



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:56 AM UTC

PDB ID : 5NAU / pdb_00005nau
Title : Torpedo californica acetylcholinesterase in complex with a non-chiral donepezil-like compound 20
Authors : Caliandro, R.; Pesaresi, A.; Lamba, D.
Deposited on : 2017-02-28
Resolution : 2.25 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

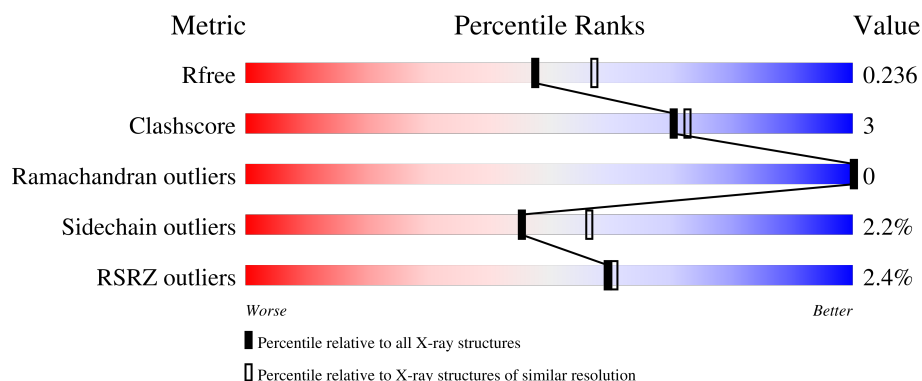
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 $\leq 5\%$. 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	543	2% 85% 12%
2	B	2	100%
3	C	4	25% 75%
3	D	4	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4634 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 Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4205	2703	710	770	22			

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



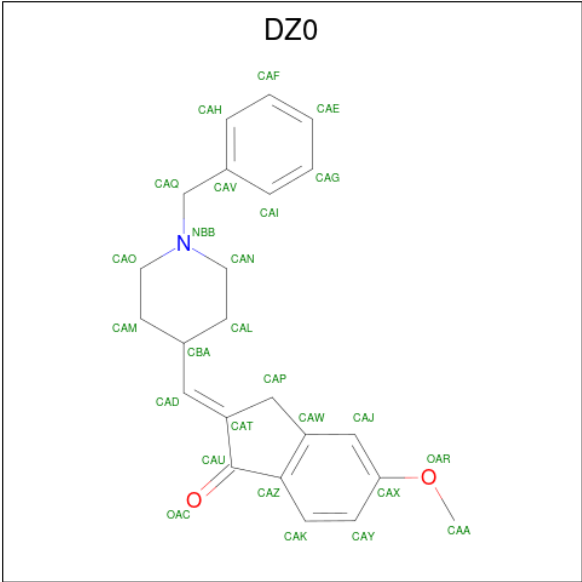
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is (2 {E})-5-methoxy-2-[[1-(phenylmethyl)piperidin-4-yl]methylidene]-3 {H}-inden-1-one (CCD ID: DZ0) (formula: C₂₃H₂₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			26	23	1	2		

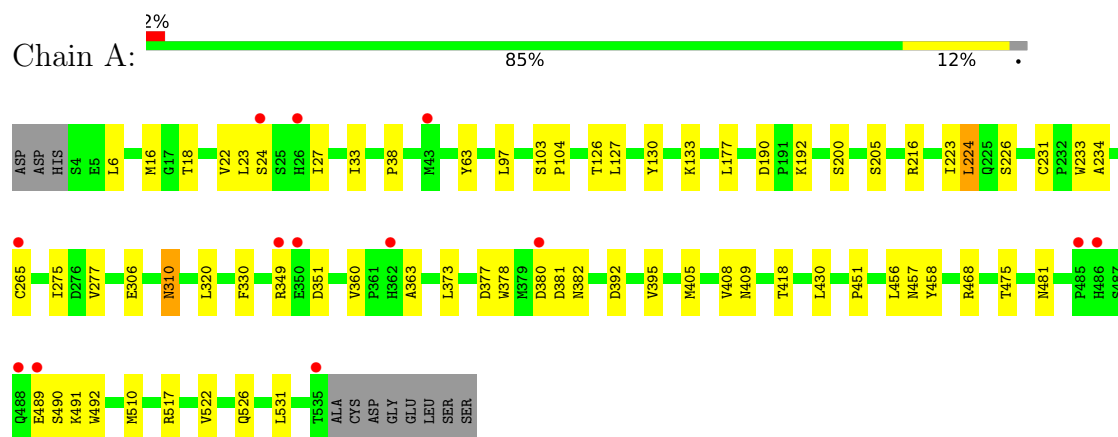
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	279	Total	O	0	0
			279	279		

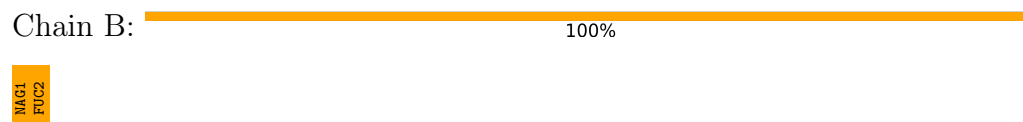
3 Residue-property plots [i](#)

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: Acetylcholinesterase



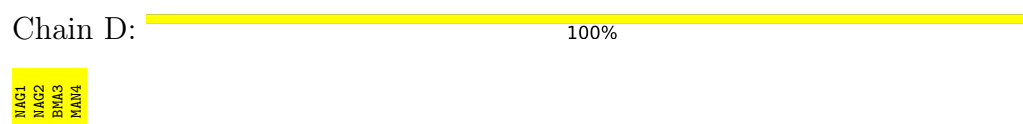
- Molecule 2: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.62Å 111.62Å 136.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.33 – 2.25 48.33 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.33-2.25) 99.5 (48.33-2.25)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.187 , 0.228 (Not available) , 0.236	Depositor DCC
R_{free} test set	2369 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4634	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 3.69% 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: NAG, DZ0, MAN, BMA, FUC

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	1.33	13/4326 (0.3%)	1.19	9/5878 (0.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	PRO	N-CD	-9.65	1.34	1.47
1	A	18	THR	CA-C	-6.68	1.44	1.52
1	A	224	LEU	CA-C	5.70	1.59	1.52
1	A	177	LEU	C-O	-5.61	1.17	1.24
1	A	97	LEU	CA-C	-5.57	1.45	1.52
1	A	517	ARG	CA-C	-5.49	1.46	1.53
1	A	38	PRO	C-O	-5.25	1.18	1.24
1	A	205	SER	CA-C	5.13	1.59	1.52
1	A	275	ILE	CA-C	5.06	1.59	1.52
1	A	234	ALA	C-O	-5.05	1.17	1.24
1	A	392	ASP	CA-C	5.04	1.59	1.52
1	A	418	THR	CA-C	-5.01	1.46	1.52
1	A	351	ASP	CA-C	5.01	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	VAL	N-CA-C	7.71	119.49	112.17
1	A	395	VAL	CA-C-N	6.63	127.49	119.99
1	A	395	VAL	C-N-CA	6.63	127.49	119.99
1	A	381	ASP	N-CA-C	-5.79	106.19	113.72
1	A	492	TRP	CA-C-N	-5.55	115.03	120.52
1	A	492	TRP	C-N-CA	-5.55	115.03	120.52
1	A	33	ILE	CB-CA-C	-5.43	105.89	110.94
1	A	216	ARG	N-CA-C	5.23	117.72	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	522	VAL	CB-CA-C	-5.16	105.18	112.14

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	4205	0	4034	26	0
2	B	24	0	22	1	0
3	C	50	0	43	1	0
3	D	50	0	43	0	0
4	A	26	0	0	1	0
5	A	279	0	0	1	0
All	All	4634	0	4142	29	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 3.

All (29) 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:405:MET:O	1:A:408:VAL:HG12	1.89	0.71
1:A:6:LEU:HB2	1:A:16:MET:HE3	1.83	0.60
1:A:223:ILE:HA	1:A:320:LEU:O	2.05	0.56
1:A:306:GLU:O	1:A:310:ASN:HB2	2.09	0.53
1:A:27:ILE:HD11	1:A:133:LYS:HB2	1.93	0.51
1:A:491:LYS:O	1:A:510:MET:HE1	2.10	0.51
1:A:405:MET:C	1:A:408:VAL:HG12	2.37	0.50
1:A:475:THR:HG22	1:A:481:ASN:O	2.12	0.50
1:A:6:LEU:CB	1:A:16:MET:HE3	2.41	0.50
3:C:1:NAG:H61	3:C:2:NAG:N2	2.27	0.49
1:A:408:VAL:HG13	1:A:409:ASN:N	2.26	0.49
1:A:451:PRO:HA	1:A:458:TYR:CD1	2.49	0.47
1:A:200:SER:HA	1:A:226:SER:O	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:CYS:HB2	5:A:871:HOH:O	2.15	0.47
1:A:456:LEU:O	1:A:457:ASN:HB2	2.14	0.47
4:A:611:DZ0:CAL	4:A:611:DZ0:CAP	2.93	0.46
1:A:360:VAL:HG12	1:A:363:ALA:HB2	1.97	0.46
1:A:531:LEU:C	1:A:531:LEU:HD23	2.42	0.45
1:A:377:ASP:O	1:A:380:ASP:O	2.34	0.45
1:A:190:ASP:OD1	1:A:192:LYS:HG2	2.17	0.45
1:A:63:TYR:CD1	1:A:126:THR:HG22	2.51	0.44
1:A:103:SER:HA	1:A:104:PRO:C	2.41	0.44
1:A:6:LEU:HB2	1:A:16:MET:CE	2.47	0.43
1:A:127:LEU:HD12	1:A:130:TYR:CE2	2.54	0.42
1:A:224:LEU:HD12	1:A:224:LEU:N	2.34	0.42
1:A:373:LEU:HD12	1:A:378:TRP:HE1	1.85	0.42
1:A:23:LEU:O	1:A:24:SER:HB2	2.20	0.42
1:A:231:CYS:HB3	1:A:233:TRP:NE1	2.34	0.42
2:B:1:NAG:H61	2:B:2:FUC:O2	2.20	0.41

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	530/543 (98%)	503 (95%)	27 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	452/474 (95%)	442 (98%)	10 (2%)	45 56

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	310	ASN
1	A	330	PHE
1	A	349	ARG
1	A	382	ASN
1	A	430	LEU
1	A	468	ARG
1	A	489	GLU
1	A	490	SER
1	A	526	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	178	GLN
1	A	409	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
3	NAG	D	2	3	14,14,15	0.59	0	17,19,21	1.57	1 (5%)
3	MAN	D	4	3	11,11,12	0.76	0	15,15,17	1.97	7 (46%)
3	NAG	C	1	3,1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	D	1	3,1	14,14,15	0.56	0	17,19,21	1.66	3 (17%)
2	NAG	B	1	2,1	14,14,15	0.73	0	17,19,21	1.66	4 (23%)
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.56	0
2	FUC	B	2	2	10,10,11	0.81	0	14,14,16	1.32	1 (7%)
3	MAN	C	4	3	11,11,12	0.86	1 (9%)	15,15,17	1.34	2 (13%)

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
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
2	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	MAN	C2-C3	2.25	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C1-O5-C5	4.25	117.88	112.19
3	D	2	NAG	C1-O5-C5	3.63	117.05	112.19
2	B	1	NAG	O5-C1-C2	-3.47	105.92	111.29
2	B	1	NAG	C1-O5-C5	3.42	116.77	112.19
3	D	4	MAN	C3-C4-C5	3.25	116.12	110.23
3	C	4	MAN	O2-C2-C3	3.24	116.87	110.15
3	D	4	MAN	O2-C2-C3	-2.86	104.23	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-C2-C3	2.61	113.45	109.64
3	D	1	NAG	C8-C7-N2	2.59	120.42	116.12
3	D	4	MAN	O3-C3-C2	-2.56	104.83	110.05
2	B	1	NAG	O4-C4-C5	2.48	115.43	109.32
3	D	4	MAN	O5-C5-C6	2.45	112.44	107.66
2	B	1	NAG	O3-C3-C2	2.42	114.43	109.40
3	D	1	NAG	O5-C5-C6	2.35	112.23	107.66
3	D	4	MAN	C6-C5-C4	-2.33	107.30	113.02
3	C	4	MAN	O5-C5-C6	2.24	112.01	107.66
2	B	2	FUC	C3-C4-C5	2.10	113.01	109.81
3	D	4	MAN	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	MAN	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
2	B	1	NAG	1	0
3	C	2	NAG	1	0
2	B	2	FUC	1	0

5.5 Carbohydrates

10 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	1	2,1	14,14,15	0.73	0	17,19,21	1.66	4 (23%)
2	FUC	B	2	2	10,10,11	0.81	0	14,14,16	1.32	1 (7%)
3	NAG	C	1	3,1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.56	0
3	BMA	C	3	3	11,11,12	0.25	0	15,15,17	0.52	0
3	MAN	C	4	3	11,11,12	0.86	1 (9%)	15,15,17	1.34	2 (13%)
3	NAG	D	1	3,1	14,14,15	0.56	0	17,19,21	1.66	3 (17%)
3	NAG	D	2	3	14,14,15	0.59	0	17,19,21	1.57	1 (5%)
3	BMA	D	3	3	11,11,12	0.85	0	15,15,17	1.35	3 (20%)
3	MAN	D	4	3	11,11,12	0.76	0	15,15,17	1.97	7 (46%)

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	-	2/6/23/26	0/1/1/1
2	FUC	B	2	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	MAN	C	4	3	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	MAN	C2-C3	2.25	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C1-O5-C5	4.25	117.88	112.19
3	D	2	NAG	C1-O5-C5	3.63	117.05	112.19
2	B	1	NAG	O5-C1-C2	-3.47	105.92	111.29
2	B	1	NAG	C1-O5-C5	3.42	116.77	112.19
3	D	4	MAN	C3-C4-C5	3.25	116.12	110.23
3	C	4	MAN	O2-C2-C3	3.24	116.87	110.15
3	D	4	MAN	O2-C2-C3	-2.86	104.23	110.15
3	D	3	BMA	C1-O5-C5	2.67	115.76	112.19
3	D	4	MAN	C1-C2-C3	2.61	113.45	109.64
3	D	1	NAG	C8-C7-N2	2.59	120.42	116.12
3	D	4	MAN	O3-C3-C2	-2.56	104.83	110.05
2	B	1	NAG	O4-C4-C5	2.48	115.43	109.32
3	D	3	BMA	O5-C5-C6	2.46	112.45	107.66
3	D	4	MAN	O5-C5-C6	2.45	112.44	107.66
2	B	1	NAG	O3-C3-C2	2.42	114.43	109.40
3	D	1	NAG	O5-C5-C6	2.35	112.23	107.66
3	D	4	MAN	C6-C5-C4	-2.33	107.30	113.02
3	C	4	MAN	O5-C5-C6	2.24	112.01	107.66
3	D	3	BMA	O4-C4-C5	2.17	114.66	109.32
2	B	2	FUC	C3-C4-C5	2.10	113.01	109.81
3	D	4	MAN	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	MAN	C4-C5-C6-O6
3	C	4	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	D	4	MAN	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6

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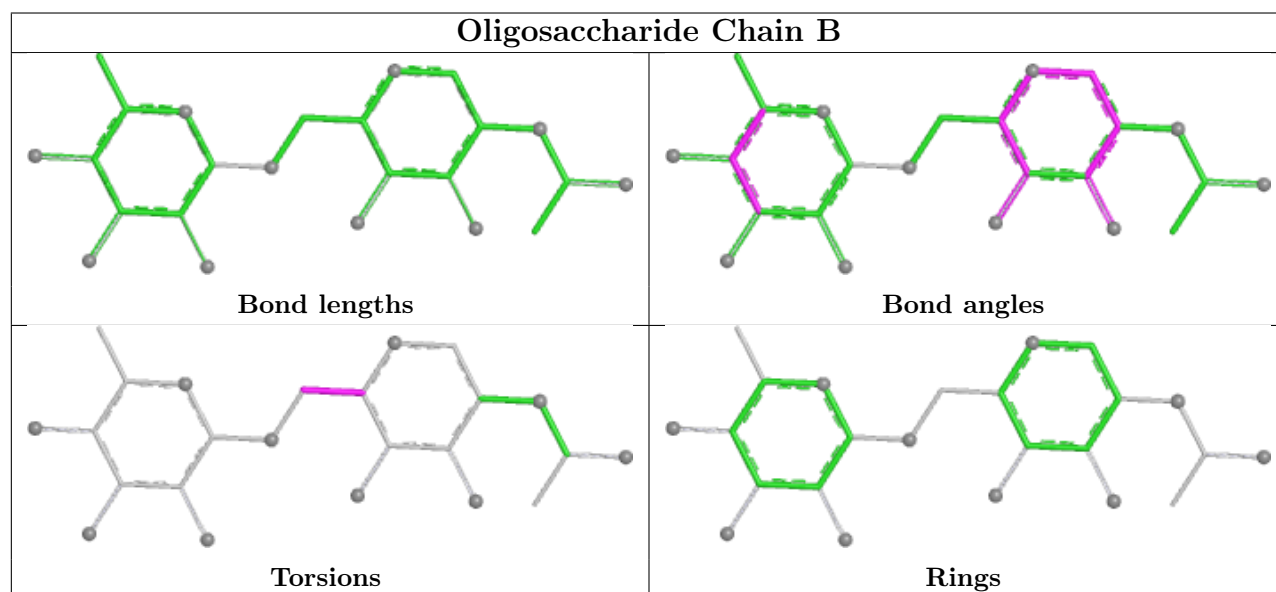
Mol	Chain	Res	Type	Atoms
3	C	3	BMA	O5-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6

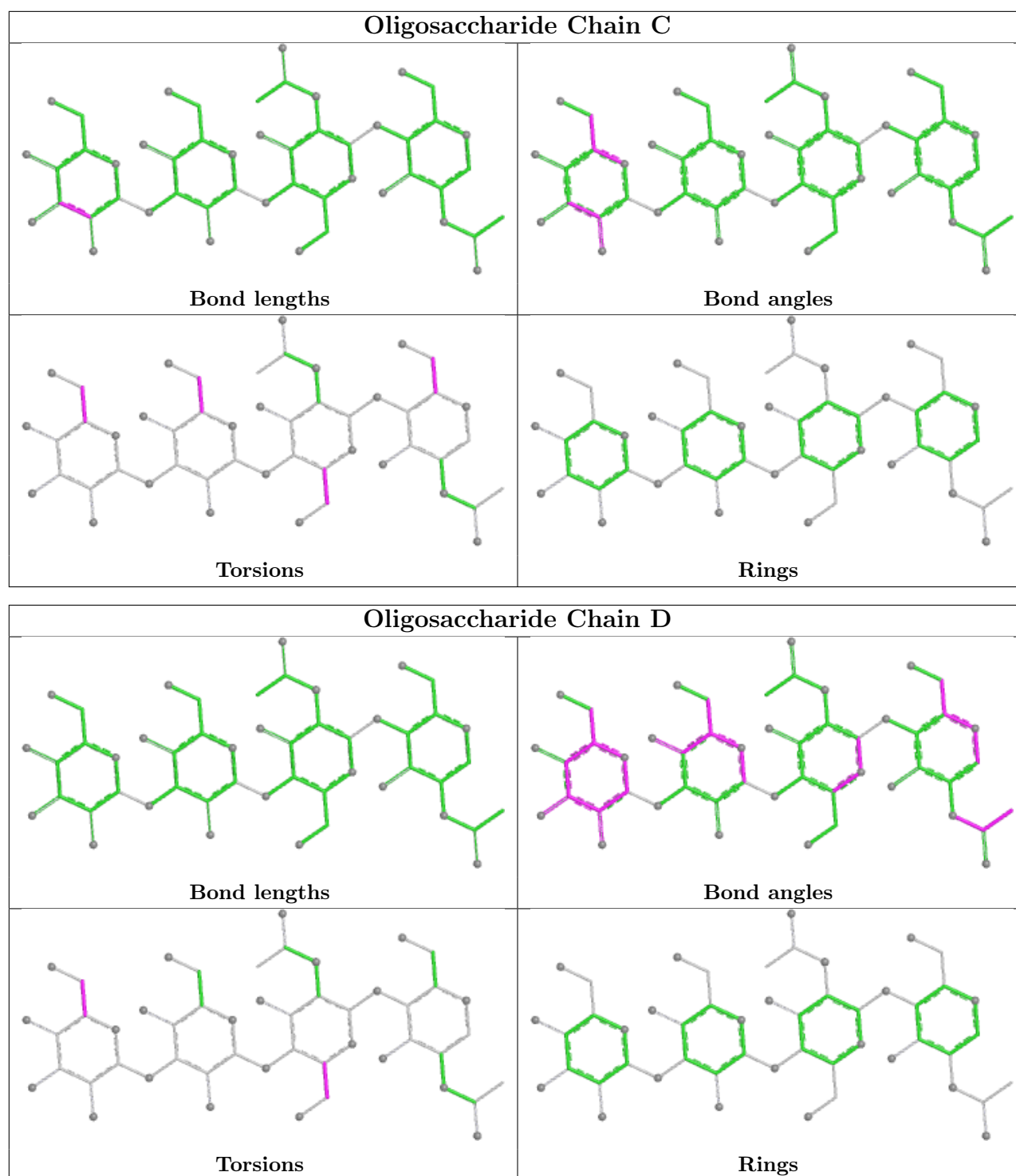
There are no ring outliers.

4 monomers are involved in 2 short contacts:

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

1 ligand 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
4	DZ0	A	611	-	29,29,29	4.59	9 (31%)	38,40,40	2.04	9 (23%)

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
4	DZ0	A	611	-	-	1/10/32/32	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	611	DZ0	CAT-CAU	-13.59	1.30	1.49
4	A	611	DZ0	CAP-CAT	-10.36	1.32	1.51
4	A	611	DZ0	CAP-CAW	-9.58	1.33	1.50
4	A	611	DZ0	CAZ-CAU	-7.85	1.31	1.48
4	A	611	DZ0	CAQ-CAV	-7.02	1.38	1.51
4	A	611	DZ0	CAZ-CAW	-6.51	1.31	1.39
4	A	611	DZ0	CAK-CAZ	-5.71	1.31	1.39
4	A	611	DZ0	CAJ-CAW	-4.74	1.32	1.39
4	A	611	DZ0	CAL-CBA	-2.30	1.48	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	611	DZ0	CAM-CBA-CAD	-6.65	102.27	111.14
4	A	611	DZ0	CAL-CBA-CAD	4.49	117.12	111.14
4	A	611	DZ0	CAW-CAP-CAT	4.42	107.47	103.49
4	A	611	DZ0	CAZ-CAU-CAT	4.29	108.67	106.64
4	A	611	DZ0	CAP-CAW-CAJ	2.60	133.57	129.66
4	A	611	DZ0	CAA-OAR-CAX	2.37	122.57	117.50
4	A	611	DZ0	CAW-CAZ-CAU	-2.35	108.25	109.52
4	A	611	DZ0	CAK-CAZ-CAW	2.16	123.57	120.88
4	A	611	DZ0	CAP-CAW-CAZ	-2.07	107.74	110.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

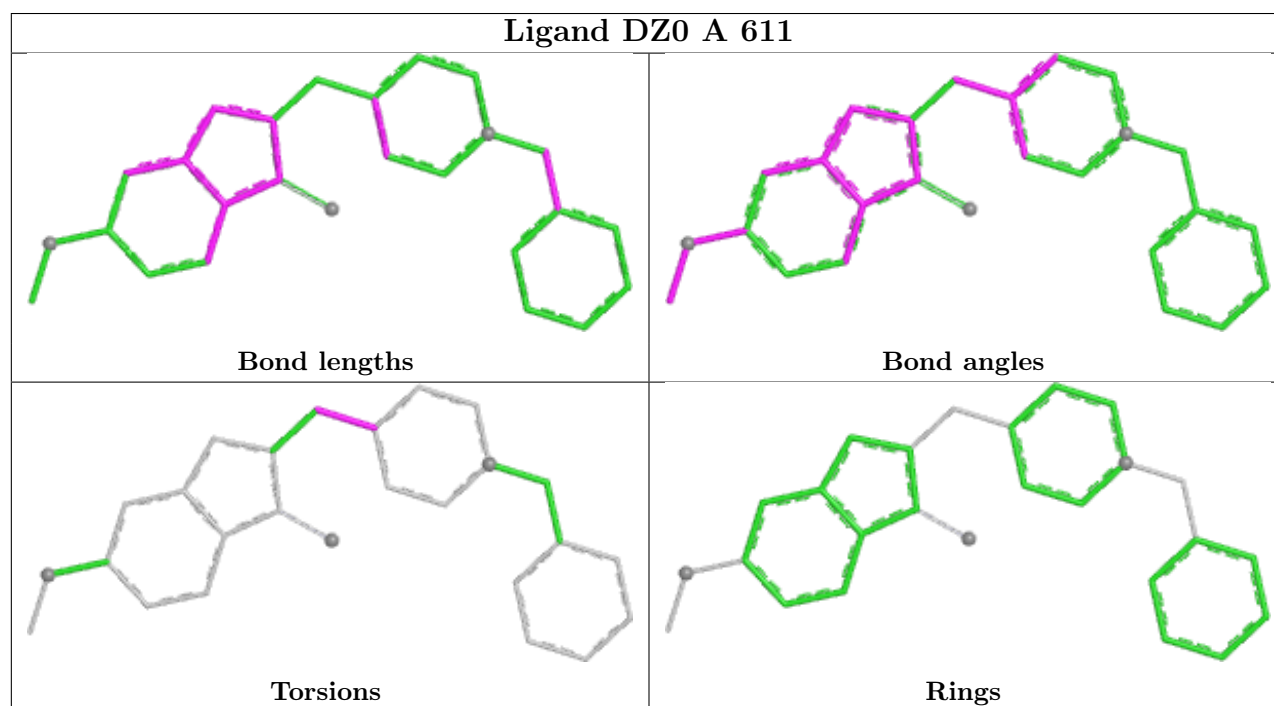
Mol	Chain	Res	Type	Atoms
4	A	611	DZ0	CAT-CAD-CBA-CAL

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	DZ0	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 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

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 [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, 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	532/543 (97%)	-0.13	13 (2%) 59 61	23, 34, 56, 87	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485	PRO	3.0
1	A	486	HIS	3.0
1	A	43	MET	2.8
1	A	535	THR	2.6
1	A	265	CYS	2.5
1	A	380	ASP	2.5
1	A	24	SER	2.4
1	A	489	GLU	2.4
1	A	26	HIS	2.3
1	A	349	ARG	2.1
1	A	350	GLU	2.1
1	A	362	HIS	2.1
1	A	488	GLN	2.1

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
3	NAG	C	2	14/15	0.66	0.21	73,91,106,107	0
3	MAN	C	4	11/12	0.70	0.15	78,100,109,113	0
3	NAG	D	2	14/15	0.72	0.16	78,92,97,100	0
3	NAG	D	1	14/15	0.73	0.16	58,75,90,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MAN	D	4	11/12	0.75	0.17	53,67,73,76	0
2	FUC	B	2	10/11	0.85	0.15	82,93,101,101	0
2	NAG	B	1	14/15	0.86	0.12	63,77,82,84	0
3	NAG	C	1	14/15	0.88	0.12	43,49,59,78	0

6.3 Carbohydrates

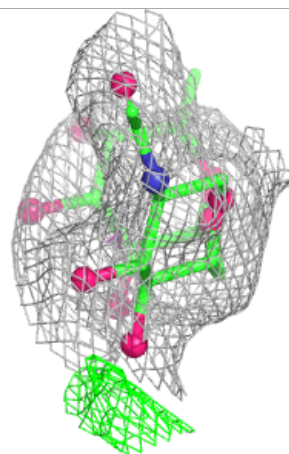
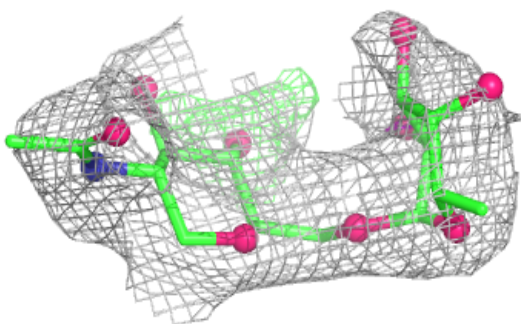
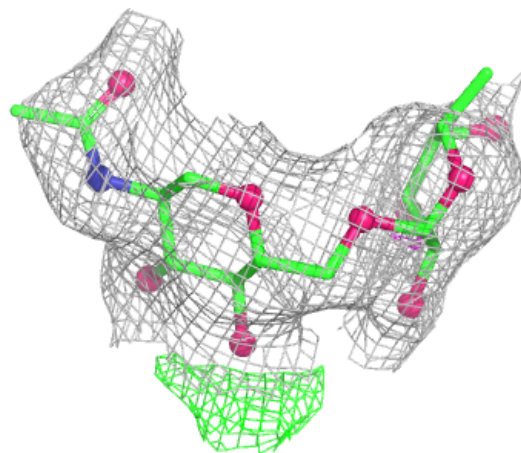
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	C	3	11/12	0.37	0.21	97,114,121,124	0
3	BMA	D	3	11/12	0.56	0.18	75,88,95,95	0
3	NAG	C	2	14/15	0.66	0.21	73,91,106,107	0
3	MAN	C	4	11/12	0.70	0.15	78,100,109,113	0
3	NAG	D	2	14/15	0.72	0.16	78,92,97,100	0
3	NAG	D	1	14/15	0.73	0.16	58,75,90,96	0
3	MAN	D	4	11/12	0.75	0.17	53,67,73,76	0
2	FUC	B	2	10/11	0.85	0.15	82,93,101,101	0
2	NAG	B	1	14/15	0.86	0.12	63,77,82,84	0
3	NAG	C	1	14/15	0.88	0.12	43,49,59,78	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.

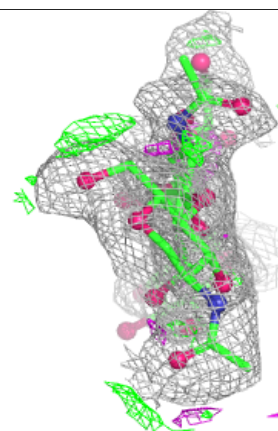
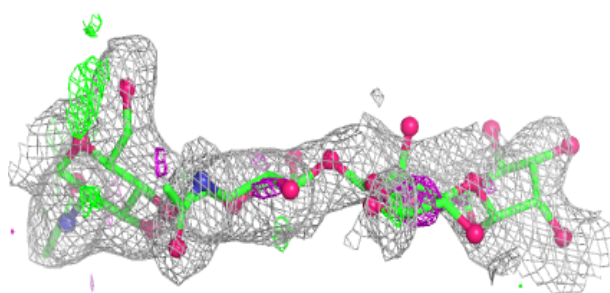
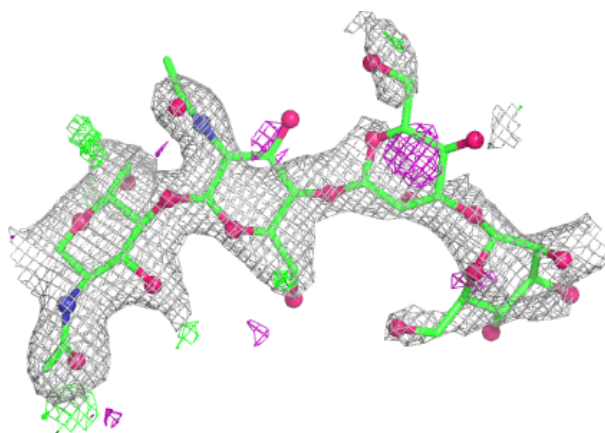
Electron density around Chain B:

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

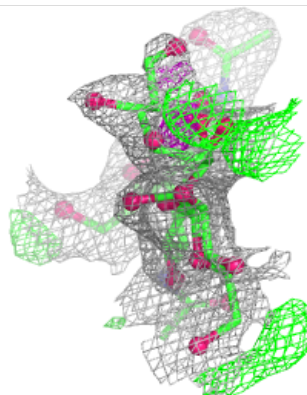
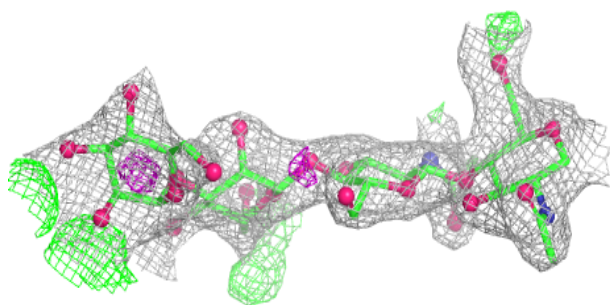
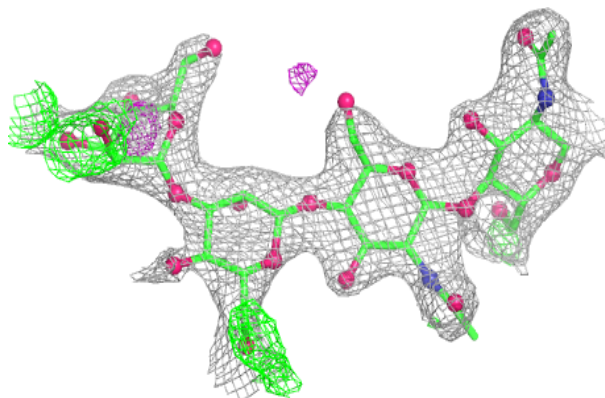


Electron density around Chain C:

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

**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)

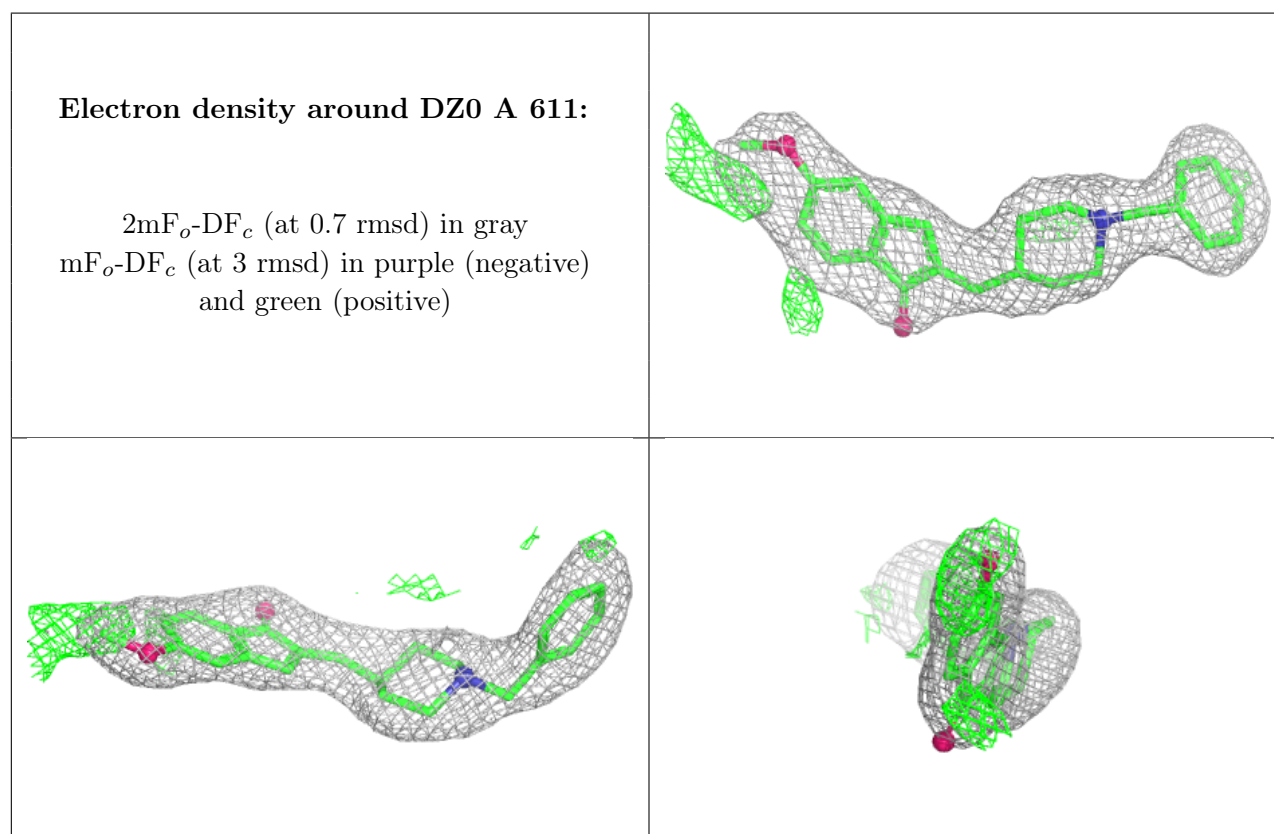


6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
4	DZ0	A	611	26/26	0.90	0.15	51,57,67,72	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 [i](#)

There are no such residues in this entry.