WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2024 – 08:19 pm BST

PDB ID	:	2WIF
Title	:	AGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY TABUN ANALOGUE TA1
Authors	:	Carletti, E.; Aurbek, N.; Gillon, E.; Loiodice, M.; Nicolet, Y.; Fontecilla, J.; Masson, P.; Thiermann, H.; Nachon, F.; Worek, F.
Deposited on	:	2009-05-11
Resolution	:	2.25 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

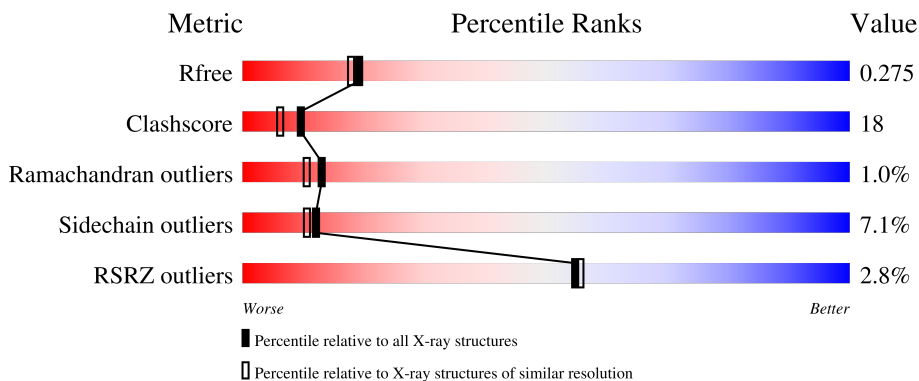|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
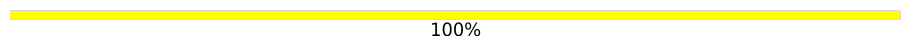*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	Percentile Ranks	Value
Rfree		0.275
Clashscore		18
Ramachandran outliers		1.0%
Sidechain outliers		7.1%
RSRZ outliers		2.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	3% / 67% / 27% / 6% ·
2	B	3	100%
2	D	3	67% / 33%
3	C	2	100%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 4747 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	S	7	2	0
			4213	2720	710	768	15			

There are 3 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

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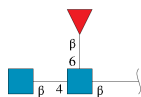
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	D	3	Total	C	N	O	0	0	0
			38	22	2	14			

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

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

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

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	Cl 3	0	0

- Molecule 6 is diethylphosphoramidic acid (three-letter code: TN6) (formula: $C_4H_{12}NO_3P$).
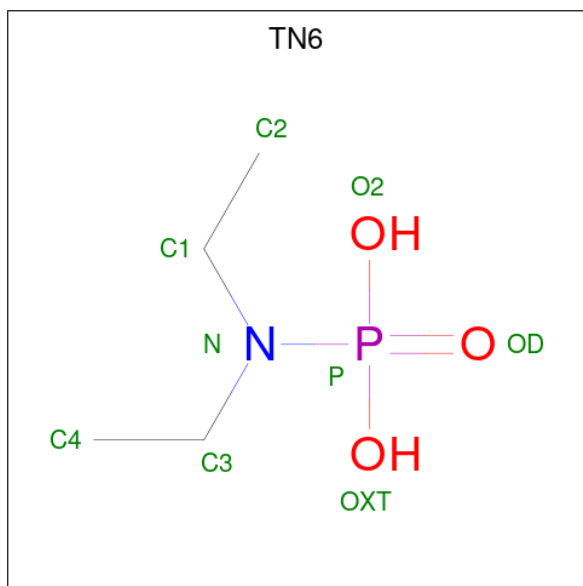
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 8	C 4	N 1	O 2	P 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

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

Continued on next page...

Continued from previous page...

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	370	Total 370	O 370	0	0

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.

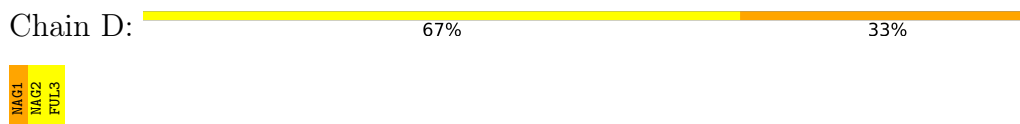• Molecule 1: CHOLINESTERASE
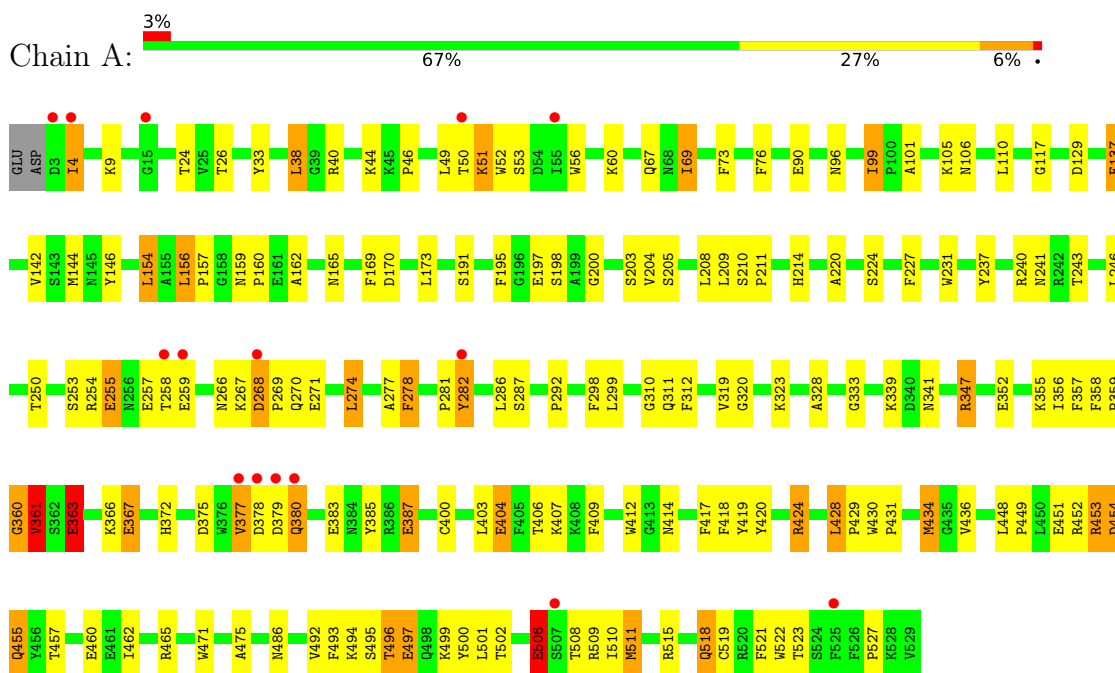
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose
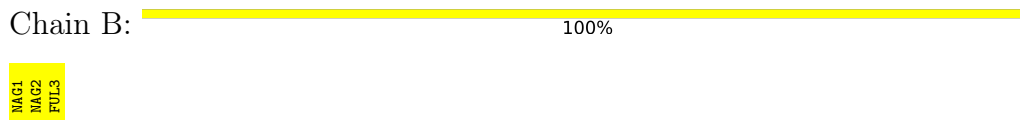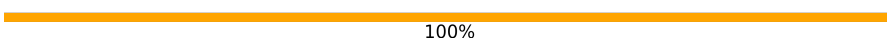

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acet amido-2-deoxy-beta-D-glucopyranose

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

Chain C:

100%

NAG1
FUL2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	154.39Å 154.39Å 126.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.25 47.67 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-2.25) 96.8 (47.67-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.207 , 0.275 0.206 , 0.275	Depositor DCC
R_{free} test set	1410 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 58.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4747	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, TN6, NA, SO4, FUL, CL

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	1.21	12/4340 (0.3%)	1.03	9/5892 (0.2%)

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	1	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	TYR	CB-CG	-10.71	1.35	1.51
1	A	497	GLU	CD-OE2	8.22	1.34	1.25
1	A	404	GLU	CG-CD	7.96	1.63	1.51
1	A	400	CYS	CB-SG	-7.70	1.69	1.82
1	A	367	GLU	CG-CD	6.02	1.60	1.51

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	515	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	A	515	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	434	MET	CG-SD-CE	6.93	111.29	100.20
1	A	274	LEU	CA-CB-CG	6.05	129.21	115.30
1	A	424	ARG	NE-CZ-NH2	-5.38	117.61	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	361	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	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	4213	0	4110	146	0
2	B	38	0	34	0	0
2	D	38	0	34	1	0
3	C	24	0	22	2	0
4	A	1	0	0	0	0
5	A	3	0	0	1	0
6	A	8	0	11	3	0
7	A	10	0	0	0	0
8	A	42	0	39	5	0
9	A	370	0	0	25	0
All	All	4747	0	4250	151	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 18.

The worst 5 of 151 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:377:VAL:O	1:A:377:VAL:HG23	1.62	0.99
1:A:320:GLY:HA3	1:A:419:TYR:CE1	1.96	0.99
1:A:282:TYR:O	1:A:282:TYR:HD1	1.45	0.97
1:A:51:LYS:N	9:A:701:HOH:O	1.96	0.96
1:A:518:GLN:HE21	1:A:518:GLN:H	1.00	0.96

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	527/529 (100%)	489 (93%)	33 (6%)	5 (1%)	14	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	VAL
1	A	453	ARG
1	A	496	THR
1	A	506	GLU
1	A	51	LYS

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	453/454 (100%)	421 (93%)	32 (7%)	12	10

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	486	ASN
1	A	506	GLU
1	A	258	THR
1	A	255	GLU
1	A	511	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	275	ASN
1	A	289	ASN
1	A	380	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	2,1	14,14,15	1.24	2 (14%)	17,19,21	1.58	5 (29%)
2	NAG	B	2	2	14,14,15	0.89	1 (7%)	17,19,21	1.83	5 (29%)
2	FUL	B	3	2	10,10,11	0.96	0	14,14,16	4.04	5 (35%)
3	NAG	C	1	3,1	14,14,15	0.84	1 (7%)	17,19,21	2.51	8 (47%)
3	FUL	C	2	3	10,10,11	0.89	0	14,14,16	2.51	7 (50%)
2	NAG	D	1	2,1	14,14,15	0.79	0	17,19,21	2.28	4 (23%)
2	NAG	D	2	2	14,14,15	0.42	0	17,19,21	1.81	4 (23%)
2	FUL	D	3	2	10,10,11	0.77	0	14,14,16	2.88	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	2,1	-	6/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	4/6/23/26	0/1/1/1
3	FUL	C	2	3	-	-	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	FUL	D	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	1	NAG	O5-C1	-2.95	1.39	1.43
2	B	2	NAG	O5-C1	-2.49	1.39	1.43
2	B	1	NAG	C2-N2	-2.36	1.42	1.46
3	C	1	NAG	C1-C2	2.28	1.55	1.52

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3	FUL	C1-C2-C3	-12.59	94.19	109.67
2	D	3	FUL	C1-C2-C3	-6.88	101.20	109.67
2	D	1	NAG	C1-O5-C5	5.52	119.67	112.19
2	D	1	NAG	O5-C1-C2	-4.95	103.47	111.29
2	D	3	FUL	C1-O5-C5	-4.75	102.00	112.78

There are no chirality outliers.

5 of 20 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	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
3	C	1	NAG	1	0
3	C	2	FUL	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.

Oligosaccharide Chain B

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings
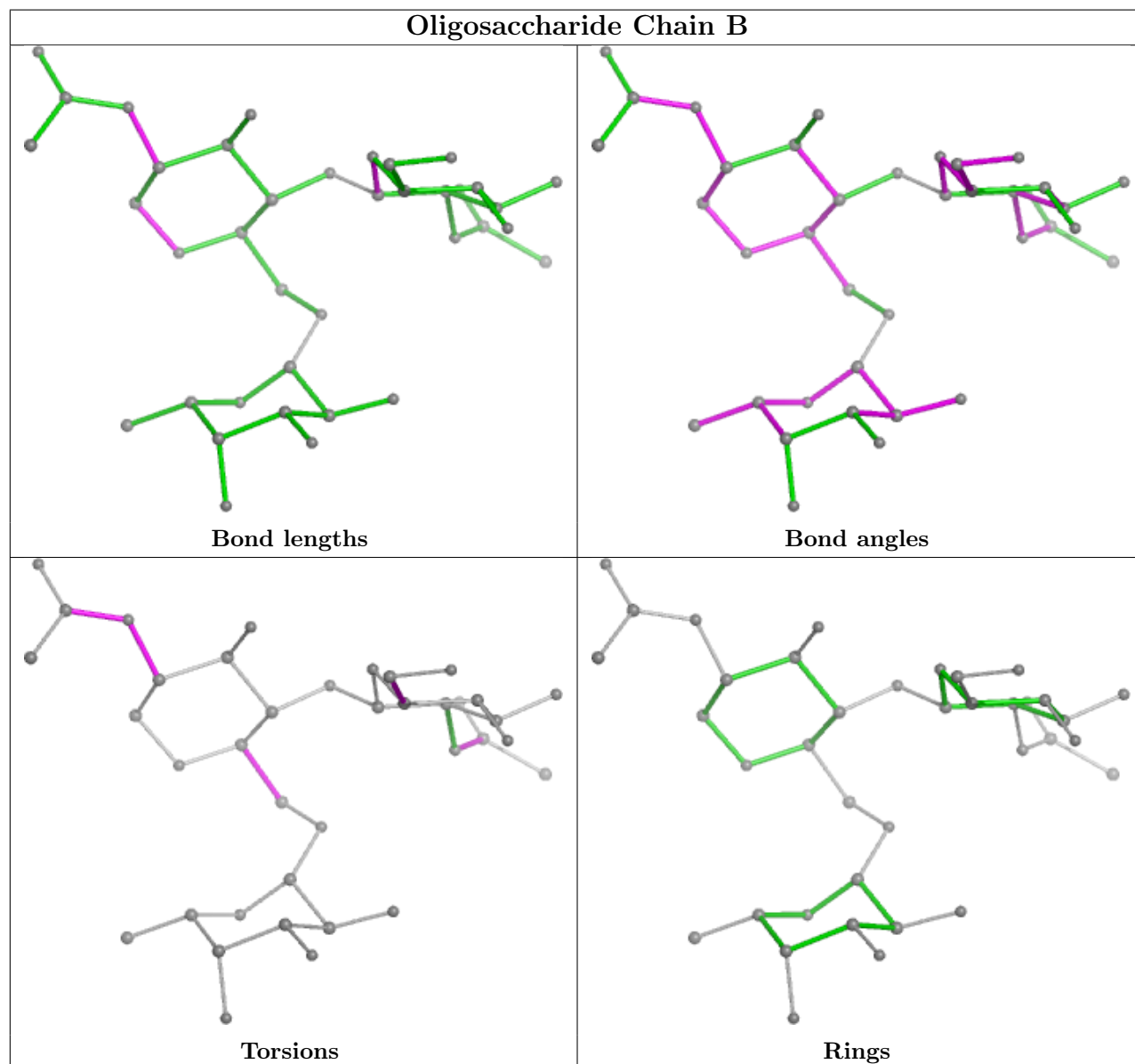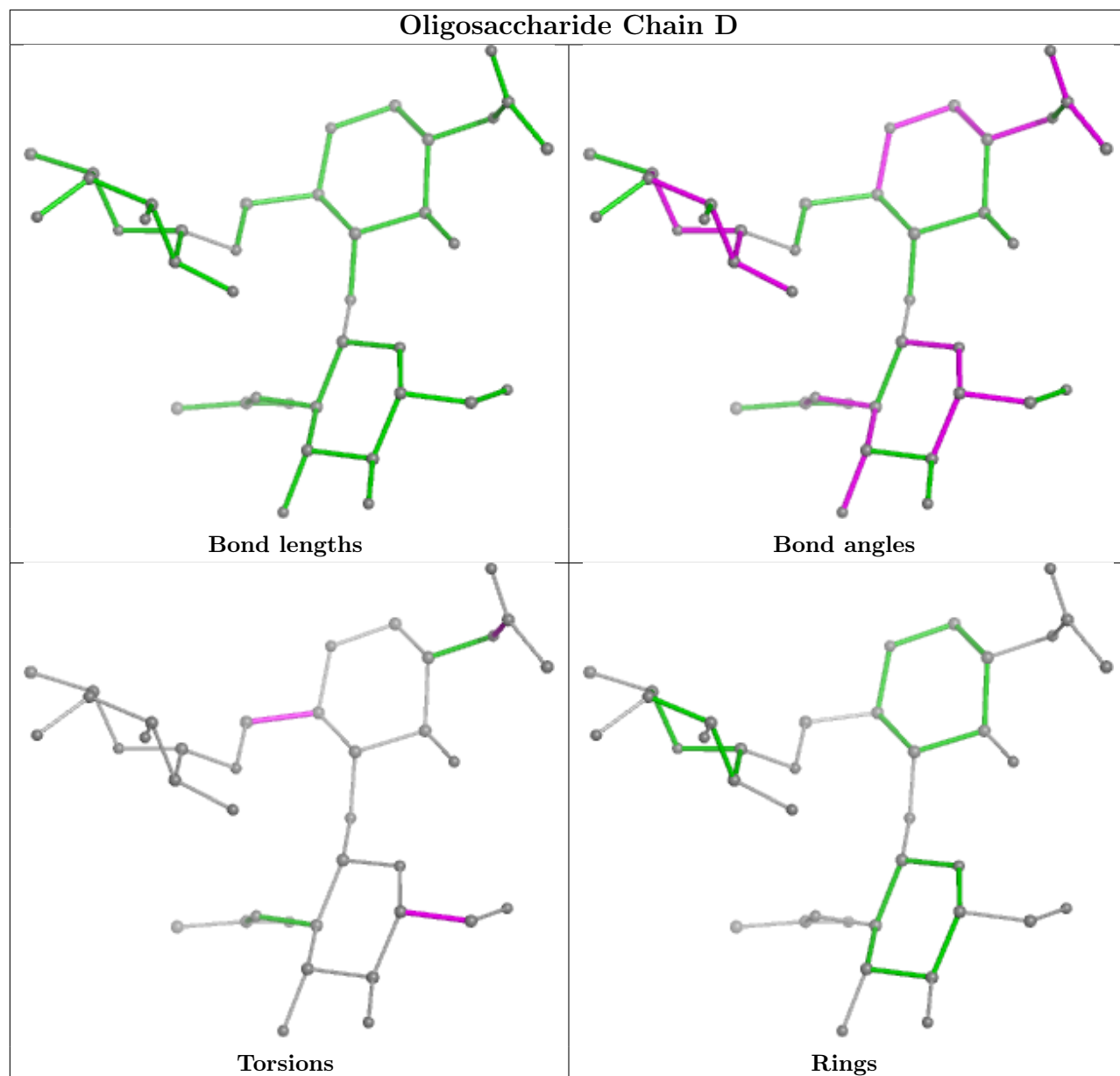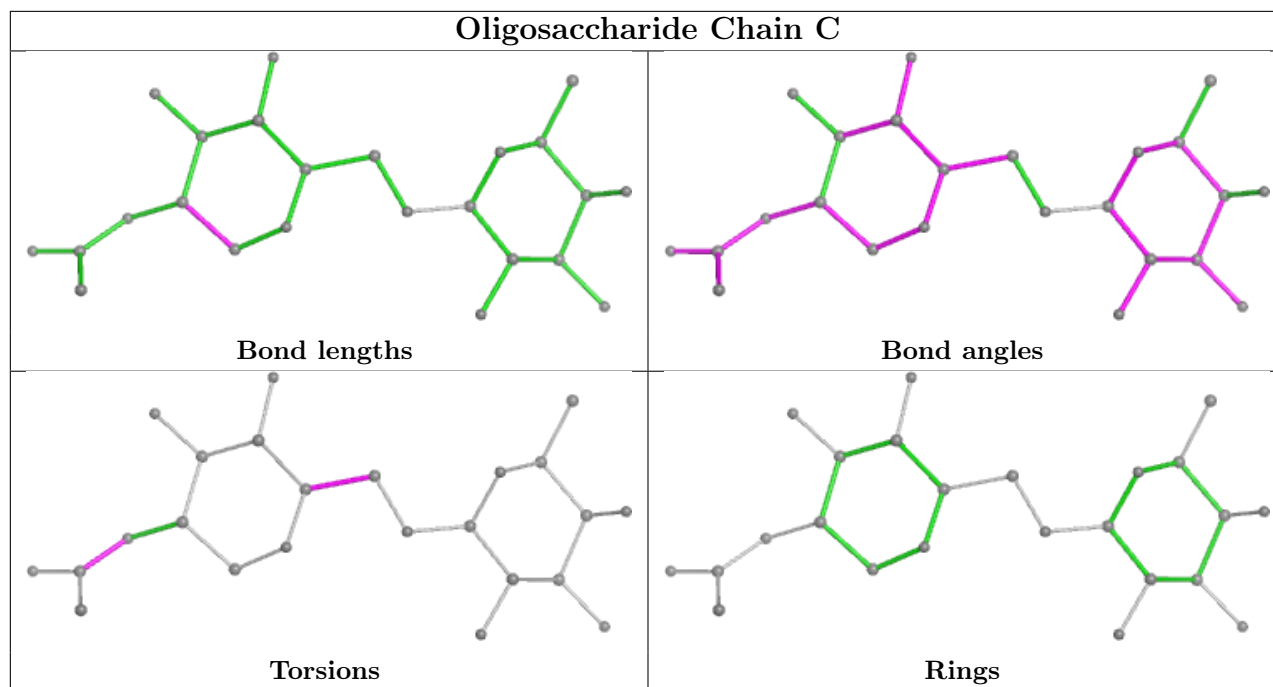
5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 4 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	#$|Z| > 2$
8	NAG	A	613	1	14,14,15	0.58	0	17,19,21	1.96	5 (29%)
7	SO4	A	605	-	4,4,4	0.15	0	6,6,6	0.29	0
8	NAG	A	615	1	14,14,15	0.48	0	17,19,21	2.03	4 (23%)
7	SO4	A	607	-	4,4,4	0.26	0	6,6,6	0.52	0
6	TN6	A	603	1	2,7,8	1.84	1 (50%)	1,8,11	0.68	0
8	NAG	A	614	1	14,14,15	0.86	0	17,19,21	1.92	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
8	NAG	A	614	1	-	2/6/23/26	0/1/1/1
6	TN6	A	603	1	-	1/4/8/10	-
8	NAG	A	615	1	-	3/6/23/26	0/1/1/1
8	NAG	A	613	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	TN6	C4-C3	2.41	1.63	1.49

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	614	NAG	C1-O5-C5	6.33	120.78	112.19
8	A	615	NAG	O5-C5-C6	4.00	113.48	107.20
8	A	615	NAG	C1-O5-C5	-3.86	106.96	112.19
8	A	613	NAG	C2-N2-C7	-3.84	117.44	122.90
8	A	615	NAG	C3-C4-C5	3.70	116.84	110.24

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	613	NAG	C8-C7-N2-C2
8	A	615	NAG	C8-C7-N2-C2
8	A	615	NAG	O7-C7-N2-C2
8	A	613	NAG	O7-C7-N2-C2
8	A	613	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	613	NAG	4	0
8	A	615	NAG	1	0
6	A	603	TN6	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	527/529 (99%)	0.06	15 (2%)	55	55	16, 33, 57, 76	11 (2%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	THR	4.4
1	A	50	THR	3.6
1	A	282	TYR	3.5
1	A	377	VAL	3.4
1	A	378	ASP	2.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.
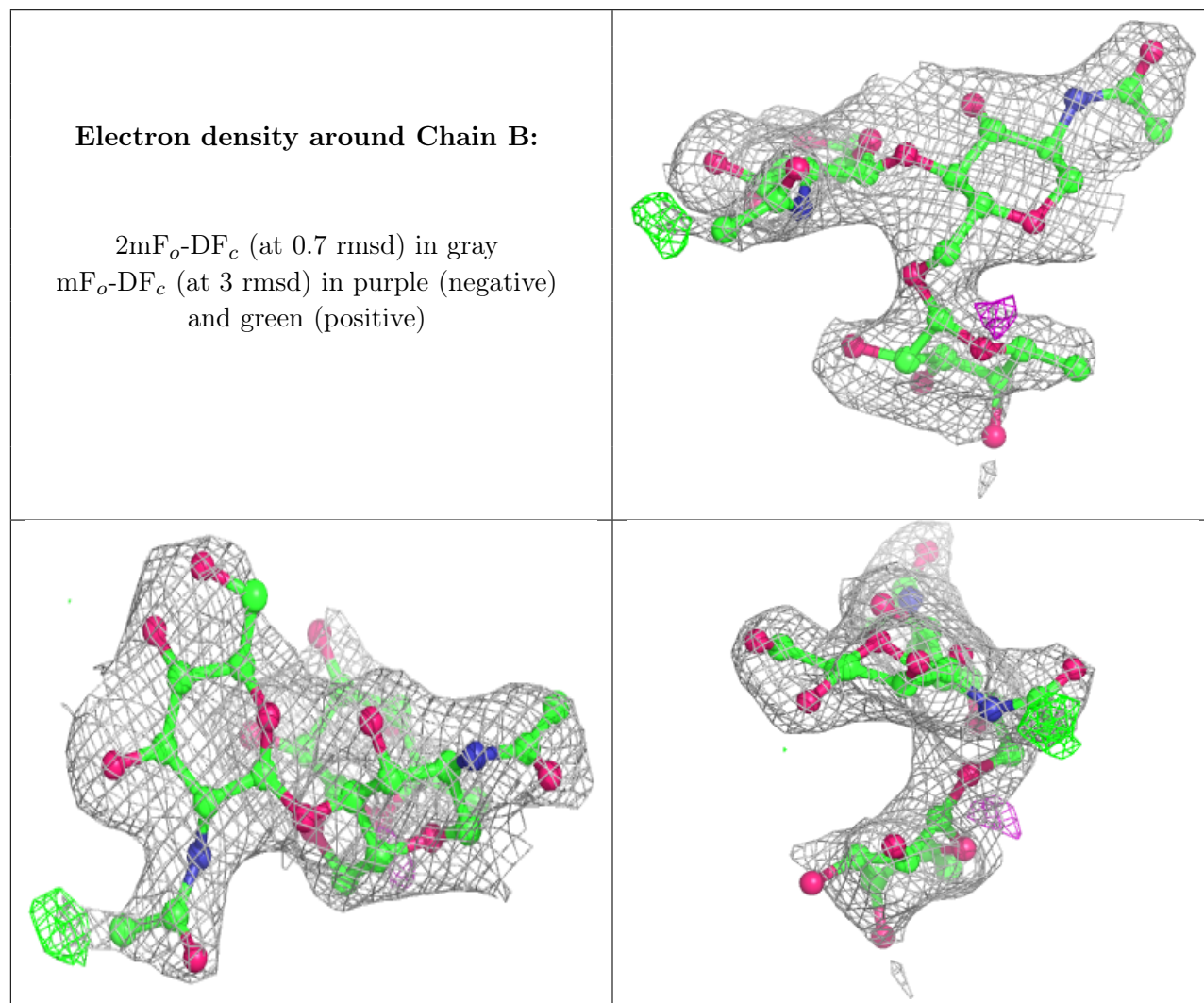
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	2	14/15	0.71	0.16	65,76,78,78	0
2	FUL	B	3	10/11	0.72	0.18	65,69,73,73	0
3	FUL	C	2	10/11	0.76	0.32	40,46,47,49	10
2	NAG	D	1	14/15	0.77	0.16	67,72,79,79	0
2	NAG	B	2	14/15	0.78	0.15	62,67,70,70	0
3	NAG	C	1	14/15	0.79	0.16	54,59,61,64	0
2	FUL	D	3	10/11	0.84	0.16	71,73,75,77	0

Continued on next page...

Continued from previous page...

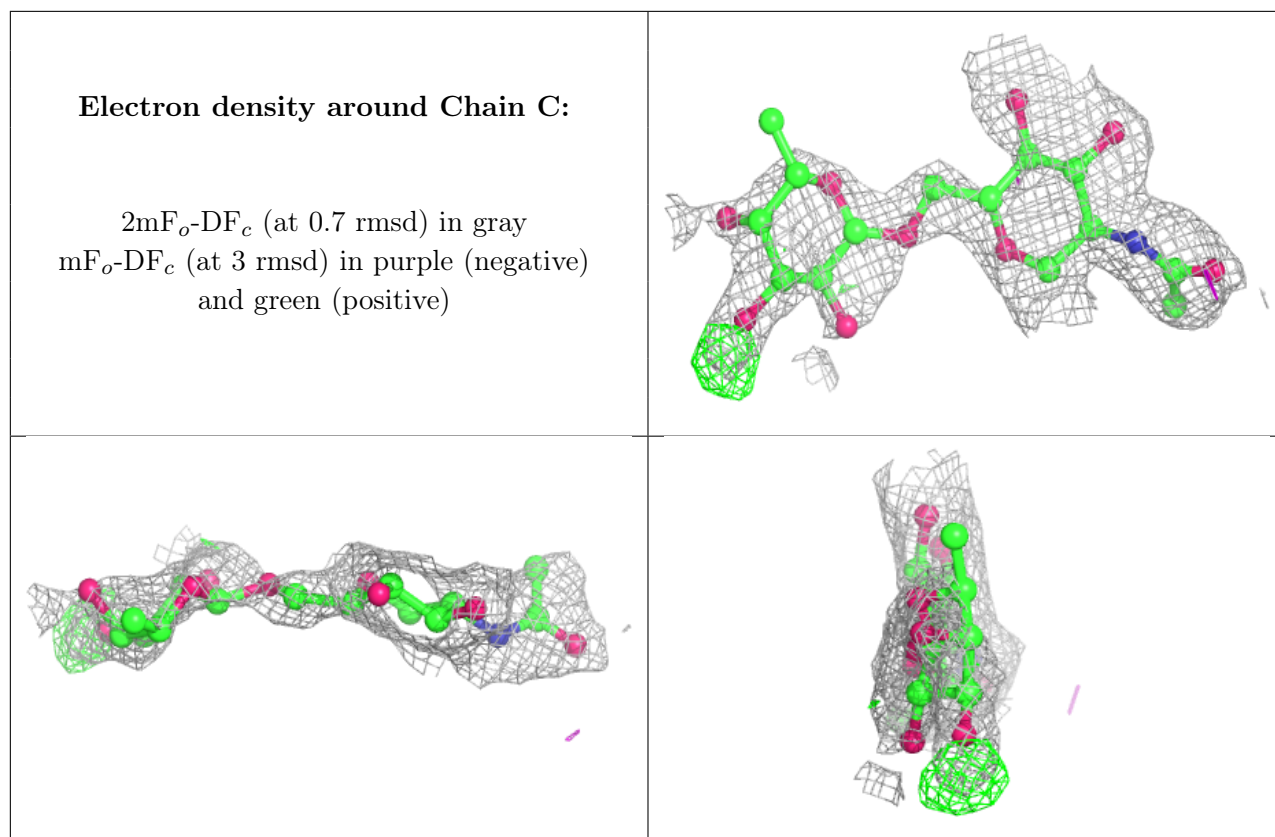| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	B	1	14/15	0.93	0.11	46,52,58,64	0

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:

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

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)
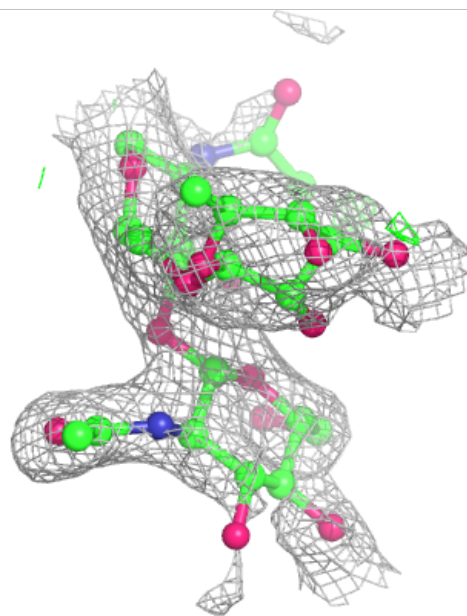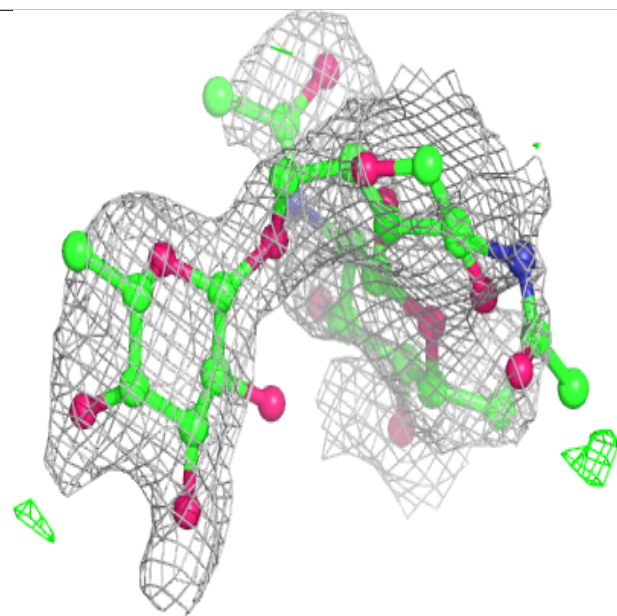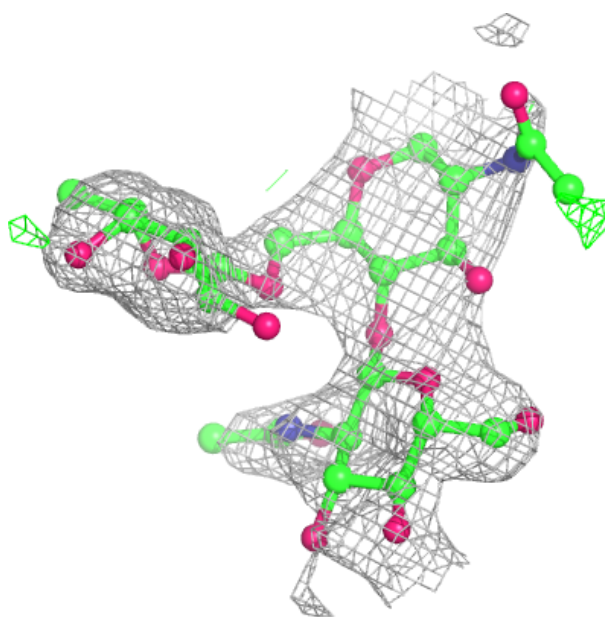
Electron density around Chain C:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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
8	NAG	A	613	14/15	0.58	0.17	73,77,79,82	0
8	NAG	A	615	14/15	0.72	0.14	82,85,88,88	0
8	NAG	A	614	14/15	0.73	0.16	45,60,64,66	0
5	CL	A	604	1/1	0.89	0.13	71,71,71,71	0
5	CL	A	606	1/1	0.91	0.10	62,62,62,62	0
7	SO4	A	605	5/5	0.92	0.10	52,52,57,58	5
5	CL	A	602	1/1	0.93	0.12	58,58,58,58	0
7	SO4	A	607	5/5	0.94	0.12	40,42,43,45	5
6	TN6	A	603	8/9	0.98	0.07	24,27,28,29	0
4	NA	A	601	1/1	0.98	0.13	41,41,41,41	1

6.5 Other polymers ⓘ

There are no such residues in this entry.