



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:39 PM BST

PDB ID : 2XMC  
Title : G117H mutant of human butyrylcholinesterase in complex with fluoride anion  
Authors : Nachon, F.; Carletti, E.; Wandhammer, M.; Nicolet, Y.; Schopfer, L.M.; Masson, P.; Lockridge, O.  
Deposited on : 2010-07-27  
Resolution : 2.40 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

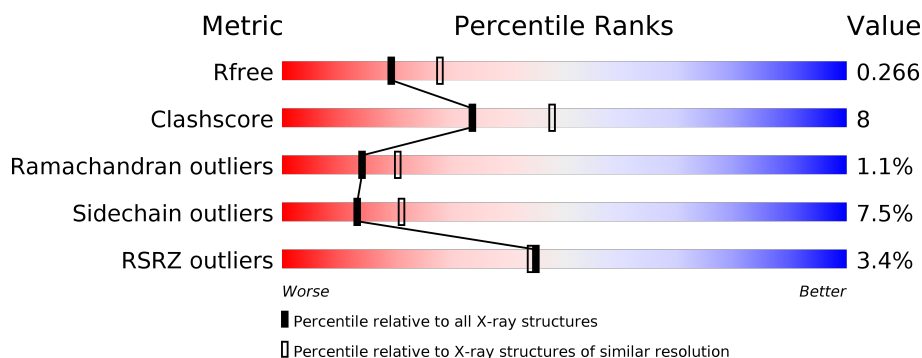
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	529	
2	B	3	
2	D	3	
3	C	2	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	B	3	X	-	-	-
2	NAG	D	2	-	-	-	X
2	FUC	D	3	X	-	-	-
3	FUC	C	2	X	-	-	-
4	UNX	A	1545	-	-	-	X
9	NAG	A	1561	X	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4616 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.

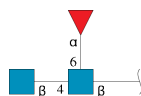
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4216	2721	710	770	15	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	engineered mutation	UNP P06276
A	117	HIS	GLY	engineered mutation	UNP P06276
A	455	GLN	ASN	engineered mutation	UNP P06276
A	481	GLN	ASN	engineered mutation	UNP P06276
A	486	GLN	ASN	engineered mutation	UNP P06276

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

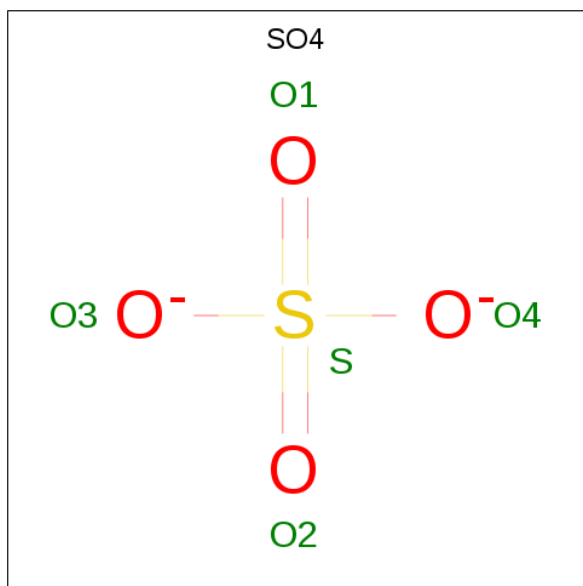
- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	X	0	0
			17	17		

- Molecule 5 is FLUORIDE ION (three-letter code: F) (formula: F).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	F	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

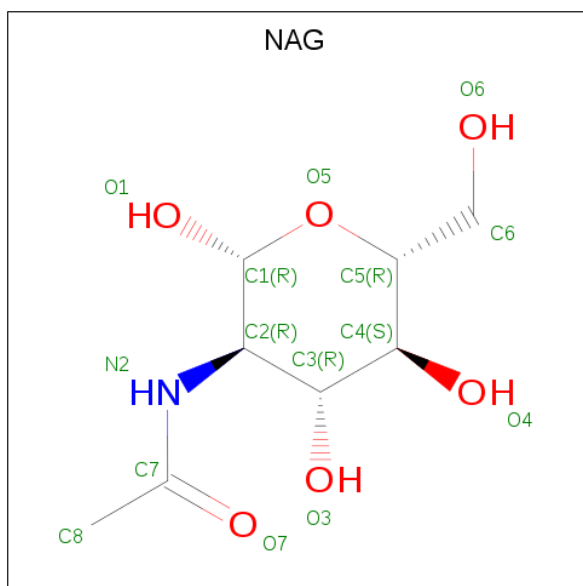
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	Cl	0	0
			5	5		

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total K 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

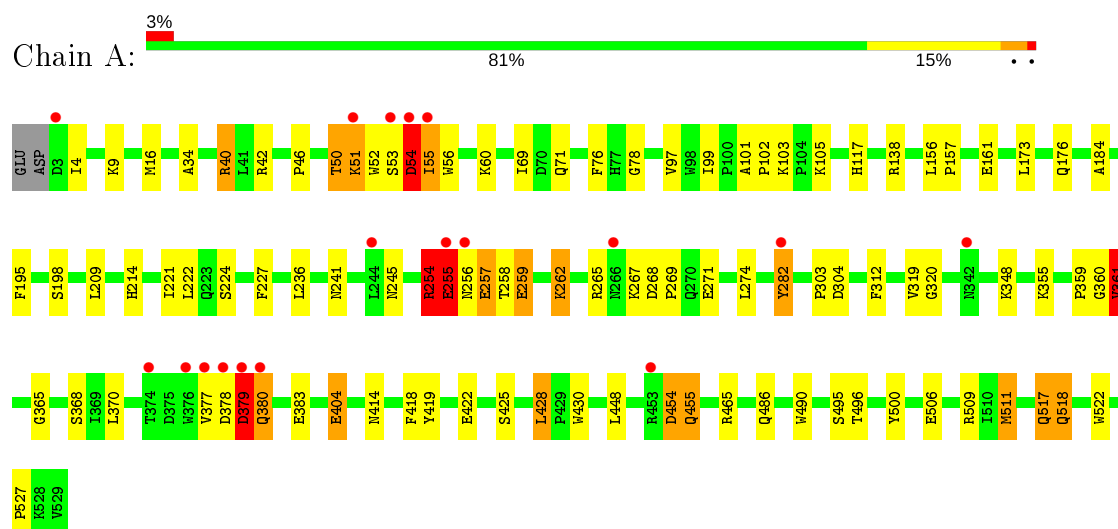
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	229	Total O 229 229	0	0

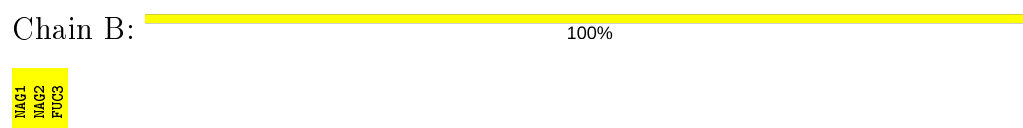
### 3 Residue-property plots [i](#)

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.

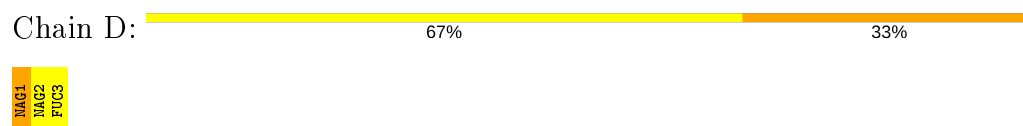
- Molecule 1: CHOLINESTERASE



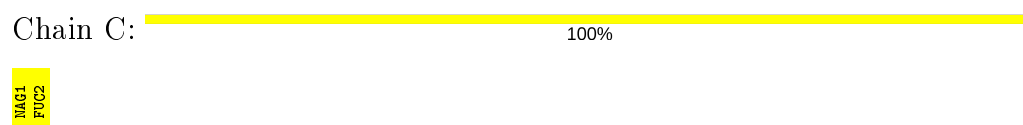
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.59 Å   155.59 Å   127.99 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	109.76 – 2.40 41.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (109.76-2.40) 96.7 (41.14-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.192   ,   0.253 0.207   ,   0.266	Depositor DCC
$R_{free}$ test set	945 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, F, UNX, K, CL, FUC, SO4

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	1.03	2/4340 (0.0%)	0.90	7/5892 (0.1%)

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	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	TRP	CG-CD1	5.39	1.44	1.36
1	A	404	GLU	CG-CD	5.33	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	465	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	511	MET	CG-SD-CE	-5.84	90.85	100.20
1	A	448	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	448	LEU	CB-CG-CD2	5.33	120.05	111.00
1	A	361	VAL	N-CA-C	5.26	125.21	111.00
1	A	465	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	254	ARG	Peptide
1	A	255	GLU	Peptide
1	A	360	GLY	Peptide
1	A	380	GLN	Peptide
1	A	53	SER	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4216	0	4111	71	0
2	B	38	0	34	0	0
2	D	38	0	34	4	0
3	C	24	0	22	0	0
4	A	17	0	0	2	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
7	A	5	0	0	0	0
8	A	1	0	0	0	0
9	A	42	0	39	0	0
10	A	229	0	0	15	0
All	All	4616	0	4240	73	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 8.

All (73) 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:40:ARG:HG2	1:A:40:ARG:HH11	1.08	1.09
1:A:518:GLN:H	1:A:518:GLN:HE21	1.20	0.89
1:A:71:GLN:HG2	10:A:2034:HOH:O	1.73	0.88
1:A:117:HIS:HD2	10:A:2120:HOH:O	1.59	0.84
1:A:40:ARG:HG2	1:A:40:ARG:NH1	1.83	0.81
1:A:454:ASP:O	1:A:455:GLN:HB2	1.83	0.79
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.22	0.75
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:HE3	10:A:2116:HOH:O	1.90	0.69
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.27	0.69
1:A:404:GLU:HG2	10:A:2107:HOH:O	1.94	0.67
1:A:157:PRO:O	10:A:2090:HOH:O	2.12	0.66
1:A:50:THR:HG22	1:A:51:LYS:HE3	1.76	0.66
1:A:241:ASN:HD22	2:D:1:NAG:H83	1.59	0.66
1:A:348:LYS:NZ	10:A:2147:HOH:O	2.30	0.65
1:A:454:ASP:O	1:A:455:GLN:CB	2.44	0.64
1:A:209:LEU:HD22	1:A:312:PHE:HB3	1.80	0.64
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.35	0.62
1:A:227:PHE:CD2	1:A:227:PHE:C	2.73	0.61
1:A:256:ASN:O	1:A:259:GLU:N	2.31	0.61
1:A:378:ASP:O	1:A:380:GLN:NE2	2.33	0.61
1:A:51:LYS:HD3	1:A:51:LYS:H	1.66	0.61
1:A:268:ASP:HB2	1:A:269:PRO:CD	2.31	0.60
1:A:117:HIS:CD2	10:A:2120:HOH:O	2.42	0.59
1:A:268:ASP:HB2	1:A:269:PRO:HD3	1.84	0.58
1:A:222:LEU:N	1:A:222:LEU:HD12	2.19	0.58
1:A:518:GLN:H	1:A:518:GLN:NE2	1.96	0.58
1:A:378:ASP:O	1:A:380:GLN:N	2.37	0.58
1:A:254:ARG:O	1:A:255:GLU:HB3	2.05	0.56
1:A:209:LEU:CD2	1:A:312:PHE:HB3	2.36	0.55
1:A:101:ALA:HA	1:A:102:PRO:C	2.26	0.55
1:A:422:GLU:OE2	1:A:509:ARG:NH2	2.39	0.55
1:A:522:TRP:O	1:A:527:PRO:HD3	2.07	0.54
1:A:282:TYR:CD2	1:A:359:PRO:HB2	2.42	0.53
1:A:40:ARG:HH11	1:A:40:ARG:CG	1.96	0.53
1:A:256:ASN:O	1:A:258:THR:N	2.42	0.53
1:A:377:VAL:HA	1:A:378:ASP:HB2	1.92	0.52
1:A:425:SER:HB3	1:A:428:LEU:HD23	1.91	0.52
1:A:245:ASN:HD21	2:D:1:NAG:H62	1.75	0.51
1:A:214[A]:HIS:HE1	10:A:2132:HOH:O	1.93	0.51
4:A:1531:UNX:UNK	4:A:1532:UNX:UNK	1.54	0.51
1:A:241:ASN:HD22	2:D:1:NAG:C8	2.23	0.51
1:A:198:SER:HA	1:A:224:SER:O	2.11	0.50
1:A:257:GLU:HG2	10:A:2110:HOH:O	2.10	0.50
1:A:267:LYS:CE	10:A:2116:HOH:O	2.53	0.50
1:A:255:GLU:N	1:A:255:GLU:OE1	2.45	0.50
1:A:319:VAL:O	1:A:418:PHE:HA	2.12	0.49
1:A:267:LYS:HD2	1:A:271:GLU:OE1	2.12	0.48
1:A:509:ARG:HD3	10:A:2206:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:NH1	10:A:2015:HOH:O	2.47	0.47
1:A:55:ILE:HD11	10:A:2003:HOH:O	2.14	0.46
4:A:1536:UNX:UNK	4:A:1537:UNX:UNK	1.61	0.45
1:A:383:GLU:CD	1:A:383:GLU:H	2.20	0.44
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.53	0.44
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.79	0.44
1:A:56:TRP:C	1:A:56:TRP:CD1	2.91	0.44
1:A:379:ASP:N	1:A:379:ASP:OD2	2.52	0.43
1:A:241:ASN:HD22	2:D:1:NAG:C7	2.29	0.43
1:A:414:ASN:OD1	10:A:2165:HOH:O	2.21	0.43
1:A:428:LEU:HD12	1:A:430:TRP:HB2	2.01	0.42
1:A:52:TRP:HD1	1:A:54:ASP:HB2	1.85	0.42
1:A:262:LYS:HG2	1:A:265:ARG:NH2	2.35	0.42
1:A:265:ARG:NE	10:A:2112:HOH:O	2.27	0.42
1:A:76:PHE:CE2	1:A:78:GLY:HA3	2.54	0.42
1:A:365:GLY:O	1:A:368:SER:HB2	2.20	0.41
1:A:34:ALA:HB2	1:A:173:LEU:HD23	2.02	0.41
1:A:517:GLN:HE21	1:A:517:GLN:HB3	1.72	0.41
1:A:103:LYS:NZ	1:A:184:ALA:O	2.53	0.41
1:A:46:PRO:HB2	1:A:173:LEU:HD22	2.03	0.41
1:A:221:ILE:C	1:A:222:LEU:HD12	2.41	0.41
1:A:97:VAL:HG12	1:A:99:ILE:HG23	2.02	0.41
1:A:268:ASP:CB	1:A:269:PRO:CD	2.99	0.40
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.56	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	526/529 (99%)	492 (94%)	28 (5%)	6 (1%)	14 20

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	255	GLU
1	A	361	VAL
1	A	379	ASP
1	A	496	THR
1	A	257	GLU

### 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	454/455 (100%)	420 (92%)	34 (8%)	13	21

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	16	MET
1	A	40	ARG
1	A	50	THR
1	A	51	LYS
1	A	54	ASP
1	A	55	ILE
1	A	60	LYS
1	A	69	ILE
1	A	105	LYS
1	A	138	ARG
1	A	156	LEU
1	A	176	GLN
1	A	195	PHE
1	A	254	ARG
1	A	255	GLU
1	A	259	GLU
1	A	262	LYS

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Mol	Chain	Res	Type
1	A	274	LEU
1	A	282	TYR
1	A	304	ASP
1	A	355	LYS
1	A	361	VAL
1	A	370	LEU
1	A	379	ASP
1	A	428	LEU
1	A	454	ASP
1	A	455	GLN
1	A	486	GLN
1	A	495	SER
1	A	506	GLU
1	A	517	GLN
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	GLN
1	A	275	ASN
1	A	380	GLN
1	A	414	ASN
1	A	517	GLN
1	A	518	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 ⓘ

8 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	1,2	14,14,15	0.88	0	17,19,21	2.61	9 (52%)
2	NAG	B	2	2	14,14,15	0.84	0	17,19,21	2.16	7 (41%)
2	FUC	B	3	2	10,10,11	1.25	1 (10%)	14,14,16	3.11	7 (50%)
3	NAG	C	1	1,3	14,14,15	1.16	1 (7%)	17,19,21	1.76	6 (35%)
3	FUC	C	2	3	10,10,11	1.15	1 (10%)	14,14,16	2.18	5 (35%)
2	NAG	D	1	1,2	14,14,15	1.02	1 (7%)	17,19,21	2.86	8 (47%)
2	NAG	D	2	2	14,14,15	1.22	1 (7%)	17,19,21	2.55	7 (41%)
2	FUC	D	3	2	10,10,11	0.87	0	14,14,16	2.45	6 (42%)

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	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUC	B	3	2	1/1/4/5	-	0/1/1/1
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	FUC	C	2	3	1/1/4/5	-	0/1/1/1
2	NAG	D	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	FUC	D	3	2	1/1/4/5	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	3.99	1.58	1.52
3	C	1	NAG	C1-C2	2.77	1.56	1.52
3	C	2	FUC	C2-C3	2.38	1.56	1.52
2	B	3	FUC	C4-C5	2.18	1.57	1.52
2	D	1	NAG	C2-N2	2.15	1.50	1.46

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	FUC	C1-C2-C3	-7.87	99.99	109.67
2	D	1	NAG	C1-O5-C5	7.65	122.56	112.19
2	D	2	NAG	C1-C2-N2	5.10	119.20	110.49
2	D	2	NAG	C3-C4-C5	-4.68	101.90	110.24
2	B	1	NAG	C1-C2-N2	-4.61	102.62	110.49
2	B	1	NAG	C2-N2-C7	4.59	129.43	122.90
2	B	3	FUC	C3-C4-C5	4.55	116.86	109.77
2	D	3	FUC	C1-C2-C3	-4.50	104.13	109.67
2	B	2	NAG	C2-N2-C7	4.42	129.19	122.90
2	D	2	NAG	O5-C5-C6	4.19	113.77	107.20
2	D	1	NAG	O7-C7-C8	-4.18	114.30	122.06
2	B	1	NAG	C3-C4-C5	-4.15	102.84	110.24
2	D	3	FUC	C3-C4-C5	4.04	116.06	109.77
2	B	3	FUC	O5-C1-C2	-3.95	104.67	110.77
2	D	3	FUC	O2-C2-C1	3.94	117.22	109.15
2	B	2	NAG	C3-C4-C5	-3.85	103.36	110.24
2	D	3	FUC	O5-C1-C2	-3.85	104.83	110.77
3	C	2	FUC	C1-C2-C3	-3.82	104.97	109.67
3	C	2	FUC	O3-C3-C2	3.79	117.25	109.99
2	B	3	FUC	C1-O5-C5	-3.77	104.23	112.78
2	D	2	NAG	C1-O5-C5	3.57	117.03	112.19
2	D	1	NAG	C1-C2-N2	3.55	116.55	110.49
2	B	2	NAG	O5-C5-C6	3.53	112.74	107.20
3	C	1	NAG	O4-C4-C5	3.48	117.94	109.30
2	D	1	NAG	O3-C3-C2	3.34	116.37	109.47
2	B	1	NAG	C8-C7-N2	3.18	121.49	116.10
3	C	1	NAG	O5-C5-C6	3.16	112.16	107.20
3	C	2	FUC	C3-C4-C5	3.14	114.66	109.77
2	B	1	NAG	O5-C5-C6	3.02	111.95	107.20
2	B	1	NAG	O6-C6-C5	3.01	121.60	111.29
3	C	2	FUC	C2-C3-C4	-2.99	105.72	110.89
2	D	1	NAG	C8-C7-N2	2.98	121.15	116.10
2	D	2	NAG	C2-N2-C7	2.98	127.15	122.90
2	D	1	NAG	O5-C5-C4	2.87	117.82	110.83
2	D	1	NAG	C4-C3-C2	-2.87	106.81	111.02
2	B	2	NAG	O5-C5-C4	-2.83	103.94	110.83
3	C	1	NAG	C8-C7-N2	2.83	120.89	116.10
2	D	3	FUC	C1-O5-C5	-2.70	106.65	112.78
2	B	1	NAG	C6-C5-C4	2.60	119.10	113.00
2	D	2	NAG	O4-C4-C5	2.60	115.75	109.30
2	D	2	NAG	O3-C3-C2	2.59	114.83	109.47
2	B	1	NAG	O7-C7-C8	-2.54	117.34	122.06
2	B	3	FUC	O2-C2-C3	2.50	115.14	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C3-C4-C5	-2.39	105.98	110.24
2	B	1	NAG	O5-C1-C2	-2.38	107.54	111.29
2	B	2	NAG	C1-O5-C5	-2.31	109.07	112.19
2	D	1	NAG	C2-N2-C7	2.26	126.11	122.90
2	B	3	FUC	C6-C5-C4	2.24	117.20	113.07
3	C	2	FUC	O2-C2-C1	2.23	113.72	109.15
3	C	1	NAG	C2-N2-C7	2.16	125.97	122.90
3	C	1	NAG	O7-C7-C8	-2.14	118.09	122.06
2	B	2	NAG	C6-C5-C4	2.13	117.99	113.00
2	B	3	FUC	C2-C3-C4	2.08	114.50	110.89
2	D	3	FUC	O3-C3-C4	2.05	115.10	110.35
2	B	2	NAG	C4-C3-C2	2.03	113.99	111.02

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	FUC	C1
2	D	3	FUC	C1
2	B	3	FUC	C1

All (14) torsion outliers are listed below:

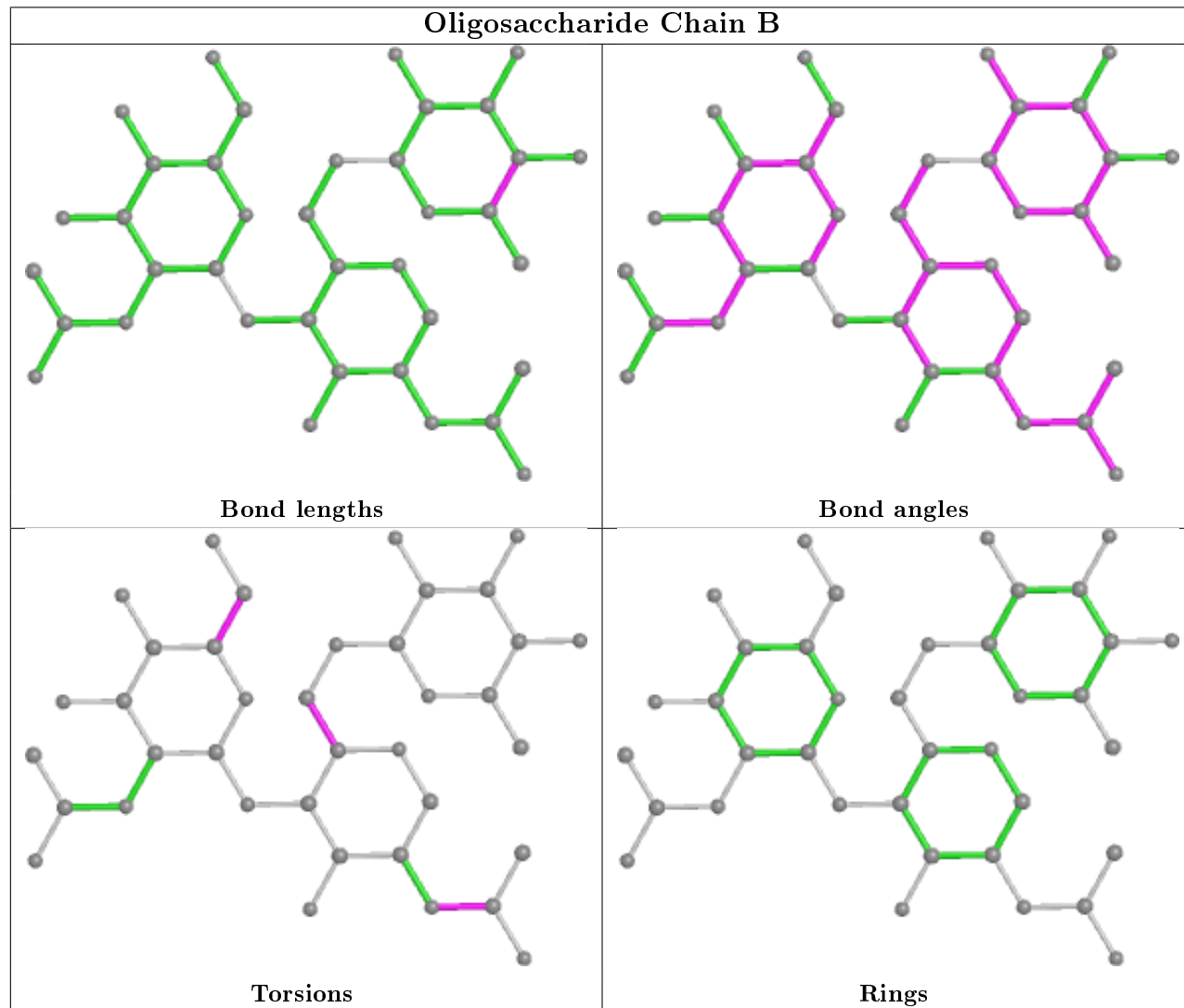
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6

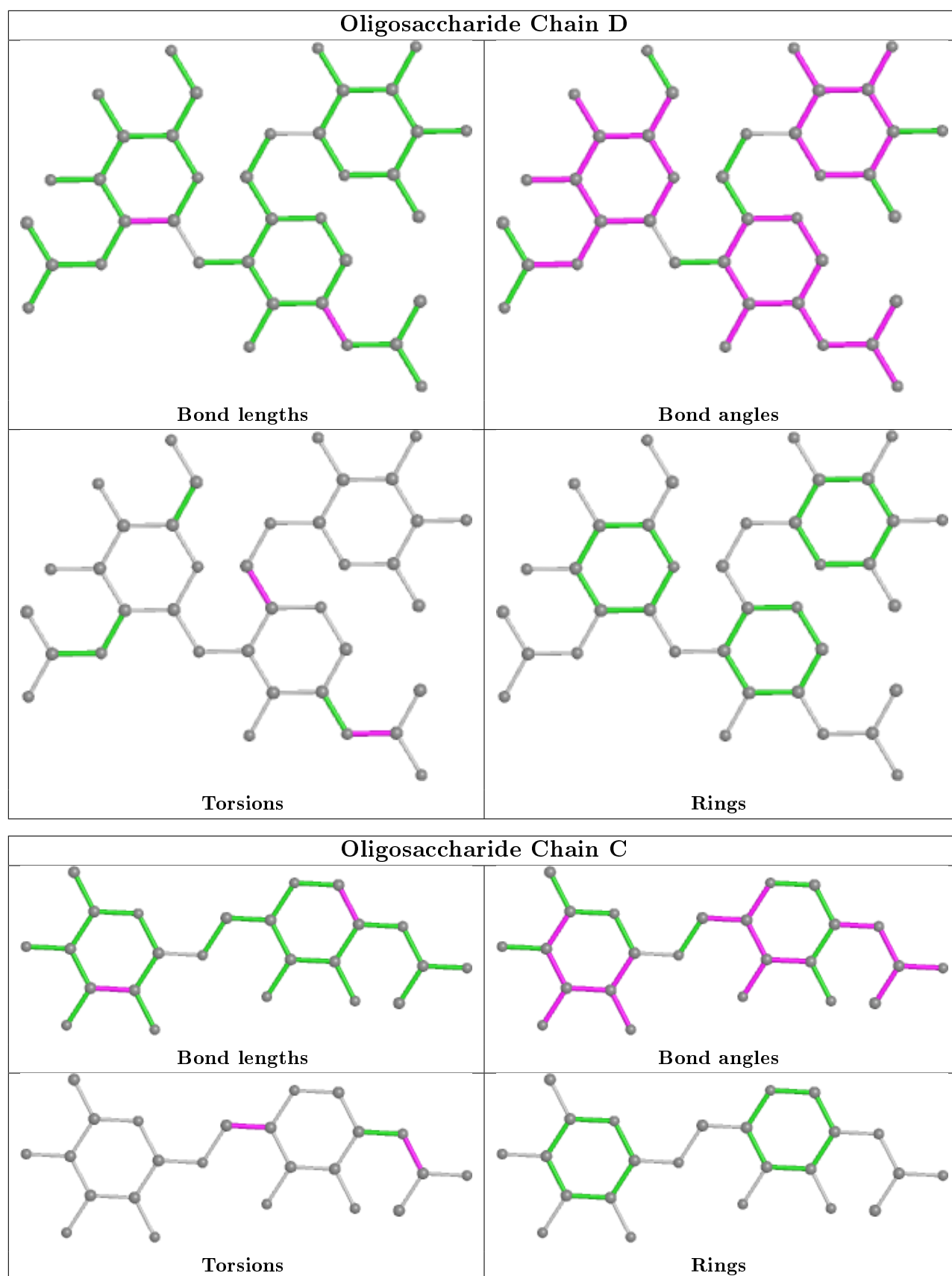
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	4	0

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 28 ligands modelled in this entry, 17 are unknown and 7 are monoatomic - leaving 4 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	$\# Z  > 2$
6	SO4	A	1548	-	4,4,4	0.38	0	6,6,6	0.52	0
9	NAG	A	1560	1	14,14,15	0.75	0	17,19,21	2.58	5 (29%)
9	NAG	A	1561	1	14,14,15	0.91	0	17,19,21	2.68	7 (41%)
9	NAG	A	1559	1	14,14,15	0.75	0	17,19,21	2.54	5 (29%)

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
9	NAG	A	1560	1	-	1/6/23/26	0/1/1/1
9	NAG	A	1561	1	1/1/5/7	4/6/23/26	0/1/1/1
9	NAG	A	1559	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1559	NAG	C1-O5-C5	7.48	122.32	112.19
9	A	1561	NAG	C2-N2-C7	7.19	133.13	122.90
9	A	1560	NAG	C1-O5-C5	6.80	121.40	112.19
9	A	1561	NAG	C1-O5-C5	5.75	119.99	112.19
9	A	1559	NAG	C4-C3-C2	-4.74	104.07	111.02
9	A	1560	NAG	O5-C5-C6	4.45	114.18	107.20
9	A	1560	NAG	C4-C3-C2	-4.01	105.14	111.02
9	A	1561	NAG	C4-C3-C2	3.51	116.16	111.02
9	A	1560	NAG	O4-C4-C3	2.96	117.19	110.35
9	A	1559	NAG	O3-C3-C4	2.74	116.68	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1559	NAG	O4-C4-C3	2.51	116.16	110.35
9	A	1561	NAG	O4-C4-C5	2.44	115.36	109.30
9	A	1561	NAG	O5-C1-C2	2.26	114.86	111.29
9	A	1559	NAG	C8-C7-N2	2.18	119.79	116.10
9	A	1560	NAG	C6-C5-C4	-2.09	108.10	113.00
9	A	1561	NAG	O7-C7-N2	2.05	125.73	121.95
9	A	1561	NAG	O7-C7-C8	-2.03	118.29	122.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1561	NAG	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1561	NAG	C1-C2-N2-C7
9	A	1559	NAG	O5-C5-C6-O6
9	A	1559	NAG	C4-C5-C6-O6
9	A	1559	NAG	C8-C7-N2-C2
9	A	1559	NAG	O7-C7-N2-C2
9	A	1561	NAG	C4-C5-C6-O6
9	A	1561	NAG	O5-C5-C6-O6
9	A	1560	NAG	C4-C5-C6-O6
9	A	1561	NAG	C3-C2-N2-C7

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	527/529 (99%)	0.05	18 (3%) 45 44	26, 42, 74, 108	9 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	ASP	4.6
1	A	255	GLU	4.1
1	A	377	VAL	4.1
1	A	282	TYR	4.0
1	A	378	ASP	3.9
1	A	53	SER	3.2
1	A	3	ASP	3.0
1	A	51	LYS	3.0
1	A	342	ASN	2.7
1	A	244	LEU	2.5
1	A	54	ASP	2.5
1	A	453	ARG	2.5
1	A	256	ASN	2.3
1	A	380	GLN	2.2
1	A	266	ASN	2.2
1	A	376	TRP	2.2
1	A	374	THR	2.1
1	A	55	ILE	2.1

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

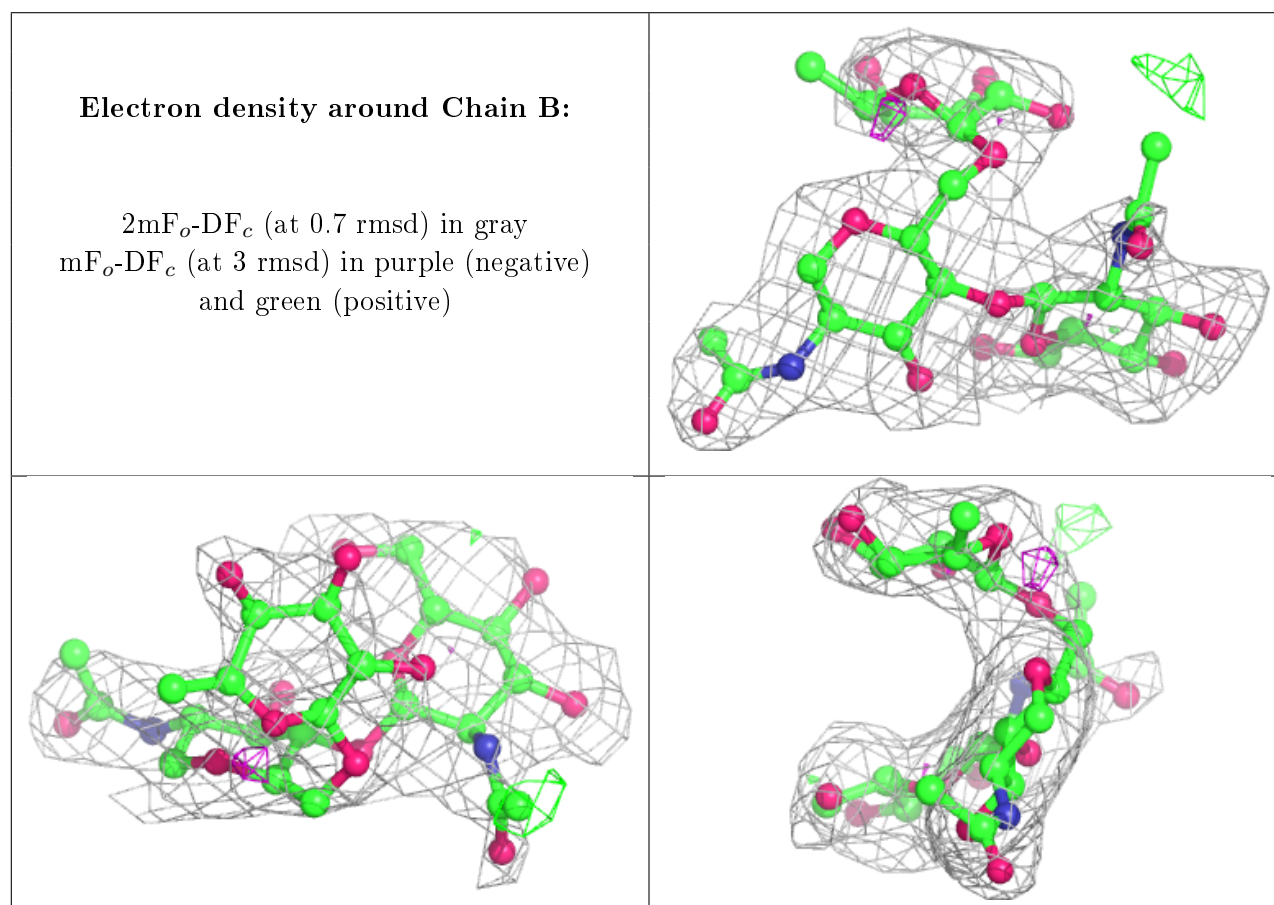
There are no non-standard protein/DNA/RNA residues in this entry.

### 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.

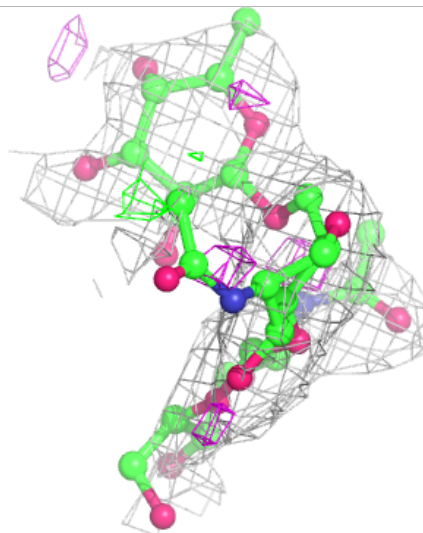
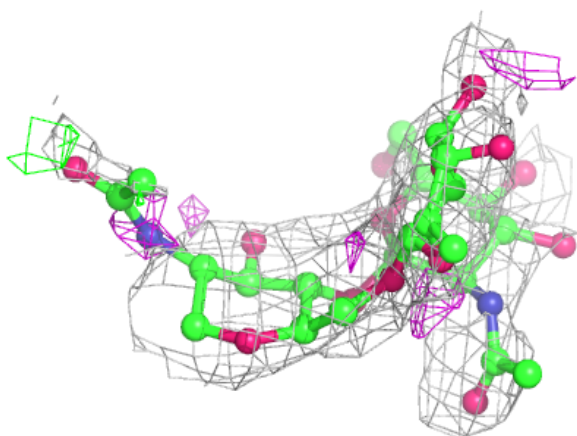
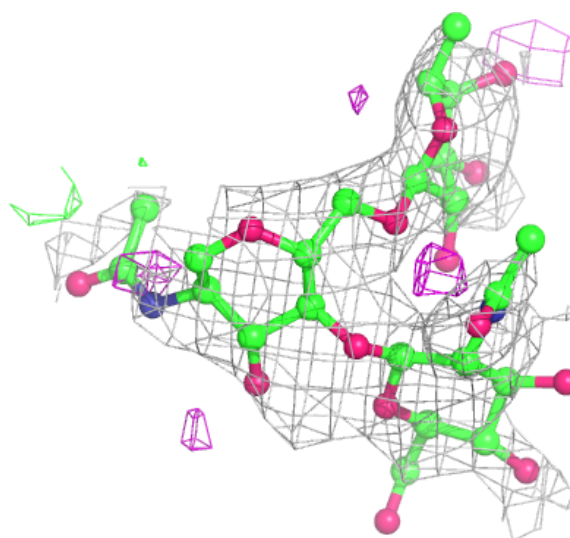
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	2	14/15	0.75	0.48	88,96,98,99	0
2	NAG	D	1	14/15	0.77	0.30	75,87,92,93	0
2	NAG	B	2	14/15	0.78	0.23	76,83,87,88	0
2	FUC	B	3	10/11	0.81	0.41	84,86,88,88	0
3	NAG	C	1	14/15	0.86	0.23	56,64,68,68	0
3	FUC	C	2	10/11	0.87	0.33	66,70,73,73	0
2	FUC	D	3	10/11	0.87	0.34	89,91,92,93	0
2	NAG	B	1	14/15	0.96	0.18	46,56,70,78	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.

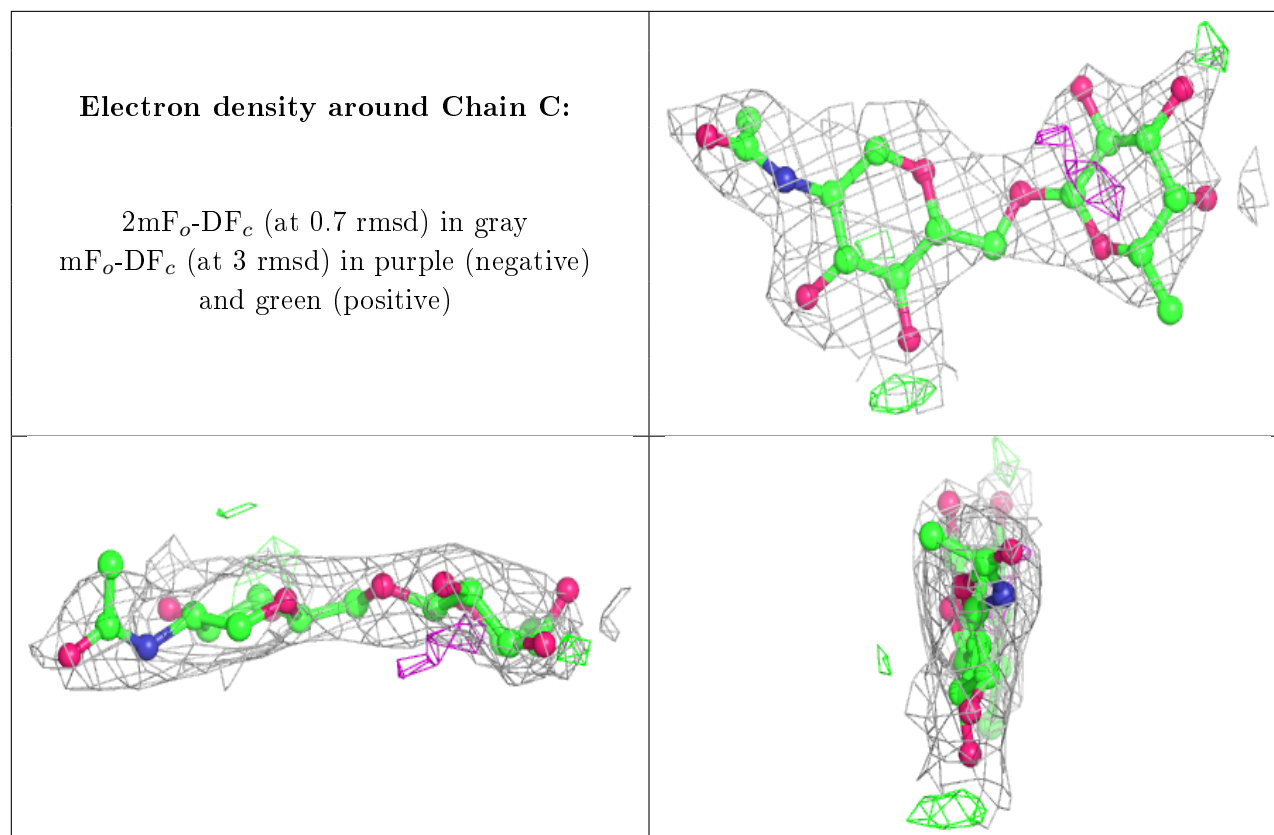


**Electron density around Chain D:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.4 Ligands ⓘ

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
4	UNX	A	1545	1/1	0.51	0.56	59,59,59,59	0
9	NAG	A	1561	14/15	0.58	0.53	80,90,95,95	0
7	CL	A	1549	1/1	0.60	0.22	91,91,91,91	0
9	NAG	A	1559	14/15	0.73	0.40	72,81,83,85	0
9	NAG	A	1560	14/15	0.77	0.22	69,77,83,85	0
7	CL	A	1550	1/1	0.81	0.19	72,72,72,72	0
4	UNX	A	1546	1/1	0.86	0.28	43,43,43,43	0
4	UNX	A	1537	1/1	0.89	0.20	28,28,28,28	0
4	UNX	A	1538	1/1	0.89	0.30	33,33,33,33	0
7	CL	A	1551	1/1	0.90	0.05	77,77,77,77	0
4	UNX	A	1531	1/1	0.92	0.35	33,33,33,33	0
4	UNX	A	1542	1/1	0.93	0.14	13,13,13,13	0
5	F	A	1530	1/1	0.93	0.23	34,34,34,34	0
4	UNX	A	1535	1/1	0.94	0.34	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	A	1548	5/5	0.94	0.33	68,68,69,71	0
7	CL	A	1565	1/1	0.94	0.12	71,71,71,71	0
8	K	A	1553	1/1	0.94	0.17	79,79,79,79	0
4	UNX	A	1536	1/1	0.94	0.23	51,51,51,51	0
4	UNX	A	1541	1/1	0.94	0.07	34,34,34,34	0
4	UNX	A	1539	1/1	0.95	0.27	22,22,22,22	0
4	UNX	A	1547	1/1	0.95	0.16	28,28,28,28	0
4	UNX	A	1543	1/1	0.95	0.16	23,23,23,23	0
7	CL	A	1552	1/1	0.95	0.24	63,63,63,63	0
4	UNX	A	1533	1/1	0.96	0.41	23,23,23,23	0
4	UNX	A	1544	1/1	0.96	0.15	12,12,12,12	0
4	UNX	A	1540	1/1	0.96	0.08	16,16,16,16	0
4	UNX	A	1532	1/1	0.96	0.35	38,38,38,38	0
4	UNX	A	1534	1/1	0.97	0.43	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.