



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 05:49 PM BST

PDB ID : 4B0P  
Title : Crystal structure of soman-aged human butyrylcholinesterase in complex with methyl 2-(pentafluorobenzyloxyimino)pyridinium  
Authors : Wandhammer, M.; de Koning, M.; van Grol, M.; Noort, D.; Goeldner, M.; Nachon, F.  
Deposited on : 2012-07-04  
Resolution : 2.50 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  
buster-report : 1.1.7 (2018)  
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

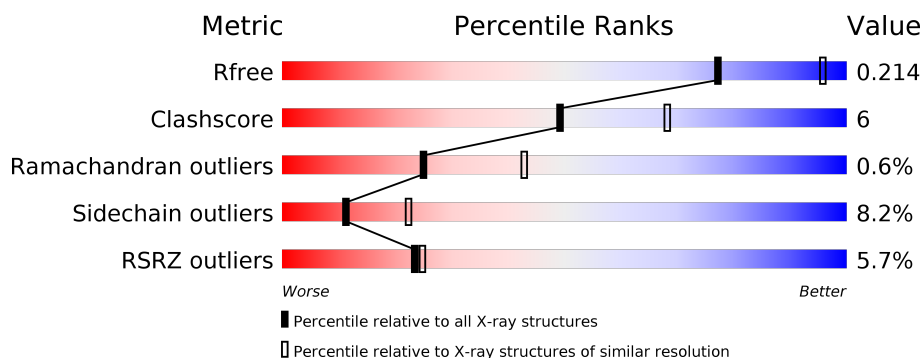
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>.</div> </div> </div>
2	B	3	<div> <div>67%</div> <div>33%</div> </div>
2	C	3	<div> <div>33%</div> <div>67%</div> </div>

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
2	NAG	B	1	X	-	-	X
2	NAG	B	2	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 4595 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.

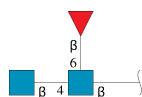
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	P	S	1	5	0
			4237	2733	710	778	1	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	conflict	UNP P06276
A	384	GLN	ASN	conflict	UNP P06276
A	455	GLN	ASN	conflict	UNP P06276
A	481	GLN	ASN	conflict	UNP P06276

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



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

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



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

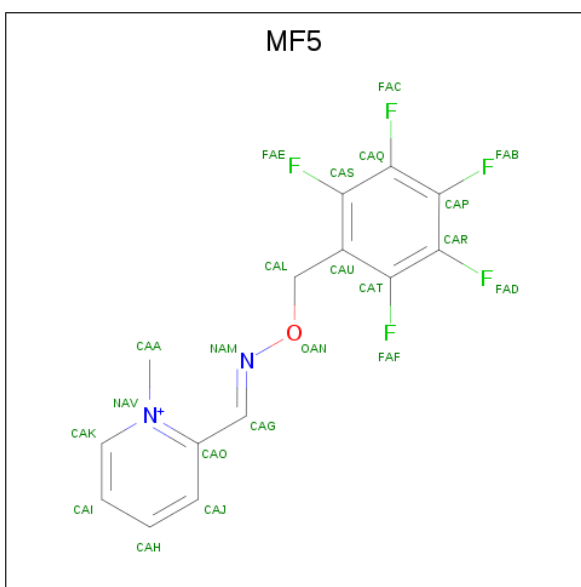
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is 1-(1-methylpyridin-1-ium-2-yl)-N-[[2,3,4,5,6-pentakis(fluoranyl)phenyl]methoxy]methanimine (three-letter code: MF5) (formula: C<sub>14</sub>H<sub>10</sub>F<sub>5</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			22	14	5	2	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	4	Total	Ca	0	0
			4	4		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

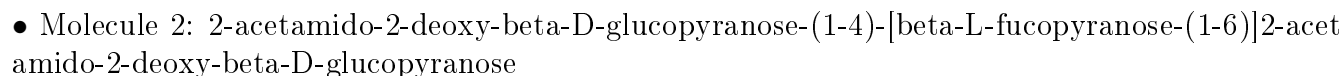
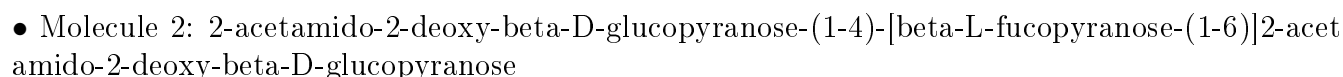
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Cl	0	0
			4	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	188	Total	O	0	0
			188	188		



- Molecule 1: CHOLINESTERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.23 Å   154.23 Å   133.86 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.88 – 2.50 42.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.88-2.50) 98.7 (42.86-2.50)	Depositor EDS
$R_{merge}$	0.01	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 2.51 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.164   ,   0.212 0.165   ,   0.214	Depositor DCC
$R_{free}$ test set	1113 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.8	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.6	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	0.96	EDS
Total number of atoms	4595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: NAG, CL, NA, K, MF5, FUL, CA, SBG

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	0.32	0/4362	0.56	0/5920

There are no bond length outliers.

There are no bond angle outliers.

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	4237	0	4130	50	0
2	B	38	0	34	1	0
2	C	38	0	34	2	0
3	A	5	0	2	1	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	22	0	10	0	0
7	A	56	0	52	0	0
8	A	4	0	0	0	0
9	A	4	0	0	0	0
10	A	188	0	0	5	0
All	All	4595	0	4262	51	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 6.

All (51) 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:240:ARG:NH1	1:A:257:GLU:OE2	2.12	0.81
1:A:257:GLU:HA	1:A:260:ILE:HD12	1.65	0.79
1:A:384:GLN:HE21	1:A:384:GLN:HA	1.51	0.75
1:A:14:ARG:NH1	1:A:57:ASN:OD1	2.20	0.73
1:A:381:ARG:O	1:A:384:GLN:HG2	1.89	0.71
1:A:270:GLN:NE2	10:A:3100:HOH:O	2.28	0.67
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.82	0.60
1:A:308:GLU:OE1	1:A:408:LYS:NZ	2.23	0.58
1:A:256:ASN:O	1:A:259:GLU:N	2.32	0.57
1:A:69:ILE:HD11	1:A:88:LEU:HD11	1.87	0.57
1:A:262:LYS:NZ	10:A:3098:HOH:O	2.19	0.56
1:A:376:TRP:O	1:A:378:ASP:HA	2.06	0.56
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.41	0.56
1:A:376:TRP:CH2	1:A:384:GLN:HB3	2.43	0.54
1:A:35:GLN:HG3	1:A:47:GLN:HB2	1.89	0.53
1:A:102:PRO:O	1:A:138:ARG:NH2	2.40	0.53
1:A:278:PHE:O	2:B:3:FUL:H4	2.09	0.52
1:A:14:ARG:HB2	1:A:55:ILE:HG21	1.92	0.51
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.46	0.51
1:A:319:VAL:O	1:A:418:PHE:HA	2.10	0.51
1:A:98:TRP:HE1	3:A:1178:GLY:N	2.09	0.51
1:A:3:ASP:N	10:A:3001:HOH:O	2.44	0.49
1:A:304:ASP:HB3	10:A:3106:HOH:O	2.12	0.49
1:A:428:LEU:HD13	1:A:430:TRP:HB2	1.94	0.49
2:C:1:NAG:H61	2:C:2:NAG:H82	1.95	0.47
1:A:119:GLN:NE2	1:A:288:VAL:HG13	2.29	0.47
1:A:350:PHE:CE2	1:A:370:LEU:HD23	2.48	0.47
1:A:384:GLN:NE2	1:A:384:GLN:HA	2.26	0.47
1:A:407:LYS:HE3	1:A:407:LYS:HB2	1.66	0.47
1:A:328:ALA:HA	1:A:434:MET:CE	2.45	0.46
1:A:321:VAL:HG11	1:A:399:ILE:HA	1.97	0.46
1:A:377:VAL:HG22	1:A:377:VAL:O	2.17	0.45
1:A:321:VAL:HG21	1:A:399:ILE:HG12	1.98	0.45
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.52	0.45
1:A:320:GLY:HA3	1:A:419:TYR:CD2	2.52	0.45
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.32	0.44
1:A:338:SER:HB2	2:C:1:NAG:H62	1.99	0.44
1:A:381:ARG:HB3	1:A:383:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:HIS:HD2	10:A:3043:HOH:O	2.01	0.43
1:A:117:GLY:H	1:A:198:SBG:H1	1.67	0.42
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.54	0.42
1:A:51:LYS:HB3	1:A:51:LYS:HE3	1.71	0.42
1:A:167:GLY:O	1:A:171:GLN:HG3	2.20	0.42
1:A:497:GLU:HG3	1:A:497:GLU:H	1.49	0.42
1:A:516:ALA:O	1:A:520:ARG:HG2	2.20	0.41
1:A:376:TRP:HA	1:A:376:TRP:CE3	2.56	0.41
1:A:282:TYR:CD1	1:A:282:TYR:O	2.74	0.41
1:A:252:CYS:SG	1:A:267:LYS:HE2	2.61	0.41
1:A:84:PRO:HG2	1:A:88:LEU:HD21	2.03	0.41
1:A:358:PHE:HB3	1:A:361:VAL:HG21	2.02	0.41
1:A:210:SER:HA	1:A:211:PRO:HD3	1.96	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	529/529 (100%)	502 (95%)	23 (4%)	4 (1%)	19	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	51	LYS
1	A	54[A]	ASP
1	A	54[B]	ASP

### 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	456/453 (101%)	417 (91%)	39 (9%)	10	20

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	16	MET
1	A	49	LEU
1	A	50	THR
1	A	51	LYS
1	A	54[A]	ASP
1	A	54[B]	ASP
1	A	99	ILE
1	A	105	LYS
1	A	195	PHE
1	A	219	ARG
1	A	236	LEU
1	A	255	GLU
1	A	259	GLU
1	A	262	LYS
1	A	272	ILE
1	A	282	TYR
1	A	286	LEU
1	A	367	GLU
1	A	370	LEU
1	A	375	ASP
1	A	377	VAL
1	A	384	GLN
1	A	411	GLU
1	A	414	ASN
1	A	428	LEU
1	A	448	LEU
1	A	454	ASP
1	A	471	TRP
1	A	489	SER

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Mol	Chain	Res	Type
1	A	496	THR
1	A	497	GLU
1	A	505	THR
1	A	506[A]	GLU
1	A	506[B]	GLU
1	A	508	THR
1	A	511	MET
1	A	520	ARG
1	A	529	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	SBG	A	198	1,5	8,9,10	2.62	3 (37%)	5,12,14	2.02	2 (40%)

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
1	SBG	A	198	1,5	-	2/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SBG	P1-O2	5.90	1.59	1.50
1	A	198	SBG	P1-O1	-3.02	1.48	1.54
1	A	198	SBG	P1-OG	2.90	1.61	1.57

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SBG	OG-CB-CA	2.72	110.80	108.14
1	A	198	SBG	OG-P1-O2	-2.70	103.25	111.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SBG	CB-OG-P1-O2
1	A	198	SBG	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SBG	1	0

## 5.5 Carbohydrates ⓘ

6 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	0.51	0	17,19,21	1.68	2 (11%)
2	NAG	B	2	2	14,14,15	0.69	0	17,19,21	1.27	2 (11%)
2	FUL	B	3	2	10,10,11	1.40	2 (20%)	14,14,16	1.55	2 (14%)
2	NAG	C	1	1,2	14,14,15	0.57	0	17,19,21	1.91	5 (29%)
2	NAG	C	2	2	14,14,15	0.54	0	17,19,21	1.23	1 (5%)
2	FUL	C	3	2	10,10,11	1.23	2 (20%)	14,14,16	1.46	2 (14%)

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	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
2	NAG	C	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	FUL	C	3	2	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	FUL	O5-C1	-3.06	1.38	1.43
2	C	3	FUL	O5-C1	-2.48	1.39	1.43
2	B	3	FUL	C4-C5	2.22	1.57	1.52
2	C	3	FUL	C4-C5	2.14	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	NAG	C1-O5-C5	4.39	118.14	112.19
2	C	2	NAG	C2-N2-C7	-4.04	117.15	122.90
2	C	3	FUL	C1-C2-C3	-3.79	105.01	109.67
2	B	1	NAG	O4-C4-C3	3.72	118.95	110.35
2	C	1	NAG	C1-C2-N2	3.72	116.84	110.49
2	C	1	NAG	C2-N2-C7	3.50	127.89	122.90
2	B	3	FUL	C3-C4-C5	3.34	114.98	109.77
2	B	3	FUL	O5-C5-C4	3.31	115.46	109.52
2	B	2	NAG	C1-O5-C5	2.86	116.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C4-C3-C2	2.85	115.19	111.02
2	C	1	NAG	O6-C6-C5	2.71	120.58	111.29
2	C	1	NAG	O5-C5-C6	2.70	111.44	107.20
2	C	1	NAG	C1-O5-C5	2.67	115.81	112.19
2	C	3	FUL	O2-C2-C1	2.53	114.33	109.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1

All (12) torsion outliers are listed below:

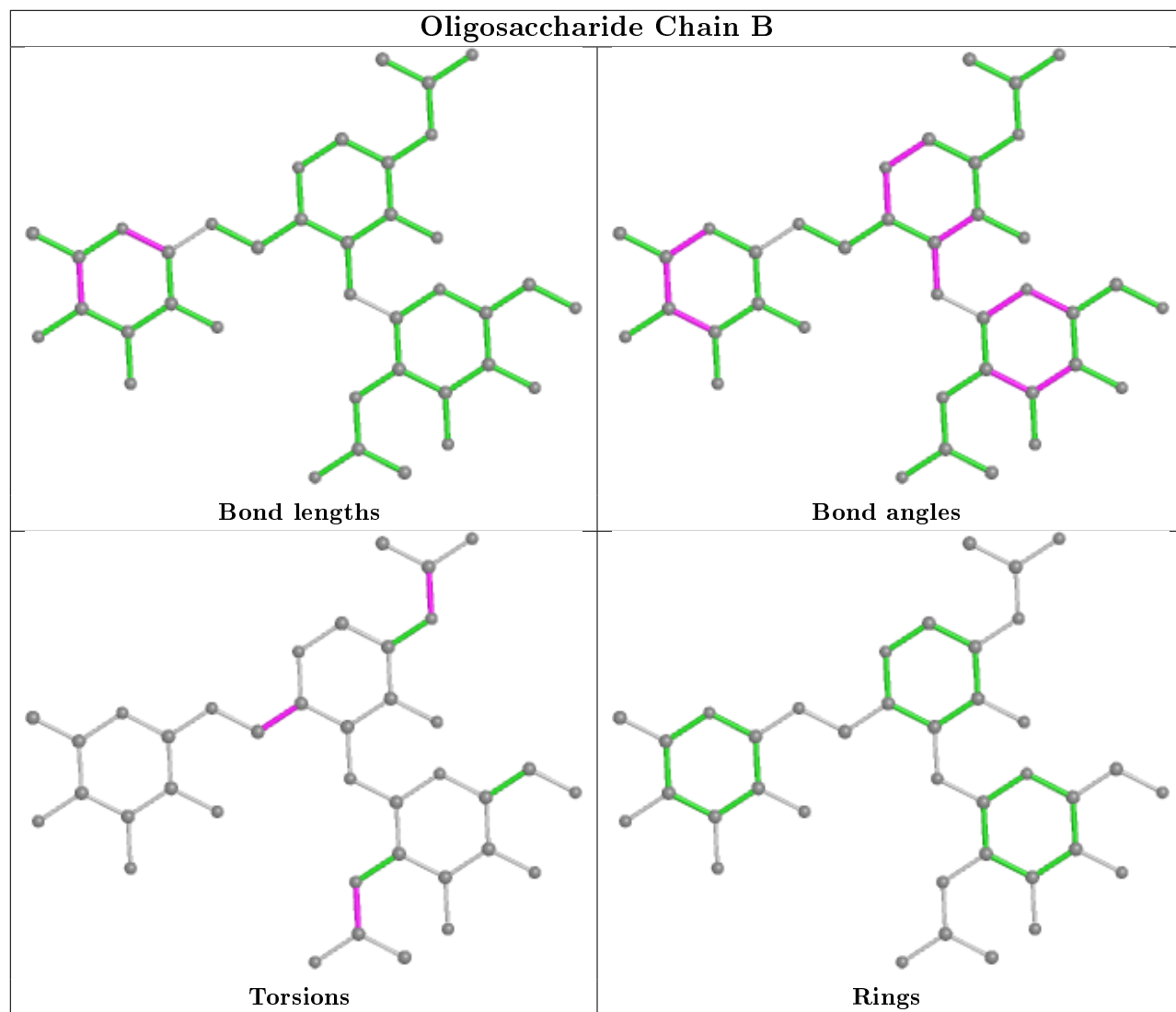
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C1-C2-N2-C7
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	B	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

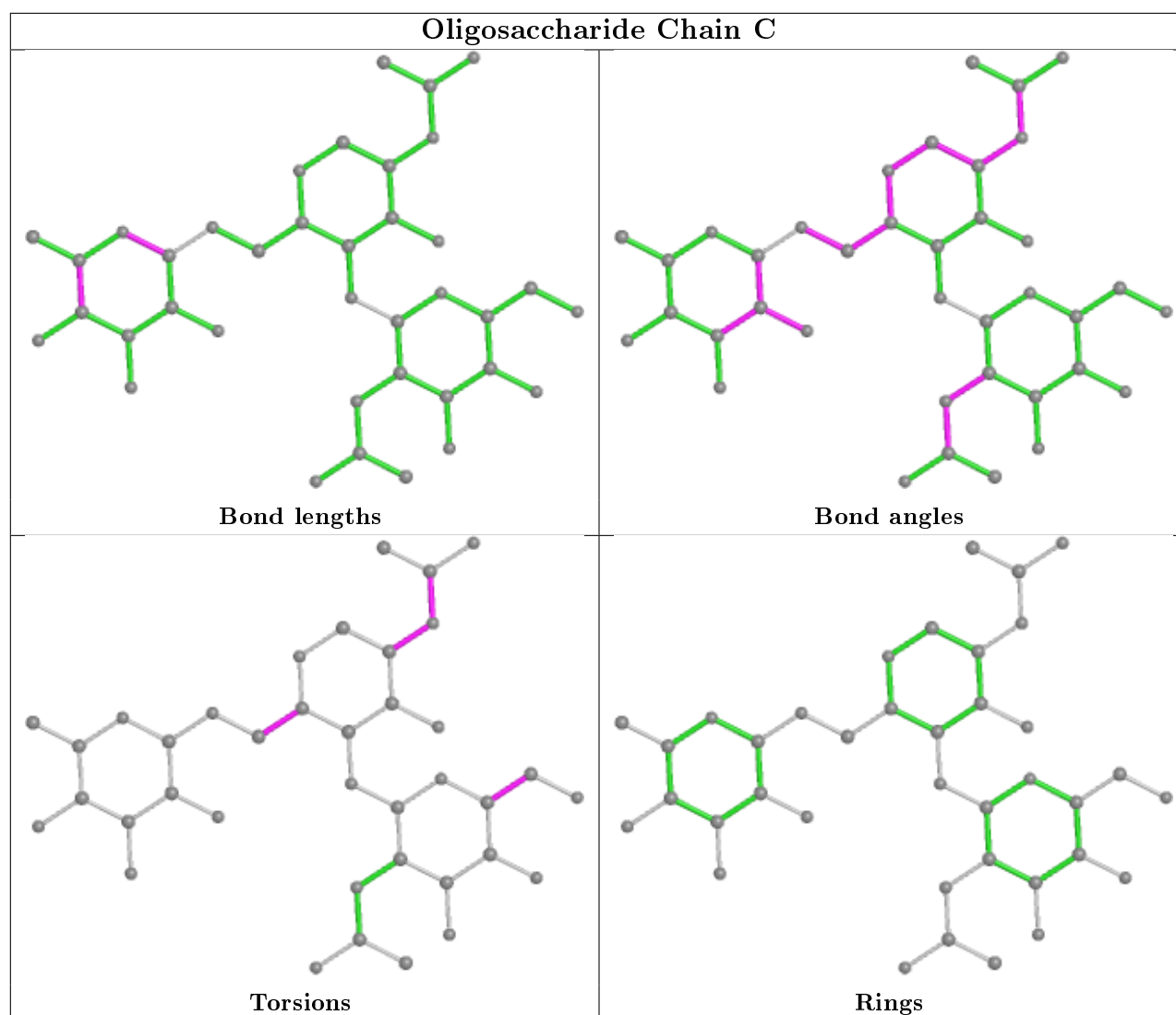
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	FUL	1	0
2	C	1	NAG	2	0
2	C	2	NAG	1	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 [i](#)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 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	MF5	A	1179	-	23,23,23	2.19	7 (30%)	31,32,32	1.53	5 (16%)
7	NAG	A	2179	1	14,14,15	0.41	0	17,19,21	2.44	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	A	2187	1	14,14,15	0.36	0	17,19,21	1.74	2 (11%)
7	NAG	A	2180	1	14,14,15	0.52	0	17,19,21	1.75	3 (17%)
7	NAG	A	2188	1	14,14,15	0.57	0	17,19,21	1.40	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
6	MF5	A	1179	-	-	0/7/7/7	0/2/2/2
7	NAG	A	2179	1	-	4/6/23/26	0/1/1/1
7	NAG	A	2187	1	-	2/6/23/26	0/1/1/1
7	NAG	A	2180	1	-	2/6/23/26	0/1/1/1
7	NAG	A	2188	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1179	MF5	CAL-CAU	-6.35	1.39	1.51
6	A	1179	MF5	FAE-CAS	-4.69	1.27	1.35
6	A	1179	MF5	CAG-NAM	3.56	1.34	1.27
6	A	1179	MF5	OAN-NAM	3.14	1.46	1.41
6	A	1179	MF5	CAO-CAG	-2.83	1.39	1.46
6	A	1179	MF5	CAO-NAV	-2.53	1.34	1.37
6	A	1179	MF5	CAK-NAV	2.43	1.40	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2179	NAG	C4-C3-C2	-6.20	101.93	111.02
7	A	2187	NAG	C1-O5-C5	5.40	119.51	112.19
7	A	2180	NAG	C1-O5-C5	5.38	119.48	112.19
6	A	1179	MF5	OAN-NAM-CAG	4.93	118.38	110.80
7	A	2179	NAG	C1-O5-C5	4.71	118.57	112.19
7	A	2179	NAG	O5-C5-C6	3.45	112.61	107.20
6	A	1179	MF5	CAT-CAU-CAS	3.16	119.65	115.90
6	A	1179	MF5	CAJ-CAO-NAV	3.03	120.15	117.46
7	A	2188	NAG	C4-C3-C2	3.02	115.45	111.02
7	A	2188	NAG	C3-C4-C5	2.94	115.49	110.24
7	A	2179	NAG	C2-N2-C7	-2.92	118.75	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1179	MF5	CAO-CAG-NAM	-2.77	112.55	117.91
7	A	2187	NAG	C4-C3-C2	-2.64	107.14	111.02
7	A	2188	NAG	O5-C1-C2	-2.56	107.24	111.29
7	A	2180	NAG	O5-C5-C6	2.35	110.89	107.20
7	A	2179	NAG	C3-C4-C5	-2.28	106.17	110.24
7	A	2180	NAG	C3-C4-C5	-2.12	106.45	110.24
6	A	1179	MF5	CAU-CAT-CAR	-2.12	119.86	122.37
7	A	2179	NAG	C1-C2-N2	2.08	114.04	110.49

There are no chirality outliers.

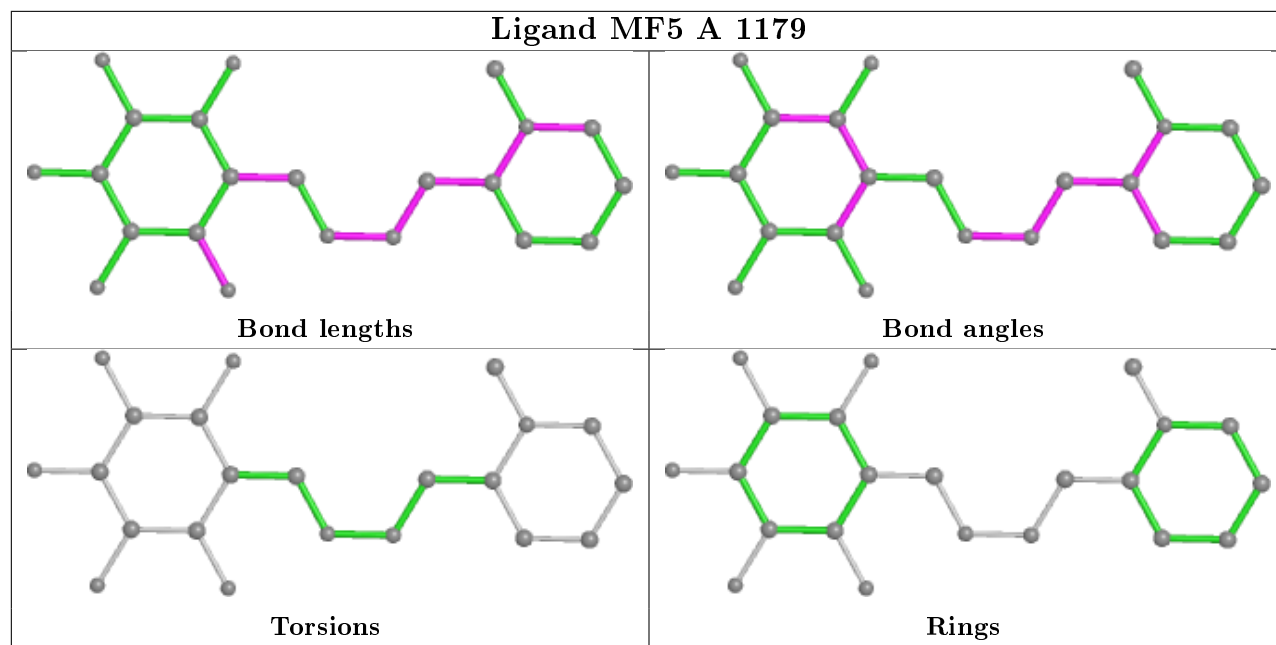
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2180	NAG	C8-C7-N2-C2
7	A	2187	NAG	O5-C5-C6-O6
7	A	2180	NAG	O7-C7-N2-C2
7	A	2187	NAG	C4-C5-C6-O6
7	A	2179	NAG	O5-C5-C6-O6
7	A	2179	NAG	C8-C7-N2-C2
7	A	2179	NAG	O7-C7-N2-C2
7	A	2179	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	526/529 (99%)	0.03	30 (5%)	23 25	24, 43, 79, 113	6 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	4.8
1	A	378	ASP	4.6
1	A	259	GLU	4.3
1	A	237	TYR	4.2
1	A	255	GLU	3.7
1	A	244	LEU	3.6
1	A	261	ILE	3.4
1	A	262	LYS	3.4
1	A	282	TYR	3.3
1	A	258	THR	3.0
1	A	376	TRP	2.8
1	A	260	ILE	2.7
1	A	52	TRP	2.6
1	A	342	ASN	2.5
1	A	53	SER	2.5
1	A	381	ARG	2.5
1	A	5	ILE	2.4
1	A	453	ARG	2.2
1	A	254	ARG	2.2
1	A	4	ILE	2.2
1	A	40	ARG	2.2
1	A	281	PRO	2.2
1	A	50	THR	2.2
1	A	55	ILE	2.2
1	A	384	GLN	2.1
1	A	458	LYS	2.1
1	A	344	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	49	LEU	2.1
1	A	385	TYR	2.0
1	A	379	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SBG	A	198	10/11	0.99	0.20	20,26,36,39	0

## 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.

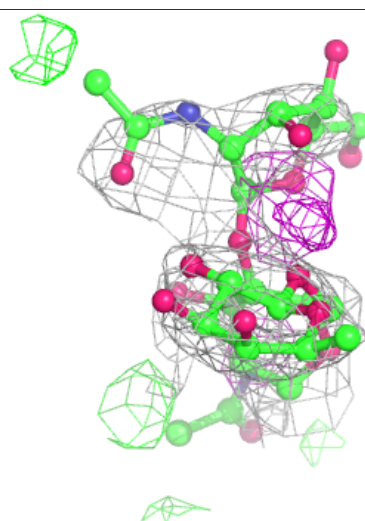
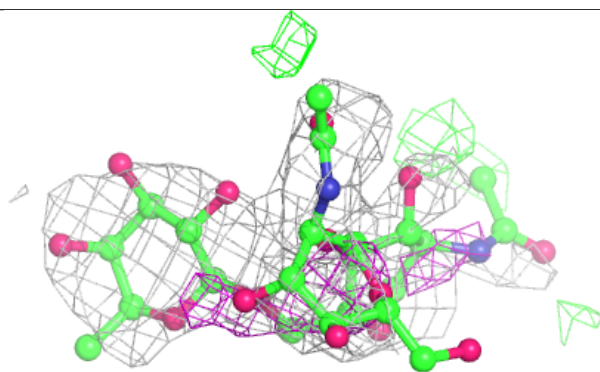
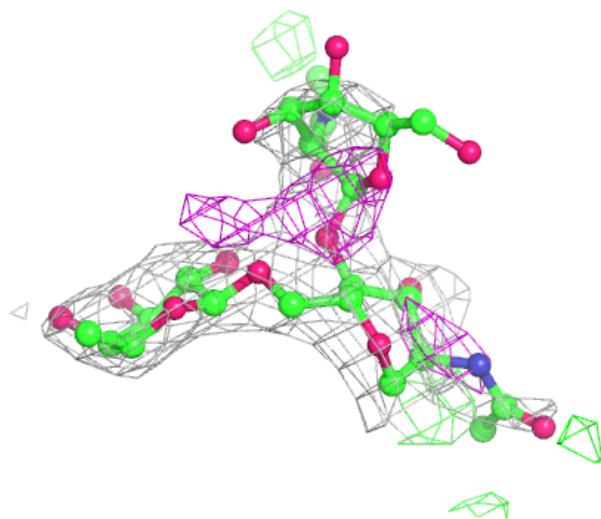
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	2	14/15	0.64	0.55	106,115,120,123	0
2	NAG	B	1	14/15	0.75	0.44	92,107,114,115	0
2	FUL	C	3	10/11	0.81	0.39	75,90,108,109	0
2	NAG	C	2	14/15	0.90	0.24	74,82,88,92	0
2	FUL	B	3	10/11	0.92	0.37	86,95,97,98	0
2	NAG	C	1	14/15	0.95	0.19	35,51,62,66	0

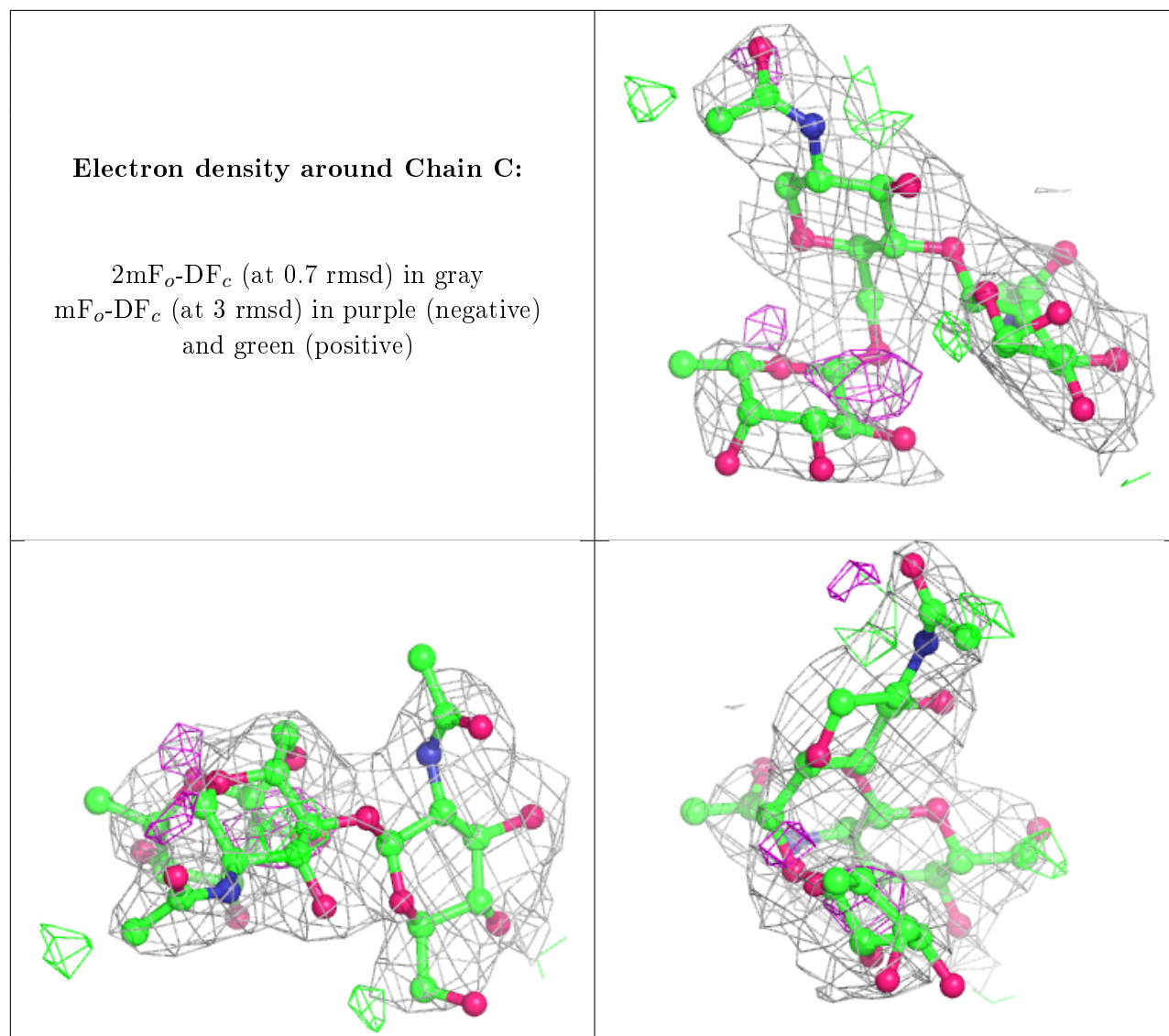
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around Chain B:**

$2mF_o-DF_c$  (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.

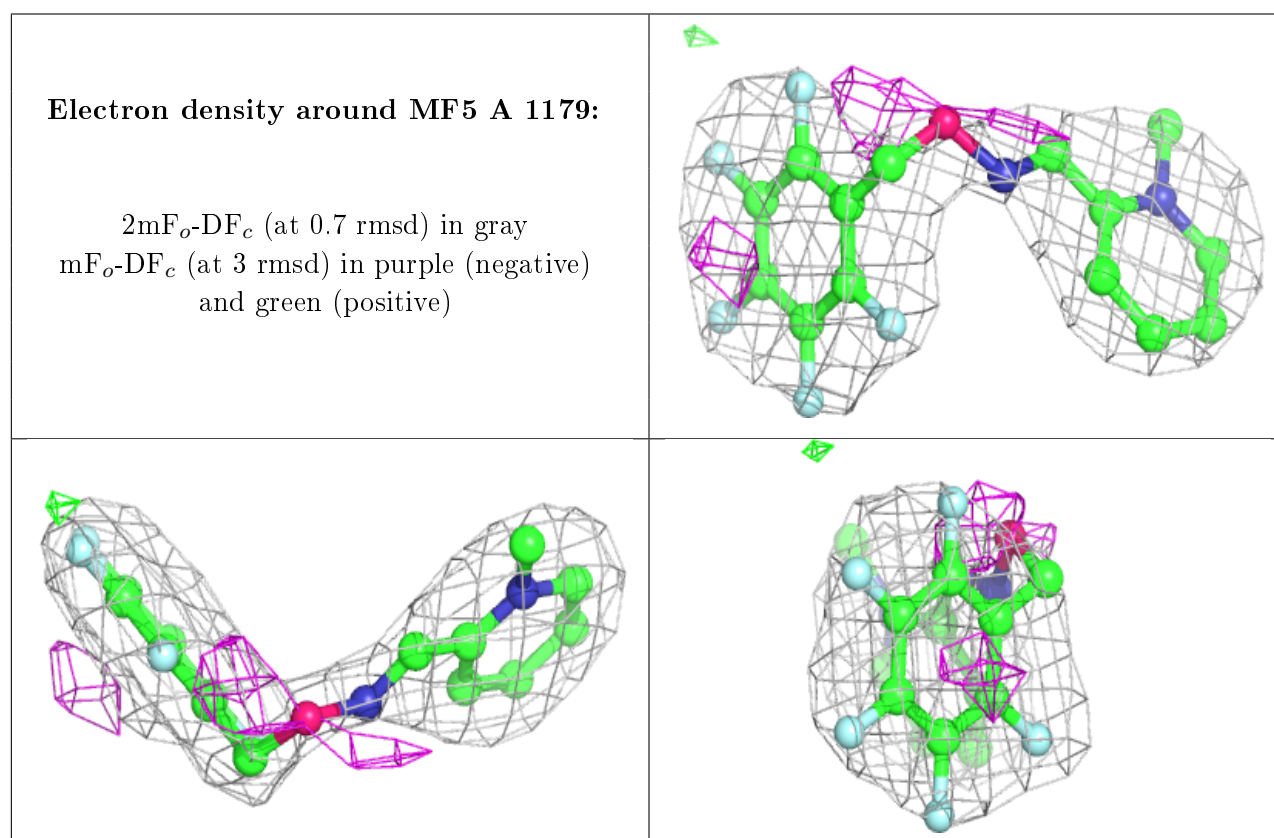
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	CL	A	2194	1/1	0.69	0.11	83,83,83,83	0
4	NA	A	1170	1/1	0.75	0.39	65,65,65,65	0
7	NAG	A	2179	14/15	0.78	0.37	72,89,91,93	0
7	NAG	A	2188	14/15	0.81	0.41	90,99,103,105	0
7	NAG	A	2187	14/15	0.83	0.18	53,71,84,84	0
7	NAG	A	2180	14/15	0.84	0.31	57,72,76,79	0
9	CL	A	2193	1/1	0.84	0.37	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CL	A	2196	1/1	0.85	0.27	76,76,76,76	0
9	CL	A	2195	1/1	0.87	0.18	86,86,86,86	0
8	CA	A	2192	1/1	0.89	0.11	80,80,80,80	0
8	CA	A	2197	1/1	0.89	0.12	84,84,84,84	0
4	NA	A	2190	1/1	0.90	0.17	50,50,50,50	0
6	MF5	A	1179	22/22	0.90	0.21	41,71,77,84	0
8	CA	A	2198	1/1	0.90	0.14	93,93,93,93	0
3	GLY	A	1178	5/5	0.91	0.18	48,56,57,62	0
5	K	A	1171	1/1	0.95	0.26	84,84,84,84	0
8	CA	A	2191	1/1	0.97	0.18	83,83,83,83	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.