



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 04:45 PM BST

PDB ID : 1F9O  
Title : Crystal structure of the cellulase Cel48F from *C. Cellulolyticum* with the thiooligosaccharide inhibitor PIPS-IG3  
Authors : Parsiegla, G.; Reverbel-Leroy, C.; Tardif, C.; Belaich, J.P.; Driguez, H.; Haser, R.  
Deposited on : 2000-07-11  
Resolution : 2.50 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	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

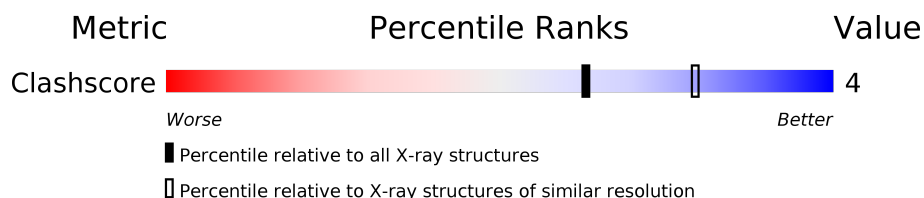
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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  $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	629	90% 10%
2	B	3	67% 33%
2	C	3	67% 33%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5316 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 ENDO-1,4-BETA-GLUCANASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	629	Total	C	N	O	S	0	0	0
			5015	3196	834	968	17			

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-4-iodophenyl 1,4-dithio-beta-D-glucopyranoside.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	3	Total	C	I	O	S	0	0	0
			41	24	1	14	2			
2	C	3	Total	C	I	O	S	0	0	0
			41	24	1	14	2			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

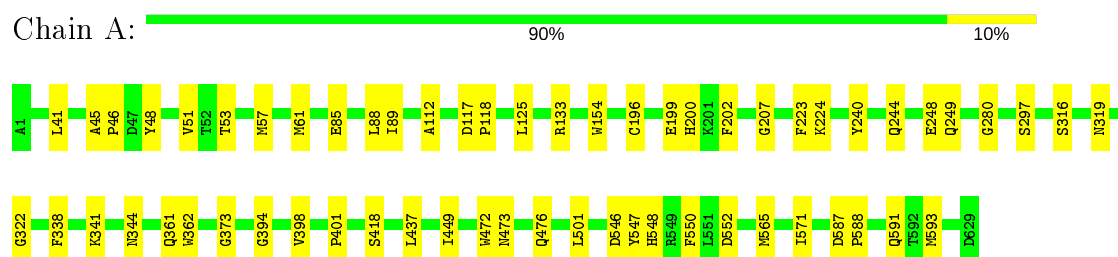
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total	O	0	0
			218	218		

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

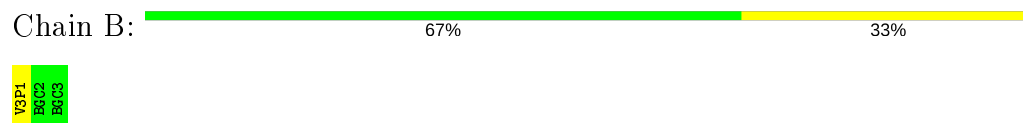
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

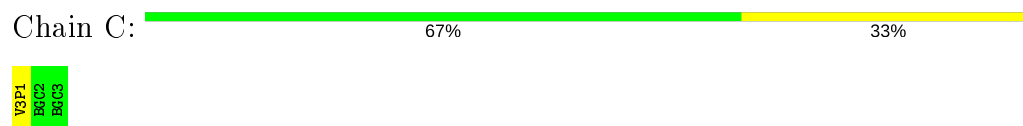
- Molecule 1: ENDO-1,4-BETA-GLUCANASE F



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-4-iodophenyl 1,4-dithio-beta-D-glucopyranoside



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-4-iodophenyl 1,4-dithio-beta-D-glucopyranoside



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.60Å 84.57Å 121.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.50	Depositor
% Data completeness (in resolution range)	99.5 (19.96-2.50)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 2.50Å)	Xtriage
Refinement program	CNS, X-PLOR 3.843	Depositor
R, $R_{free}$	0.179 , 0.243	Depositor
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.293	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5316	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V3P, CA, BGC

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	0.36	0/5179	0.62	0/7048

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

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	5015	0	4653	42	0
2	B	41	0	19	0	0
2	C	41	0	19	0	0
3	A	1	0	0	0	0
4	A	218	0	0	3	0
All	All	5316	0	4691	42	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 4.

All (42) 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:57:MET:HG3	1:A:88:LEU:HD12	1.68	0.76
1:A:45:ALA:HB3	1:A:46:PRO:CD	2.17	0.75
1:A:547:TYR:O	1:A:550:PHE:HB2	1.94	0.68
1:A:112:ALA:HB2	1:A:125:LEU:HD23	1.74	0.67
1:A:133:ARG:HH11	1:A:133:ARG:HG2	1.59	0.67
1:A:48:TYR:HB3	1:A:51:VAL:HG13	1.83	0.59
1:A:565:MET:SD	1:A:571:ILE:HD11	2.45	0.57
1:A:297:SER:HB2	1:A:316:SER:HB3	1.89	0.54
1:A:202:PHE:O	1:A:207:GLY:HA2	2.09	0.53
1:A:57:MET:HG3	1:A:88:LEU:CD1	2.37	0.52
1:A:45:ALA:HB3	1:A:46:PRO:HD3	1.89	0.50
1:A:46:PRO:HB2	1:A:51:VAL:CG2	2.41	0.50
1:A:398:VAL:HG23	1:A:401:PRO:HG3	1.94	0.50
1:A:196:CYS:O	1:A:223:PHE:HA	2.12	0.50
1:A:199:GLU:O	1:A:200:HIS:HB2	2.12	0.49
1:A:591:GLN:HG2	4:A:1174:HOH:O	2.12	0.49
1:A:297:SER:CB	1:A:316:SER:HB3	2.42	0.49
1:A:473:ASN:HB3	1:A:476:GLN:HB3	1.94	0.48
1:A:244:GLN:O	1:A:248:GLU:HG3	2.16	0.47
1:A:322:GLY:HA2	1:A:418:SER:HB2	1.97	0.46
1:A:341:LYS:HB3	1:A:341:LYS:HE2	1.60	0.45
1:A:344:ASN:N	1:A:344:ASN:HD22	2.13	0.45
1:A:362:TRP:CD1	1:A:472:TRP:HB2	2.52	0.45
1:A:45:ALA:HB3	1:A:46:PRO:HD2	1.98	0.45
1:A:319:ASN:O	1:A:373:GLY:HA3	2.18	0.44
1:A:546:ASP:HB2	4:A:1050:HOH:O	2.18	0.44
1:A:53:THR:HA	1:A:154:TRP:O	2.18	0.44
1:A:280:GLY:HA2	1:A:394:GLY:HA3	1.99	0.44
1:A:133:ARG:HH11	1:A:133:ARG:CG	2.28	0.43
1:A:361:GLN:HA	1:A:437:LEU:HD21	1.99	0.43
1:A:41:LEU:HD21	1:A:593:MET:HG3	1.99	0.43
1:A:240:TYR:HA	1:A:338:PHE:CZ	2.53	0.43
1:A:249:GLN:HG2	4:A:1124:HOH:O	2.18	0.42
1:A:548:HIS:HD2	1:A:552:ASP:OD2	2.01	0.42
1:A:85:GLU:HA	1:A:89:ILE:HD12	2.02	0.42
1:A:117:ASP:HA	1:A:118:PRO:HD3	1.91	0.42
1:A:449:ILE:HD11	1:A:501:LEU:HD21	2.01	0.42
1:A:297:SER:OG	1:A:316:SER:HB3	2.20	0.41
1:A:587:ASP:HA	1:A:588:PRO:HD3	1.92	0.41
1:A:57:MET:O	1:A:61:MET:HG3	2.20	0.41
1:A:48:TYR:HB3	1:A:51:VAL:CG1	2.51	0.40
1:A:196:CYS:O	1:A:224:LYS:HE3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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	V3P	B	1	2	19,20,20	1.58	3 (15%)	24,28,28	3.14	3 (12%)
2	BGC	B	2	2	11,11,12	0.40	0	15,15,17	0.54	0
2	BGC	B	3	2	11,11,12	0.49	0	15,15,17	0.62	0
2	V3P	C	1	2	19,20,20	1.07	2 (10%)	24,28,28	1.00	1 (4%)
2	BGC	C	2	2	11,11,12	0.28	0	15,15,17	0.33	0
2	BGC	C	3	2	11,11,12	0.36	0	15,15,17	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
2	V3P	B	1	2	-	4/6/26/26	0/2/2/2
2	BGC	B	2	2	-	2/2/19/22	0/1/1/1
2	BGC	B	3	2	-	0/2/19/22	0/1/1/1
2	V3P	C	1	2	-	0/6/26/26	0/2/2/2
2	BGC	C	2	2	-	0/2/19/22	0/1/1/1
2	BGC	C	3	2	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	V3P	C61-I6	-4.20	1.99	2.10
2	B	1	V3P	C1-S1	3.78	1.88	1.82
2	C	1	V3P	C31-S1	3.68	1.84	1.77
2	B	1	V3P	C21-C11	-2.55	1.34	1.38
2	C	1	V3P	C5-C4	2.19	1.54	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	V3P	C2-C1-S1	14.05	133.36	109.37
2	C	1	V3P	C2-C1-S1	-4.36	101.92	109.37
2	B	1	V3P	O5-C1-S1	-4.04	99.00	110.43
2	B	1	V3P	C31-S1-C1	-2.33	96.88	101.54

There are no chirality outliers.

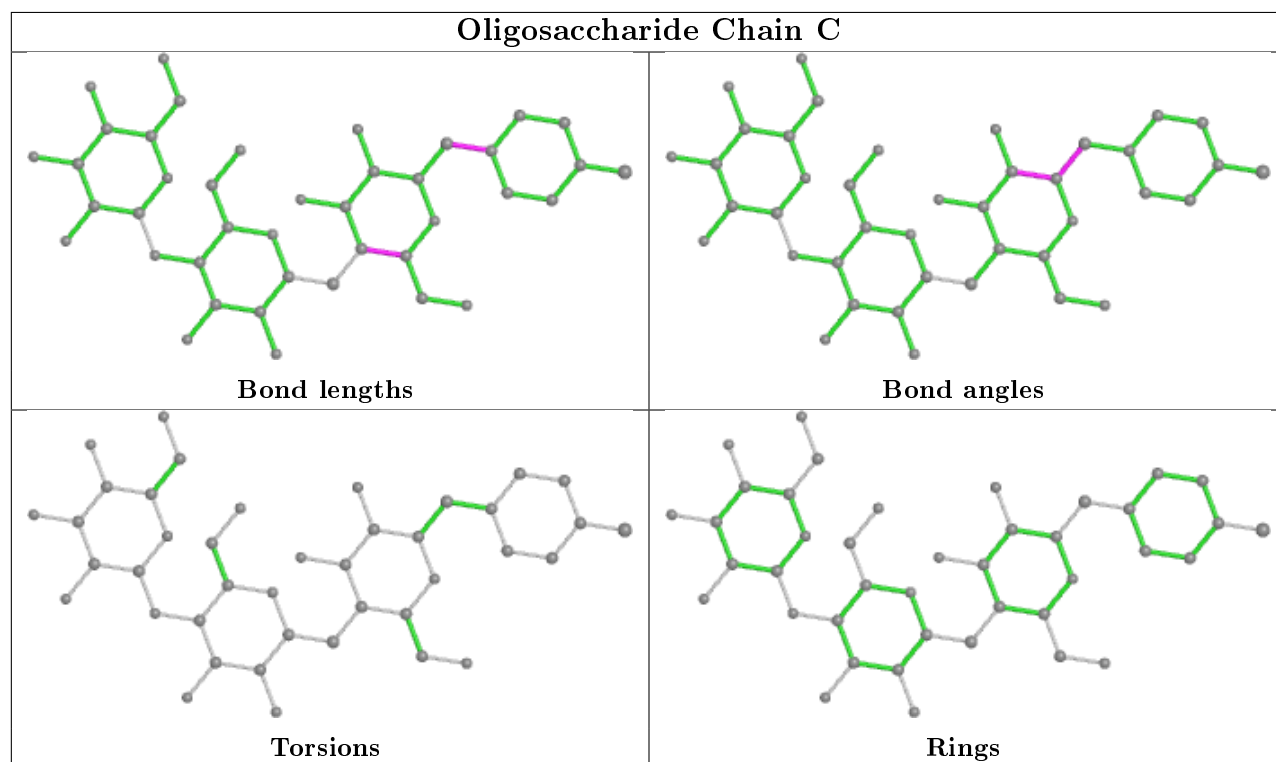
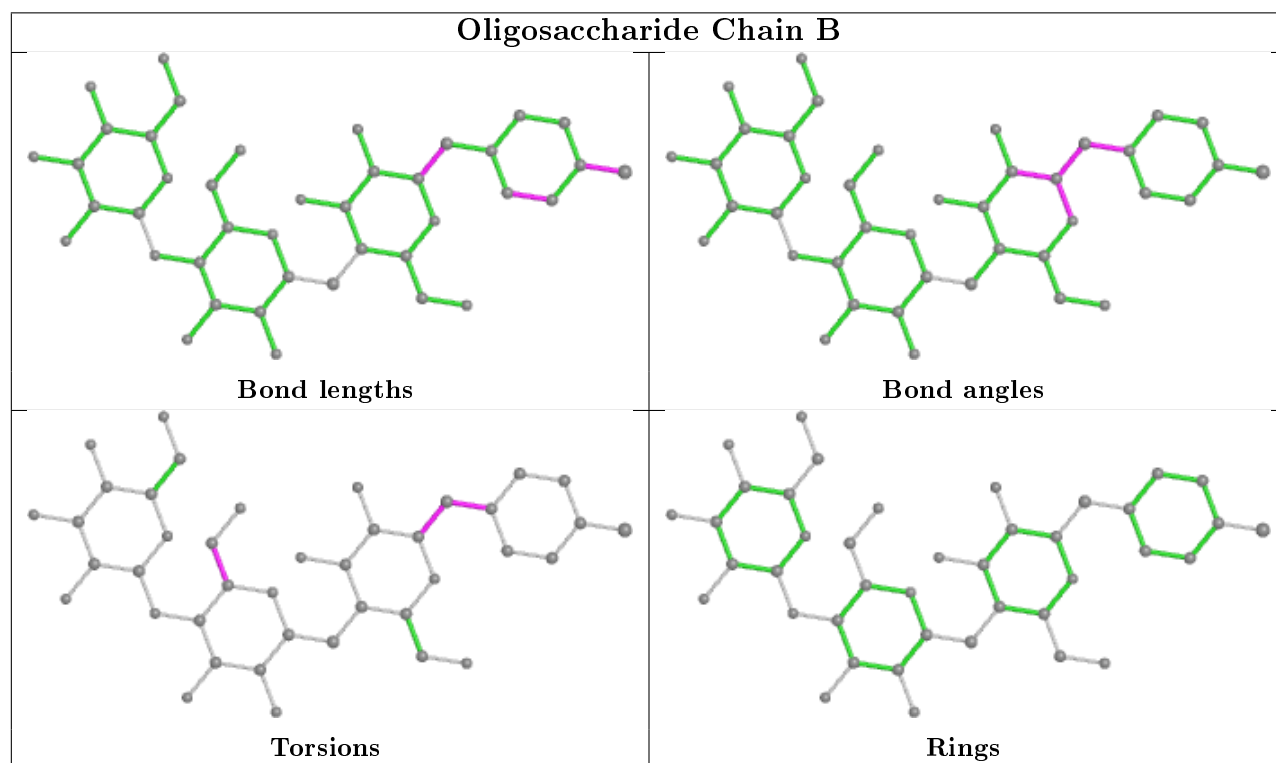
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	BGC	O5-C5-C6-O6
2	B	2	BGC	C4-C5-C6-O6
2	B	1	V3P	O5-C1-S1-C31
2	B	1	V3P	C2-C1-S1-C31
2	B	1	V3P	C21-C31-S1-C1
2	B	1	V3P	C41-C31-S1-C1

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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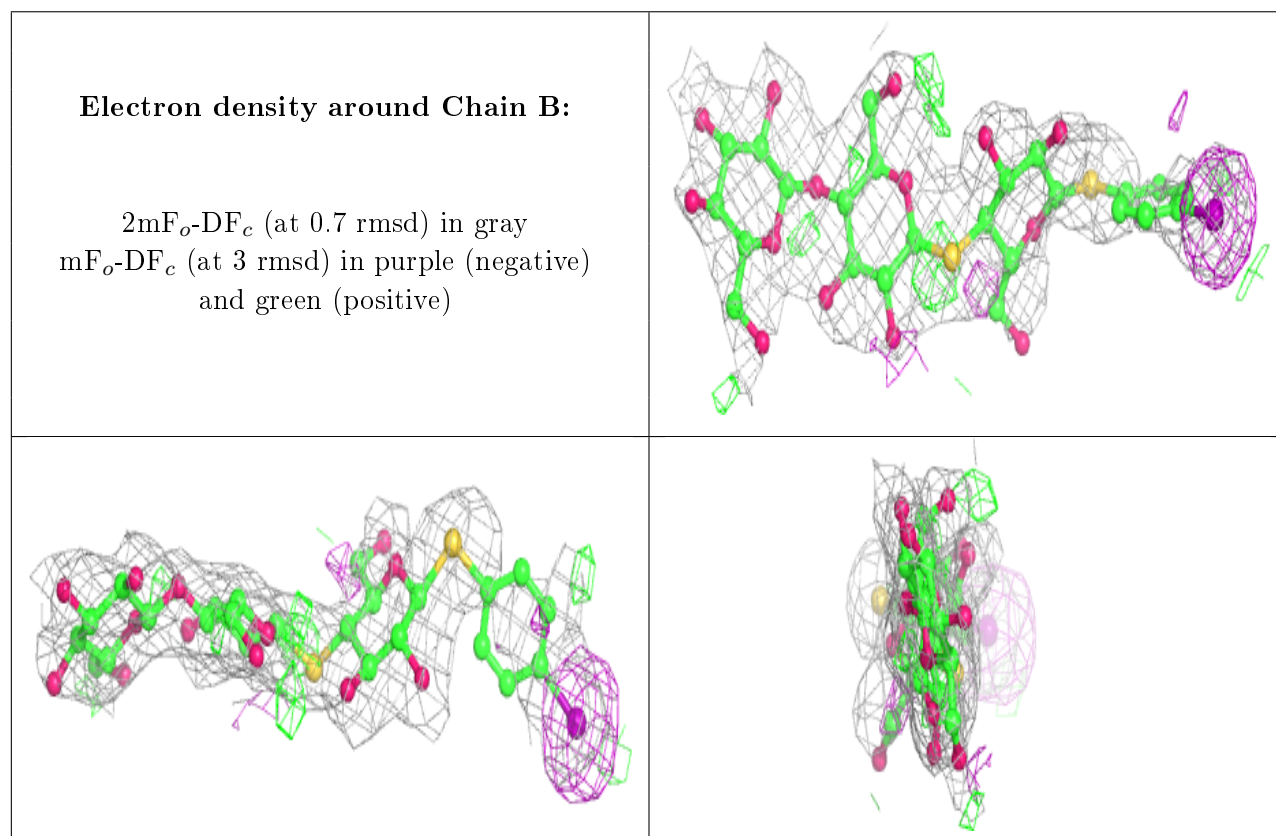
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

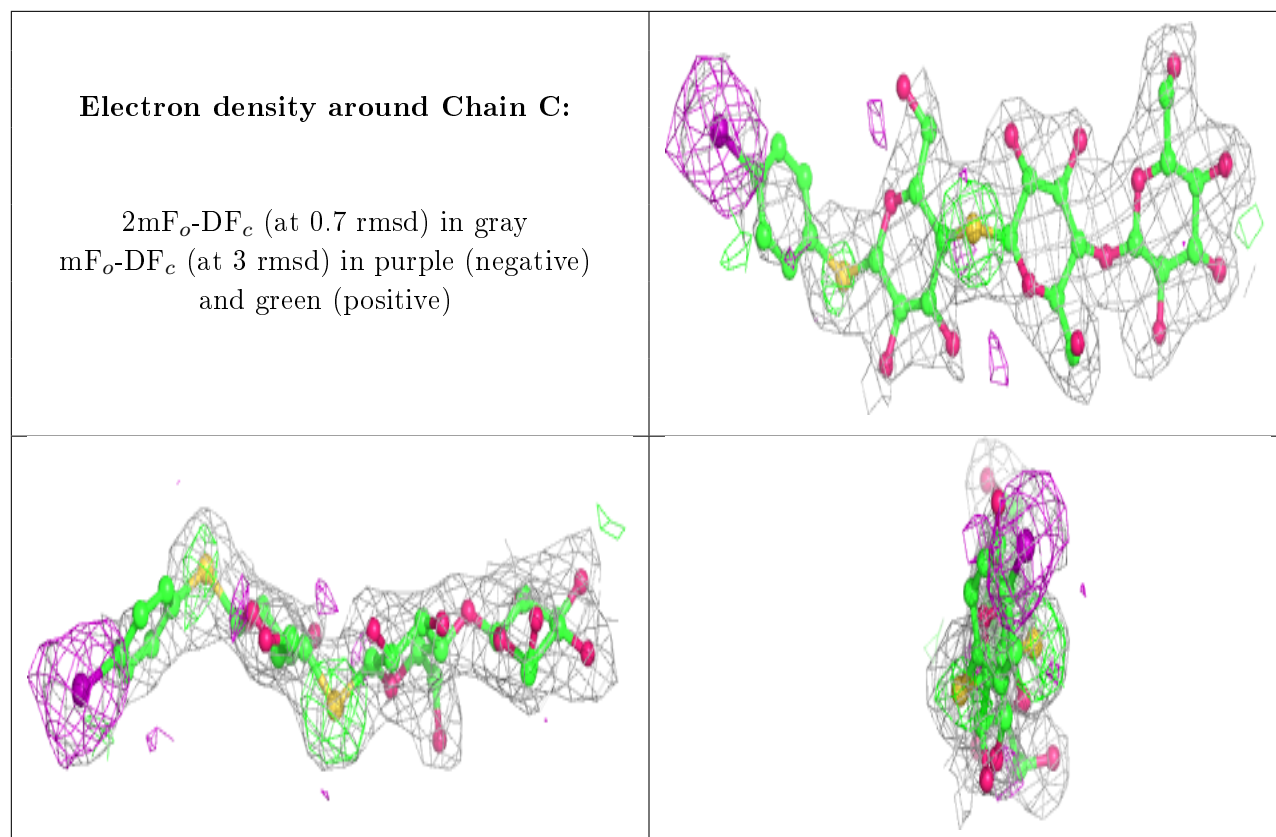
EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

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](#)

EDS failed to run properly - this section is therefore empty.

## 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.