:O1	2.34	0.45
5:B:1509:EDO:H22	7:B:2121:HOH:O	2.18	0.44
1:B:377:ASP:HA	1:B:381[B]:MET:HB2	2.00	0.44
4:A:1511:BTB:O8	4:A:1511:BTB:C3	2.61	0.43
1:B:215:GLN:HG3	1:B:228:TRP:CD2	2.54	0.43
1:A:163:VAL:HG23	1:A:206:VAL:CG2	2.49	0.42
1:B:251:HIS:NE2	3:D:1:GLO:H1	2.35	0.41
1:B:296:ASN:HD21	3:D:1:GLO:C1	2.34	0.41
1:B:125:LYS:HD3	5:B:1509:EDO:H11	2.04	0.40

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	A	474/475 (100%)	457 (96%)	17 (4%)	0	100	100
1	B	474/475 (100%)	460 (97%)	14 (3%)	0	100	100
All	All	948/950 (100%)	917 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	391/394 (99%)	388 (99%)	3 (1%)	81	61
1	B	393/394 (100%)	390 (99%)	3 (1%)	81	61
All	All	784/788 (100%)	778 (99%)	6 (1%)	81	61

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	214	HIS
1	A	478	GLU
1	B	103	GLN
1	B	214	HIS
1	B	478	GLU

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

### 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](#)

14 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	BGC	C	1[B]	2	11,11,12	0.68	0	15,15,17	2.10	4 (26%)
2	BGC	C	2	6,2	11,11,12	0.66	0	15,15,17	1.16	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BGC	C	3	2	11,11,12	0.56	0	15,15,17	0.87	0
2	BGC	C	4	2	11,11,12	0.46	0	15,15,17	1.05	0
2	XYS	C	5	2	9,9,10	0.65	0	10,12,14	0.71	0
2	XYS	C	6	2	9,9,10	0.48	0	10,12,14	1.49	1 (10%)
2	XYS	C	7	2	9,9,10	0.85	0	10,12,14	1.81	3 (30%)
3	GLO	D	1	3	10,11,11	1.47	1 (10%)	13,14,14	4.10	8 (61%)
3	BGC	D	2	3	11,11,12	1.48	2 (18%)	15,15,17	1.75	4 (26%)
3	BGC	D	3	3	11,11,12	0.51	0	15,15,17	1.05	0
3	BGC	D	4	3	11,11,12	0.64	0	15,15,17	0.75	0
3	XYS	D	5	3	9,9,10	0.85	0	10,12,14	0.75	0
3	XYS	D	6	3	9,9,10	0.67	0	10,12,14	1.07	1 (10%)
3	XYS	D	7	3	9,9,10	0.92	0	10,12,14	1.33	2 (20%)

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	C	1[B]	2	-	0/2/19/22	0/1/1/1
2	BGC	C	2	6,2	-	1/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4	2	-	0/2/19/22	0/1/1/1
2	XYS	C	5	2	-	-	0/1/1/1
2	XYS	C	6	2	-	-	0/1/1/1
2	XYS	C	7	2	-	-	0/1/1/1
3	GLO	D	1	3	-	13/14/16/16	-
3	BGC	D	2	3	-	2/2/19/22	0/1/1/1
3	BGC	D	3	3	-	0/2/19/22	0/1/1/1
3	BGC	D	4	3	-	0/2/19/22	0/1/1/1
3	XYS	D	5	3	-	-	0/1/1/1
3	XYS	D	6	3	-	-	0/1/1/1
3	XYS	D	7	3	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	BGC	C1-C2	2.97	1.59	1.52
3	D	2	BGC	C2-C3	2.95	1.56	1.52
3	D	1	GLO	O4-C4	2.75	1.49	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	GLO	C5-C4-C3	-9.96	96.88	112.47
3	D	1	GLO	O4-C4-C5	6.44	124.38	108.81
2	C	1[B]	BGC	C1-C2-C3	5.82	116.82	109.67
3	D	1	GLO	O4-C4-C3	-5.03	97.77	109.47
3	D	1	GLO	O3-C3-C2	4.05	116.59	109.17
2	C	6	XYS	C5-O5-C1	3.55	116.98	111.52
3	D	2	BGC	O2-C2-C1	3.18	115.66	109.15
2	C	1[B]	BGC	C1-O5-C5	3.13	116.43	112.19
2	C	1[B]	BGC	C3-C4-C5	-3.12	104.67	110.24
3	D	1	GLO	O5-C5-C6	-3.04	102.02	109.14
3	D	1	GLO	C4-C3-C2	-2.94	108.41	113.54
2	C	7	XYS	O2-C2-C1	2.89	115.06	109.15
3	D	2	BGC	O5-C1-C2	-2.83	106.40	110.77
2	C	7	XYS	C5-O5-C1	2.79	115.82	111.52
3	D	7	XYS	C5-C4-C3	2.76	113.06	109.67
2	C	7	XYS	C5-C4-C3	2.68	112.96	109.67
3	D	1	GLO	C3-C2-C1	-2.57	103.03	111.10
3	D	2	BGC	O6-C6-C5	-2.49	102.75	111.29
3	D	2	BGC	O3-C3-C2	2.44	114.68	109.99
3	D	7	XYS	C5-O5-C1	2.42	115.24	111.52
2	C	1[B]	BGC	O4-C4-C5	2.33	115.09	109.30
3	D	1	GLO	C6-C5-C4	2.18	117.14	112.41
3	D	6	XYS	C1-C2-C3	-2.06	107.13	109.67
2	C	2	BGC	O5-C1-C2	-2.02	107.66	110.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	GLO	C1-C2-C3-C4
3	D	1	GLO	C2-C3-C4-C5
3	D	1	GLO	C2-C3-C4-O4
3	D	1	GLO	O3-C3-C4-C5
3	D	1	GLO	O4-C4-C5-C6
3	D	1	GLO	O4-C4-C5-O5
3	D	1	GLO	O5-C5-C6-O6
3	D	1	GLO	C4-C5-C6-O6
3	D	1	GLO	O3-C3-C4-O4
3	D	2	BGC	C4-C5-C6-O6
3	D	1	GLO	O2-C2-C3-O3
2	C	2	BGC	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	D	1	GLO	O2-C2-C3-C4
3	D	2	BGC	O5-C5-C6-O6
3	D	1	GLO	C1-C2-C3-O3
3	D	1	GLO	C3-C4-C5-C6

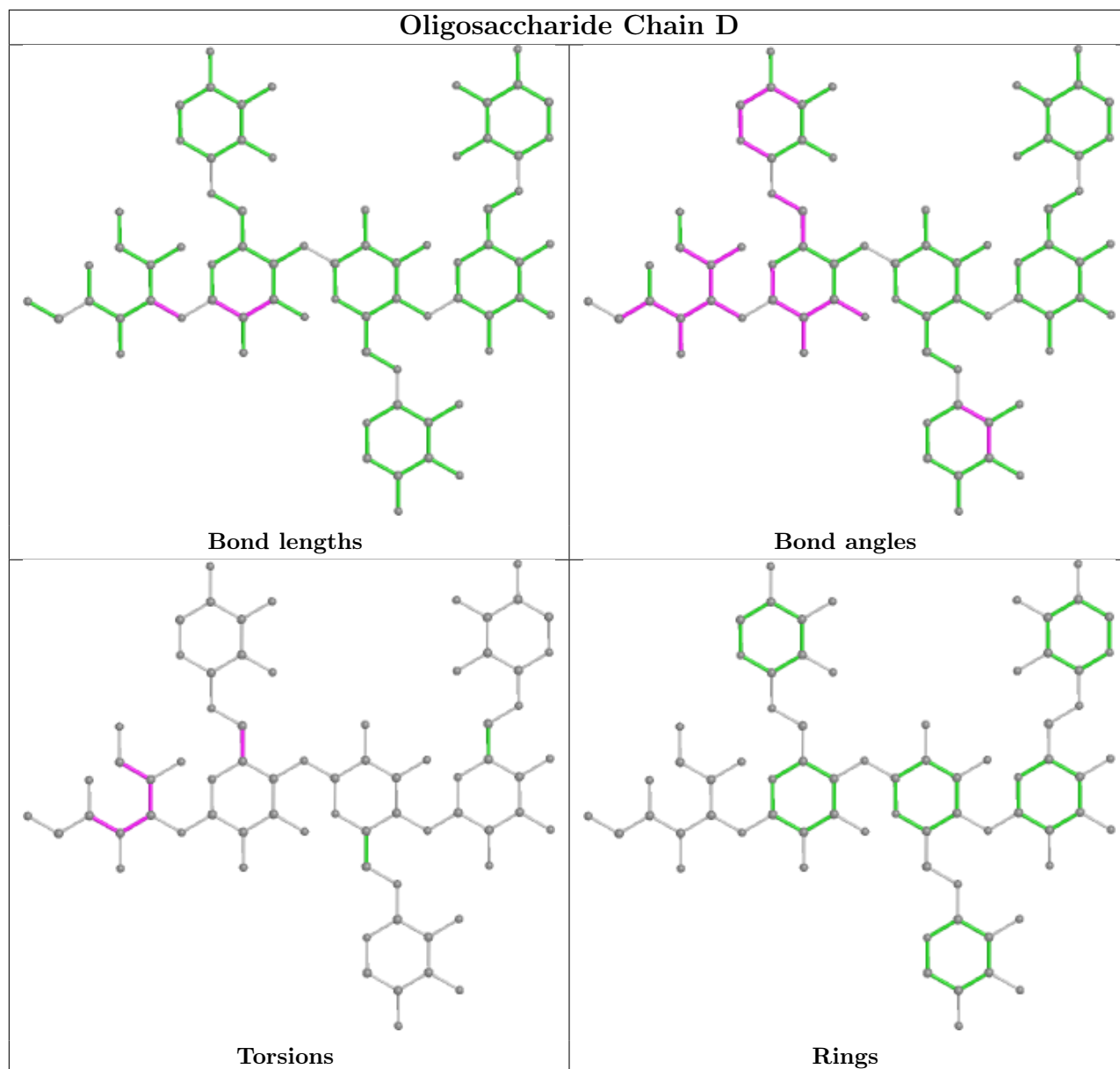
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1[B]	BGC	1	0
3	D	1	GLO	3	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](#)

16 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
5	EDO	A	1512	-	3,3,3	0.53	0	2,2,2	0.41	0
5	EDO	B	1506	-	3,3,3	0.47	0	2,2,2	0.25	0
5	EDO	B	1504	-	3,3,3	0.54	0	2,2,2	0.30	0
5	EDO	A	1600	-	3,3,3	0.48	0	2,2,2	0.23	0
5	EDO	A	1515	-	3,3,3	0.42	0	2,2,2	0.56	0
4	BTB	A	1511	-	13,13,13	0.72	0	7,16,16	0.94	0
5	EDO	A	1513	-	3,3,3	0.47	0	2,2,2	0.23	0
5	EDO	B	1509	-	3,3,3	0.56	0	2,2,2	0.21	0
5	EDO	B	1510	-	3,3,3	0.45	0	2,2,2	0.16	0
5	EDO	A	1516	-	3,3,3	0.60	0	2,2,2	0.22	0
5	EDO	A	1517	-	3,3,3	0.37	0	2,2,2	0.22	0
5	EDO	B	1508	-	3,3,3	0.43	0	2,2,2	0.22	0
6	GLC	A	1519[A]	2	11,11,12	0.89	0	15,15,17	1.41	2 (13%)
5	EDO	B	1507	-	3,3,3	0.39	0	2,2,2	0.43	0
5	EDO	A	1514	-	3,3,3	0.41	0	2,2,2	0.42	0
5	EDO	B	1505	-	3,3,3	0.45	0	2,2,2	0.32	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
5	EDO	A	1512	-	-	0/1/1/1	-
5	EDO	B	1506	-	-	0/1/1/1	-
5	EDO	B	1504	-	-	0/1/1/1	-
5	EDO	A	1600	-	-	0/1/1/1	-
5	EDO	A	1515	-	-	0/1/1/1	-
4	BTB	A	1511	-	-	1/21/21/21	-
5	EDO	A	1513	-	-	1/1/1/1	-
5	EDO	B	1509	-	-	1/1/1/1	-
5	EDO	B	1510	-	-	1/1/1/1	-
5	EDO	A	1516	-	-	0/1/1/1	-
5	EDO	A	1517	-	-	1/1/1/1	-
5	EDO	B	1508	-	-	0/1/1/1	-
6	GLC	A	1519[A]	2	-	2/2/19/22	0/1/1/1
5	EDO	B	1507	-	-	1/1/1/1	-
5	EDO	A	1514	-	-	0/1/1/1	-
5	EDO	B	1505	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1519[A]	GLC	O5-C1-C2	-2.37	107.11	110.77
6	A	1519[A]	GLC	C2-C3-C4	-2.15	107.17	110.89

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1519[A]	GLC	O5-C5-C6-O6
6	A	1519[A]	GLC	C4-C5-C6-O6
5	A	1513	EDO	O1-C1-C2-O2
5	B	1505	EDO	O1-C1-C2-O2
5	B	1510	EDO	O1-C1-C2-O2
4	A	1511	BTB	C6-C5-N-C7
5	B	1507	EDO	O1-C1-C2-O2
5	B	1509	EDO	O1-C1-C2-O2
5	A	1517	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1511	BTB	2	0
5	B	1509	EDO	3	0
5	B	1510	EDO	1	0
5	B	1507	EDO	1	0
5	B	1505	EDO	3	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	A	469/475 (98%)	-0.29	6 (1%) 77 77	8, 14, 44, 111	0
1	B	462/475 (97%)	-0.26	7 (1%) 73 73	8, 14, 45, 95	0
All	All	931/950 (98%)	-0.28	13 (1%) 75 75	8, 14, 45, 111	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	503	LEU	3.7
1	B	68	PRO	3.1
1	B	42	SER	2.8
1	A	503	LEU	2.7
1	A	509	HIS	2.7
1	B	71	TRP	2.6
1	A	506	HIS	2.6
1	A	510	HIS	2.6
1	B	174	ASN	2.6
1	B	88	GLU	2.6
1	B	69	ALA	2.2
1	A	508	HIS	2.1
1	A	504	GLU	2.1

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

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

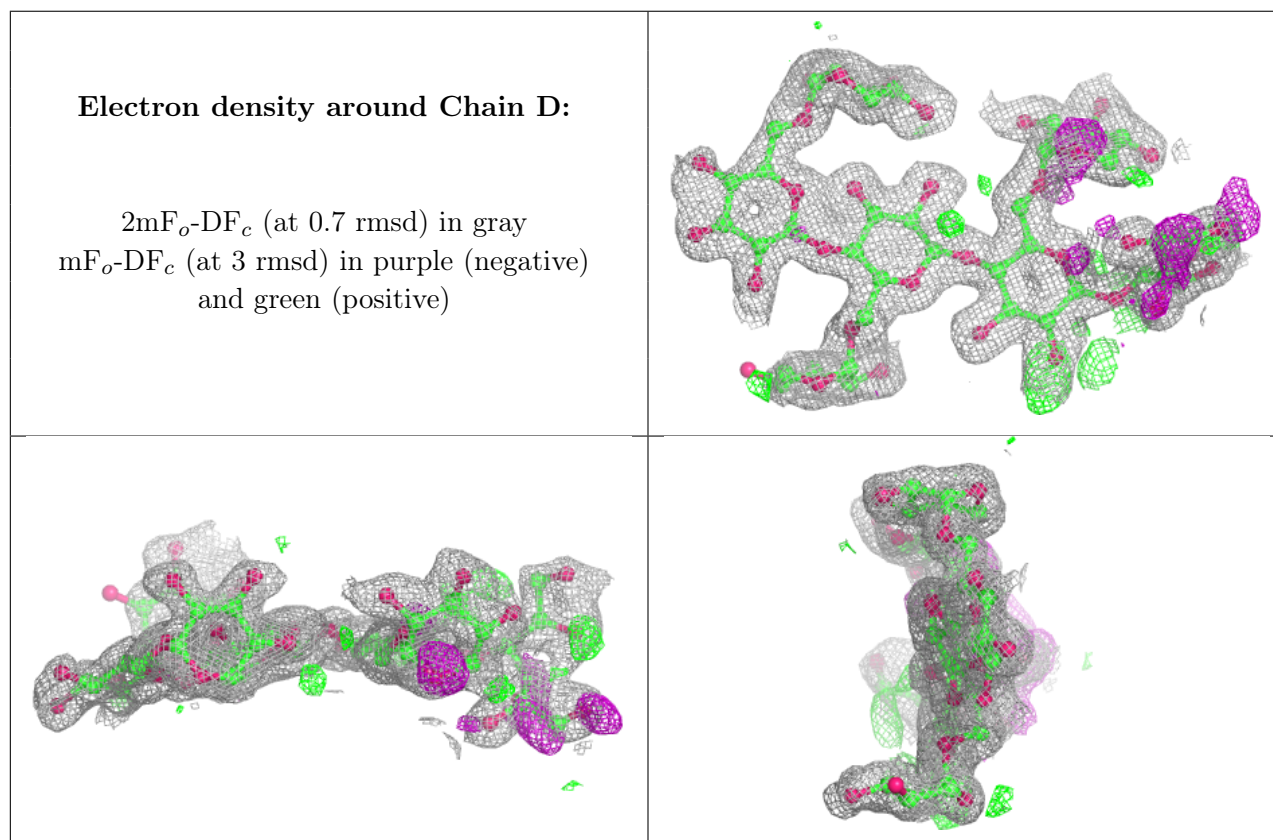
### 6.3 Carbohydrates [i](#)

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
3	BGC	D	2	11/12	0.77	0.14	19,27,48,68	0
3	XYS	D	7	9/10	0.81	0.18	26,33,44,104	0
3	XYS	D	5	9/10	0.88	0.22	28,35,42,45	0
3	GLO	D	1	12/12	0.88	0.22	17,41,76,136	0
3	BGC	D	4	11/12	0.91	0.22	29,33,58,67	0
2	XYS	C	7	9/10	0.92	0.16	19,24,32,48	0
2	XYS	C	5	9/10	0.92	0.10	16,18,24,26	0
3	XYS	D	6	9/10	0.93	0.18	28,43,90,152	0
2	BGC	C	2	11/12	0.94	0.11	17,21,28,30	0
2	XYS	C	6	9/10	0.94	0.13	37,42,162,212	0
2	BGC	C	4	11/12	0.94	0.12	19,23,32,35	0
2	BGC	C	3	11/12	0.95	0.09	17,21,24,29	0
3	BGC	D	3	11/12	0.95	0.13	20,25,36,37	0
2	BGC	C	1[B]	11/12	0.95	0.08	15,25,41,61	11

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<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
5	EDO	B	1509	4/4	0.75	0.26	36,40,48,58	0
5	EDO	B	1505	4/4	0.87	0.11	23,44,52,79	0
5	EDO	B	1510	4/4	0.89	0.12	21,39,42,56	0
5	EDO	A	1600	4/4	0.90	0.27	35,36,41,77	0
4	BTB	A	1511	14/14	0.90	0.12	17,29,70,97	0
5	EDO	B	1507	4/4	0.92	0.16	18,40,51,96	0
5	EDO	B	1504	4/4	0.92	0.10	31,46,50,57	0
5	EDO	B	1506	4/4	0.92	0.19	26,30,32,39	0
5	EDO	A	1513	4/4	0.94	0.26	24,30,35,64	0
5	EDO	A	1516	4/4	0.95	0.12	21,28,30,53	0
5	EDO	A	1515	4/4	0.95	0.12	29,31,34,44	0
6	GLC	A	1519[A]	11/12	0.96	0.07	7,18,70,90	11
5	EDO	B	1508	4/4	0.97	0.12	26,26,36,47	0
5	EDO	A	1512	4/4	0.97	0.07	20,21,21,22	0
5	EDO	A	1517	4/4	0.98	0.07	28,29,30,42	0
5	EDO	A	1514	4/4	0.98	0.07	19,23,36,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.