



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 10:19 PM UTC

PDB ID : 7EOX / pdb\_00007eox  
Title : Protease structure from Euphorbia resinifera  
Authors : Siritapetawee, J.; Attarataya, J.; Charoenwattanasatien, R.  
Deposited on : 2021-04-24  
Resolution : 1.70 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](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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

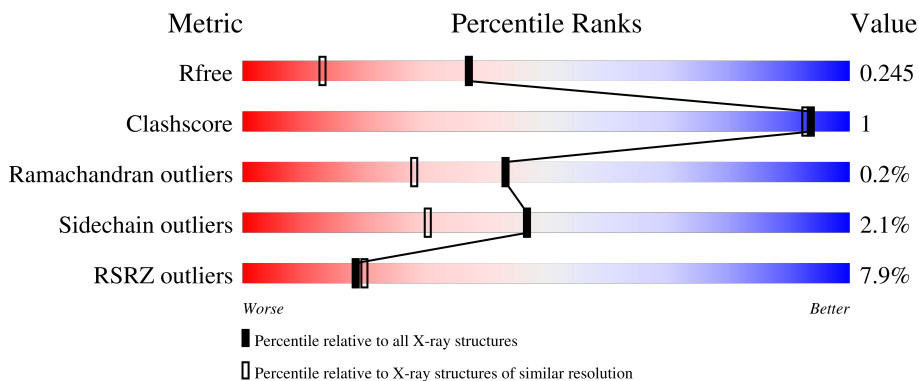
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	654	
1	B	654	
2	C	7	

## 2 Entry composition [i](#)

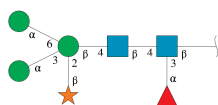
There are 5 unique types of molecules in this entry. The entry contains 10263 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	634	4719	2963	783	956	17	0	0	0
1	B	634	4719	2963	783	956	17	0	0	0

- Molecule 2 is an oligosaccharide called beta-D-xylopyranose-(1-2)-[alpha-D-mannopyranose-(1-3)][alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	7	80	45	2	33	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	I		
4	A	2	2	2	0	0
4	B	2	2	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	277	277	277	0	0
5	B	422	422	422	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.67Å 112.88Å 201.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.01 – 1.70 60.01 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (60.01-1.70) 98.6 (60.01-1.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.203 , 0.237 0.214 , 0.245	Depositor DCC
$R_{free}$ test set	8569 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 26.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10263	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: IOD, NAG, XYP, BMA, FUC, MAN

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	1.10	1/4836 (0.0%)	1.34	10/6601 (0.2%)
1	B	1.08	2/4836 (0.0%)	1.26	9/6601 (0.1%)
All	All	1.09	3/9672 (0.0%)	1.30	19/13202 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	477	ILE	C-O	6.36	1.30	1.24
1	B	289	VAL	N-CA	5.07	1.50	1.46
1	A	289	VAL	N-CA	5.04	1.50	1.46

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ASP	CA-CB-CG	8.94	121.54	112.60
1	B	1	ASP	CA-CB-CG	8.30	120.90	112.60
1	B	654	TRP	CA-C-O	-8.12	107.00	120.80
1	A	654	TRP	CA-C-O	-7.20	108.56	120.80
1	A	407	ALA	CA-C-N	6.71	126.71	120.34

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	4719	0	4495	17	0
1	B	4719	0	4493	9	0
2	C	80	0	60	0	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	277	0	0	1	0
5	B	422	0	0	5	0
All	All	10263	0	9087	26	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 1.

The worst 5 of 26 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:108:THR:O	1:A:112:THR:HB	1.76	0.85
1:A:112:THR:HG21	1:A:408:GLY:H	1.44	0.80
1:A:112:THR:HG21	1:A:408:GLY:N	2.15	0.60
1:A:112:THR:HG22	1:A:407:ALA:HB1	1.84	0.60
1:B:247:ARG:NH1	5:B:801:HOH:O	2.23	0.57

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	628/654 (96%)	604 (96%)	23 (4%)	1 (0%)	43 28
1	B	628/654 (96%)	608 (97%)	19 (3%)	1 (0%)	43 28
All	All	1256/1308 (96%)	1212 (96%)	42 (3%)	2 (0%)	43 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	GLY
1	B	330	GLY

### 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	517/528 (98%)	504 (98%)	13 (2%)	42	24
1	B	517/528 (98%)	508 (98%)	9 (2%)	53	38
All	All	1034/1056 (98%)	1012 (98%)	22 (2%)	47	30

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	53	SER
1	B	298	ASN
1	B	199	LYS
1	B	392	GLN
1	A	199	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	611	ASN
1	B	591	ASN
1	B	196	ASN
1	B	131	GLN
1	B	497	HIS

### 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](#)

7 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	NAG	C	1	1,2	14,14,15	0.60	0	17,19,21	1.41	1 (5%)
2	NAG	C	2	2	14,14,15	0.66	0	17,19,21	1.42	2 (11%)
2	BMA	C	3	2	11,11,12	0.83	0	15,15,17	1.31	2 (13%)
2	XYP	C	4	2	9,9,10	0.69	0	10,12,14	1.12	1 (10%)
2	MAN	C	5	2	11,11,12	0.51	0	15,15,17	1.00	1 (6%)
2	MAN	C	6	2	11,11,12	0.75	0	15,15,17	1.00	0
2	FUC	C	7	2	10,10,11	0.40	0	14,14,16	1.11	1 (7%)

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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	XYP	C	4	2	-	-	0/1/1/1
2	MAN	C	5	2	-	2/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	FUC	C	7	2	-	-	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-C2-N2	-3.27	105.28	110.43
2	C	2	NAG	C1-O5-C5	3.02	116.23	112.19
2	C	3	BMA	O2-C2-C3	2.96	116.29	110.15
2	C	2	NAG	O6-C6-C5	-2.42	103.10	111.33
2	C	4	XYP	C4-C3-C2	-2.22	108.28	110.92

There are no chirality outliers.

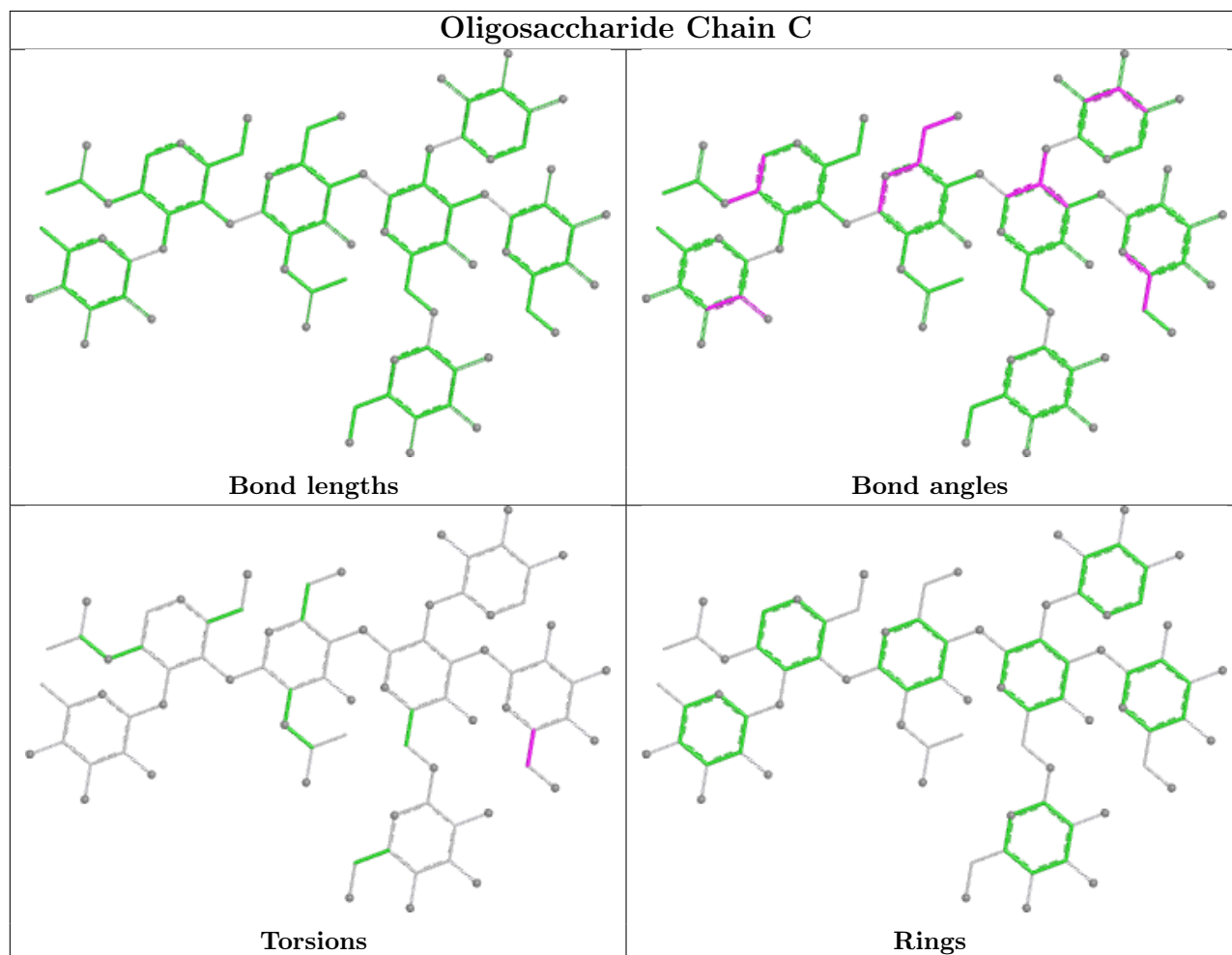
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	5	MAN	C4-C5-C6-O6
2	C	5	MAN	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](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	NAG	A	701	1	14,14,15	1.14	1 (7%)	17,19,21	0.89	0
3	NAG	B	701	1	14,14,15	0.82	1 (7%)	17,19,21	1.47	3 (17%)
3	NAG	B	702	1	14,14,15	1.34	1 (7%)	17,19,21	1.32	3 (17%)

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	701	1	-	0/6/23/26	0/1/1/1
3	NAG	B	701	1	-	2/6/23/26	0/1/1/1
3	NAG	B	702	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NAG	C1-C2	3.72	1.57	1.52
3	A	701	NAG	C1-C2	2.43	1.55	1.52
3	B	701	NAG	C1-C2	2.27	1.55	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	NAG	C4-C3-C2	-3.18	106.36	111.02
3	B	702	NAG	O3-C3-C4	2.70	116.74	110.38
3	B	701	NAG	C1-O5-C5	2.24	115.19	112.19
3	B	702	NAG	O5-C1-C2	-2.21	107.87	111.29
3	B	701	NAG	O3-C3-C2	2.21	114.00	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	NAG	O5-C5-C6-O6
3	B	701	NAG	C4-C5-C6-O6
3	B	702	NAG	C4-C5-C6-O6
3	B	702	NAG	O5-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<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	634/654 (96%)	0.82	84 (13%) <b>7</b> <b>7</b>	16, 29, 51, 76	0
1	B	634/654 (96%)	0.16	16 (2%) 58 62	15, 23, 41, 71	0
All	All	1268/1308 (96%)	0.49	100 (7%) <b>18</b> <b>20</b>	15, 26, 48, 76	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	ILE	6.3
1	A	566	THR	4.7
1	B	565	ASP	4.1
1	A	58	CYS	3.9
1	A	260	LEU	3.8

### 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.

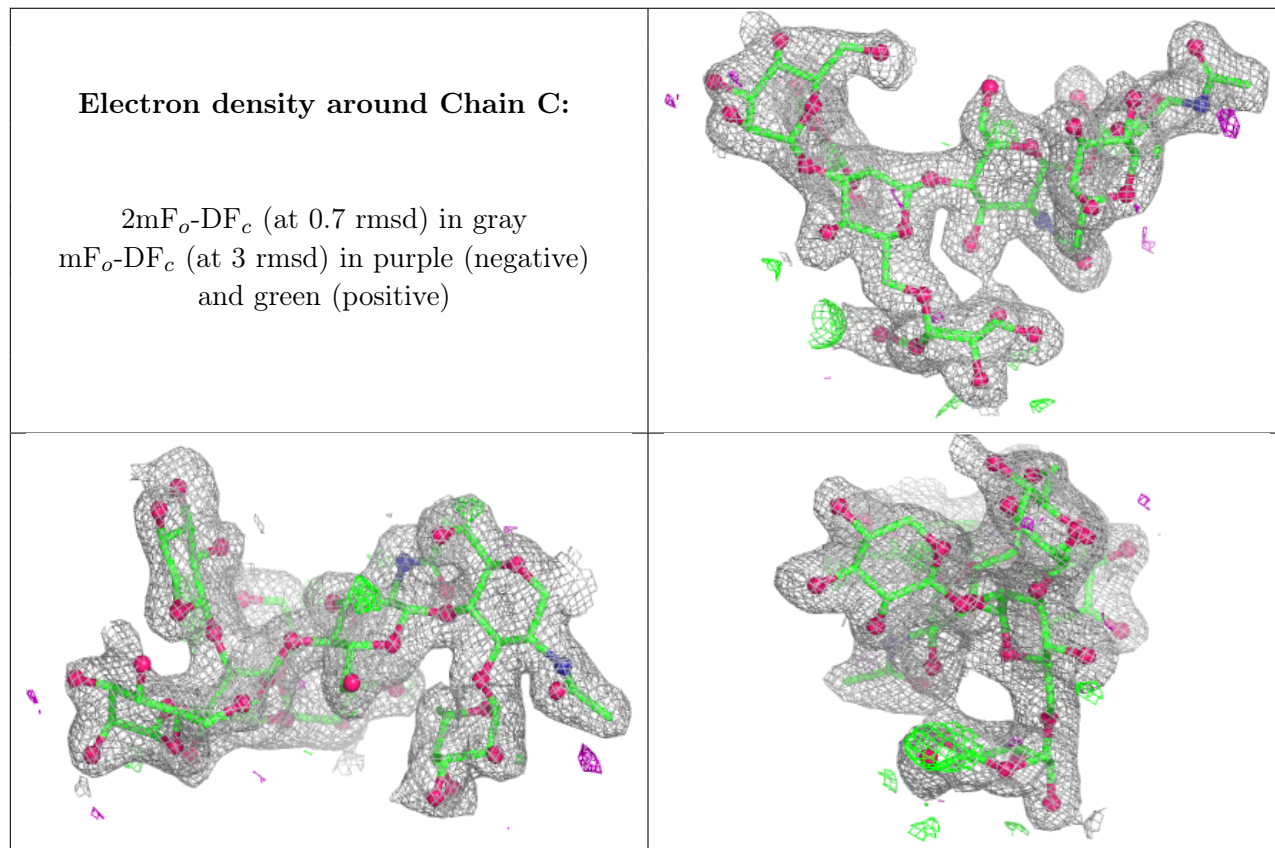
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MAN	C	5	11/12	0.80	0.15	50,54,57,64	0
2	FUC	C	7	10/11	0.87	0.12	35,38,40,41	0
2	NAG	C	1	14/15	0.93	0.09	27,28,32,36	0
2	NAG	C	2	14/15	0.93	0.10	25,30,37,47	0
2	MAN	C	6	11/12	0.94	0.09	25,26,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	XYP	C	4	9/10	0.95	0.09	31,31,36,37	0
2	BMA	C	3	11/12	0.95	0.08	27,30,37,43	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 [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	NAG	B	702	14/15	0.80	0.15	40,46,51,51	0
3	NAG	B	701	14/15	0.81	0.14	44,50,54,57	0
3	NAG	A	701	14/15	0.82	0.13	37,44,47,52	0
4	IOD	A	702	1/1	0.99	0.03	25,25,25,25	0
4	IOD	A	703	1/1	0.99	0.04	31,31,31,31	0
4	IOD	B	704	1/1	0.99	0.03	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IOD	B	703	1/1	1.00	0.02	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.