Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 08:00 PM EDT

PDB ID	:	2XMG
Title	:	G117H mutant of human butyrylcholinesterase in complex with VX
Authors	:	Nachon, F.; Carletti, E.; Wandhammer, M.; Nicolet, Y.; Schopfer, L.M.; Masson, P.; Lockridge, O.
Deposited on	:	2010-07-27
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

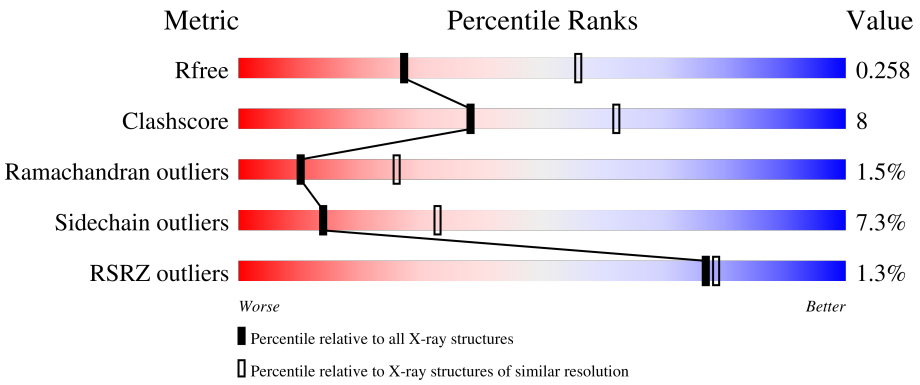
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	% 81% 15% • •
2	B	3	67% 33%
2	D	3	67% 33%
3	C	2	50% 50%

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
8	NH4	A	1543	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 4544 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.

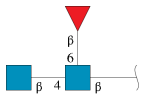
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4226	2727	713	771	15	0	2	0

There are 5 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[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
2	D	3	38	22	2	14	0	0	0

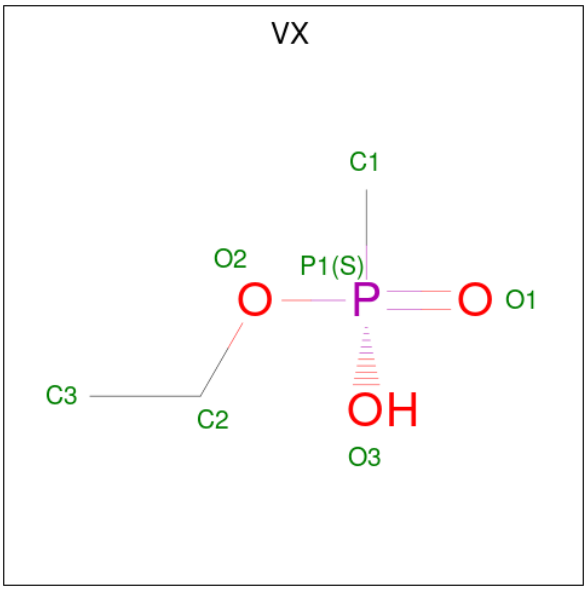
- Molecule 3 is an oligosaccharide called beta-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

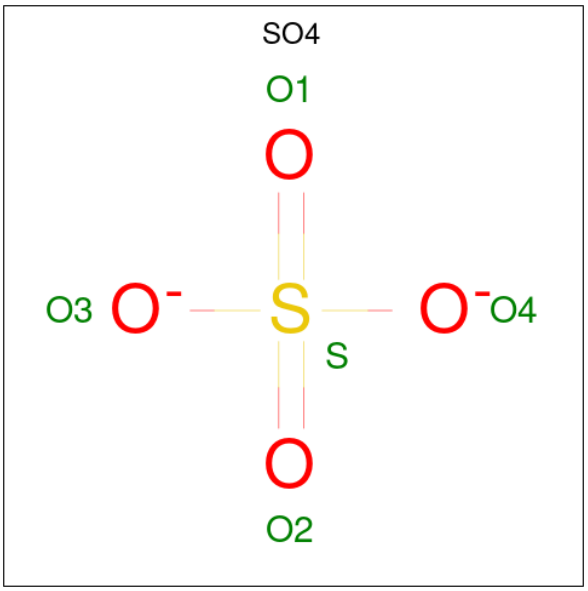
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
4	A	7	7	7	0	0

- Molecule 5 is O-ETHYLMETHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: VX) (formula: $C_3H_9O_3P$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

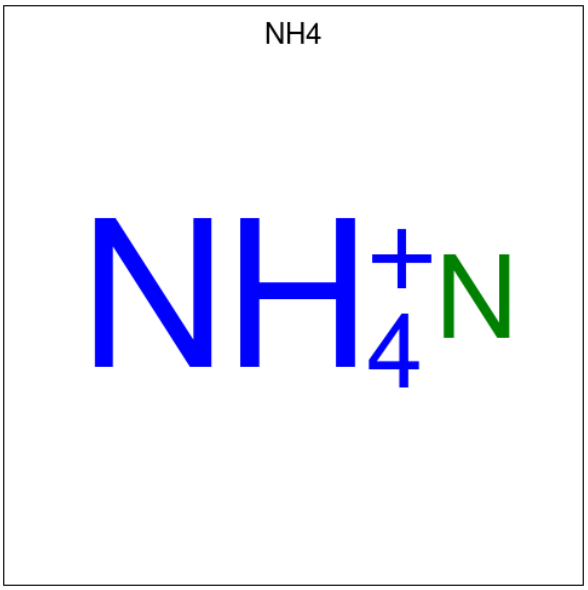


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0

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

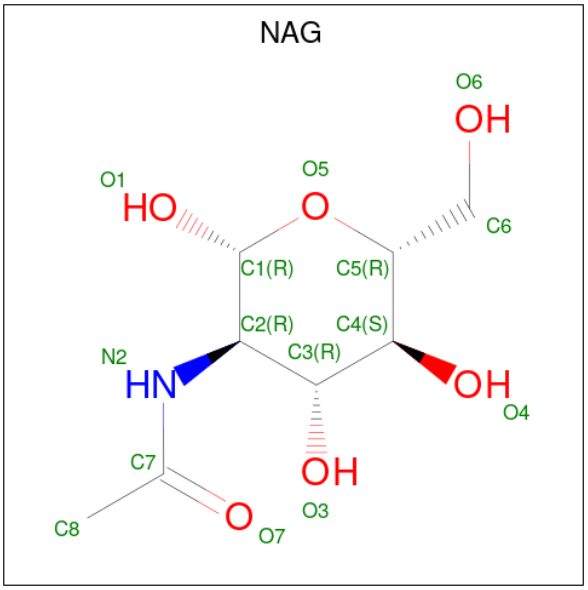
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total Cl 5 5	0	0

- Molecule 8 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



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

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is water.

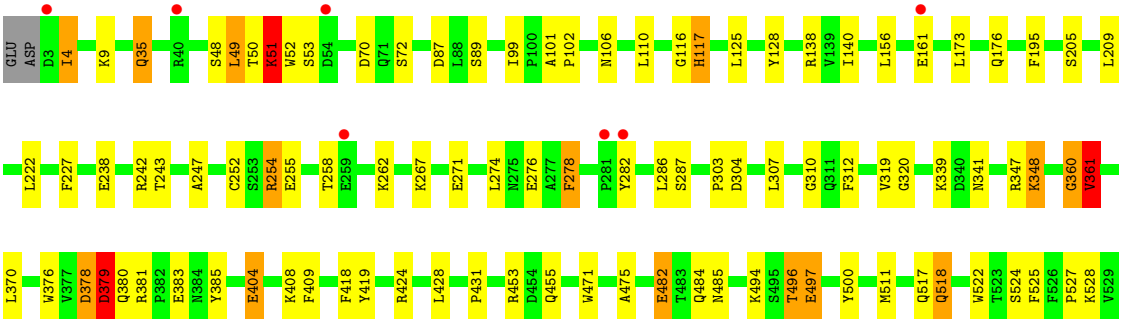
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	151	Total O 151 151	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CHOLINESTERASE

Chain A:



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

Chain B:

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

Chain D:

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

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	156.57Å 156.57Å 128.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.43 – 2.70 61.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.3 (110.43-2.70) 94.3 (61.47-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.250 0.185 , 0.258	Depositor DCC
R_{free} test set	880 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å^2)	55.1	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.9	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	4544	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, FUL, SO4, UNX, CL, VX, NAG

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	0.87	1/4351 (0.0%)	0.83	2/5907 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	GLU	CG-CD	6.07	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	424	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	GLY	Peptide

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	4226	0	4117	65	0
2	B	38	0	34	2	0
2	D	38	0	34	1	0
3	C	24	0	22	1	0
4	A	7	0	0	0	0
5	A	6	0	8	2	0
6	A	5	0	0	0	0
7	A	5	0	0	0	0
8	A	2	0	0	0	0
9	A	42	0	39	1	0
10	A	151	0	0	4	0
All	All	4544	0	4254	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:156:LEU:HD13	1:A:243:THR:HG21	1.47	0.97
1:A:518:GLN:HE21	1:A:518:GLN:N	1.62	0.96
1:A:50:THR:O	1:A:51:LYS:HB3	1.67	0.94
1:A:518:GLN:H	1:A:518:GLN:NE2	1.72	0.87
1:A:518:GLN:HE21	1:A:518:GLN:H	0.86	0.82
1:A:117:HIS:HB3	5:A:1530:VX:H33	1.62	0.79
9:A:1550:NAG:H5	10:A:2151:HOH:O	1.82	0.79
1:A:341:ASN:HD22	2:B:1:NAG:H83	1.52	0.74
1:A:380:GLN:N	1:A:381:ARG:HB2	2.03	0.74
1:A:341:ASN:ND2	2:B:1:NAG:H83	2.03	0.73
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.30	0.66
1:A:380:GLN:H	1:A:381:ARG:HB2	1.61	0.65
1:A:267:LYS:HE3	1:A:271:GLU:OE1	1.98	0.64
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.82	0.62
1:A:4:ILE:HD12	1:A:4:ILE:N	2.14	0.62
1:A:524:SER:O	1:A:528:LYS:HE3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:GLU:OE2	1:A:485:ASN:HB2	2.03	0.59
1:A:319:VAL:O	1:A:418:PHE:HA	2.03	0.59
1:A:227:PHE:CD2	1:A:227:PHE:C	2.80	0.55
1:A:173:LEU:O	1:A:176:GLN:HB3	2.07	0.55
1:A:50:THR:HA	10:A:2011:HOH:O	2.08	0.54
1:A:4:ILE:HD12	1:A:4:ILE:H	1.73	0.54
1:A:496:THR:OG1	1:A:497:GLU:HG2	2.08	0.54
1:A:482:GLU:OE1	1:A:484:GLN:N	2.33	0.53
1:A:525:PHE:C	1:A:525:PHE:CD1	2.82	0.53
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.44	0.52
1:A:101:ALA:HA	1:A:102:PRO:C	2.29	0.51
1:A:35:GLN:NE2	1:A:48:SER:O	2.43	0.51
1:A:278:PHE:CD2	1:A:278:PHE:N	2.77	0.51
1:A:376:TRP:HA	1:A:376:TRP:CE3	2.45	0.51
1:A:227:PHE:CE2	1:A:303:PRO:HB2	2.46	0.50
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.46	0.50
1:A:347:ARG:HD2	1:A:385:TYR:OH	2.11	0.49
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.48	0.49
1:A:238:GLU:O	1:A:242:ARG:HG3	2.13	0.49
1:A:35:GLN:NE2	1:A:49:LEU:HA	2.29	0.47
1:A:116:GLY:C	1:A:117:HIS:CD2	2.87	0.47
1:A:361:VAL:HA	10:A:2090:HOH:O	2.14	0.47
1:A:99:ILE:HG22	1:A:140:ILE:HG12	1.96	0.47
1:A:404:GLU:OE2	1:A:408:LYS:HE2	2.14	0.47
1:A:125:LEU:HD12	1:A:128:TYR:CE2	2.50	0.47
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.51	0.46
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.98	0.46
1:A:110:LEU:HD11	1:A:475:ALA:CB	2.46	0.45
1:A:49:LEU:HD12	1:A:50:THR:H	1.80	0.45
1:A:247:ALA:O	1:A:252:CYS:N	2.40	0.44
1:A:339:LYS:O	1:A:431:PRO:HG3	2.17	0.44
1:A:117:HIS:CB	5:A:1530:VX:H33	2.42	0.44
1:A:379:ASP:HB2	1:A:381:ARG:HG3	1.99	0.44
1:A:380:GLN:CA	1:A:381:ARG:HB2	2.47	0.44
1:A:376:TRP:HA	1:A:376:TRP:HE3	1.81	0.44
1:A:381:ARG:NE	1:A:383:GLU:OE1	2.51	0.43
1:A:278:PHE:O	2:D:3:FUL:H4	2.18	0.42
1:A:4:ILE:N	1:A:4:ILE:CD1	2.80	0.42
1:A:348:LYS:HD3	1:A:348:LYS:HA	1.82	0.42
1:A:378:ASP:O	1:A:380:GLN:NE2	2.53	0.42
1:A:209:LEU:HD11	1:A:227:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:TRP:O	1:A:378:ASP:OD1	2.37	0.42
1:A:254:ARG:HA	1:A:254:ARG:HD3	1.55	0.41
1:A:227:PHE:HZ	1:A:307:LEU:HB2	1.85	0.41
1:A:205:SER:HB3	1:A:222:LEU:HD21	2.02	0.41
1:A:51:LYS:HG3	1:A:52:TRP:N	2.34	0.41
1:A:106:ASN:ND2	3:C:1:NAG:H83	2.35	0.40
1:A:522:TRP:O	1:A:527:PRO:HD3	2.21	0.40
1:A:312:PHE:CD1	1:A:409:PHE:CE1	3.10	0.40
1:A:348:LYS:HB2	10:A:2088:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	527/529 (100%)	483 (92%)	36 (7%)	8 (2%)	10 26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	VAL
1	A	379	ASP
1	A	51	LYS
1	A	496	THR
1	A	87	ASP
1	A	378	ASP
1	A	276	GLU
1	A	360	GLY

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	455/455 (100%)	422 (93%)	33 (7%)	14 33

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	35	GLN
1	A	49	LEU
1	A	51	LYS
1	A	53	SER
1	A	72	SER
1	A	89	SER
1	A	117	HIS
1	A	138	ARG
1	A	195	PHE
1	A	254	ARG
1	A	255	GLU
1	A	262	LYS
1	A	274	LEU
1	A	278	PHE
1	A	282	TYR
1	A	286	LEU
1	A	287	SER
1	A	304	ASP
1	A	348	LYS
1	A	361	VAL
1	A	370	LEU
1	A	379	ASP
1	A	428	LEU
1	A	453	ARG
1	A	455	GLN
1	A	471	TRP
1	A	482	GLU
1	A	494	LYS

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Mol	Chain	Res	Type
1	A	497	GLU
1	A	517	GLN
1	A	518	GLN

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

Mol	Chain	Res	Type
1	A	17	GLN
1	A	35	GLN
1	A	117	HIS
1	A	380	GLN
1	A	517	GLN
1	A	518	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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	0.71	0	17,19,21	2.05	8 (47%)
2	NAG	B	2	2	14,14,15	0.82	0	17,19,21	2.68	8 (47%)
2	FUL	B	3	2	10,10,11	0.94	0	14,14,16	2.79	4 (28%)
3	NAG	C	1	1,3	14,14,15	1.31	1 (7%)	17,19,21	2.14	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FUL	C	2	3	10,10,11	0.76	0	14,14,16	2.31	5 (35%)
2	NAG	D	1	1,2	14,14,15	0.78	0	17,19,21	2.65	4 (23%)
2	NAG	D	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.85	5 (29%)
2	FUL	D	3	2	10,10,11	0.92	0	14,14,16	2.13	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
3	NAG	C	1	1,3	-	4/6/23/26	0/1/1/1
3	FUL	C	2	3	-	-	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	NAG	C1-C2	3.86	1.57	1.52
2	D	2	NAG	C1-C2	2.65	1.56	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	9.09	124.37	112.19
2	B	3	FUL	C1-C2-C3	-8.41	97.40	109.64
2	B	2	NAG	C1-C2-N2	5.99	119.87	110.43
2	B	2	NAG	C2-N2-C7	5.74	130.59	122.90
3	C	2	FUL	C1-C2-C3	-5.39	101.80	109.64
2	D	3	FUL	C1-C2-C3	-5.12	102.19	109.64
2	D	2	NAG	C1-O5-C5	4.61	118.37	112.19
3	C	1	NAG	C2-N2-C7	4.47	128.89	122.90
2	B	2	NAG	C3-C4-C5	4.14	117.73	110.23
2	D	3	FUL	O2-C2-C1	3.89	118.12	109.22
2	B	1	NAG	O7-C7-C8	-3.54	115.74	122.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	FUL	O2-C2-C1	3.44	117.09	109.22
2	B	3	FUL	C1-O5-C5	-3.43	104.88	112.97
3	C	1	NAG	C8-C7-N2	3.41	121.77	116.12
3	C	1	NAG	C1-C2-N2	3.34	115.69	110.43
3	C	1	NAG	O5-C5-C6	3.06	113.62	107.66
2	D	2	NAG	C1-C2-N2	2.94	115.06	110.43
2	D	1	NAG	O5-C5-C4	2.86	117.80	110.83
2	B	2	NAG	C4-C3-C2	2.86	115.20	111.02
2	B	1	NAG	C1-C2-N2	-2.85	105.94	110.43
2	B	1	NAG	O5-C1-C2	-2.84	106.89	111.29
2	B	2	NAG	C1-O5-C5	2.74	115.86	112.19
3	C	2	FUL	C2-C3-C4	-2.67	106.16	110.86
2	D	2	NAG	O4-C4-C5	2.67	115.90	109.32
2	D	1	NAG	O7-C7-C8	-2.66	117.33	122.05
2	B	1	NAG	O5-C5-C6	2.61	112.75	107.66
3	C	1	NAG	C3-C4-C5	-2.61	105.50	110.23
2	B	1	NAG	C8-C7-N2	2.61	120.45	116.12
2	B	1	NAG	C3-C4-C5	-2.59	105.54	110.23
2	B	1	NAG	C6-C5-C4	2.52	119.20	113.02
2	D	1	NAG	O7-C7-N2	2.51	126.42	121.98
2	D	2	NAG	C4-C3-C2	-2.48	107.38	111.02
3	C	2	FUL	O3-C3-C2	2.46	115.07	110.05
3	C	2	FUL	O5-C1-C2	-2.36	105.17	110.79
2	D	3	FUL	C3-C4-C5	2.35	113.38	109.81
2	B	2	NAG	O7-C7-N2	2.34	126.12	121.98
2	B	1	NAG	O6-C6-C5	2.31	119.20	111.33
2	B	3	FUL	O5-C5-C6	2.29	112.37	107.40
2	B	3	FUL	C6-C5-C4	2.26	117.21	113.08
2	D	2	NAG	C3-C4-C5	-2.25	106.16	110.23
3	C	1	NAG	O4-C4-C5	2.20	114.75	109.32
2	B	2	NAG	O5-C1-C2	-2.18	107.92	111.29
2	B	2	NAG	O5-C5-C4	2.05	115.81	110.83
2	D	3	FUL	O5-C1-C2	-2.04	105.92	110.79

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

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

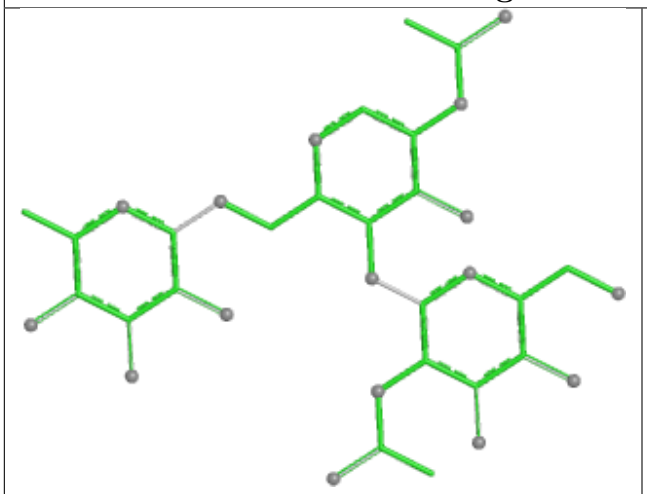
There are no ring outliers.

3 monomers are involved in 4 short contacts:

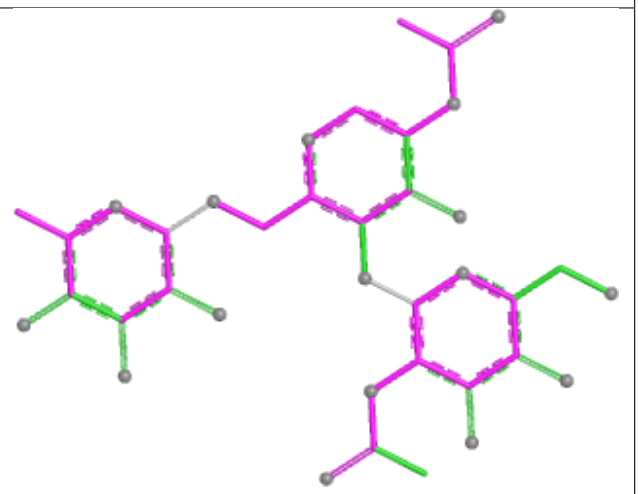
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	FUL	1	0
2	B	1	NAG	2	0
3	C	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

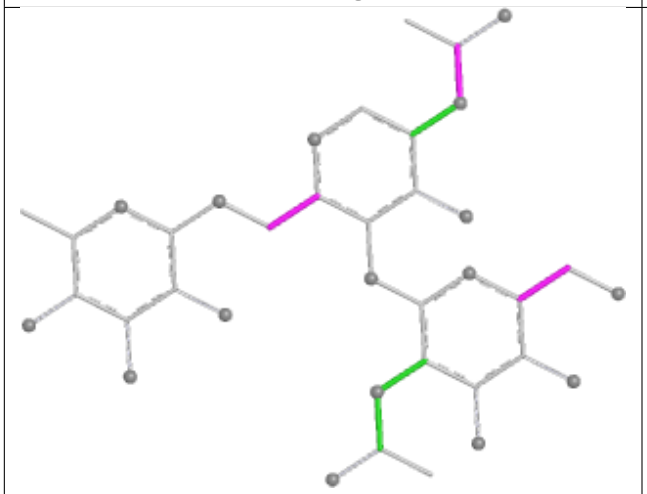
Oligosaccharide Chain B



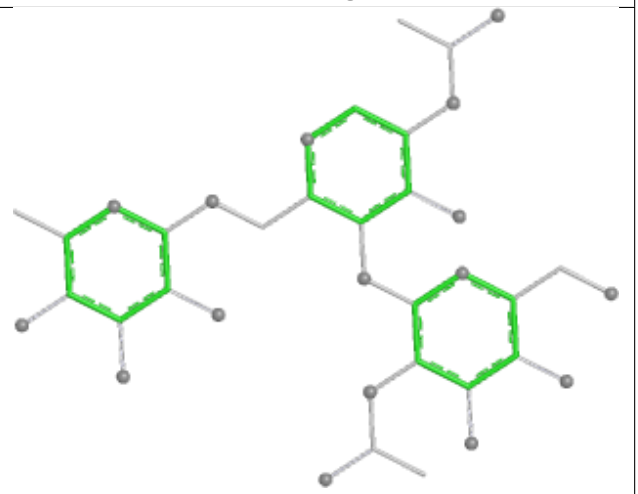
Bond lengths



Bond angles

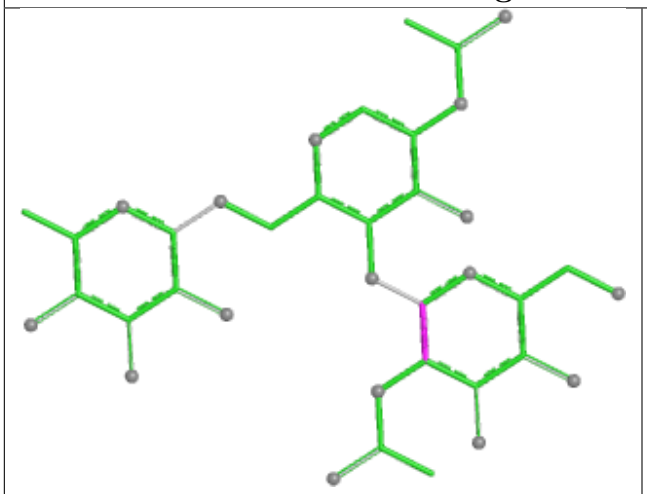


Torsions

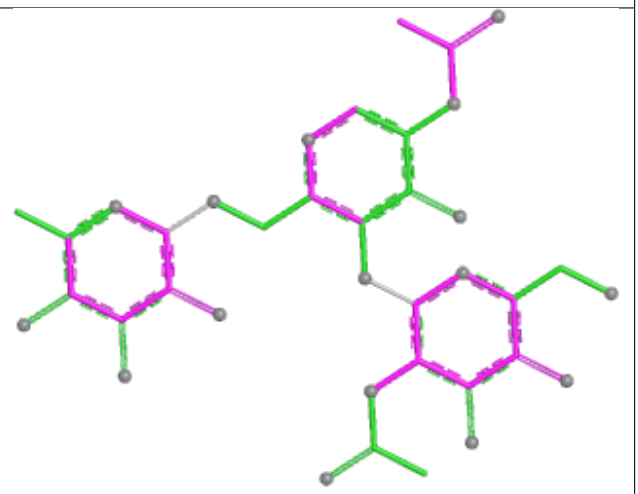


Rings

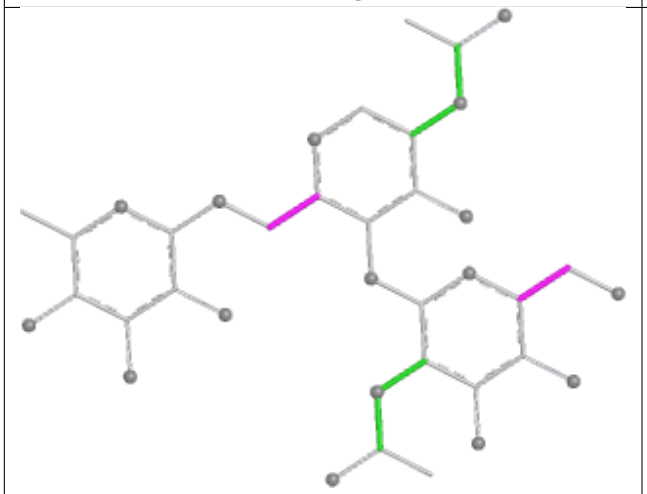
Oligosaccharide Chain D



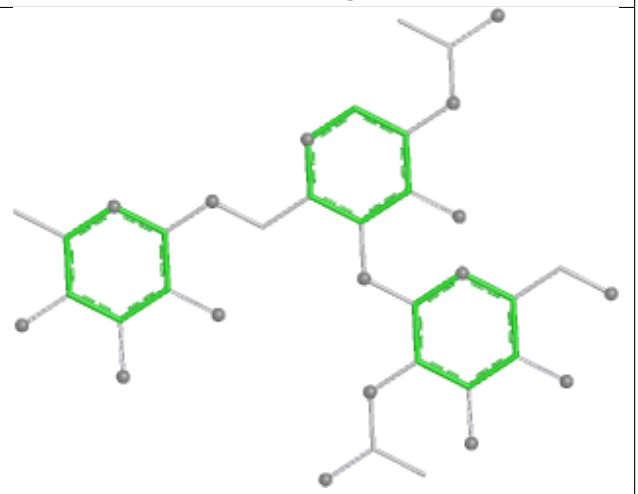
Bond lengths



Bond angles

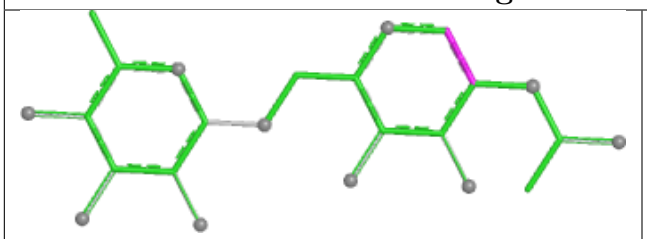


Torsions

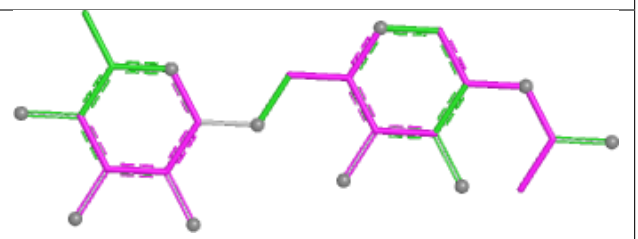


Rings

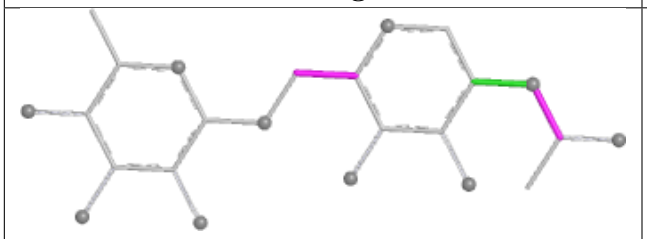
Oligosaccharide Chain C



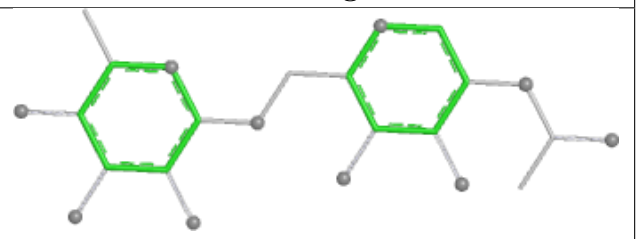
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 7 are unknown, 5 are monoatomic and 2 are modelled with single atom - 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	$\#\|Z\| > 2$
9	NAG	A	1551	1	14,14,15	1.00	0	17,19,21	1.79	4 (23%)
9	NAG	A	1549	1	14,14,15	0.80	0	17,19,21	2.97	6 (35%)
5	VX	A	1530	1	2,5,6	0.85	0	1,5,8	0.53	0
9	NAG	A	1550	1	14,14,15	0.84	1 (7%)	17,19,21	2.87	4 (23%)
6	SO4	A	1531	-	4,4,4	0.53	0	6,6,6	0.34	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
9	NAG	A	1549	1	-	4/6/23/26	0/1/1/1
9	NAG	A	1551	1	-	2/6/23/26	0/1/1/1
5	VX	A	1530	1	-	0/1/3/4	-
9	NAG	A	1550	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1550	NAG	O5-C1	2.03	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1549	NAG	C1-O5-C5	9.62	125.08	112.19
9	A	1550	NAG	O5-C1-C2	6.43	121.24	111.29
9	A	1550	NAG	C1-O5-C5	6.35	120.69	112.19
9	A	1550	NAG	C1-C2-N2	-5.85	101.22	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1549	NAG	C4-C3-C2	-3.90	105.30	111.02
9	A	1549	NAG	C8-C7-N2	3.83	122.48	116.12
9	A	1551	NAG	O5-C1-C2	-2.93	106.76	111.29
9	A	1551	NAG	O5-C5-C6	2.77	113.06	107.66
9	A	1551	NAG	C2-N2-C7	2.74	126.58	122.90
9	A	1551	NAG	C6-C5-C4	2.57	119.32	113.02
9	A	1549	NAG	O4-C4-C3	2.37	115.97	110.38
9	A	1549	NAG	O3-C3-C4	2.08	115.29	110.38
9	A	1549	NAG	O7-C7-C8	-2.07	118.37	122.05
9	A	1550	NAG	C2-N2-C7	2.01	125.59	122.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1549	NAG	O5-C5-C6-O6
9	A	1551	NAG	C4-C5-C6-O6
9	A	1551	NAG	O5-C5-C6-O6
9	A	1549	NAG	C8-C7-N2-C2
9	A	1549	NAG	O7-C7-N2-C2
9	A	1549	NAG	C4-C5-C6-O6
9	A	1550	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1530	VX	2	0
9	A	1550	NAG	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 (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	527/529 (99%)	-0.12	7 (1%) 77 78	31, 52, 90, 123	10 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	4.0
1	A	282	TYR	3.8
1	A	40	ARG	3.2
1	A	54	ASP	2.9
1	A	259	GLU	2.6
1	A	161	GLU	2.2
1	A	281	PRO	2.2

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

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

6.3 Carbohydrates (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
2	NAG	D	2	14/15	0.78	0.32	91,98,101,101	0
3	NAG	C	1	14/15	0.79	0.20	63,67,68,68	0
2	NAG	B	2	14/15	0.87	0.30	79,85,88,88	0
2	FUL	D	3	10/11	0.88	0.33	90,92,94,96	0
2	NAG	D	1	14/15	0.90	0.25	76,87,91,92	0

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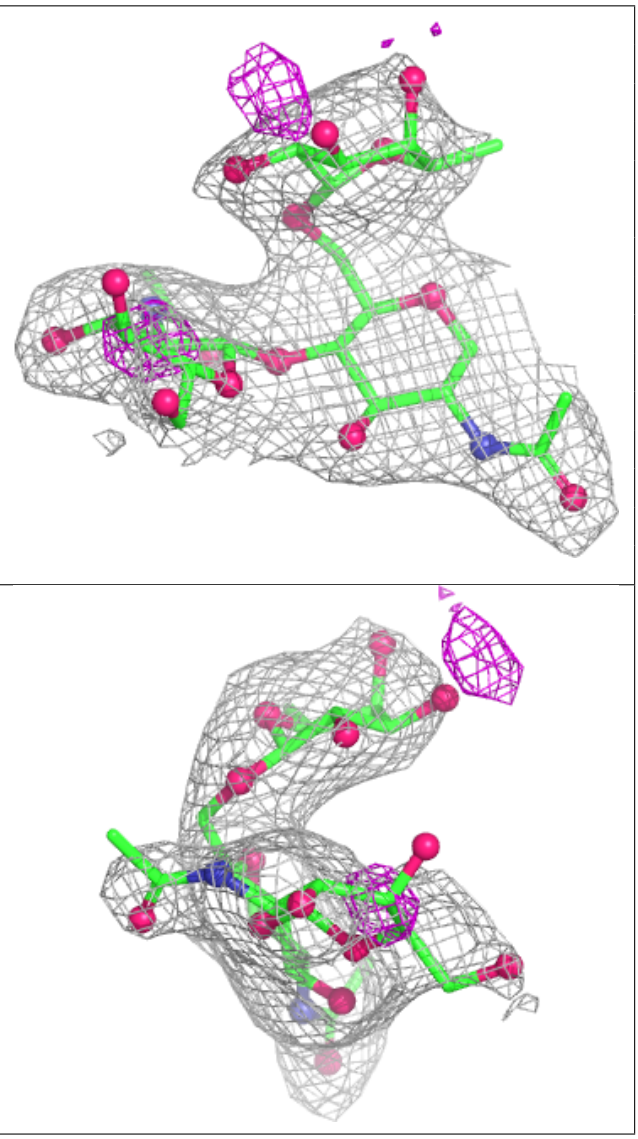
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUL	C	2	10/11	0.92	0.27	66,70,75,76	0
2	FUL	B	3	10/11	0.93	0.26	73,75,78,78	0
2	NAG	B	1	14/15	0.95	0.16	51,59,72,73	0

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.

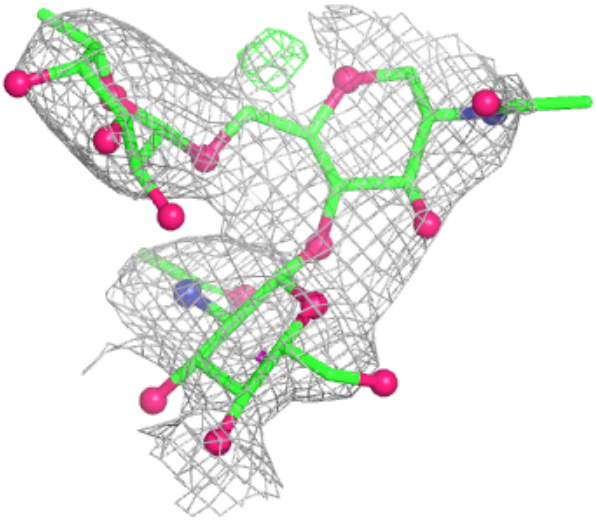
Electron density around Chain B:

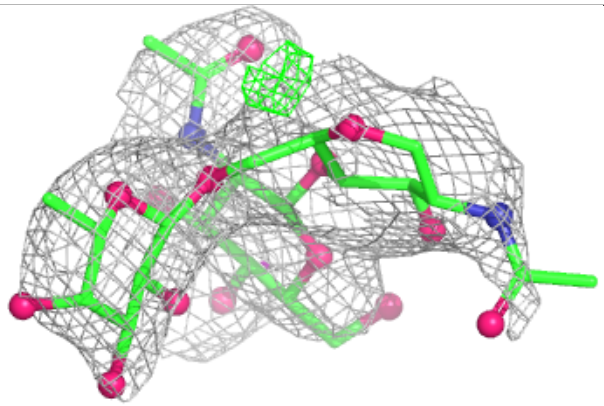
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

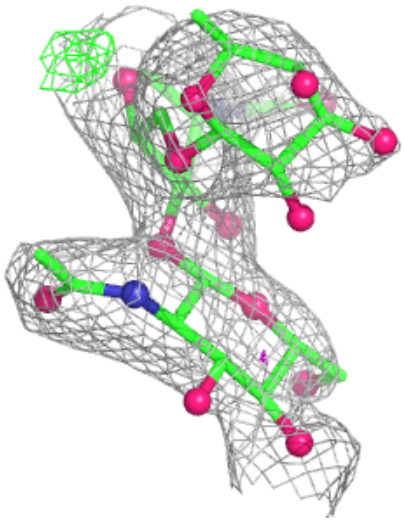


Electron density around Chain D:

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

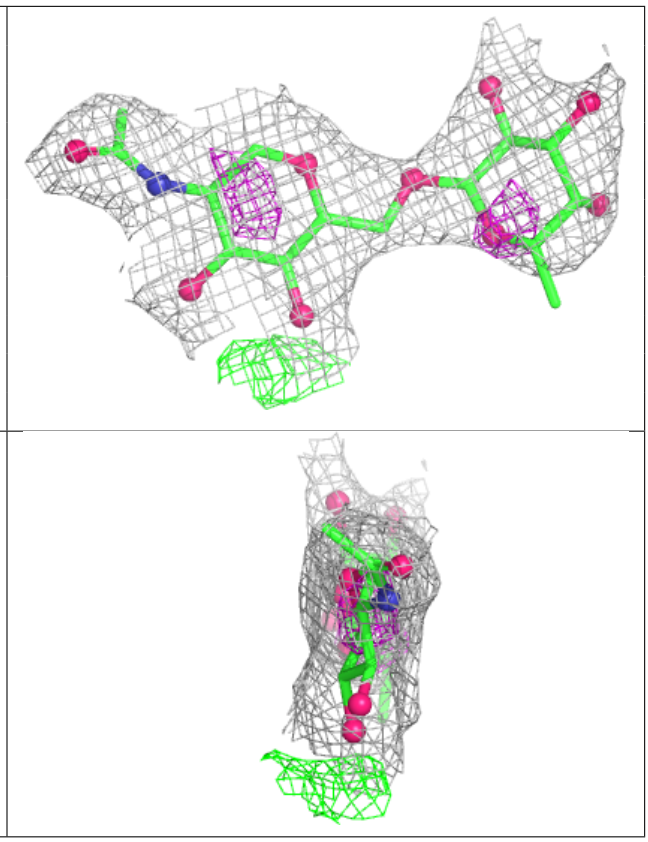






Electron density around Chain C:

$2mF_o$-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(Å^2)	Q<0.9
8	NH4	A	1543	1/1	0.59	0.50	48,48,48,48	0
4	UNX	A	1538	1/1	0.81	0.17	13,13,13,13	0
7	CL	A	1532	1/1	0.82	0.20	72,72,72,72	0
9	NAG	A	1549	14/15	0.83	0.17	76,82,84,84	0
9	NAG	A	1550	14/15	0.87	0.19	63,76,81,82	0
9	NAG	A	1551	14/15	0.89	0.25	72,79,84,86	0
4	UNX	A	1540	1/1	0.90	0.19	24,24,24,24	0
4	UNX	A	1542	1/1	0.91	0.18	23,23,23,23	0
4	UNX	A	1539	1/1	0.92	0.28	36,36,36,36	0
4	UNX	A	1541	1/1	0.93	0.32	28,28,28,28	0
7	CL	A	1533	1/1	0.93	0.08	74,74,74,74	0
8	NH4	A	1556	1/1	0.94	0.55	40,40,40,40	0
7	CL	A	1534	1/1	0.94	0.16	75,75,75,75	0
4	UNX	A	1536	1/1	0.95	0.19	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CL	A	1555	1/1	0.96	0.15	62,62,62,62	0
7	CL	A	1535	1/1	0.96	0.24	67,67,67,67	0
4	UNX	A	1537	1/1	0.97	0.08	15,15,15,15	0
6	SO4	A	1531	5/5	0.97	0.10	67,68,69,71	0
5	VX	A	1530	6/7	0.98	0.13	53,55,56,57	0

6.5 Other polymers (i)

There are no such residues in this entry.