



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 05:44 PM BST

PDB ID : 5XSW  
Title : Crystal structure of an archaeal chitinase in the substrate-complex form (P63)  
Authors : Nishitani, Y.; Miki, K.  
Deposited on : 2017-06-15  
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 : 2.13.1  
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) : 2.13.1

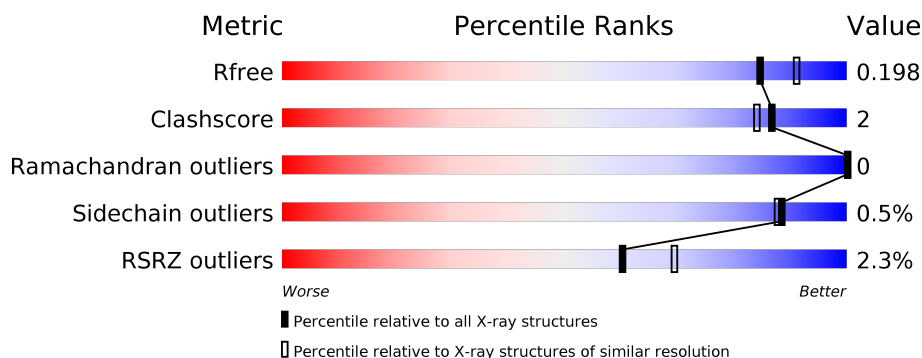
# 1 Overall quality at a glance

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 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	486	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 94%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>94%</span> <span>6%</span> </div> </div>
1	B	486	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 94%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>94%</span> <span>6%</span> </div> </div>
2	C	2	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>100%</span> </div> </div>
2	D	2	<div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>100%</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9068 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.

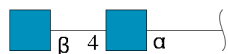
- Molecule 1 is a protein called Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	4	0
			4003	2602	650	738	13			
1	B	485	Total	C	N	O	S	0	5	0
			4017	2613	652	739	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	MET	-	initiating methionine	UNP A0A161KIT4
B	320	MET	-	initiating methionine	UNP A0A161KIT4

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			29	16	2	11			
2	D	2	Total	C	N	O	0	0	0
			29	16	2	11			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

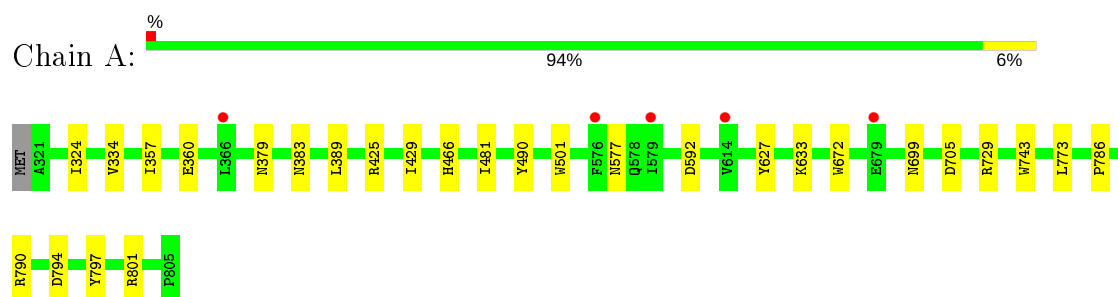
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	466	Total O 466 466	0	0
5	B	432	Total O 432 432	0	0

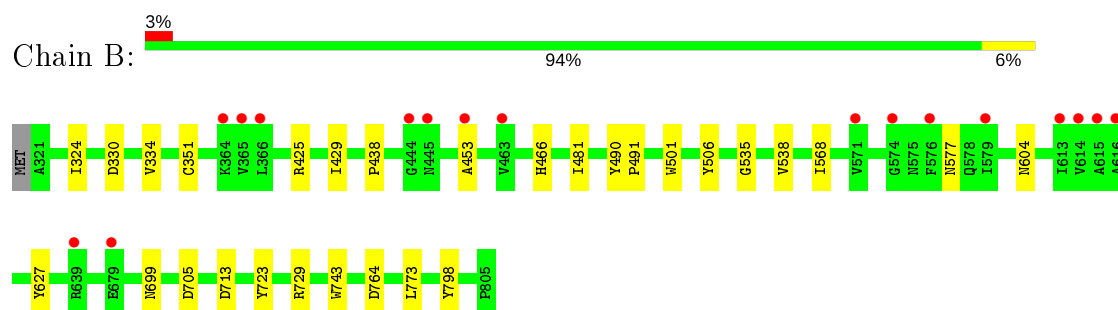
### 3 Residue-property plots [i](#)

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.

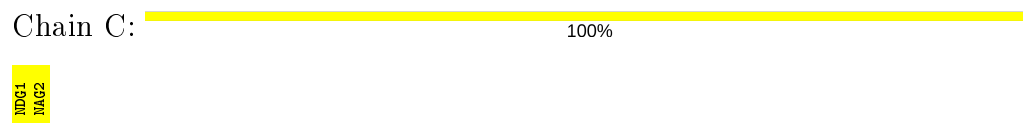
- Molecule 1: Chitinase



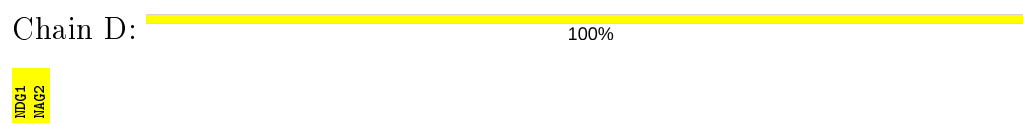
- Molecule 1: Chitinase



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.25Å 182.25Å 110.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.52 – 1.95 47.53 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.52-1.95) 99.5 (47.53-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.167 , 0.196 0.169 , 0.198	Depositor DCC
$R_{free}$ test set	7614 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9068	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: GOL, PO4, NAG, NDG

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	0.90	0/4136	0.75	0/5648
1	B	0.89	2/4152 (0.0%)	0.76	1/5671 (0.0%)
All	All	0.89	2/8288 (0.0%)	0.75	1/11319 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	351	CYS	CB-SG	-5.60	1.72	1.81
1	B	506	TYR	CD1-CE1	5.10	1.47	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	713	ASP	CB-CG-OD1	5.18	122.96	118.30

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	4003	0	3821	16	0
1	B	4017	0	3830	17	0
2	C	29	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	29	0	24	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	36	0	48	4	0
4	B	36	0	48	3	0
5	A	466	0	0	3	0
5	B	432	0	0	1	0
All	All	9068	0	7795	34	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 (34) 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)
4:B:905:GOL:H2	5:B:1215:HOH:O	1.65	0.96
1:B:764:ASP:N	1:B:764:ASP:OD1	2.30	0.61
1:A:379:ASN:HB3	5:A:1446:HOH:O	2.04	0.57
4:A:905:GOL:H2	5:A:1111:HOH:O	2.05	0.56
1:B:324:ILE:HD13	1:B:334:VAL:HG22	1.88	0.55
1:A:490[A]:TYR:CE1	1:A:699:ASN:ND2	2.78	0.52
1:A:797:TYR:O	1:A:801:ARG:HG3	2.09	0.52
1:B:481:ILE:HG13	1:B:773:LEU:HG	1.93	0.51
1:B:466:HIS:O	1:B:705:ASP:HB3	2.11	0.50
1:B:723:TYR:CG	4:B:904:GOL:H11	2.47	0.50
1:A:786:PRO:HB2	4:A:907:GOL:H32	1.93	0.50
1:B:729:ARG:HB2	1:B:743:TRP:CZ2	2.47	0.50
1:A:324:ILE:HD13	1:A:334:VAL:HG22	1.94	0.49
1:B:490[B]:TYR:CE2	1:B:699:ASN:ND2	2.79	0.49
1:B:438:PRO:HG3	1:B:453:ALA:HB2	1.94	0.49
1:B:604:ASN:OD1	4:B:904:GOL:O1	2.33	0.47
1:A:729:ARG:HD2	1:A:743:TRP:CE2	2.48	0.47
1:B:490[B]:TYR:CG	1:B:491[B]:PRO:HD2	2.51	0.45
1:A:429:ILE:HA	1:A:627:TYR:CE1	2.52	0.45
1:A:633:LYS:HE2	1:A:672:TRP:CE3	2.52	0.44
4:A:905:GOL:H2	5:A:1244:HOH:O	2.16	0.43
1:A:357:ILE:HD11	1:A:389:LEU:HD11	2.01	0.43
1:A:360:GLU:HA	1:A:383:ASN:O	2.18	0.43
1:B:330:ASP:OD1	1:B:330:ASP:N	2.50	0.42
1:B:535:GLY:HA3	1:B:568:ILE:HB	2.00	0.42
1:A:577:ASN:OD1	1:B:577:ASN:ND2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:HIS:O	1:A:705:ASP:HB3	2.19	0.42
1:B:501[B]:TRP:CD1	1:B:538:VAL:HG13	2.54	0.42
1:A:797:TYR:CZ	1:A:801:ARG:HD2	2.55	0.41
1:A:790:ARG:HH12	4:A:906:GOL:H2	1.85	0.41
1:B:429:ILE:HA	1:B:627:TYR:CE1	2.56	0.41
1:A:481:ILE:HG13	1:A:773:LEU:HG	2.03	0.41
1:A:592:ASP:HB2	1:B:798:TYR:HB3	2.03	0.40
1:B:481:ILE:CG1	1:B:773:LEU:HG	2.51	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	487/486 (100%)	471 (97%)	16 (3%)	0	100	100
1	B	488/486 (100%)	473 (97%)	15 (3%)	0	100	100
All	All	975/972 (100%)	944 (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	424/421 (101%)	421 (99%)	3 (1%)	84	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	425/421 (101%)	424 (100%)	1 (0%)	93	93
All	All	849/842 (101%)	845 (100%)	4 (0%)	88	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	425	ARG
1	A	501	TRP
1	A	794	ASP
1	B	425	ARG

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 ⓘ

4 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	NDG	C	1	2	15,15,15	1.44	3 (20%)	21,21,21	1.67	5 (23%)
2	NAG	C	2	2	14,14,15	1.60	6 (42%)	17,19,21	1.31	3 (17%)
2	NDG	D	1	2	15,15,15	1.36	3 (20%)	21,21,21	1.54	3 (14%)
2	NAG	D	2	2	14,14,15	1.62	4 (28%)	17,19,21	1.30	2 (11%)

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	NDG	C	1	2	-	0/6/26/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NDG	D	1	2	-	0/6/26/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NDG	C8-C7	3.37	1.57	1.50
2	D	2	NAG	O5-C1	3.02	1.48	1.43
2	D	1	NDG	C7-N2	2.87	1.44	1.34
2	C	1	NDG	O5-C1	2.66	1.49	1.42
2	C	1	NDG	C7-N2	2.63	1.43	1.34
2	D	1	NDG	C8-C7	2.55	1.55	1.50
2	C	2	NAG	O5-C1	2.51	1.47	1.43
2	C	2	NAG	C1-C2	-2.51	1.48	1.52
2	D	2	NAG	C7-N2	2.46	1.42	1.34
2	C	2	NAG	C4-C5	-2.46	1.47	1.53
2	C	2	NAG	C8-C7	2.43	1.55	1.50
2	D	1	NDG	O5-C1	2.20	1.48	1.42
2	D	2	NAG	O4-C4	2.13	1.48	1.43
2	D	2	NAG	C8-C7	2.03	1.54	1.50
2	C	2	NAG	O5-C5	2.02	1.47	1.43
2	C	2	NAG	C7-N2	2.01	1.41	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NDG	C1-C2-C3	3.44	115.23	110.54
2	C	1	NDG	O4-C4-C5	-3.20	101.35	109.30
2	C	1	NDG	C4-C3-C2	2.98	114.70	110.34
2	D	1	NDG	C1-C2-N2	-2.90	107.37	110.73
2	C	1	NDG	C1-C2-N2	-2.84	107.44	110.73
2	C	1	NDG	C8-C7-N2	2.70	120.67	116.10
2	D	1	NDG	O4-C4-C5	-2.59	102.86	109.30
2	C	1	NDG	O7-C7-N2	-2.59	117.19	121.95
2	C	2	NAG	O6-C6-C5	-2.57	102.49	111.29
2	C	2	NAG	O7-C7-N2	-2.36	117.62	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-C2-N2	-2.34	106.48	110.49
2	D	2	NAG	C8-C7-N2	2.08	119.62	116.10
2	C	2	NAG	O4-C4-C5	-2.02	104.28	109.30

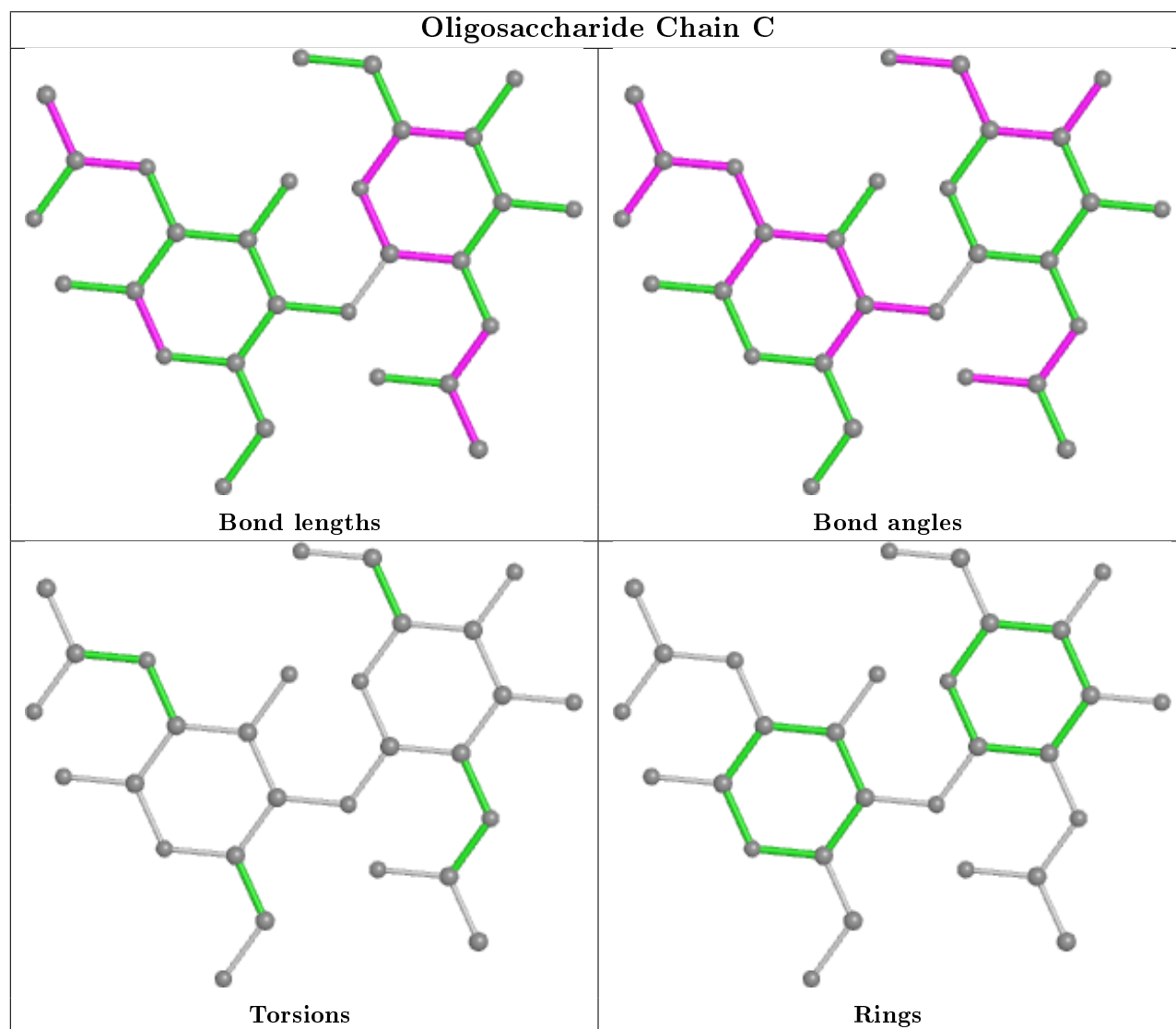
There are no chirality outliers.

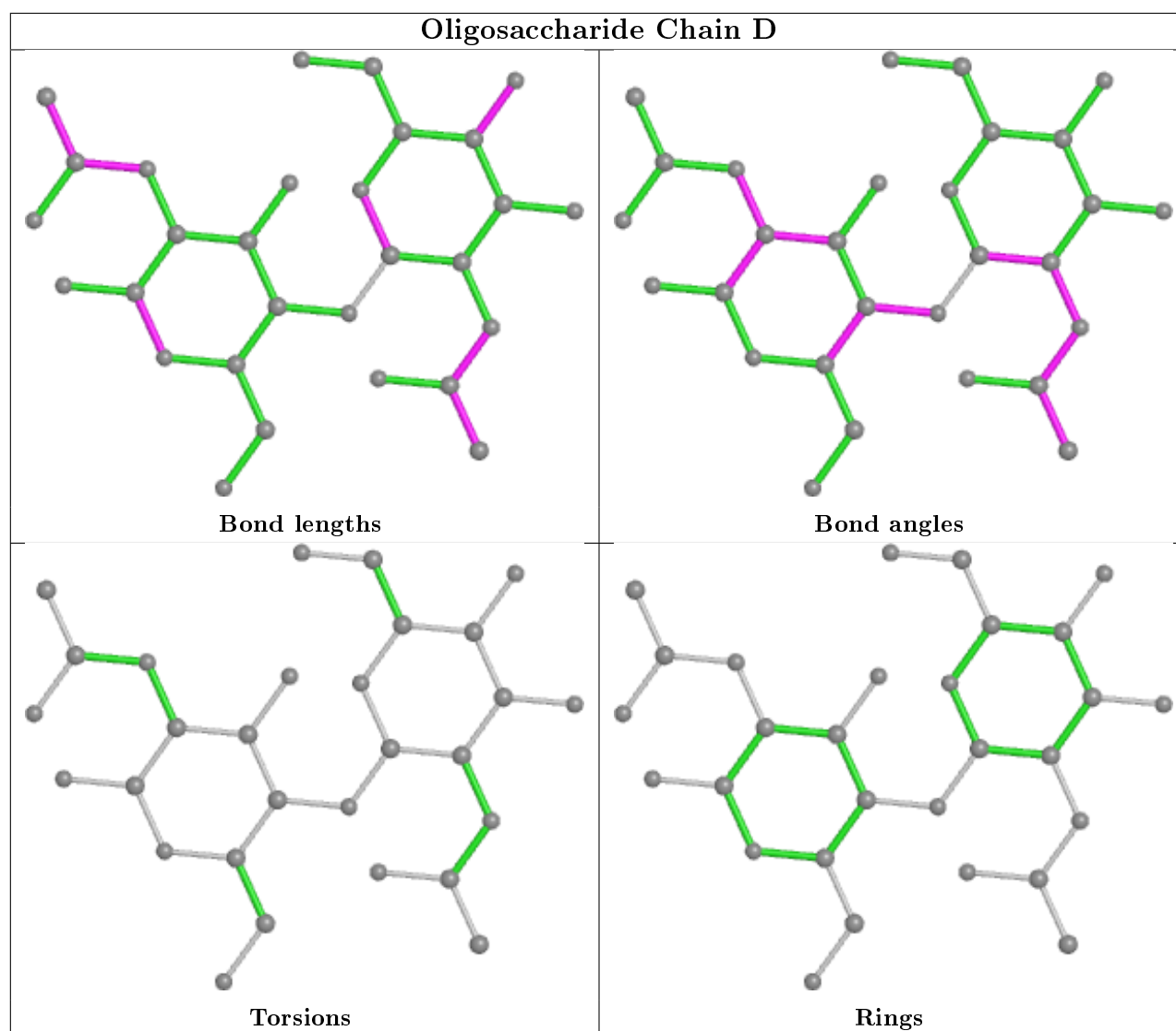
There are no torsion outliers.

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](#)

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	$\# Z  > 2$
4	GOL	A	904	-	5,5,5	0.44	0	5,5,5	0.62	0
4	GOL	B	904	-	5,5,5	0.16	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PO4	B	902	-	4,4,4	1.50	1 (25%)	6,6,6	0.81	0
4	GOL	B	903	-	5,5,5	0.31	0	5,5,5	0.80	0
4	GOL	A	905	-	5,5,5	0.24	0	5,5,5	1.07	0
4	GOL	A	908	-	5,5,5	0.24	0	5,5,5	0.28	0
3	PO4	B	901	-	4,4,4	1.42	1 (25%)	6,6,6	1.15	0
4	GOL	A	906	-	5,5,5	0.30	0	5,5,5	0.45	0
4	GOL	B	908	-	5,5,5	0.23	0	5,5,5	0.28	0
3	PO4	A	901	-	4,4,4	1.52	1 (25%)	6,6,6	1.38	1 (16%)
4	GOL	B	907	-	5,5,5	0.23	0	5,5,5	0.39	0
4	GOL	B	906	-	5,5,5	0.29	0	5,5,5	0.48	0
3	PO4	A	902	-	4,4,4	1.31	0	6,6,6	1.05	1 (16%)
4	GOL	B	905	-	5,5,5	0.28	0	5,5,5	0.78	0
4	GOL	A	907	-	5,5,5	0.18	0	5,5,5	0.53	0
4	GOL	A	903	-	5,5,5	0.33	0	5,5,5	0.58	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
4	GOL	A	904	-	-	4/4/4/4	-
4	GOL	B	904	-	-	2/4/4/4	-
4	GOL	B	907	-	-	3/4/4/4	-
4	GOL	A	908	-	-	4/4/4/4	-
4	GOL	A	905	-	-	1/4/4/4	-
4	GOL	B	903	-	-	0/4/4/4	-
4	GOL	A	906	-	-	2/4/4/4	-
4	GOL	B	908	-	-	2/4/4/4	-
4	GOL	B	906	-	-	0/4/4/4	-
4	GOL	B	905	-	-	2/4/4/4	-
4	GOL	A	907	-	-	1/4/4/4	-
4	GOL	A	903	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	PO4	P-O4	-2.37	1.47	1.54
3	B	902	PO4	P-O1	2.26	1.56	1.50
3	B	901	PO4	P-O4	-2.16	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	PO4	O4-P-O2	-2.37	100.35	107.97
3	A	902	PO4	O4-P-O2	2.30	115.36	107.97

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	904	GOL	O1-C1-C2-O2
4	A	904	GOL	O1-C1-C2-C3
4	A	904	GOL	C1-C2-C3-O3
4	B	904	GOL	O1-C1-C2-C3
4	A	908	GOL	C1-C2-C3-O3
4	A	906	GOL	O1-C1-C2-C3
4	B	908	GOL	C1-C2-C3-O3
4	B	908	GOL	O2-C2-C3-O3
4	B	907	GOL	C1-C2-C3-O3
4	B	905	GOL	O1-C1-C2-C3
4	B	904	GOL	O1-C1-C2-O2
4	A	905	GOL	O1-C1-C2-C3
4	A	907	GOL	O1-C1-C2-C3
4	A	904	GOL	O2-C2-C3-O3
4	A	908	GOL	O2-C2-C3-O3
4	A	906	GOL	O1-C1-C2-O2
4	B	905	GOL	O1-C1-C2-O2
4	A	908	GOL	O1-C1-C2-O2
4	B	907	GOL	O2-C2-C3-O3
4	A	908	GOL	O1-C1-C2-C3
4	A	903	GOL	O1-C1-C2-C3
4	B	907	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	904	GOL	2	0
4	A	905	GOL	2	0
4	A	906	GOL	1	0
4	B	905	GOL	1	0
4	A	907	GOL	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	485/486 (99%)	-0.04	5 (1%) 82 87	20, 31, 51, 74	0
1	B	485/486 (99%)	0.08	17 (3%) 44 53	21, 33, 52, 70	0
All	All	970/972 (99%)	0.02	22 (2%) 60 69	20, 32, 52, 74	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	571	VAL	3.5
1	B	445	ASN	3.2
1	A	579	ILE	3.1
1	B	579	ILE	3.0
1	B	365	VAL	2.7
1	B	453	ALA	2.6
1	B	679	GLU	2.6
1	A	366	LEU	2.5
1	B	576	PHE	2.3
1	B	444	GLY	2.3
1	A	679	GLU	2.2
1	B	616	ALA	2.2
1	A	614	VAL	2.2
1	B	366	LEU	2.2
1	B	639	ARG	2.2
1	B	615	ALA	2.2
1	A	576	PHE	2.1
1	B	613	ILE	2.1
1	B	614	VAL	2.1
1	B	364	LYS	2.1
1	B	574	GLY	2.0
1	B	463	VAL	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 ⓘ

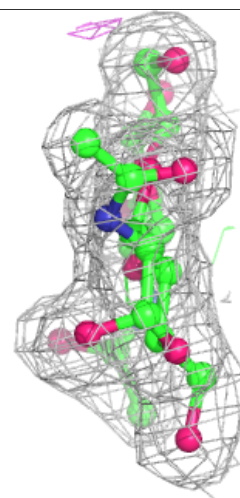
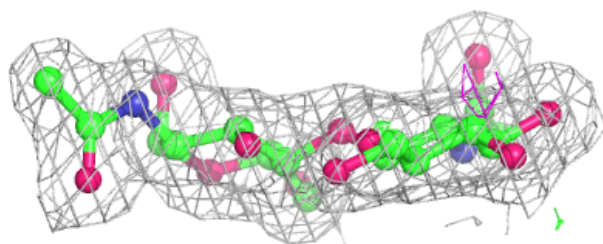
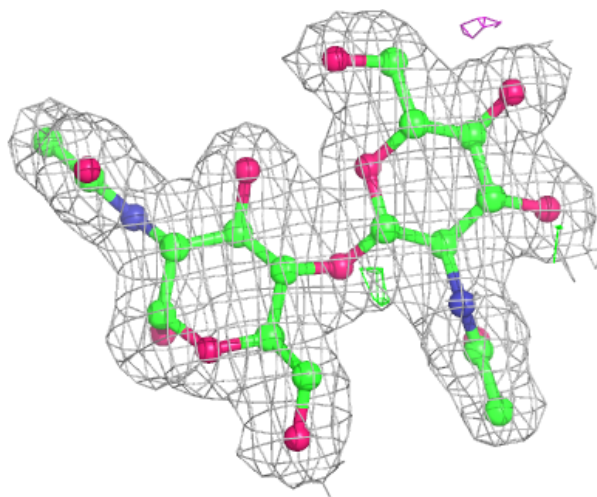
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

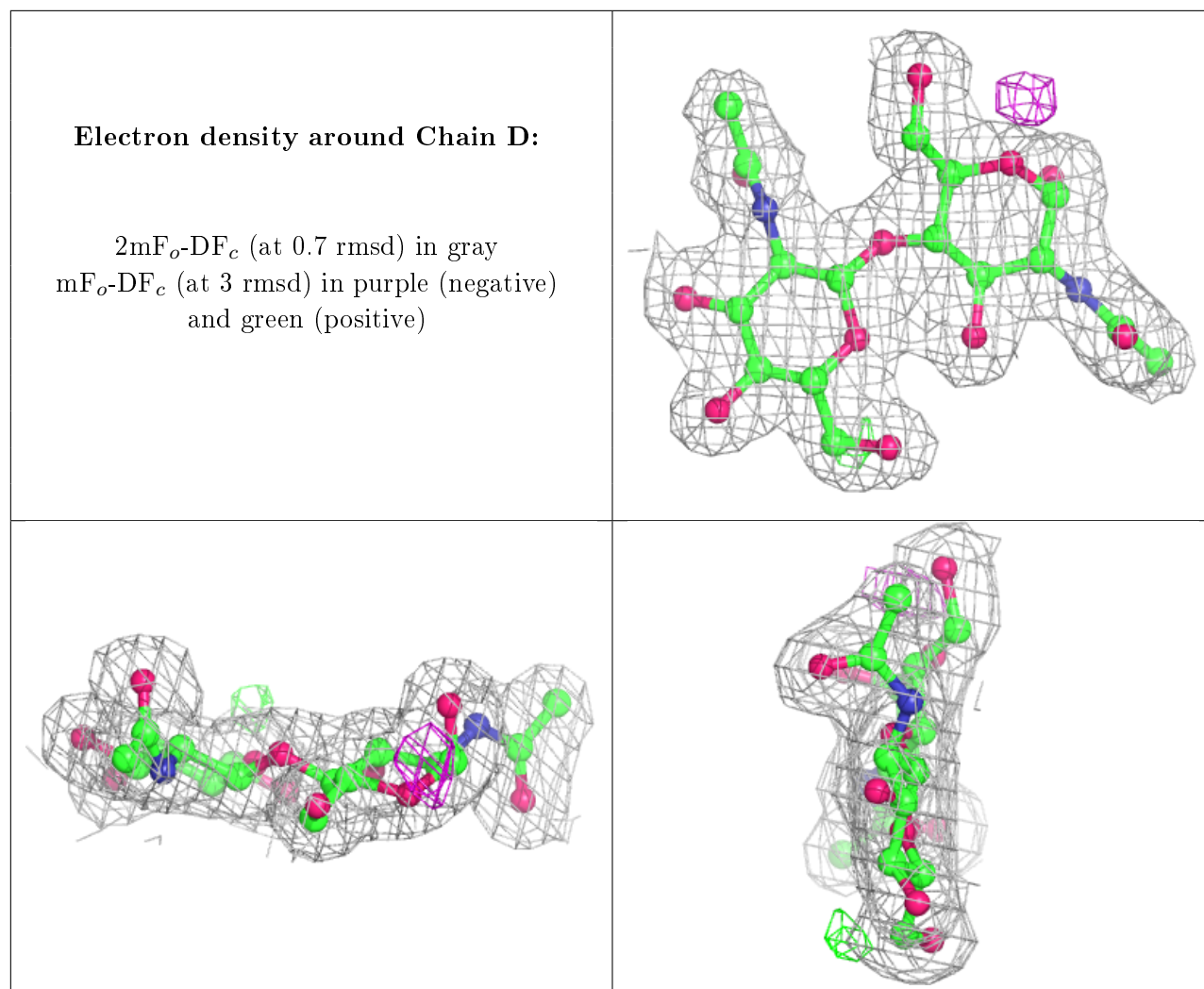
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	2	14/15	0.98	0.09	22,24,30,31	0
2	NDG	D	1	15/15	0.98	0.08	21,27,34,34	0
2	NDG	C	1	15/15	0.98	0.07	25,27,32,37	0
2	NAG	D	2	14/15	0.99	0.11	21,23,29,33	0

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)





## 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
4	GOL	B	906	6/6	0.78	0.18	37,44,55,61	6
4	GOL	B	907	6/6	0.85	0.15	32,37,50,61	0
4	GOL	A	904	6/6	0.88	0.14	49,55,62,63	6
4	GOL	B	908	6/6	0.89	0.13	48,61,67,77	0
4	GOL	B	903	6/6	0.89	0.19	24,39,46,47	6
4	GOL	A	906	6/6	0.89	0.15	36,41,47,62	0
4	GOL	A	908	6/6	0.90	0.15	53,65,66,69	6
4	GOL	B	904	6/6	0.92	0.11	43,50,52,56	6
4	GOL	A	903	6/6	0.93	0.13	30,37,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	907	6/6	0.95	0.11	28,43,48,53	0
4	GOL	A	905	6/6	0.97	0.21	23,37,42,45	0
3	PO4	A	902	5/5	0.97	0.06	24,26,38,38	5
4	GOL	B	905	6/6	0.98	0.19	24,37,40,54	0
3	PO4	B	902	5/5	0.99	0.07	25,26,36,37	5
3	PO4	A	901	5/5	0.99	0.19	26,28,33,35	5
3	PO4	B	901	5/5	1.00	0.18	25,28,34,34	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.