



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2021 – 04:09 PM EDT

PDB ID : 7KN8  
Title : Crystal structure of the GH74 xyloglucanase from *Xanthomonas campestris* (Xcc1752)  
Authors : Araujo, E.A.; Vieira, P.S.; Murakami, M.T.; Polikarpov, I.  
Deposited on : 2020-11-04  
Resolution : 1.95 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

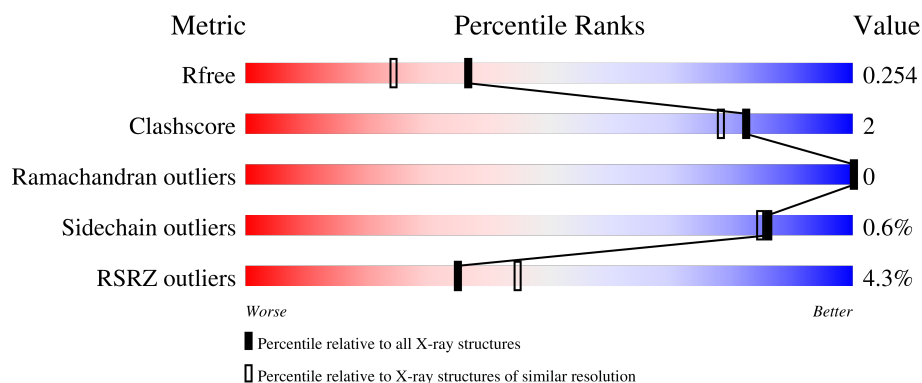
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	715	<div> <div>5%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	B	715	<div> <div>4%</div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
2	C	3	<div> <div>33%</div> <div>67%</div> </div>
2	D	3	<div> <div>100%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12052 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.

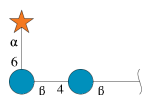
- Molecule 1 is a protein called Cellulase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	707	Total	C	N	O	S	0	2	0
			5428	3403	1017	1000	8			
1	B	708	Total	C	N	O	S	0	1	0
			5424	3401	1017	998	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP Q8P9U5
B	37	MET	-	initiating methionine	UNP Q8P9U5

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	3	Total	C	O	0	0	0
			32	17	15			
2	D	3	Total	C	O	0	0	0
			32	17	15			

- Molecule 3 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
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	I 7	0	0
5	B	7	Total 7	I 7	0	0

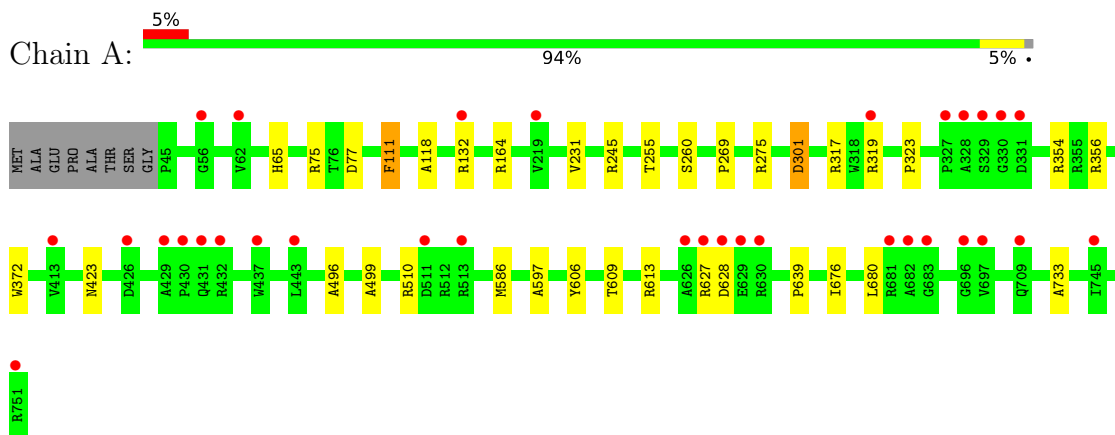
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	525	Total 525	O 525	0	0
6	B	559	Total 559	O 559	0	0

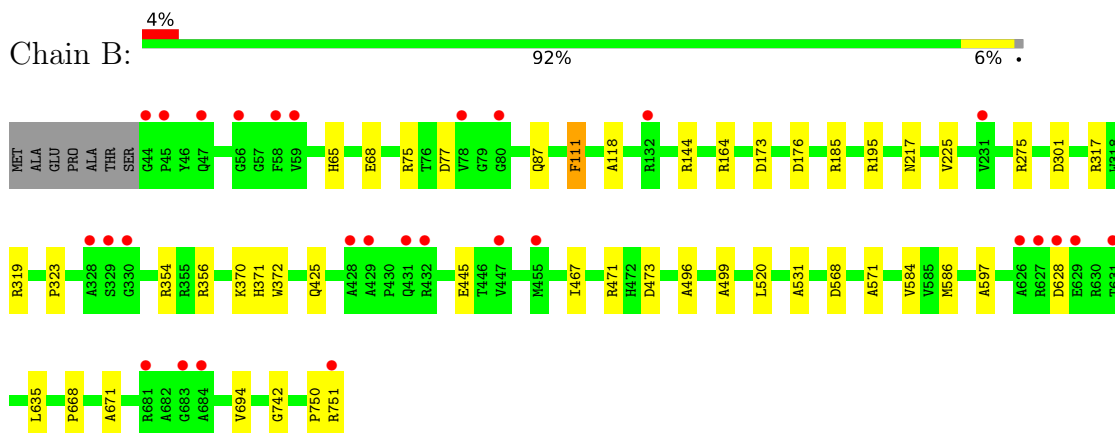
### 3 Residue-property plots

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



- Molecule 1: Cellulase



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



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

Chain D:

100%

BGC1  
BGC2  
XTS3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.79Å 100.43Å 168.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.95 38.80 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.99-1.95) 98.1 (38.80-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 1.95Å)	Xtriage
Refinement program	PHENIX dev_3139	Depositor
R, $R_{free}$	0.216 , 0.252 0.217 , 0.254	Depositor DCC
$R_{free}$ test set	5054 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 33.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0573e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: XYZ, BGC, EDO, IOD, NA

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	0.40	0/5586	0.60	0/7615
1	B	0.39	0/5582	0.60	0/7610
All	All	0.40	0/11168	0.60	0/15225

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5428	0	5149	23	0
1	B	5424	0	5148	27	0
2	C	32	0	27	3	0
2	D	32	0	27	0	0
3	A	20	0	30	4	0
3	B	16	0	24	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	7	0	0	2	0
5	B	7	0	0	3	0
6	A	525	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	559	0	0	0	0
All	All	12052	0	10405	53	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 (53) 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:A:586:MET:HG3	3:A:802:EDO:H11	1.60	0.83
1:B:471:ARG:NH1	1:B:473:ASP:OD1	2.20	0.74
1:A:132:ARG:HH21	1:A:627:ARG:HH12	1.40	0.68
1:B:520:LEU:HD23	1:B:531:ALA:HA	1.77	0.66
1:A:231:VAL:HG13	3:A:805:EDO:H11	1.81	0.63
1:B:467:ILE:HG22	3:B:801:EDO:H22	1.83	0.60
1:A:356:ARG:NH1	2:C:1:BGC:O1	2.34	0.60
1:A:132:ARG:NH2	1:A:627:ARG:HH12	2.06	0.54
1:B:68:GLU:OE2	1:B:144:ARG:NH1	2.31	0.54
3:A:802:EDO:H21	6:A:1116:HOH:O	2.09	0.52
1:B:195:ARG:HG3	5:B:808:IOD:I	2.80	0.52
1:A:597:ALA:HB3	1:A:606:TYR:HB2	1.93	0.51
1:A:323:PRO:HG3	1:A:372:TRP:CD2	2.47	0.49
1:A:609:THR:OG1	3:A:804:EDO:H11	2.13	0.49
1:B:668:PRO:HB3	1:B:694:VAL:HG22	1.95	0.49
1:B:370:LYS:HG2	1:B:371:HIS:CE1	2.47	0.49
1:B:87:GLN:HA	5:B:810:IOD:I	2.83	0.48
1:B:317:ARG:HH12	1:B:319:ARG:HE	1.63	0.47
1:B:750:PRO:O	1:B:751:ARG:HB3	2.16	0.46
1:A:496:ALA:HB3	1:A:499:ALA:O	2.16	0.46
1:B:668:PRO:HG2	1:B:671:ALA:HB2	1.97	0.46
1:B:354:ARG:NH1	1:B:356:ARG:HH21	2.15	0.45
1:A:275:ARG:HD3	5:B:806:IOD:I	2.87	0.44
2:C:1:BGC:O3	2:C:3:XYS:H3	2.18	0.44
1:A:301:ASP:N	1:A:301:ASP:OD1	2.51	0.43
1:A:354:ARG:NH1	1:A:356:ARG:HH21	2.16	0.43
1:A:639:PRO:HD3	1:A:676:ILE:HD13	2.00	0.43
1:B:75:ARG:HD3	1:B:111:PHE:CD1	2.54	0.43
1:A:255:THR:HG21	1:A:269:PRO:HB3	2.01	0.43
1:B:586:MET:HB2	1:B:635:LEU:HD22	2.01	0.43
1:A:77:ASP:HB3	1:A:164:ARG:HD2	2.01	0.43
1:A:510:ARG:NH1	6:A:905:HOH:O	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:807:IOD:I	1:B:275:ARG:HD3	2.89	0.43
1:B:445:GLU:HA	1:B:742:GLY:O	2.19	0.43
1:A:317:ARG:HH11	1:A:319:ARG:HG3	1.83	0.42
1:A:680:LEU:HA	1:A:733:ALA:HB1	2.00	0.42
1:A:613:ARG:HD2	1:A:613:ARG:HA	1.81	0.42
1:B:568:ASP:CG	1:B:571:ALA:HB3	2.39	0.42
1:A:65:HIS:NE2	1:A:118:ALA:HA	2.35	0.42
1:B:217:ASN:HB2	1:B:301:ASP:OD2	2.20	0.42
1:B:323:PRO:HG3	1:B:372:TRP:CD2	2.54	0.42
1:B:370:LYS:HG2	1:B:371:HIS:ND1	2.34	0.42
1:B:77:ASP:HB3	1:B:164:ARG:HD2	2.02	0.41
1:B:68:GLU:CD	1:B:144:ARG:HH12	2.20	0.41
1:B:496:ALA:HB3	1:B:499:ALA:O	2.21	0.41
1:B:173:ASP:HB3	1:B:176:ASP:O	2.20	0.41
1:A:75:ARG:HD3	1:A:111:PHE:CD1	2.56	0.40
1:A:423:ASN:N	1:A:423:ASN:OD1	2.54	0.40
1:B:65:HIS:NE2	1:B:118:ALA:HA	2.36	0.40
5:A:812:IOD:I	2:C:1:BGC:H1	2.91	0.40
1:A:245:ARG:HA	1:A:260:SER:O	2.21	0.40
1:B:185:ARG:HD2	1:B:225:VAL:O	2.21	0.40
1:B:584:VAL:O	1:B:597:ALA:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	706/715 (99%)	682 (97%)	24 (3%)	0	100	100
1	B	706/715 (99%)	684 (97%)	22 (3%)	0	100	100
All	All	1412/1430 (99%)	1366 (97%)	46 (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	522/526 (99%)	519 (99%)	3 (1%)	86	85
1	B	521/526 (99%)	518 (99%)	3 (1%)	86	85
All	All	1043/1052 (99%)	1037 (99%)	6 (1%)	86	85

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

Mol	Chain	Res	Type
1	A	111	PHE
1	A	301	ASP
1	A	628	ASP
1	B	111	PHE
1	B	425	GLN
1	B	628	ASP

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](#)

6 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	2	12,12,12	1.05	1 (8%)	17,17,17	1.25	1 (5%)
2	BGC	C	2	2	11,11,12	1.48	2 (18%)	15,15,17	0.91	0
2	XYS	C	3	2	9,9,10	1.82	2 (22%)	10,12,14	0.93	1 (10%)
2	BGC	D	1	2	12,12,12	1.28	1 (8%)	17,17,17	1.00	0
2	BGC	D	2	2	11,11,12	1.52	2 (18%)	15,15,17	0.93	0
2	XYS	D	3	2	9,9,10	1.82	2 (22%)	10,12,14	0.95	1 (10%)

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	2	-	2/2/22/22	0/1/1/1
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	XYS	C	3	2	-	-	0/1/1/1
2	BGC	D	1	2	-	2/2/22/22	0/1/1/1
2	BGC	D	2	2	-	1/2/19/22	0/1/1/1
2	XYS	D	3	2	-	-	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	BGC	O5-C1	3.98	1.50	1.43
2	C	3	XYS	O5-C1	3.98	1.50	1.42
2	D	3	XYS	O5-C1	3.78	1.50	1.42
2	C	2	BGC	O5-C1	3.76	1.49	1.43
2	D	1	BGC	O5-C1	3.15	1.50	1.42
2	D	3	XYS	O5-C5	2.88	1.48	1.42
2	C	3	XYS	O5-C5	2.73	1.48	1.42
2	C	1	BGC	O5-C1	2.63	1.49	1.42
2	D	2	BGC	C2-C3	-2.20	1.49	1.52
2	C	2	BGC	C2-C3	-2.05	1.49	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	XYS	C5-C4-C3	2.36	112.57	109.67
2	C	3	XYS	C5-C4-C3	2.23	112.40	109.67
2	C	1	BGC	C4-C3-C2	2.08	114.45	110.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	BGC	O5-C5-C6-O6
2	D	1	BGC	C4-C5-C6-O6
2	C	1	BGC	C4-C5-C6-O6
2	C	1	BGC	O5-C5-C6-O6
2	D	2	BGC	O5-C5-C6-O6

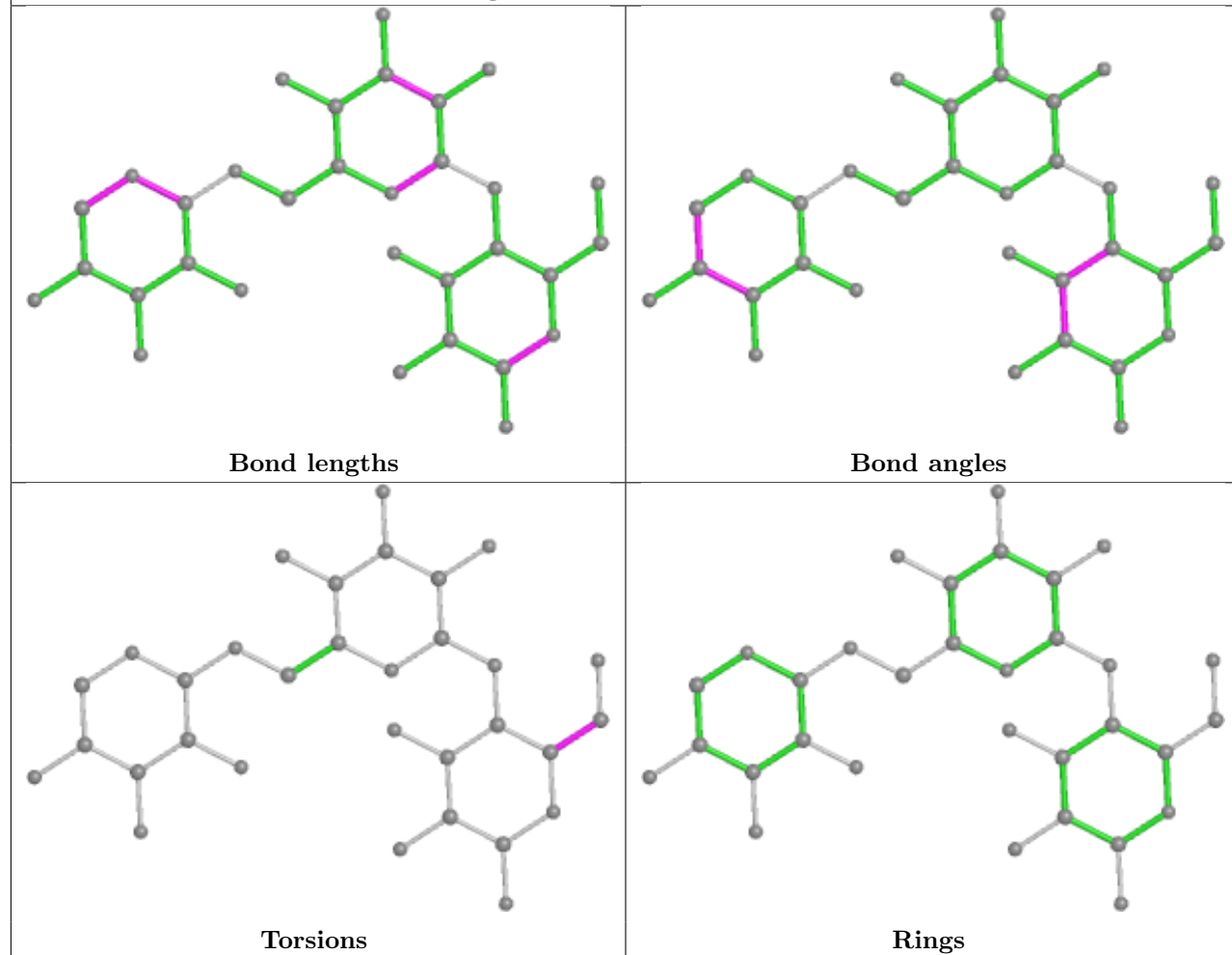
There are no ring outliers.

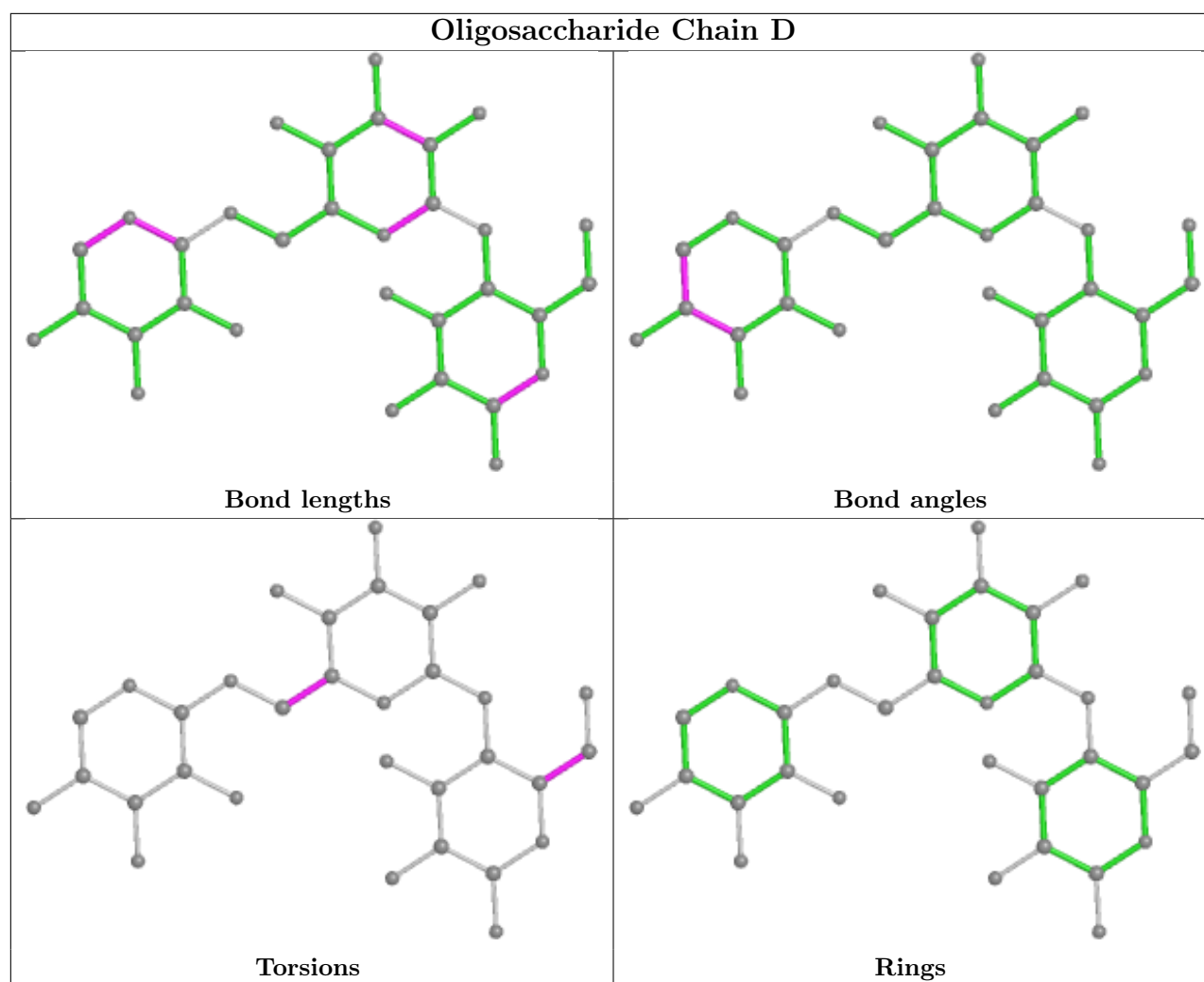
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	XYS	1	0
2	C	1	BGC	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.

## Oligosaccharide Chain C





## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 16 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	EDO	A	805	-	3,3,3	0.46	0	2,2,2	0.05	0
3	EDO	B	802	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	B	803	-	3,3,3	0.41	0	2,2,2	0.47	0
3	EDO	A	801	-	3,3,3	0.46	0	2,2,2	0.50	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	804	-	3,3,3	0.50	0	2,2,2	0.53	0
3	EDO	B	804	-	3,3,3	0.50	0	2,2,2	0.27	0
3	EDO	A	802	-	3,3,3	0.49	0	2,2,2	0.47	0
3	EDO	B	801	-	3,3,3	0.43	0	2,2,2	0.75	0
3	EDO	A	803	-	3,3,3	0.42	0	2,2,2	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	805	-	-	0/1/1/1	-
3	EDO	B	802	-	-	1/1/1/1	-
3	EDO	B	803	-	-	1/1/1/1	-
3	EDO	A	801	-	-	0/1/1/1	-
3	EDO	A	804	-	-	0/1/1/1	-
3	EDO	B	804	-	-	1/1/1/1	-
3	EDO	A	802	-	-	0/1/1/1	-
3	EDO	B	801	-	-	0/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	EDO	O1-C1-C2-O2
3	B	803	EDO	O1-C1-C2-O2
3	B	804	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	805	EDO	1	0
3	A	804	EDO	1	0
3	A	802	EDO	2	0
3	B	801	EDO	1	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

### 6.1 Protein, DNA and RNA chains

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	707/715 (98%)	0.35	33 (4%) 31 41	14, 19, 23, 31	0
1	B	708/715 (99%)	0.33	28 (3%) 38 48	15, 19, 23, 28	0
All	All	1415/1430 (98%)	0.34	61 (4%) 35 45	14, 19, 23, 31	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	329	SER	8.2
1	A	328	ALA	6.5
1	A	330	GLY	5.9
1	A	132	ARG	4.0
1	B	681	ARG	4.0
1	A	751	ARG	3.8
1	B	328	ALA	3.7
1	B	751	ARG	3.7
1	A	513	ARG	3.7
1	A	629	GLU	3.5
1	A	628	ASP	3.4
1	A	626	ALA	3.4
1	B	45	PRO	3.1
1	B	428	ALA	3.1
1	B	329	SER	3.0
1	A	627	ARG	2.9
1	A	430	PRO	2.9
1	A	682	ALA	2.7
1	A	429	ALA	2.7
1	B	626	ALA	2.7
1	A	696	GLY	2.6
1	B	44	GLY	2.6
1	A	331	ASP	2.6
1	B	455	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	630	ARG	2.6
1	A	437	TRP	2.6
1	B	631	THR	2.6
1	B	78	VAL	2.4
1	A	709	GLN	2.4
1	B	683	GLY	2.4
1	A	683	GLY	2.4
1	A	511[A]	ASP	2.3
1	B	231	VAL	2.3
1	B	429	ALA	2.3
1	B	59	VAL	2.3
1	A	327	PRO	2.3
1	A	681	ARG	2.3
1	B	47	GLN	2.3
1	B	58	PHE	2.2
1	A	413	VAL	2.2
1	A	56	GLY	2.2
1	B	330	GLY	2.2
1	B	629	GLU	2.2
1	A	697	VAL	2.2
1	B	432	ARG	2.2
1	B	628	ASP	2.2
1	A	745	ILE	2.2
1	A	426	ASP	2.1
1	B	684	ALA	2.1
1	B	627	ARG	2.1
1	A	443	LEU	2.1
1	B	80	GLY	2.1
1	B	56	GLY	2.1
1	A	319	ARG	2.1
1	B	132	ARG	2.1
1	A	219	VAL	2.0
1	B	447	VAL	2.0
1	A	62	VAL	2.0
1	A	432	ARG	2.0
1	A	431	GLN	2.0
1	B	431	GLN	2.0

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

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

### 6.3 Carbohydrates

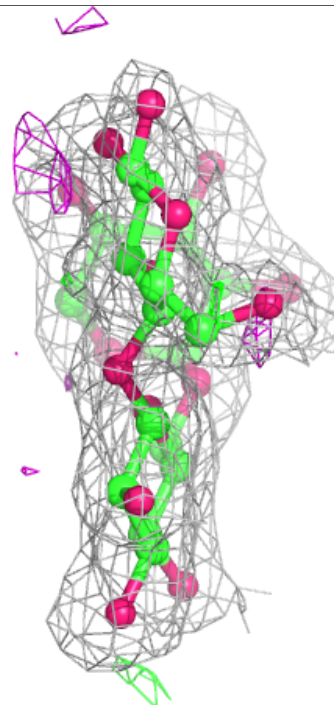
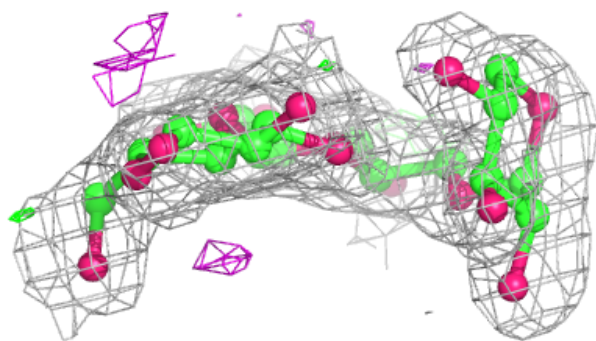
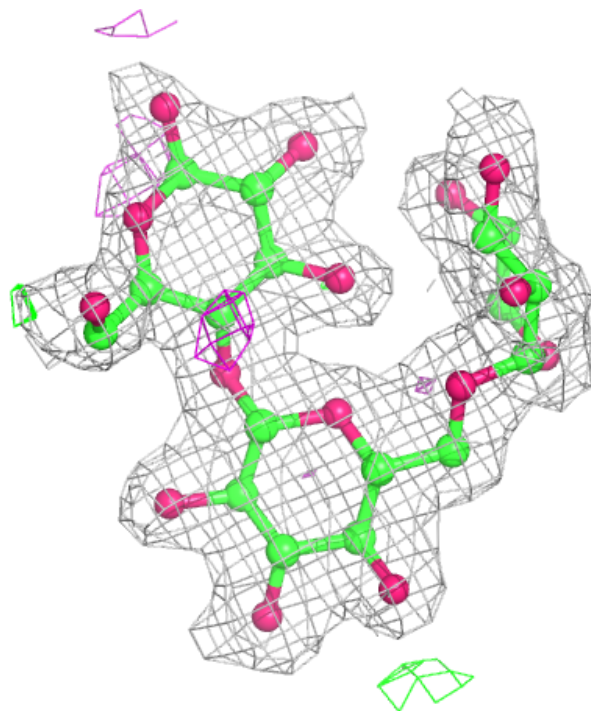
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	C	1	12/12	0.90	0.13	18,22,24,26	0
2	XYS	C	3	9/10	0.90	0.12	20,21,22,23	0
2	BGC	D	1	12/12	0.93	0.11	20,21,22,24	0
2	BGC	C	2	11/12	0.94	0.12	15,18,20,22	0
2	BGC	D	2	11/12	0.94	0.12	16,19,20,21	0
2	XYS	D	3	9/10	0.94	0.09	20,21,22,23	0

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

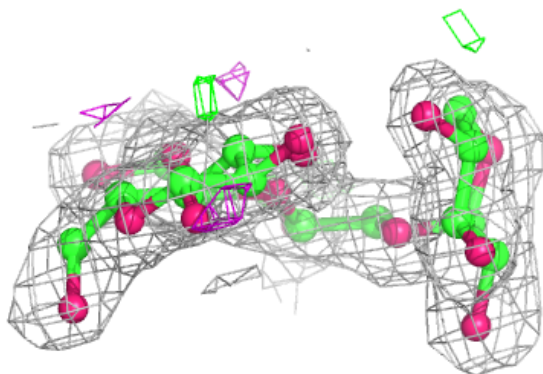
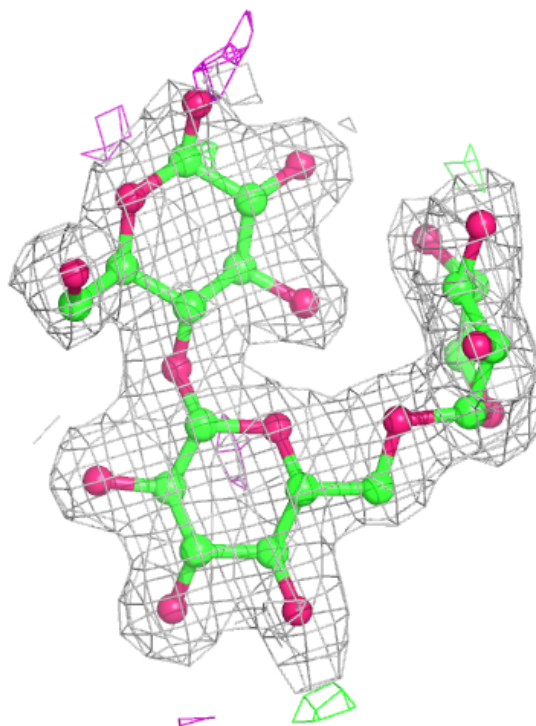
**Electron density around Chain C:**

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



### Electron density around Chain D:

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



## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	803	4/4	0.87	0.21	19,20,20,20	0
4	NA	A	806	1/1	0.87	0.23	19,19,19,19	0
3	EDO	B	801	4/4	0.89	0.17	16,18,19,20	0
3	EDO	A	801	4/4	0.90	0.16	16,18,19,20	0
3	EDO	A	804	4/4	0.93	0.20	19,20,21,22	0
3	EDO	A	802	4/4	0.93	0.19	18,18,19,19	0
5	IOD	B	808	1/1	0.93	0.27	62,62,62,62	0
5	IOD	A	810	1/1	0.95	0.28	64,64,64,64	0
5	IOD	A	811	1/1	0.95	0.33	61,61,61,61	0
3	EDO	B	804	4/4	0.95	0.12	20,20,21,21	0
5	IOD	B	810	1/1	0.95	0.36	60,60,60,60	0
3	EDO	A	803	4/4	0.96	0.09	20,20,20,20	0
3	EDO	A	805	4/4	0.96	0.12	17,18,18,18	0
3	EDO	B	802	4/4	0.97	0.11	18,19,19,19	0
4	NA	B	805	1/1	0.97	0.11	18,18,18,18	0
5	IOD	B	812	1/1	0.97	0.21	54,54,54,54	0
5	IOD	A	813	1/1	0.98	0.30	53,53,53,53	0
5	IOD	B	811	1/1	0.98	0.20	46,46,46,46	0
5	IOD	A	812	1/1	0.98	0.19	48,48,48,48	0
5	IOD	B	807	1/1	0.99	0.19	49,49,49,49	0
5	IOD	A	808	1/1	0.99	0.18	47,47,47,47	0
5	IOD	B	809	1/1	0.99	0.17	47,47,47,47	0
5	IOD	A	809	1/1	0.99	0.29	60,60,60,60	0
5	IOD	A	807	1/1	0.99	0.11	34,34,34,34	0
5	IOD	B	806	1/1	0.99	0.10	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.