



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 06:17 PM BST

PDB ID : 2WSL
Title : Aged Form of Human Butyrylcholinesterase Inhibited by Tabun Analogue TA4
Authors : Carletti, E.; Aurbek, N.; Gillon, E.; Loiodice, M.; Nicolet, Y.; Fontecilla, J.; Masson, P.; Thiermann, H.; Nachon, F.; Worek, F.
Deposited on : 2009-09-08
Resolution : 2.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

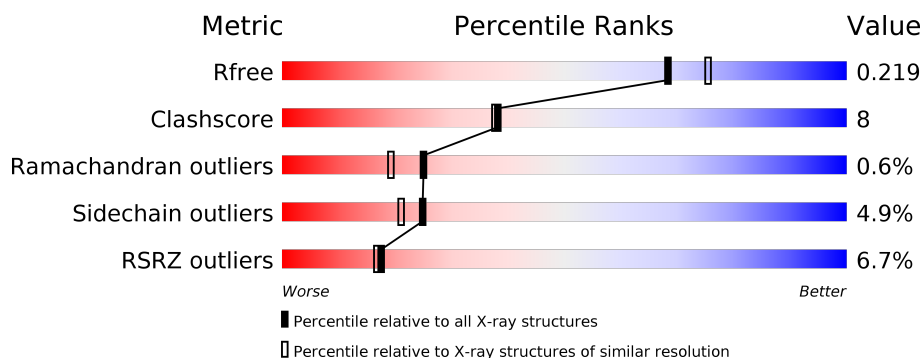
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 ≥ 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>7%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>
2	B	3	<div> <div>33%</div> <div>67%</div> </div>
3	C	2	<div> <div>50%</div> <div>50%</div> </div>
4	D	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	D	2	-	-	-	X
5	NAG	A	1537	X	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4817 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.

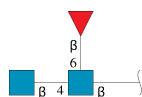
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4264	2756	714	777	17	0	10	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	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)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



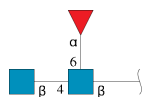
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0

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



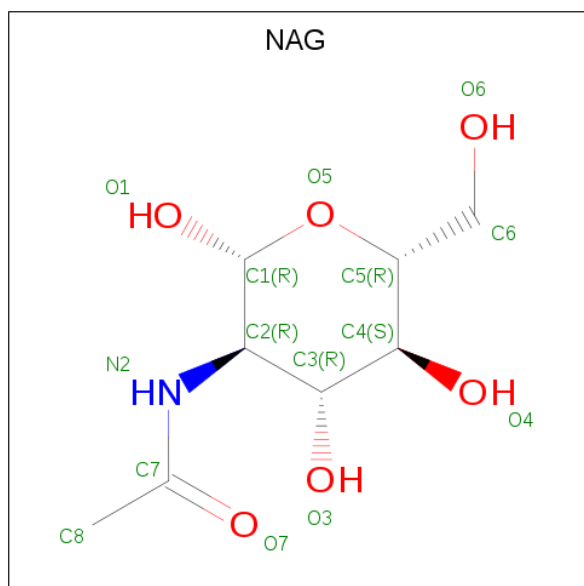
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is 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
4	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $\text{C}_8\text{H}_{15}\text{NO}_6$).



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

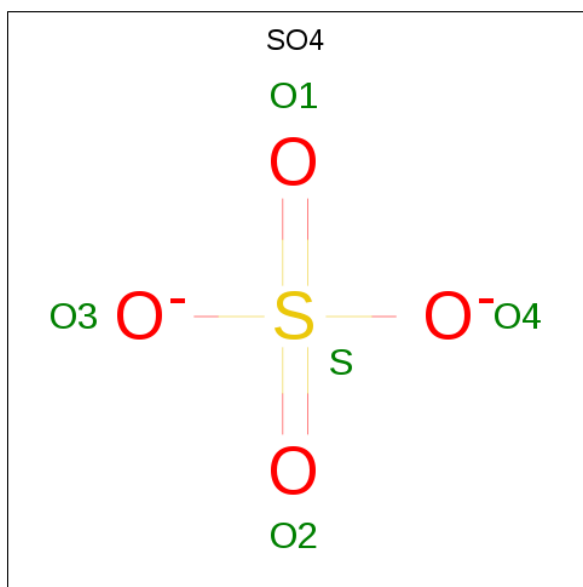
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

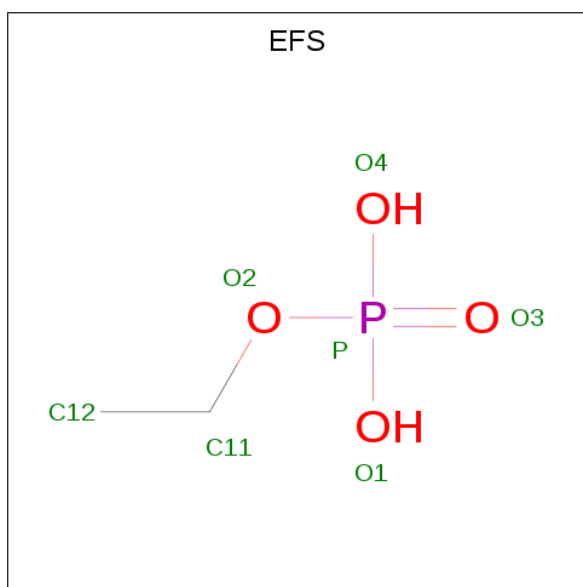
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 9 is ETHYL DIHYDROGEN PHOSPHATE (three-letter code: EFS) (formula: C₂H₇O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O	P	0	0
			6	2	3	1		

- Molecule 10 is FLUORIDE ION (three-letter code: F) (formula: F).

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

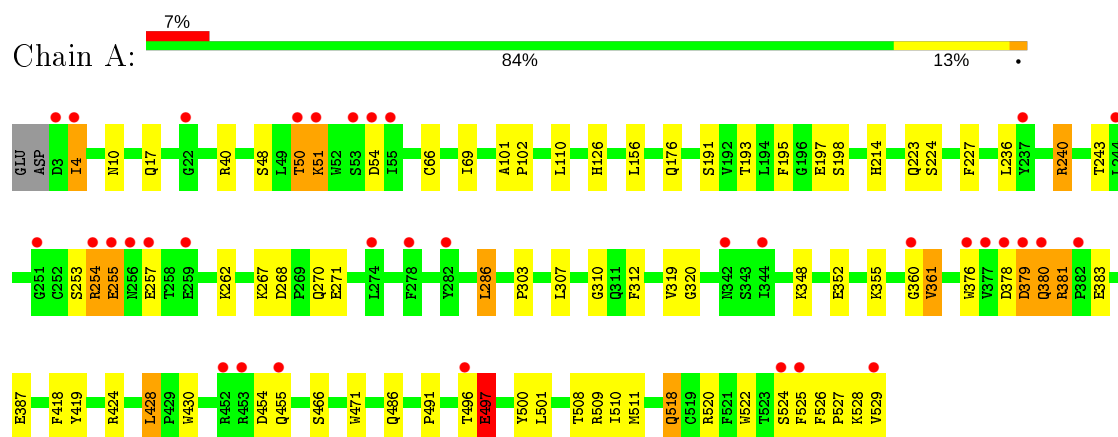
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	397	Total	O	0	0
			397	397		

3 Residue-property plots

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)-[beta-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



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[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, α , β , γ	154.86 Å 154.86 Å 126.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 2.00 48.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.87-2.00) 99.8 (48.87-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.55 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.184 , 0.220 0.184 , 0.219	Depositor DCC
R_{free} test set	1543 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4817	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CL, NAG, F, NA, EFS, FUC, FUL, CSS, 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	0.58	0/4408	0.62	0/5982

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

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	4264	0	4173	65	0
2	B	38	0	34	0	0
3	C	24	0	22	1	0
4	D	38	0	34	0	0
5	A	42	0	39	0	0
6	A	1	0	0	1	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	A	6	0	5	1	0
10	A	1	0	0	1	0
11	A	397	0	0	13	0
All	All	4817	0	4307	66	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 (66) 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:48:SER:HB3	11:A:2041:HOH:O	1.44	1.18
1:A:496:THR:O	1:A:497:GLU:HB2	1.37	1.14
1:A:509[B]:ARG:HH11	1:A:509[B]:ARG:CG	1.71	1.03
1:A:496:THR:O	1:A:497:GLU:CB	2.19	0.90
1:A:501:LEU:HD11	1:A:508:THR:CG2	2.04	0.88
1:A:509[B]:ARG:HH11	1:A:509[B]:ARG:HG3	1.37	0.86
1:A:518:GLN:H	1:A:518:GLN:HE21	1.25	0.84
6:A:1541:CL:CL	11:A:2241:HOH:O	2.32	0.84
1:A:509[B]:ARG:NH1	1:A:509[B]:ARG:CG	2.42	0.78
1:A:501:LEU:HD11	1:A:508:THR:HG23	1.66	0.77
1:A:509[B]:ARG:NH1	1:A:509[B]:ARG:HG3	1.97	0.77
1:A:509[B]:ARG:HH11	1:A:509[B]:ARG:HG2	1.51	0.76
1:A:522:TRP:O	1:A:527:PRO:HD3	1.88	0.73
1:A:253:SER:O	1:A:254:ARG:HD3	1.97	0.64
1:A:497:GLU:HG2	11:A:2351:HOH:O	1.96	0.63
1:A:240:ARG:NH1	1:A:257:GLU:OE2	2.32	0.62
1:A:54:ASP:HB2	11:A:2046:HOH:O	1.99	0.62
1:A:176:GLN:NE2	11:A:2145:HOH:O	2.31	0.61
1:A:268[A]:ASP:OD2	1:A:270:GLN:HB3	2.00	0.61
1:A:255:GLU:CD	1:A:255:GLU:H	2.06	0.59
1:A:267:LYS:HE3	1:A:271:GLU:OE1	2.01	0.59
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.84	0.58
1:A:227[A]:PHE:CE1	1:A:303:PRO:HB2	2.41	0.56
1:A:379:ASP:CG	11:A:2254:HOH:O	2.44	0.56
1:A:520:ARG:NH2	11:A:2381:HOH:O	2.39	0.55
1:A:126:HIS:HE1	11:A:2309:HOH:O	1.89	0.55
1:A:428:LEU:HD13	1:A:430:TRP:HB2	1.89	0.55
1:A:380:GLN:N	1:A:381:ARG:HB2	2.21	0.54
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.43	0.53
1:A:526:PHE:HA	1:A:529:VAL:HG22	1.90	0.53
1:A:352:GLU:HA	1:A:355:LYS:HE3	1.91	0.52
1:A:4:ILE:HD12	1:A:4:ILE:H	1.75	0.51
1:A:491:PRO:CD	1:A:510[B]:ILE:HD12	2.41	0.51
1:A:518:GLN:H	1:A:518:GLN:NE2	2.02	0.50
1:A:50:THR:O	1:A:51:LYS:HG2	2.12	0.50
1:A:520:ARG:NH1	11:A:2382:HOH:O	2.45	0.49
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.28	0.48
1:A:497:GLU:HA	11:A:2349:HOH:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:HA	1:A:102:PRO:C	2.34	0.47
1:A:466:SER:OG	10:A:1546:F:F	2.16	0.47
1:A:268[A]:ASP:OD2	1:A:270:GLN:CB	2.61	0.46
1:A:191:SER:HB2	3:C:2:FUC:H3	1.96	0.46
1:A:319:VAL:O	1:A:418:PHE:HA	2.15	0.46
1:A:198:SER:HA	1:A:224:SER:O	2.16	0.45
1:A:380:GLN:N	1:A:380:GLN:HE21	2.14	0.45
1:A:491:PRO:HD3	1:A:510[B]:ILE:HD12	1.99	0.45
1:A:500:TYR:CZ	1:A:511[A]:MET:HB2	2.52	0.45
1:A:509[B]:ARG:NH1	11:A:2367:HOH:O	2.50	0.45
1:A:227[B]:PHE:HZ	1:A:307:LEU:HB2	1.82	0.44
1:A:214:HIS:HE1	11:A:2216:HOH:O	2.01	0.44
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.53	0.44
1:A:197:GLU:HA	1:A:223:GLN:O	2.19	0.42
1:A:4:ILE:N	1:A:4:ILE:HD12	2.34	0.42
1:A:360:GLY:HA2	1:A:361:VAL:O	2.20	0.42
1:A:383:GLU:O	1:A:387:GLU:HG3	2.19	0.42
1:A:376:TRP:C	1:A:378:ASP:HA	2.40	0.42
1:A:286:LEU:HD23	9:A:1544:EFS:H123	2.02	0.42
1:A:509[A]:ARG:HA	1:A:509[A]:ARG:HD2	1.82	0.42
1:A:227[A]:PHE:CD1	1:A:303:PRO:HB2	2.55	0.41
1:A:10:ASN:ND2	11:A:2002:HOH:O	2.55	0.40
1:A:4:ILE:HD11	1:A:17:GLN:HG2	2.03	0.40
1:A:525:PHE:CE2	1:A:529:VAL:HG21	2.57	0.40
1:A:110:LEU:HD23	1:A:193:THR:HB	2.03	0.40
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.57	0.40
1:A:524:SER:O	1:A:528:LYS:HE3	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	534/529 (101%)	515 (96%)	16 (3%)	3 (1%)	25 19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	GLU
1	A	379	ASP
1	A	361	VAL

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	461/453 (102%)	439 (95%)	22 (5%)	25 22

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	40	ARG
1	A	50	THR
1	A	51	LYS
1	A	69	ILE
1	A	195	PHE
1	A	236	LEU
1	A	240	ARG
1	A	254	ARG
1	A	255	GLU
1	A	262	LYS
1	A	286	LEU
1	A	348	LYS
1	A	380	GLN
1	A	381	ARG
1	A	428	LEU
1	A	454	ASP
1	A	455	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	471	TRP
1	A	486	GLN
1	A	497	GLU
1	A	518	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	126	HIS
1	A	172	GLN
1	A	214	HIS
1	A	275	ASN
1	A	289	ASN
1	A	380	GLN
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 ⓘ

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	CSS	A	66	1	4,6,7	1.12	1 (25%)	1,6,8	0.10	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
1	CSS	A	66	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CSS	CB-SG	-2.01	1.75	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

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	0.73	0	17,19,21	1.73	4 (23%)
2	NAG	B	2	2	14,14,15	0.46	0	17,19,21	0.98	0
2	FUL	B	3	2	10,10,11	0.76	0	14,14,16	1.70	2 (14%)
3	NAG	C	1	1,3	14,14,15	0.71	0	17,19,21	1.30	3 (17%)
3	FUC	C	2	3	10,10,11	0.68	0	14,14,16	1.10	1 (7%)
4	NAG	D	1	1,4	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
4	NAG	D	2	4	14,14,15	0.48	0	17,19,21	1.15	1 (5%)
4	FUC	D	3	4	10,10,11	0.62	0	14,14,16	0.59	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
2	NAG	B	1	1,2	-	3/6/23/26	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	FUC	D	3	4	-	-	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	3	FUL	C1-C2-C3	-4.41	104.25	109.67
2	B	1	NAG	C2-N2-C7	3.84	128.37	122.90
4	D	2	NAG	C1-O5-C5	3.69	117.19	112.19
3	C	2	FUC	C1-C2-C3	3.17	113.56	109.67
2	B	1	NAG	C8-C7-N2	2.86	120.94	116.10
2	B	3	FUL	O5-C1-C2	-2.67	106.64	110.77
2	B	1	NAG	O5-C5-C6	2.50	111.12	107.20
3	C	1	NAG	C1-C2-N2	2.21	114.27	110.49
3	C	1	NAG	C8-C7-N2	2.13	119.70	116.10
4	D	1	NAG	C8-C7-N2	2.11	119.67	116.10
2	B	1	NAG	C6-C5-C4	2.08	117.88	113.00
3	C	1	NAG	O5-C1-C2	-2.05	108.05	111.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

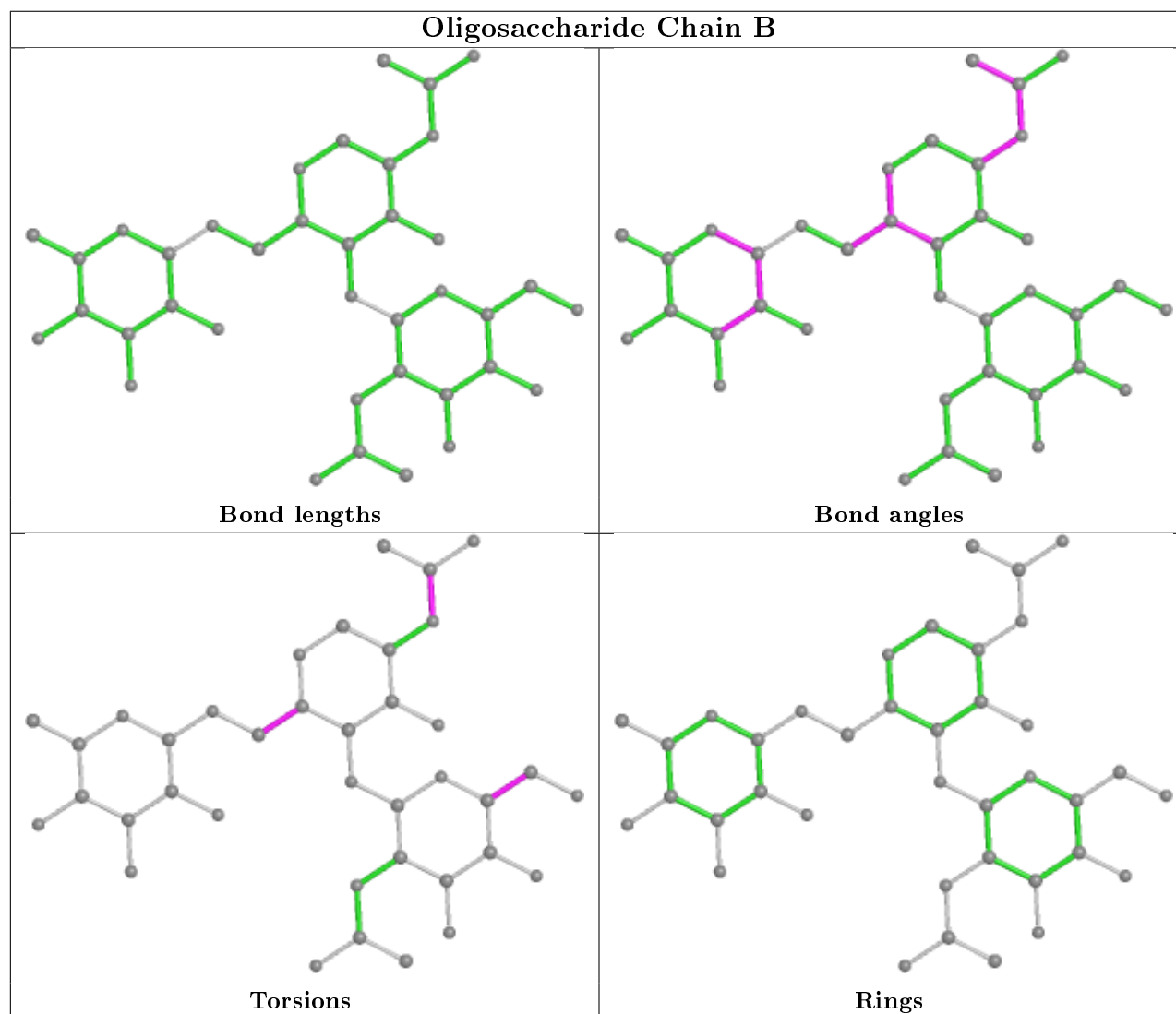
Mol	Chain	Res	Type	Atoms
2	B	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6

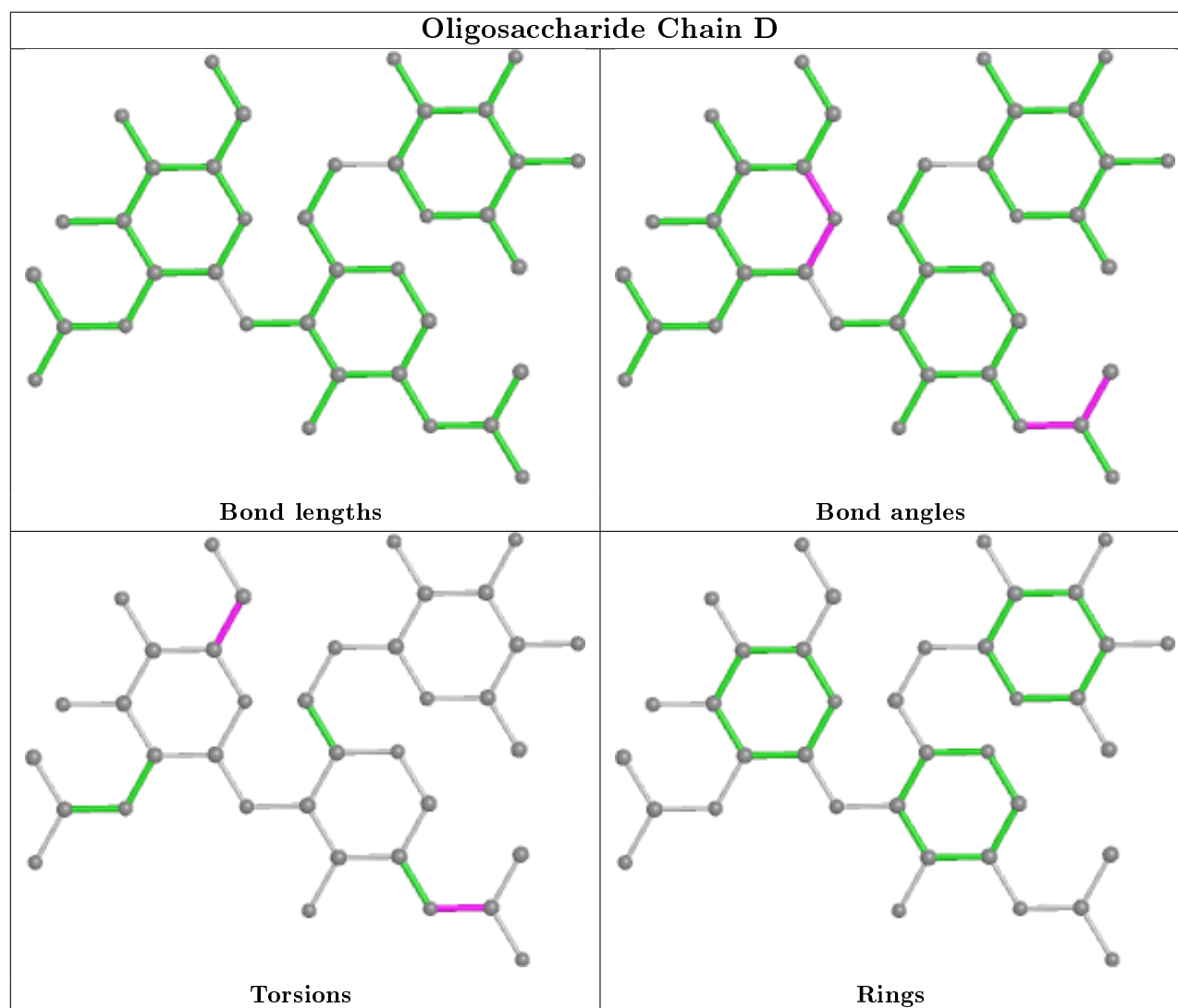
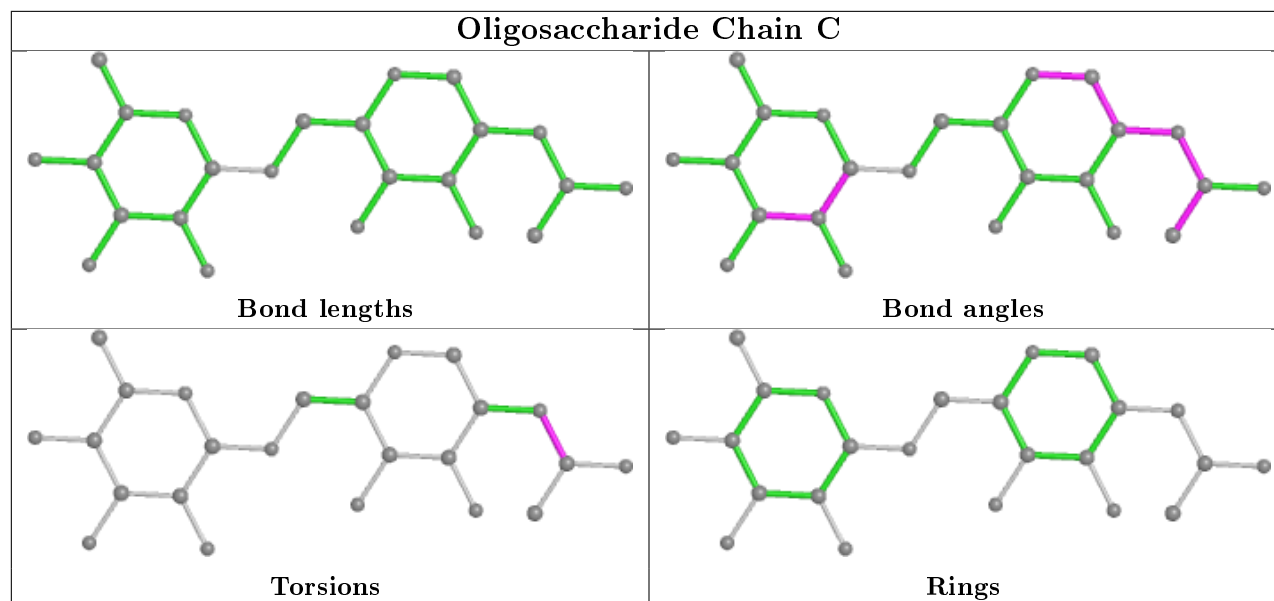
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	FUC	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

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\# Z > 2$
5	NAG	A	1536	1	14,14,15	0.56	0	17,19,21	1.45	2 (11%)
5	NAG	A	1535	1	14,14,15	0.42	0	17,19,21	1.35	3 (17%)
9	EFS	A	1544	1	2,5,6	0.59	0	0,5,8	0.00	-
8	SO4	A	1543	-	4,4,4	0.20	0	6,6,6	0.28	0
5	NAG	A	1537	1	14,14,15	0.69	0	17,19,21	1.54	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
5	NAG	A	1536	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1535	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1537	1	1/1/5/7	1/6/23/26	0/1/1/1
9	EFS	A	1544	1	-	0/1/3/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1537	NAG	C4-C3-C2	4.47	117.57	111.02
5	A	1536	NAG	C1-O5-C5	3.32	116.69	112.19
5	A	1535	NAG	C1-O5-C5	3.29	116.65	112.19
5	A	1537	NAG	C3-C4-C5	2.75	115.15	110.24
5	A	1535	NAG	O5-C1-C2	-2.21	107.80	111.29
5	A	1535	NAG	C8-C7-N2	2.13	119.71	116.10
5	A	1536	NAG	C4-C3-C2	2.03	113.99	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1537	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1535	NAG	O5-C5-C6-O6
5	A	1535	NAG	C4-C5-C6-O6
5	A	1535	NAG	C8-C7-N2-C2
5	A	1535	NAG	O7-C7-N2-C2
5	A	1537	NAG	O5-C5-C6-O6
5	A	1536	NAG	O5-C5-C6-O6
5	A	1536	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1544	EFS	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, 95th 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 ²)	Q<0.9
1	A	526/529 (99%)	0.18	35 (6%) 17 17	16, 24, 42, 55	6 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	ASP	4.8
1	A	255	GLU	4.7
1	A	377	VAL	4.7
1	A	3	ASP	4.6
1	A	50	THR	4.2
1	A	529	VAL	4.1
1	A	54	ASP	4.0
1	A	282	TYR	4.0
1	A	453	ARG	3.9
1	A	380	GLN	3.5
1	A	53	SER	3.3
1	A	378	ASP	3.2
1	A	259	GLU	3.1
1	A	525	PHE	3.1
1	A	455	GLN	3.0
1	A	51	LYS	2.8
1	A	254	ARG	2.8
1	A	237	TYR	2.6
1	A	360	GLY	2.6
1	A	376	TRP	2.6
1	A	496	THR	2.5
1	A	342	ASN	2.4
1	A	452	ARG	2.4
1	A	256	ASN	2.3
1	A	274	LEU	2.3
1	A	524	SER	2.3
1	A	4	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	344	ILE	2.2
1	A	278	PHE	2.2
1	A	251	GLY	2.2
1	A	55	ILE	2.2
1	A	382	PRO	2.1
1	A	22	GLY	2.1
1	A	257	GLU	2.1
1	A	244	LEU	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, 95th 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 ²)	Q<0.9
1	CSS	A	66	7/8	0.97	0.11	20,21,25,28	1

6.3 Carbohydrates [i](#)

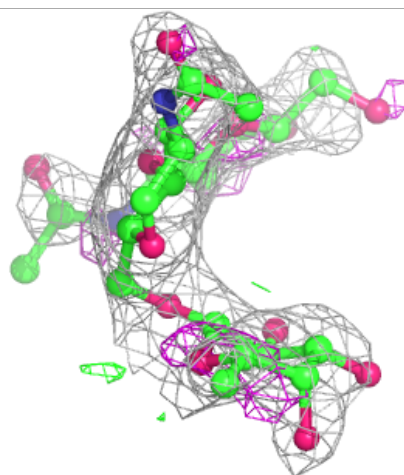
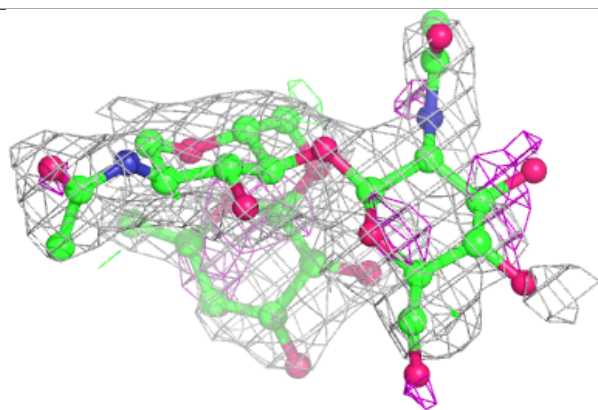
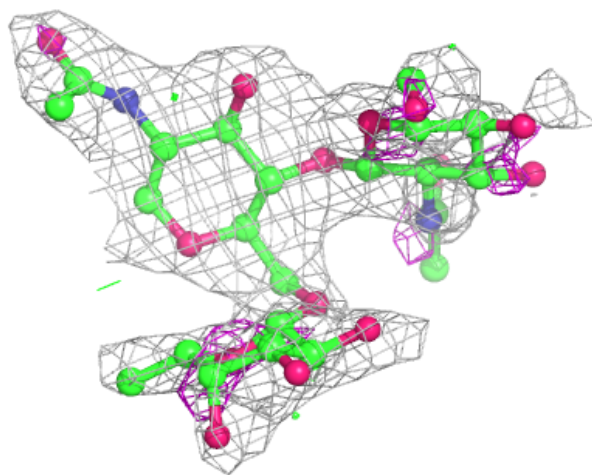
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	D	2	14/15	0.77	0.49	63,64,65,66	0
2	FUL	B	3	10/11	0.78	0.38	52,53,54,54	0
2	NAG	B	2	14/15	0.84	0.52	53,57,58,58	0
3	FUC	C	2	10/11	0.86	0.22	27,29,31,31	10
4	NAG	D	1	14/15	0.89	0.31	52,57,60,60	0
4	FUC	D	3	10/11	0.91	0.44	56,56,56,57	0
2	NAG	B	1	14/15	0.91	0.18	36,40,49,50	0
3	NAG	C	1	14/15	0.92	0.21	33,37,39,41	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.

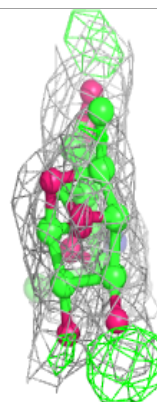
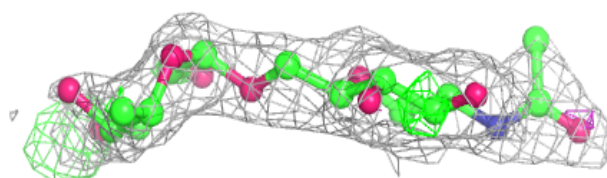
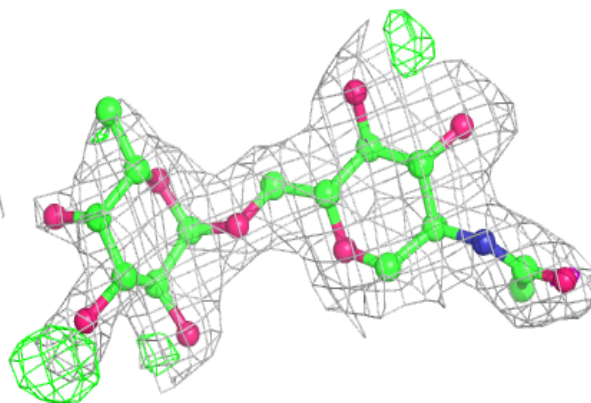
Electron density around Chain B:

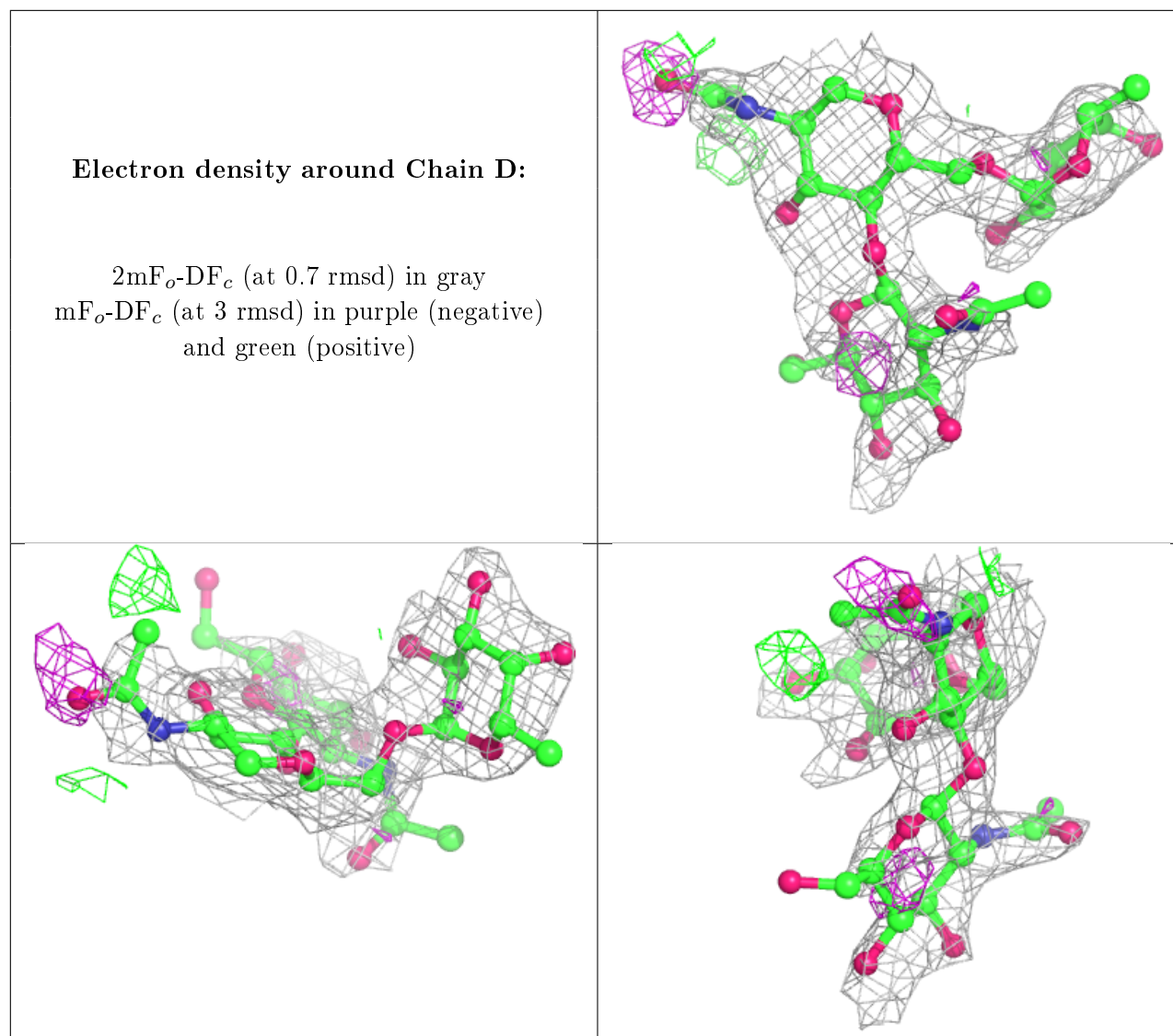
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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, 95th 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 ²)	Q<0.9
5	NAG	A	1537	14/15	0.43	0.58	58,61,62,62	0
5	NAG	A	1536	14/15	0.69	0.27	43,45,49,51	0
5	NAG	A	1535	14/15	0.71	0.30	48,52,53,53	0
10	F	A	1546	1/1	0.85	0.34	46,46,46,46	0
6	CL	A	1541	1/1	0.92	0.06	52,52,52,52	0
7	NA	A	1542	1/1	0.93	0.33	47,47,47,47	1
8	SO4	A	1543	5/5	0.97	0.17	27,31,32,33	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	EFS	A	1544	6/7	0.99	0.20	21,24,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.