



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2021 – 01:21 PM EDT

PDB ID : 2OK5  
Title : Human Complement factor B  
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Deposited on : 2007-01-16  
Resolution : 2.30 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.

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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 : 2.17.1  
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) : 2.17.1

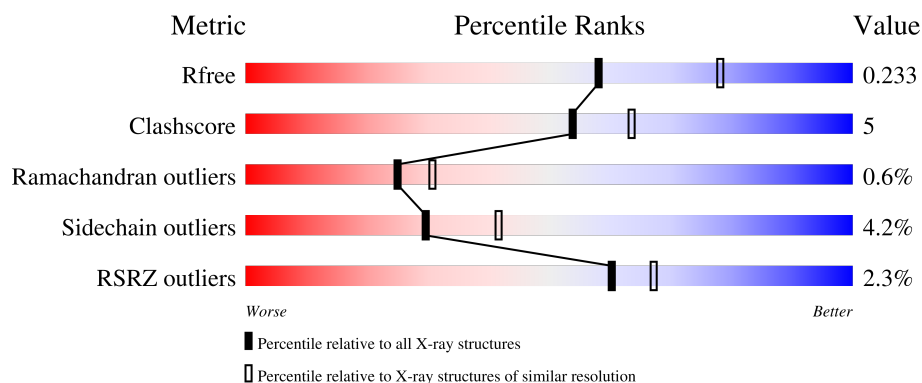
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

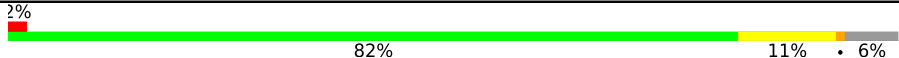
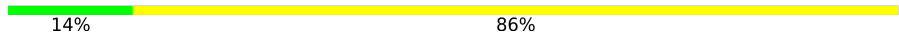
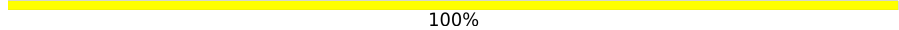
The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	752	 2% 82% 11% • 6%
2	B	7	 14% 86%
3	C	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	1354	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6118 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.

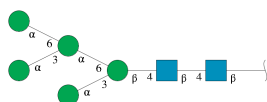
- Molecule 1 is a protein called Complement factor B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	710	5606	3526	978	1069	33	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	cloning artifact	UNP P00751
A	-8	SER	-	cloning artifact	UNP P00751
A	-7	HIS	-	expression tag	UNP P00751
A	-6	HIS	-	expression tag	UNP P00751
A	-5	HIS	-	expression tag	UNP P00751
A	-4	HIS	-	expression tag	UNP P00751
A	-3	HIS	-	expression tag	UNP P00751
A	-2	HIS	-	expression tag	UNP P00751
A	-1	GLY	-	cloning artifact	UNP P00751
A	0	SER	-	cloning artifact	UNP P00751
A	740	ALA	-	cloning artifact	UNP P00751
A	741	ALA	-	cloning artifact	UNP P00751
A	742	ALA	-	cloning artifact	UNP P00751

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	7	83	46	2	35	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

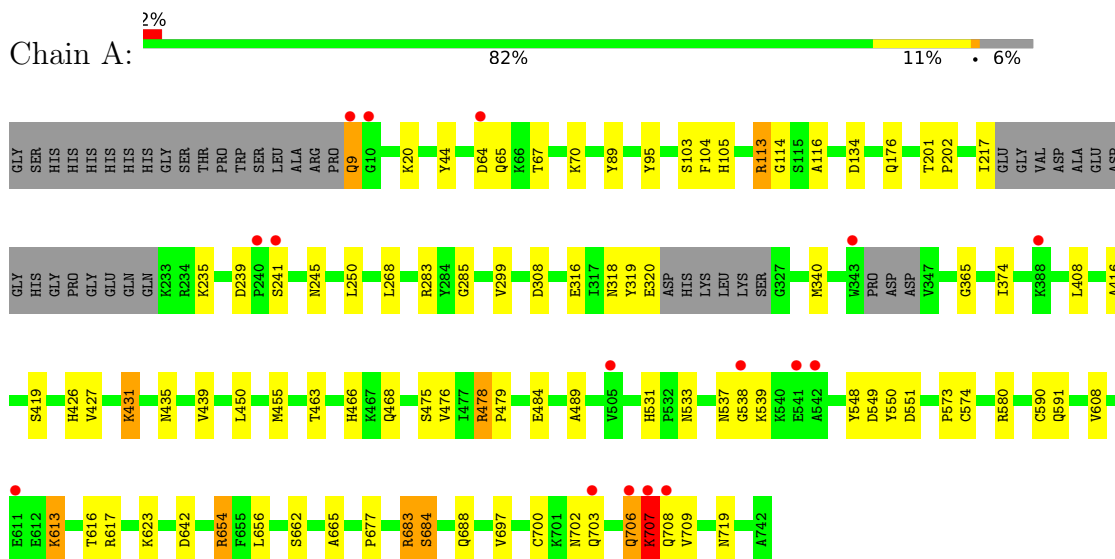
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	295	Total 295	O 295	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.

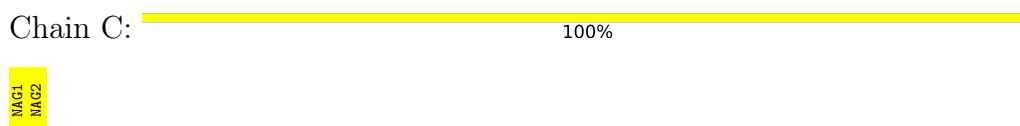
- Molecule 1: Complement factor B



- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.03Å 104.03Å 151.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 – 2.30 57.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (60.00-2.30) 99.8 (57.89-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, $R_{free}$	0.195 , 0.241 0.190 , 0.233	Depositor DCC
$R_{free}$ test set	2147 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, MAN, NAG, BMA

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	0.50	0/5730	0.61	1/7752 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	LYS	Peptide
1	A	537	ASN	Peptide

### 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	5606	0	5478	61	0
2	B	83	0	70	0	0
3	C	28	0	25	0	0
4	A	28	0	26	0	0
5	A	78	0	104	11	0
6	A	295	0	0	4	0
All	All	6118	0	5703	61	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 5.

All (61) 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:706:GLN:HA	1:A:707:LYS:CB	1.77	1.13
1:A:574:CYS:HB3	6:A:1411:HOH:O	1.49	1.12
1:A:706:GLN:HA	1:A:707:LYS:HB3	1.29	1.05
1:A:201:THR:HA	5:A:1354:GOL:H31	1.43	1.01
1:A:468:GLN:HE21	1:A:617:ARG:HE	1.20	0.84
1:A:202:PRO:HD3	5:A:1354:GOL:H32	1.64	0.78
1:A:435:ASN:HD22	5:A:1354:GOL:H32	1.48	0.77
1:A:202:PRO:HD3	5:A:1354:GOL:C3	2.16	0.76
1:A:531:HIS:HD2	1:A:533:ASN:H	1.35	0.74
1:A:463:THR:H	1:A:466:HIS:CD2	2.09	0.71
1:A:706:GLN:HA	1:A:707:LYS:HB2	1.70	0.70
1:A:463:THR:H	1:A:466:HIS:HD2	1.42	0.67
1:A:435:ASN:ND2	5:A:1354:GOL:H32	2.10	0.67
1:A:299:VAL:HG22	1:A:340:MET:HE2	1.82	0.61
1:A:550:TYR:CE2	1:A:654:ARG:HD3	2.37	0.59
1:A:250:LEU:HD21	1:A:268:LEU:HD11	1.86	0.57
1:A:707:LYS:HG2	1:A:709:VAL:HG23	1.86	0.57
1:A:706:GLN:CA	1:A:707:LYS:HB3	2.20	0.56
1:A:616:THR:HG23	6:A:1610:HOH:O	2.07	0.54
1:A:374:ILE:HD11	1:A:416:ALA:HB1	1.90	0.54
1:A:468:GLN:NE2	1:A:617:ARG:HE	1.99	0.54
1:A:549:ASP:OD1	1:A:654:ARG:HD2	2.09	0.53
1:A:623:LYS:HE2	1:A:662:SER:O	2.08	0.53
1:A:245:ASN:HD21	1:A:283:ARG:HH21	1.56	0.53
1:A:202:PRO:HD3	5:A:1354:GOL:H31	1.89	0.53
1:A:538:GLY:HA3	6:A:1471:HOH:O	2.08	0.52
1:A:103:SER:OG	1:A:105:HIS:HE1	1.94	0.51
1:A:217:ILE:HD11	1:A:235:LYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:GLY:HA3	1:A:340:MET:HE1	1.91	0.50
1:A:531:HIS:CD2	1:A:533:ASN:H	2.23	0.50
1:A:550:TYR:CZ	1:A:654:ARG:HD3	2.47	0.50
1:A:707:LYS:HA	1:A:708:GLN:C	2.32	0.48
1:A:613:LYS:HE3	1:A:613:LYS:HA	1.95	0.48
1:A:702:ASN:O	1:A:707:LYS:HB2	2.13	0.47
1:A:468:GLN:HG2	1:A:608:VAL:HG21	1.96	0.47
1:A:285:GLY:HA3	1:A:340:MET:CE	2.45	0.47
1:A:573:PRO:HD3	1:A:688:GLN:O	2.15	0.46
1:A:20:LYS:HB2	1:A:70:LYS:HE3	1.97	0.46
1:A:468:GLN:HE21	1:A:617:ARG:NE	2.00	0.46
1:A:476:VAL:HB	1:A:484:GLU:HB3	1.96	0.46
1:A:538:GLY:CA	1:A:539:LYS:HB2	2.44	0.46
1:A:665:ALA:HB3	5:A:1361:GOL:H11	1.98	0.46
1:A:548:TYR:O	1:A:551:ASP:HB2	2.15	0.45
1:A:574:CYS:CB	6:A:1411:HOH:O	2.28	0.45
1:A:489:ALA:HB2	1:A:677:PRO:HG3	1.99	0.45
1:A:706:GLN:CA	1:A:707:LYS:CB	2.67	0.44
1:A:44:TYR:CE1	5:A:1362:GOL:H2	2.53	0.44
1:A:656:LEU:HG	1:A:719:ASN:HB2	2.00	0.43
1:A:113:ARG:NH2	1:A:134:ASP:OD2	2.52	0.43
1:A:683:ARG:O	1:A:684:SER:HB2	2.18	0.43
1:A:431:LYS:HE3	5:A:1354:GOL:H2	2.01	0.43
1:A:419:SER:HB2	1:A:426:HIS:CD2	2.55	0.42
1:A:9:GLN:HE21	1:A:9:GLN:N	2.17	0.42
1:A:478:ARG:HA	1:A:479:PRO:HD2	1.90	0.42
1:A:319:TYR:HA	1:A:320:GLU:HA	1.81	0.41
1:A:590:CYS:SG	5:A:1358:GOL:H31	2.60	0.41
1:A:114:GLY:HA2	5:A:1364:GOL:H12	2.01	0.41
1:A:89:TYR:HB3	1:A:104:PHE:CD1	2.55	0.41
1:A:202:PRO:HA	1:A:439:VAL:HG22	2.04	0.40
1:A:95:TYR:CD2	1:A:95:TYR:C	2.95	0.40
1:A:103:SER:HA	1:A:116:ALA:O	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	702/752 (93%)	682 (97%)	16 (2%)	4 (1%)	25	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	GLY
1	A	707	LYS
1	A	703	GLN
1	A	706	GLN

### 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	618/652 (95%)	592 (96%)	26 (4%)	30	42

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	64	ASP
1	A	65	GLN
1	A	67	THR
1	A	176	GLN
1	A	239	ASP
1	A	241	SER

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Mol	Chain	Res	Type
1	A	308	ASP
1	A	316	GLU
1	A	318	ASN
1	A	408	LEU
1	A	427	VAL
1	A	450	LEU
1	A	455	MET
1	A	475	SER
1	A	478	ARG
1	A	580	ARG
1	A	591	GLN
1	A	613	LYS
1	A	642	ASP
1	A	654	ARG
1	A	683	ARG
1	A	684	SER
1	A	697	VAL
1	A	700	CYS
1	A	707	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	165	HIS
1	A	176	GLN
1	A	318	ASN
1	A	357	HIS
1	A	367	HIS
1	A	435	ASN
1	A	466	HIS
1	A	468	GLN
1	A	531	HIS
1	A	601	GLN

### 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 ⓘ

9 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	B	1	2,1	14,14,15	0.82	0	17,19,21	0.96	1 (5%)
2	NAG	B	2	2	14,14,15	0.62	0	17,19,21	1.17	2 (11%)
2	BMA	B	3	2	11,11,12	0.71	0	15,15,17	0.77	0
2	MAN	B	4	2	11,11,12	0.63	0	15,15,17	1.14	1 (6%)
2	MAN	B	5	2	11,11,12	0.61	0	15,15,17	1.25	2 (13%)
2	MAN	B	6	2	11,11,12	0.65	0	15,15,17	1.12	1 (6%)
2	MAN	B	7	2	11,11,12	0.69	0	15,15,17	1.58	2 (13%)
3	NAG	C	1	1,3	14,14,15	0.66	0	17,19,21	1.35	1 (5%)
3	NAG	C	2	3	14,14,15	0.55	0	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	NAG	B	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
2	MAN	B	4	2	-	1/2/19/22	0/1/1/1
2	MAN	B	5	2	-	2/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	0/1/1/1
2	MAN	B	7	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	MAN	C3-C4-C5	4.18	117.69	110.24
2	B	6	MAN	O5-C5-C6	3.34	112.44	107.20
3	C	2	NAG	C2-N2-C7	3.22	127.48	122.90
2	B	4	MAN	C1-O5-C5	2.89	116.10	112.19
2	B	2	NAG	C1-O5-C5	2.77	115.94	112.19
2	B	7	MAN	O5-C5-C6	2.76	111.52	107.20
2	B	5	MAN	C1-O5-C5	2.51	115.59	112.19
3	C	1	NAG	O5-C1-C2	-2.48	107.36	111.29
3	C	2	NAG	C4-C3-C2	2.36	114.47	111.02
2	B	5	MAN	C3-C4-C5	2.20	114.17	110.24
2	B	1	NAG	O5-C1-C2	-2.20	107.82	111.29
2	B	2	NAG	C8-C7-N2	2.19	119.81	116.10

There are no chirality outliers.

All (16) torsion outliers are listed below:

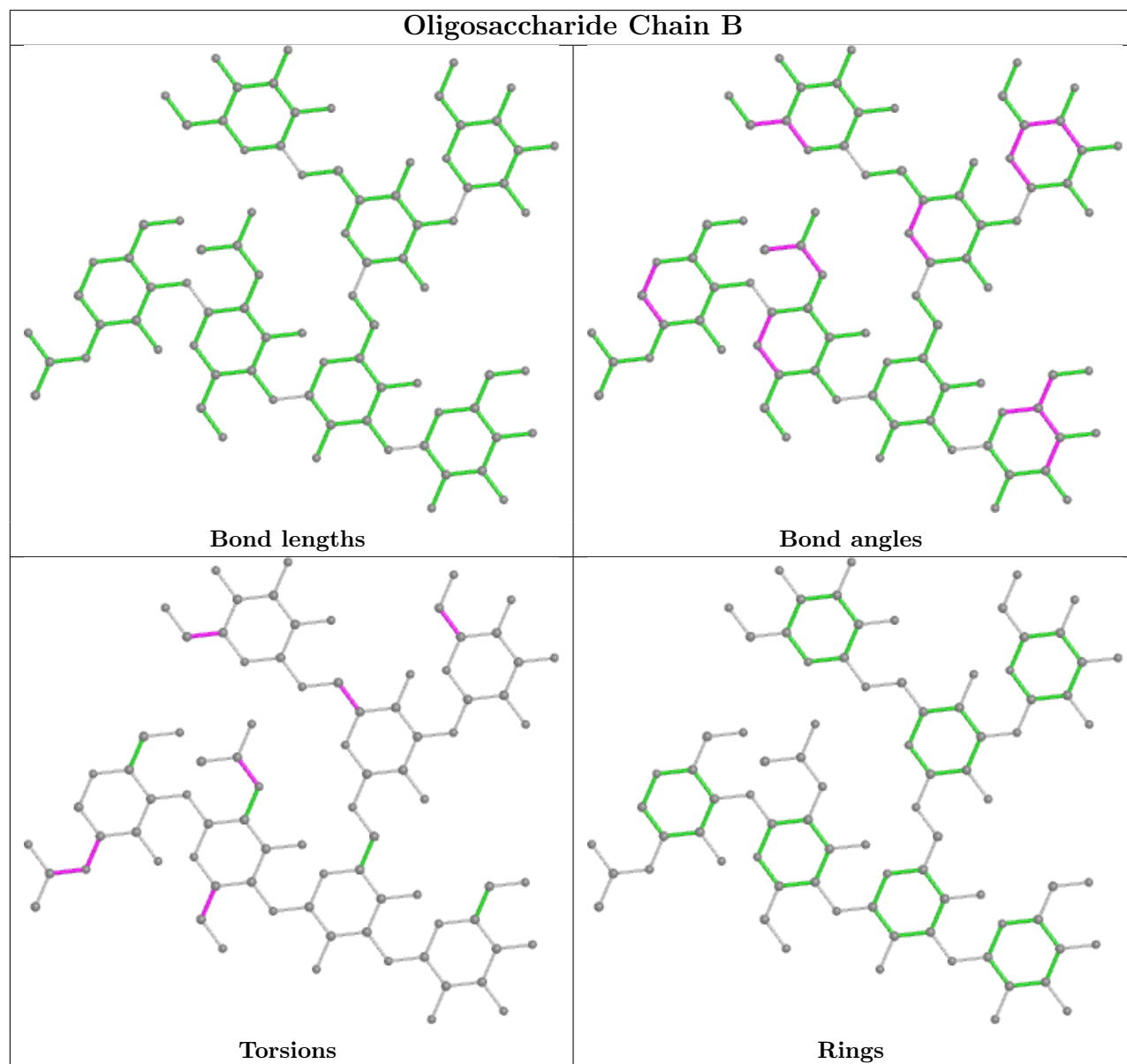
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	5	MAN	C4-C5-C6-O6
2	B	5	MAN	O5-C5-C6-O6
2	B	1	NAG	O7-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	6	MAN	C4-C5-C6-O6
2	B	6	MAN	O5-C5-C6-O6
2	B	1	NAG	C1-C2-N2-C7
2	B	2	NAG	C4-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6

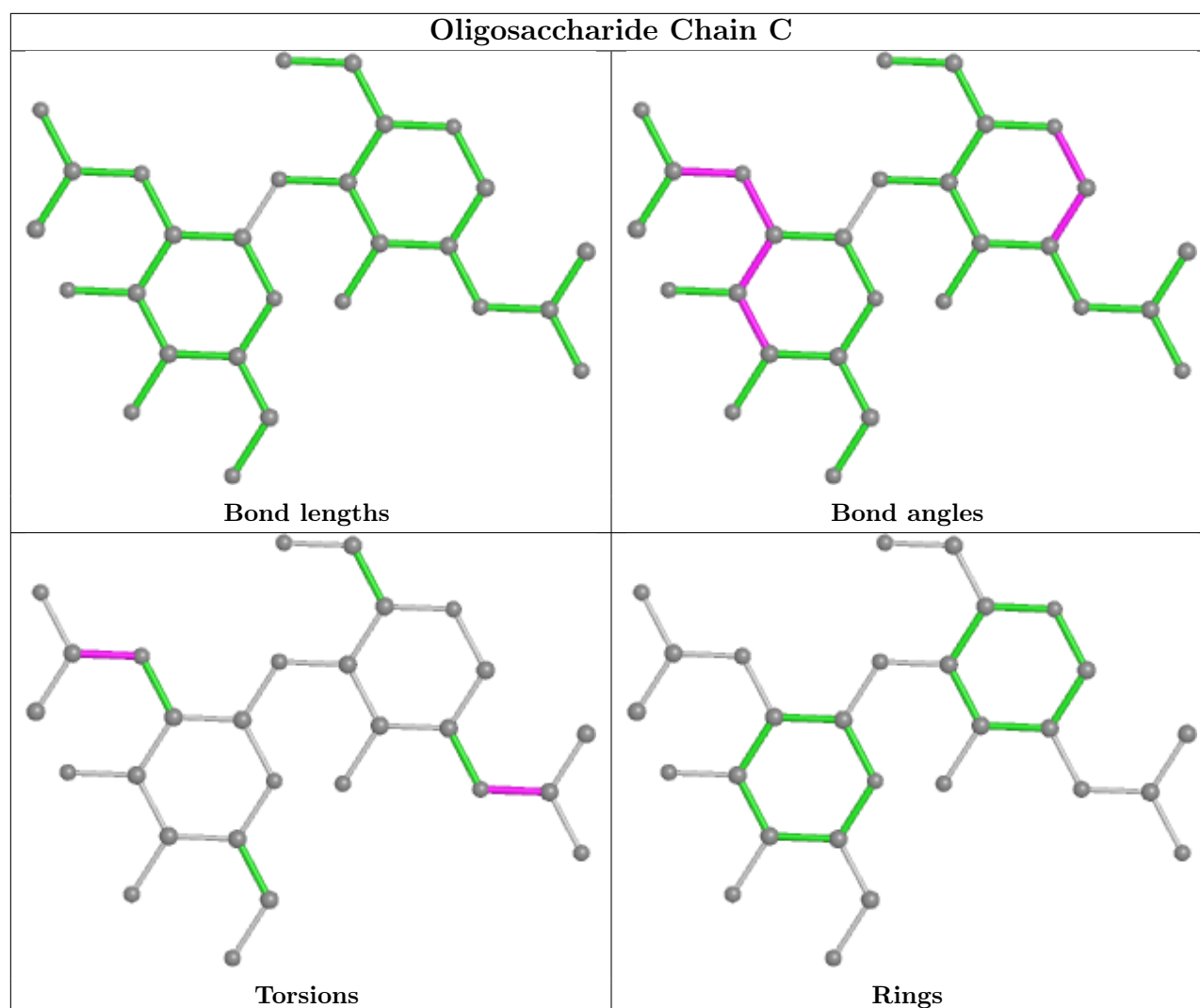
There are no ring outliers.



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](#)

15 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	$\# Z  > 2$
5	GOL	A	1366	-	5,5,5	0.38	0	5,5,5	0.33	0
5	GOL	A	1354	-	5,5,5	0.34	0	5,5,5	0.71	0
5	GOL	A	1361	-	5,5,5	0.37	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1260	1	14,14,15	0.52	0	17,19,21	1.51	3 (17%)
5	GOL	A	1364	-	5,5,5	0.37	0	5,5,5	0.33	0
5	GOL	A	1365	-	5,5,5	0.37	0	5,5,5	0.39	0
5	GOL	A	1359	-	5,5,5	0.35	0	5,5,5	0.27	0
5	GOL	A	1360	-	5,5,5	0.39	0	5,5,5	0.34	0
5	GOL	A	1356	-	5,5,5	0.36	0	5,5,5	0.23	0
5	GOL	A	1357	-	5,5,5	0.37	0	5,5,5	0.41	0
5	GOL	A	1355	-	5,5,5	0.30	0	5,5,5	0.34	0
5	GOL	A	1358	-	5,5,5	0.38	0	5,5,5	0.41	0
5	GOL	A	1362	-	5,5,5	0.42	0	5,5,5	0.36	0
5	GOL	A	1363	-	5,5,5	0.34	0	5,5,5	0.37	0
4	NAG	A	1353	1	14,14,15	0.42	0	17,19,21	1.12	1 (5%)

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
5	GOL	A	1366	-	-	4/4/4/4	-
5	GOL	A	1354	-	-	0/4/4/4	-
5	GOL	A	1361	-	-	0/4/4/4	-
4	NAG	A	1260	1	-	4/6/23/26	0/1/1/1
5	GOL	A	1364	-	-	2/4/4/4	-
5	GOL	A	1365	-	-	3/4/4/4	-
5	GOL	A	1359	-	-	3/4/4/4	-
5	GOL	A	1360	-	-	4/4/4/4	-
5	GOL	A	1356	-	-	0/4/4/4	-
5	GOL	A	1357	-	-	4/4/4/4	-
5	GOL	A	1355	-	-	2/4/4/4	-
5	GOL	A	1358	-	-	4/4/4/4	-
5	GOL	A	1362	-	-	2/4/4/4	-
5	GOL	A	1363	-	-	4/4/4/4	-
4	NAG	A	1353	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1260	NAG	C3-C4-C5	3.34	116.19	110.24
4	A	1353	NAG	C1-O5-C5	2.94	116.17	112.19
4	A	1260	NAG	C4-C3-C2	2.92	115.30	111.02
4	A	1260	NAG	O5-C1-C2	-2.16	107.87	111.29

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1353	NAG	C8-C7-N2-C2
4	A	1353	NAG	O7-C7-N2-C2
5	A	1355	GOL	C1-C2-C3-O3
5	A	1358	GOL	C1-C2-C3-O3
5	A	1359	GOL	C1-C2-C3-O3
5	A	1359	GOL	O2-C2-C3-O3
5	A	1360	GOL	O1-C1-C2-C3
5	A	1362	GOL	O1-C1-C2-C3
5	A	1363	GOL	O1-C1-C2-C3
5	A	1365	GOL	C1-C2-C3-O3
5	A	1366	GOL	O1-C1-C2-O2
5	A	1366	GOL	O1-C1-C2-C3
4	A	1260	NAG	O5-C5-C6-O6
4	A	1260	NAG	C4-C5-C6-O6
4	A	1260	NAG	C8-C7-N2-C2
4	A	1260	NAG	O7-C7-N2-C2
5	A	1357	GOL	O1-C1-C2-C3
5	A	1357	GOL	C1-C2-C3-O3
5	A	1358	GOL	O1-C1-C2-C3
5	A	1359	GOL	O1-C1-C2-C3
5	A	1360	GOL	C1-C2-C3-O3
5	A	1363	GOL	C1-C2-C3-O3
5	A	1364	GOL	C1-C2-C3-O3
5	A	1366	GOL	C1-C2-C3-O3
5	A	1355	GOL	O2-C2-C3-O3
5	A	1358	GOL	O1-C1-C2-O2
5	A	1360	GOL	O1-C1-C2-O2
5	A	1360	GOL	O2-C2-C3-O3
5	A	1363	GOL	O1-C1-C2-O2
5	A	1365	GOL	O2-C2-C3-O3
5	A	1358	GOL	O2-C2-C3-O3
5	A	1362	GOL	O1-C1-C2-O2
5	A	1365	GOL	O1-C1-C2-C3
5	A	1357	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	1363	GOL	O2-C2-C3-O3
5	A	1364	GOL	O2-C2-C3-O3
5	A	1366	GOL	O2-C2-C3-O3
5	A	1357	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1354	GOL	7	0
5	A	1361	GOL	1	0
5	A	1364	GOL	1	0
5	A	1358	GOL	1	0
5	A	1362	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 [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	710/752 (94%)	0.11	16 (2%) 60 67	22, 32, 44, 60	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	505	VAL	4.4
1	A	703	GLN	3.0
1	A	706	GLN	2.8
1	A	10	GLY	2.6
1	A	9	GLN	2.6
1	A	538	GLY	2.4
1	A	388	LYS	2.4
1	A	241	SER	2.4
1	A	64	ASP	2.3
1	A	707	LYS	2.2
1	A	542	ALA	2.2
1	A	343	TRP	2.2
1	A	708	GLN	2.1
1	A	611	GLU	2.1
1	A	240	PRO	2.1
1	A	541	GLU	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.

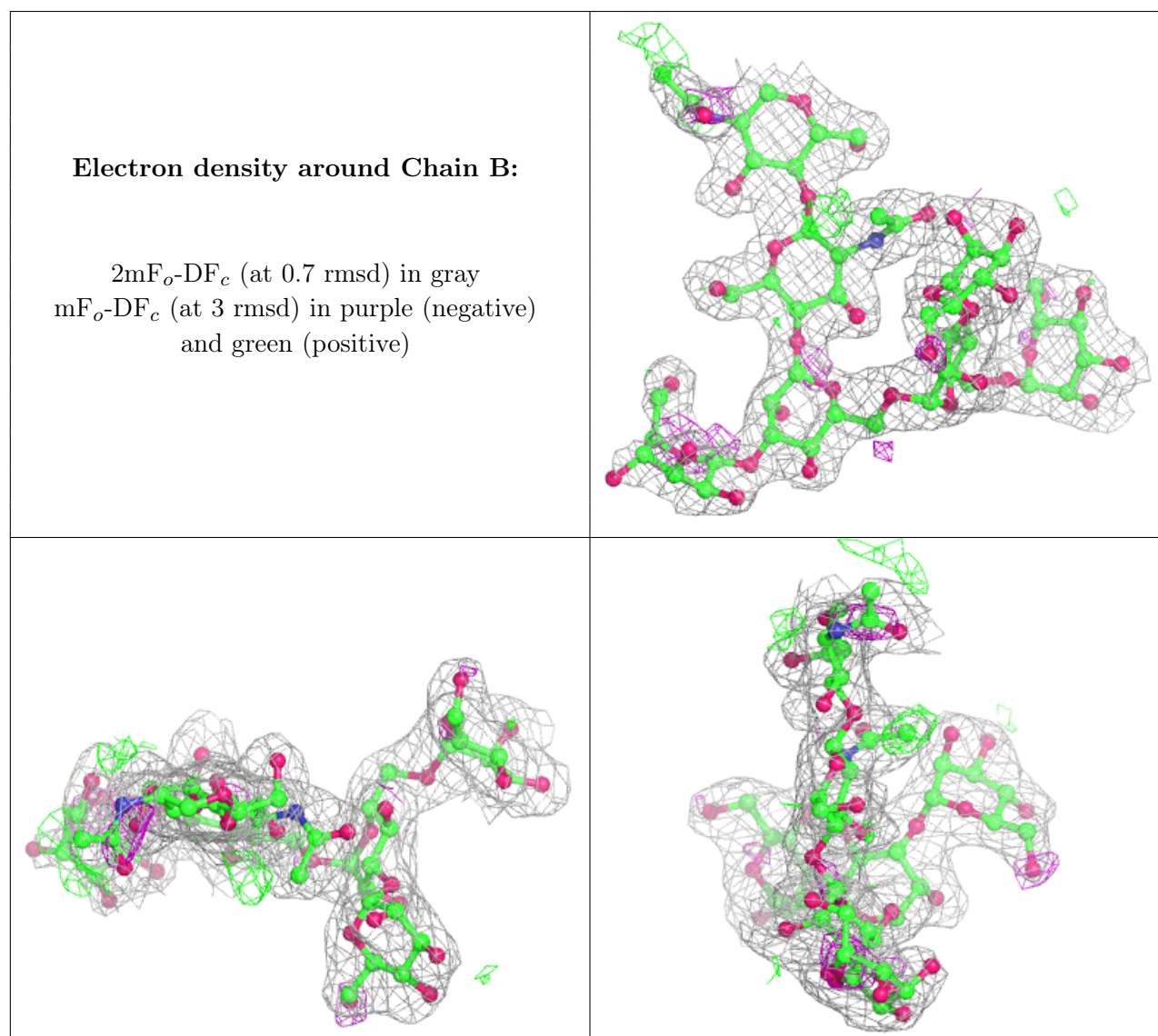
### 6.3 Carbohydrates [i](#)

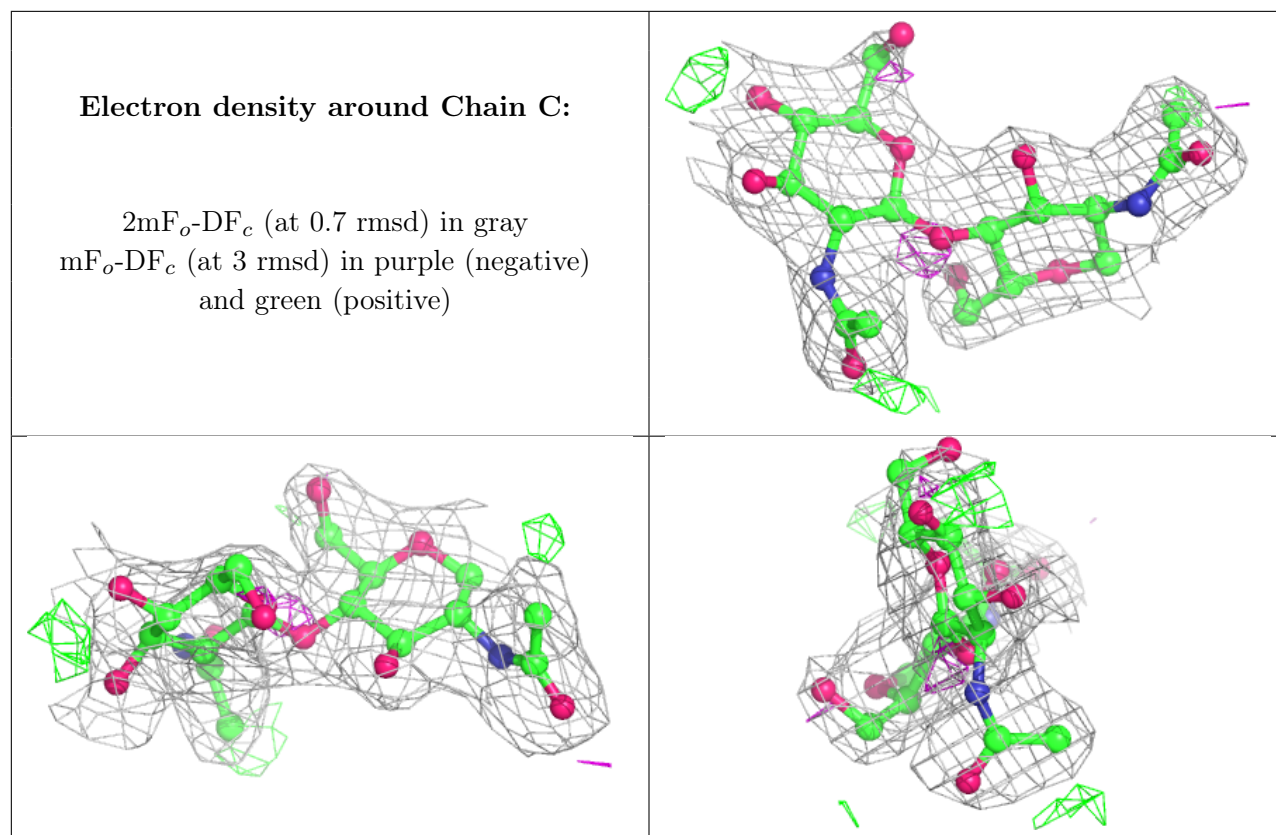
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	B	7	11/12	0.75	0.33	62,65,65,66	0
3	NAG	C	2	14/15	0.80	0.17	53,56,57,58	0
2	BMA	B	3	11/12	0.86	0.15	35,49,52,57	0
2	NAG	B	2	14/15	0.90	0.11	41,44,46,48	0
3	NAG	C	1	14/15	0.91	0.12	38,41,45,50	0
2	NAG	B	1	14/15	0.91	0.12	32,40,46,47	0
2	MAN	B	5	11/12	0.94	0.14	38,40,42,44	0
2	MAN	B	6	11/12	0.95	0.09	25,28,31,34	0
2	MAN	B	4	11/12	0.97	0.09	28,34,36,38	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( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	1364	6/6	0.70	0.34	78,78,79,79	0
5	GOL	A	1362	6/6	0.83	0.33	56,58,58,58	0
5	GOL	A	1358	6/6	0.84	0.18	63,64,64,64	0
4	NAG	A	1353	14/15	0.86	0.28	56,60,61,61	0
5	GOL	A	1360	6/6	0.86	0.24	62,62,62,63	0
5	GOL	A	1359	6/6	0.87	0.29	64,67,67,67	0
5	GOL	A	1365	6/6	0.87	0.25	55,56,57,57	0
5	GOL	A	1354	6/6	0.88	0.35	36,40,41,42	0
5	GOL	A	1356	6/6	0.89	0.33	61,62,62,62	0
5	GOL	A	1366	6/6	0.90	0.20	70,71,71,71	0
4	NAG	A	1260	14/15	0.91	0.16	50,54,55,56	0
5	GOL	A	1357	6/6	0.91	0.22	45,46,46,47	0
5	GOL	A	1355	6/6	0.91	0.22	40,45,45,46	0
5	GOL	A	1363	6/6	0.94	0.28	55,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	1361	6/6	0.94	0.25	43,47,47,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.