



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2020 – 04:52 PM BST

PDB ID : 1OCJ  
Title : Mutant D416A of the CELLOBIOHYDROLASE CEL6A FROM HUMICOLA INSOLENS in complex with a THIOPENTASACCHARIDE at 1.3 angstrom resolution  
Authors : Varrot, A.; Frandsen, T.P.; Von Ossowski, I.; Boyer, V.; Driguez, H.; Schulein, M.; Davies, G.J.  
Deposited on : 2003-02-07  
Resolution : 1.30 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 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	:	2.14.6
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)	:	2.14.6

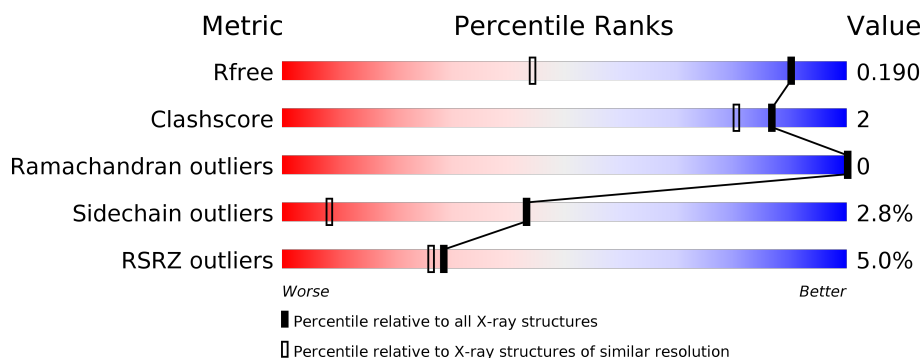
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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  $\leq 5\%$ . 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	362	<div> <div>5%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	B	5	<div> <div>20%</div> <div>80%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3331 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 CELLOBIOHYDROLASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	8	0
			2835	1804	490	530	11			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	5	Total	C	O	S	0	0	0
			57	31	22	4			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

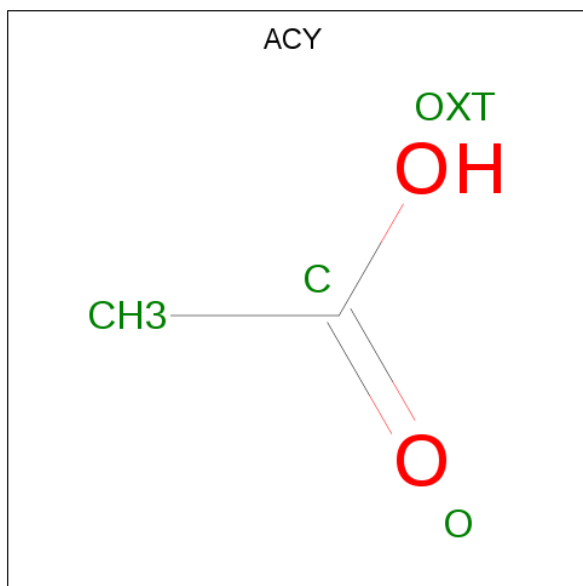


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

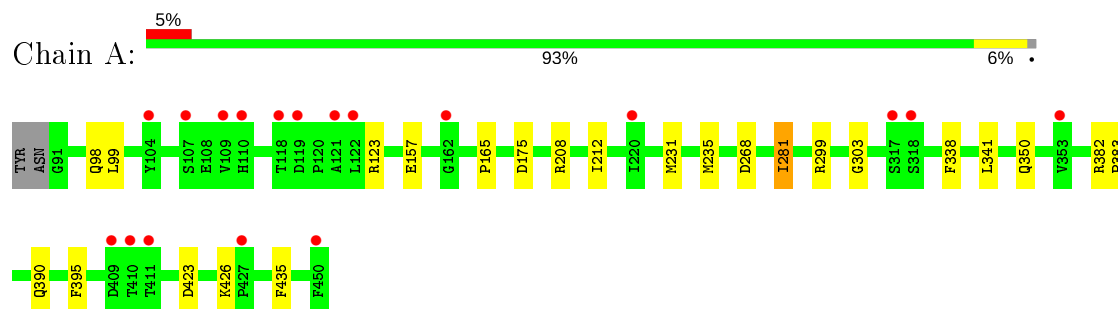
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	402	Total	O	0	18
			420	420		

### 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: CELLOBIOHYDROLASE II



#### • Molecule 2: beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose-(1-4)-1,4-dithio-beta-D-glucopyranose-(1-4)-4-thio-beta-D-glucopyranose-(1-4)-methyl 4-thio-alpha-D-glucopyranoside



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.44Å 67.55Å 53.66Å 90.00° 110.87° 90.00°	Depositor
Resolution (Å)	30.00 – 1.30 28.01 – 1.30	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-1.30) 91.0 (28.01-1.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.145 , 0.174 0.160 , 0.190	Depositor DCC
$R_{free}$ test set	6647 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.6	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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: MG, BGC, NAG, SSG, MA3, ACY, SGC

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	0.72	0/2944	0.84	6/4027 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	235	MET	CG-SD-CE	-5.76	90.99	100.20
1	A	299	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	423	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	175	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	338	PHE	CB-CG-CD1	5.02	124.31	120.80

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	2835	0	2720	11	0
2	B	57	0	50	0	0
3	A	14	0	13	0	0
4	A	1	0	0	0	0
5	A	4	0	3	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	420	0	0	0	0
All	All	3331	0	2786	11	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 (11) 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:208:ARG:NH1	1:A:212:ILE:HD11	1.98	0.79
1:A:281:ILE:HG22	1:A:341[B]:LEU:CD1	2.17	0.74
1:A:281:ILE:CG2	1:A:341[B]:LEU:HD12	2.26	0.66
1:A:281:ILE:HG22	1:A:341[B]:LEU:HD12	1.80	0.63
1:A:281:ILE:CG2	1:A:341[B]:LEU:CD1	2.83	0.56
1:A:208:ARG:NH1	1:A:212:ILE:CD1	2.69	0.53
1:A:303:GLY:HA3	1:A:350:GLN:O	2.10	0.52
1:A:281:ILE:HG22	1:A:341[B]:LEU:HD13	1.93	0.50
1:A:98:GLN:HG3	1:A:165:PRO:HG2	1.93	0.49
1:A:99:LEU:HG	5:A:507:ACY:H3	2.03	0.40
1:A:383:PRO:HA	1:A:395:PHE:O	2.21	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	366/362 (101%)	355 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	294/288 (102%)	286 (97%)	8 (3%)	44 9

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	157	GLU
1	A	231	MET
1	A	281	ILE
1	A	382	ARG
1	A	390	GLN
1	A	426	LYS
1	A	435	PHE

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

5 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	MA3	B	1	2	12,13,13	1.47	1 (8%)	14,18,18	2.76	5 (35%)
2	SGC	B	2	2	10,11,12	1.40	2 (20%)	12,15,17	2.60	6 (50%)
2	SSG	B	3	2	10,11,12	1.67	4 (40%)	12,15,17	3.57	7 (58%)
2	SSG	B	4	2	10,11,12	1.91	4 (40%)	12,15,17	3.08	7 (58%)
2	BGC	B	5	2	11,11,12	0.50	0	15,15,17	0.87	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	MA3	B	1	2	-	1/4/24/24	0/1/1/1
2	SGC	B	2	2	-	0/2/19/22	0/1/1/1
2	SSG	B	3	2	-	1/2/19/22	0/1/1/1
2	SSG	B	4	2	-	0/2/19/22	0/1/1/1
2	BGC	B	5	2	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	MA3	O1-C1	4.46	1.47	1.40
2	B	4	SSG	C5-C4	-3.62	1.50	1.53
2	B	3	SSG	O5-C1	-3.21	1.38	1.43
2	B	4	SSG	C3-C4	-2.39	1.51	1.53
2	B	4	SSG	C2-C3	-2.39	1.49	1.52
2	B	2	SGC	C2-C3	-2.38	1.49	1.52
2	B	4	SSG	O3-C3	-2.14	1.37	1.43
2	B	2	SGC	O5-C1	-2.08	1.40	1.43
2	B	3	SSG	C3-C4	-2.04	1.51	1.53
2	B	3	SSG	C5-C4	-2.01	1.51	1.53
2	B	3	SSG	C2-C3	-2.00	1.49	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	SSG	C1-O5-C5	7.63	122.53	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	MA3	O1-C1-C2	-7.26	99.64	108.15
2	B	4	SSG	O5-C1-C2	5.90	119.88	110.77
2	B	4	SSG	C1-O5-C5	5.60	119.77	112.19
2	B	3	SSG	C1-C2-C3	5.12	115.96	109.67
2	B	2	SGC	C1-O5-C5	5.11	119.11	112.19
2	B	3	SSG	O3-C3-C4	4.56	118.50	109.12
2	B	3	SSG	O5-C1-C2	4.37	117.52	110.77
2	B	2	SGC	O5-C1-C2	4.18	117.22	110.77
2	B	3	SSG	C6-C5-C4	3.45	120.27	112.69
2	B	1	MA3	C1-O5-C5	3.42	120.40	113.69
2	B	4	SSG	O3-C3-C4	3.33	115.97	109.12
2	B	1	MA3	O5-C1-O1	-3.12	103.73	110.97
2	B	2	SGC	C1-C2-C3	3.01	113.37	109.67
2	B	4	SSG	O2-C2-C3	2.90	115.94	110.14
2	B	1	MA3	O5-C5-C6	2.77	113.32	106.44
2	B	2	SGC	O3-C3-C4	2.76	114.79	109.12
2	B	2	SGC	O2-C2-C3	2.74	115.62	110.14
2	B	1	MA3	O5-C1-C2	2.71	116.08	110.35
2	B	4	SSG	O5-C5-C6	2.68	111.40	107.20
2	B	4	SSG	C1-C2-C3	2.58	112.84	109.67
2	B	4	SSG	C6-C5-C4	2.38	117.91	112.69
2	B	2	SGC	O2-C2-C1	2.31	113.87	109.15
2	B	3	SSG	O2-C2-C3	2.27	114.68	110.14
2	B	3	SSG	O5-C5-C6	2.04	110.40	107.20

There are no chirality outliers.

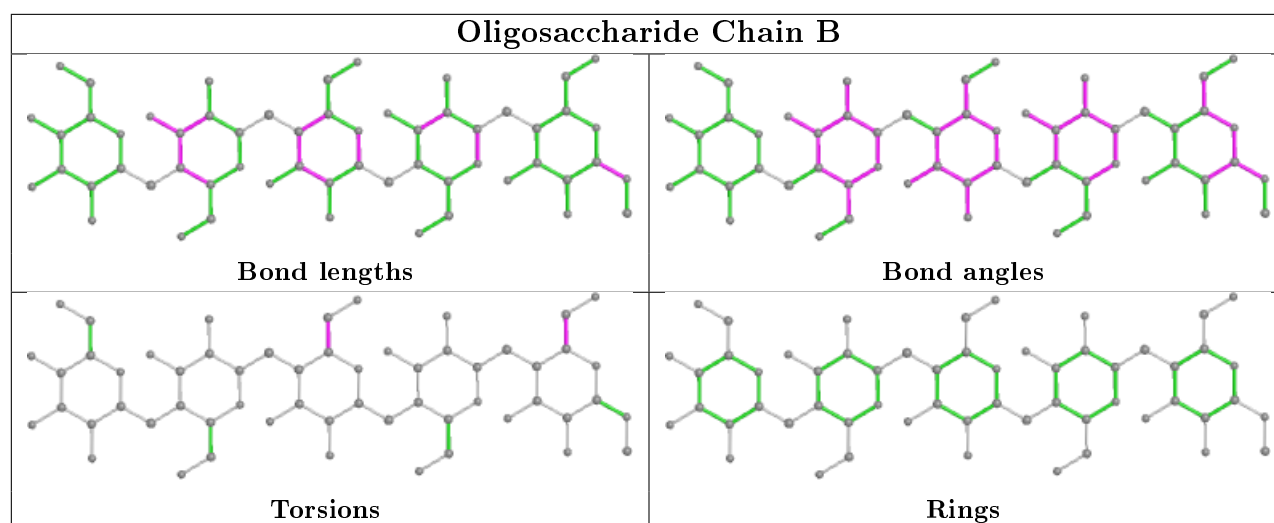
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3	SSG	O5-C5-C6-O6
2	B	1	MA3	C4-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 ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
5	ACY	A	507	-	1,3,3	0.74	0	0,3,3	0.00	-
3	NAG	A	500	1	14,14,15	0.49	0	17,19,21	0.70	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	NAG	A	500	1	-	0/6/23/26	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	ACY	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 [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	360/362 (99%)	0.34	18 (5%)	28 26	7, 12, 26, 33	10 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	PHE	4.9
1	A	104	TYR	3.1
1	A	317	SER	2.9
1	A	118	THR	2.8
1	A	121	ALA	2.6
1	A	411	THR	2.5
1	A	110	HIS	2.4
1	A	318	SER	2.4
1	A	162	GLY	2.4
1	A	119	ASP	2.3
1	A	109	VAL	2.3
1	A	427	PRO	2.2
1	A	410	THR	2.2
1	A	220	ILE	2.2
1	A	353	VAL	2.1
1	A	409	ASP	2.0
1	A	107	SER	2.0
1	A	122	LEU	2.0

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

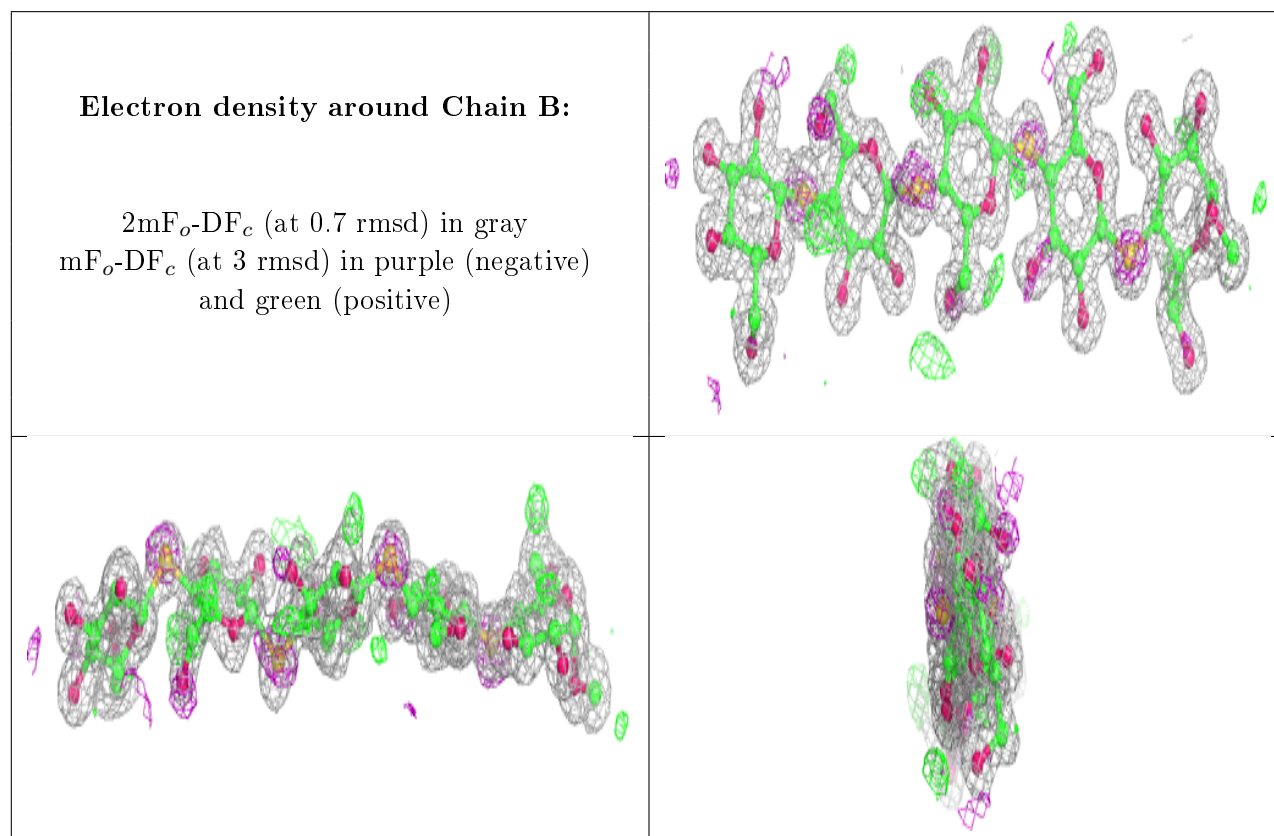
There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SSG	B	3	11/12	0.92	0.11	15,19,21,27	0
2	SSG	B	4	11/12	0.95	0.11	13,16,18,22	0
2	BGC	B	5	11/12	0.95	0.09	12,13,15,15	0
2	SGC	B	2	11/12	0.96	0.08	11,12,13,17	0
2	MA3	B	1	13/13	0.97	0.10	11,13,17,23	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.



### 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
5	ACY	A	507	4/4	0.80	0.26	17,18,18,19	0
3	NAG	A	500	14/15	0.97	0.07	9,11,15,17	0
4	MG	A	506	1/1	0.98	0.24	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.