Full wwPDB X-ray Structure Validation Report (i)

Dec 5, 2023 – 06:26 am GMT

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)

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:

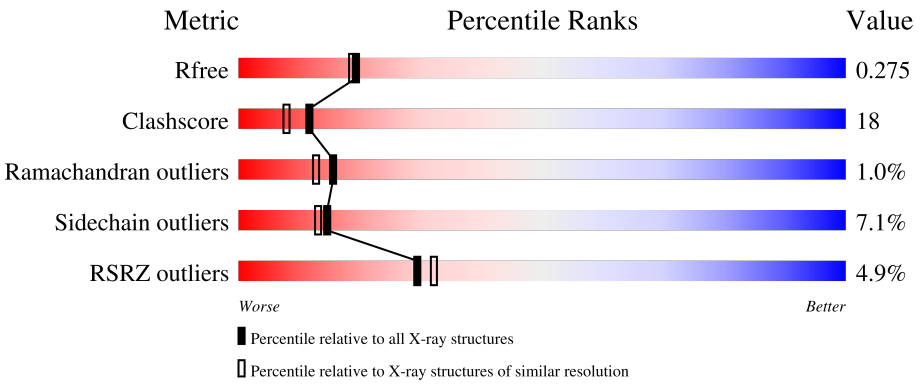
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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	5%; 67%; 27%; 6% •
2	B	3	100%
2	D	3	67%; 33%
3	C	2	100%

2 Entry composition (i)

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.

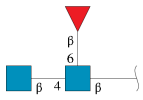
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4213	2720	710	768	15	7	2	0

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
			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

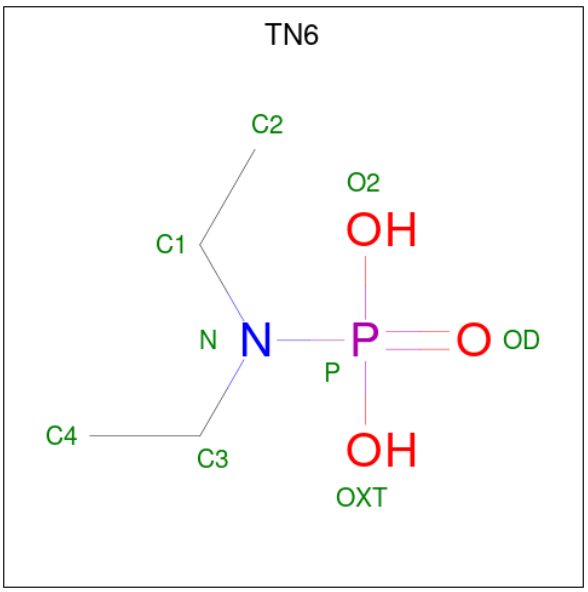
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

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

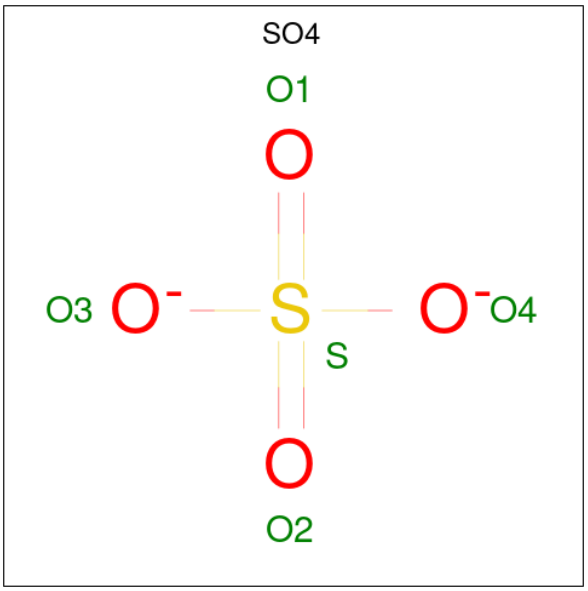
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	3	3	3	0	0

- Molecule 6 is diethylphosphoramidic acid (three-letter code: TN6) (formula: $C_4H_{12}NO_3P$).



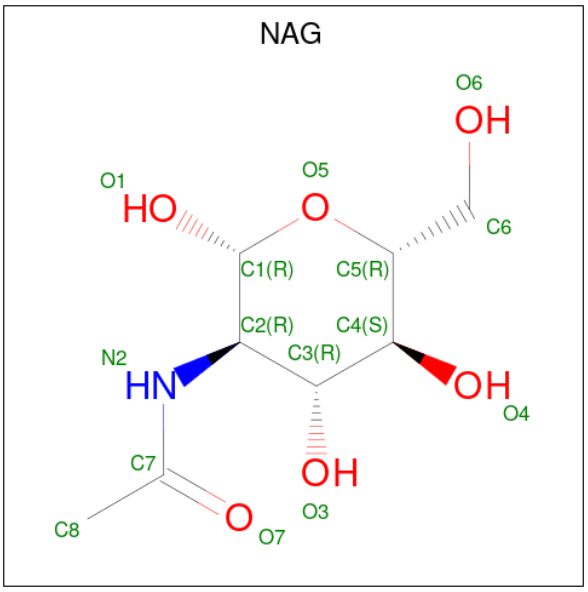
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	8	4	1	2	1	0	0

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



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

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



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

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

- Molecule 9 is water.

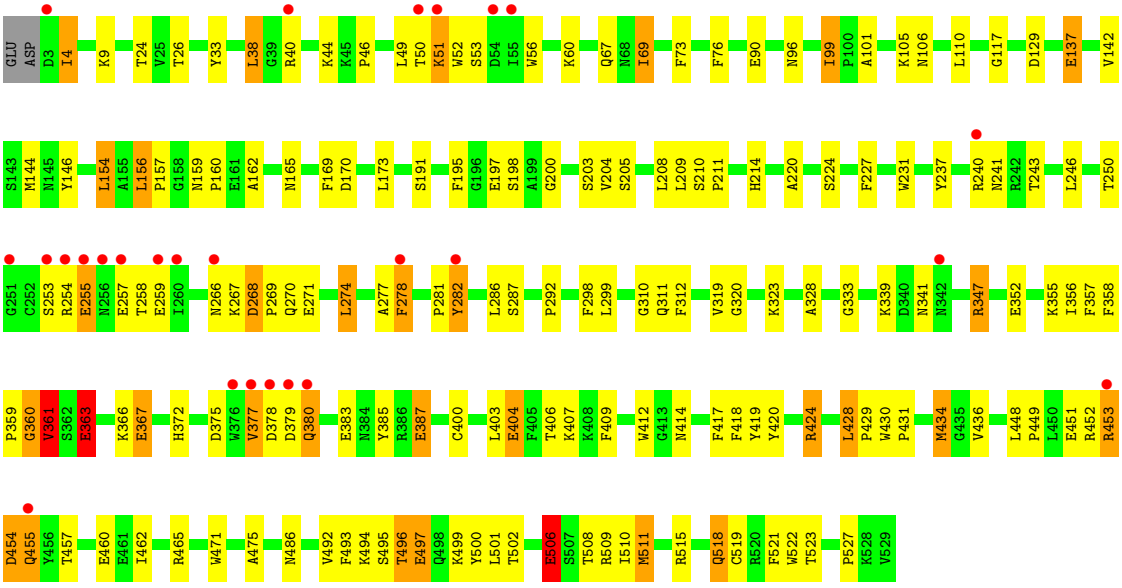
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	370	370	370	0	0

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.

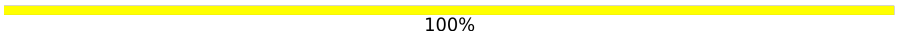
• Molecule 1: CHOLINESTERASE

Chain A:



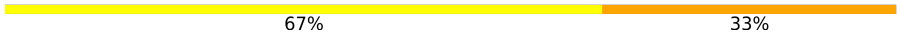
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

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: 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 , 61.2	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, CL, NA, NAG, SO4, TN6

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

All (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
1	A	137	GLU	CG-CD	5.97	1.60	1.51
1	A	471	TRP	CB-CG	5.84	1.60	1.50
1	A	146	TYR	CD1-CE1	5.56	1.47	1.39
1	A	521	PHE	CE1-CZ	5.49	1.47	1.37
1	A	363	GLU	CG-CD	5.35	1.59	1.51
1	A	420	TYR	CD1-CE1	-5.27	1.31	1.39
1	A	197	GLU	CD-OE2	5.24	1.31	1.25

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	A	360	GLY	C-N-CA	5.31	134.97	121.70
1	A	347	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	424	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	129	ASP	CB-CG-OD2	-5.04	113.77	118.30

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 (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	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.

All (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
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.06	0.91
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.36	0.88
1:A:361:VAL:O	1:A:366:LYS:NZ	2.11	0.83
1:A:380:GLN:HB2	5:A:604:CL:CL	2.16	0.83
1:A:367:GLU:HB3	9:A:847:HOH:O	1.79	0.83
1:A:518:GLN:H	1:A:518:GLN:NE2	1.77	0.81
1:A:328:ALA:HA	1:A:434:MET:CE	2.13	0.79
1:A:377:VAL:O	1:A:377:VAL:CG2	2.31	0.77
1:A:282:TYR:O	1:A:282:TYR:CD1	2.37	0.76
1:A:509:ARG:HG2	1:A:509:ARG:NH1	1.97	0.76
1:A:117:GLY:HA2	6:A:603:TN6:H22C	1.68	0.76
1:A:250:THR:HB	1:A:267:LYS:HE2	1.67	0.76
1:A:454:ASP:O	1:A:455:GLN:HB2	1.85	0.75
1:A:495:SER:HA	9:A:704:HOH:O	1.87	0.75
1:A:50:THR:O	1:A:51:LYS:HG2	1.88	0.74
1:A:452:ARG:HD2	9:A:714:HOH:O	1.88	0.74
1:A:4:ILE:HD12	1:A:4:ILE:N	2.04	0.73
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.72	0.72
1:A:494:LYS:NZ	9:A:706:HOH:O	2.22	0.71
1:A:267:LYS:HE3	1:A:271:GLU:OE1	1.89	0.71
1:A:270:GLN:O	1:A:274:LEU:HB2	1.91	0.71
1:A:424:ARG:NH1	1:A:428:LEU:HD12	2.05	0.70
1:A:24:THR:O	1:A:101:ALA:HB3	1.92	0.70
1:A:451:GLU:OE1	1:A:453:ARG:HG2	1.92	0.70
1:A:428:LEU:HD13	1:A:430:TRP:HB2	1.73	0.69
1:A:518:GLN:HE21	1:A:518:GLN:N	1.83	0.69
1:A:257:GLU:OE1	9:A:702:HOH:O	2.14	0.66
1:A:452:ARG:C	1:A:454:ASP:H	1.99	0.65
1:A:522:TRP:O	1:A:527:PRO:HD3	1.96	0.65
1:A:4:ILE:HD12	1:A:4:ILE:H	1.63	0.63
1:A:277:ALA:HB2	9:A:885:HOH:O	1.98	0.63
1:A:191:SER:HB2	3:C:2:FUL:H3	1.82	0.62
1:A:495:SER:CA	9:A:704:HOH:O	2.46	0.61
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.36	0.61
1:A:383:GLU:O	1:A:387:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ARG:O	1:A:454:ASP:N	2.34	0.60
1:A:154:LEU:HD23	1:A:162:ALA:HB1	1.84	0.60
1:A:403:LEU:O	1:A:407:LYS:HG3	2.02	0.60
1:A:404:GLU:HG2	9:A:914:HOH:O	2.01	0.59
1:A:198:SER:HA	1:A:224:SER:O	2.03	0.59
1:A:496:THR:N	9:A:704:HOH:O	2.21	0.59
1:A:428:LEU:CD1	1:A:430:TRP:HB2	2.32	0.58
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.38	0.58
1:A:358:PHE:N	1:A:359:PRO:HD3	2.19	0.58
8:A:615:NAG:H62	9:A:1013:HOH:O	2.03	0.57
1:A:417:PHE:CE2	1:A:492:VAL:HG12	2.38	0.57
1:A:372[A]:HIS:CE1	9:A:781:HOH:O	2.58	0.56
1:A:319:VAL:O	1:A:418:PHE:HA	2.06	0.56
1:A:500:TYR:CE1	1:A:511:MET:HB2	2.41	0.55
1:A:110:LEU:HD21	1:A:475:ALA:CB	2.36	0.55
1:A:495:SER:O	1:A:496:THR:OG1	2.19	0.55
1:A:452:ARG:C	1:A:454:ASP:N	2.58	0.55
1:A:4:ILE:N	1:A:4:ILE:CD1	2.67	0.55
1:A:274:LEU:O	1:A:278:PHE:CE2	2.61	0.54
1:A:383:GLU:OE2	1:A:383:GLU:N	2.39	0.54
1:A:357:PHE:C	1:A:359:PRO:HD3	2.28	0.53
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.38	0.53
1:A:208:LEU:O	1:A:214[B]:HIS:HE1	1.91	0.53
1:A:428:LEU:HD22	1:A:429:PRO:HD2	1.92	0.52
8:A:613:NAG:C6	9:A:960:HOH:O	2.56	0.52
1:A:497:GLU:CD	1:A:499:LYS:HE3	2.30	0.52
8:A:613:NAG:H61	9:A:960:HOH:O	2.08	0.52
1:A:96:ASN:O	1:A:142:VAL:HA	2.10	0.52
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.92	0.52
1:A:277:ALA:CB	9:A:885:HOH:O	2.55	0.51
1:A:378:ASP:C	1:A:380:GLN:H	2.13	0.51
1:A:157:PRO:HD2	1:A:240:ARG:HD3	1.92	0.51
1:A:60:LYS:HE3	9:A:1007:HOH:O	2.09	0.51
1:A:255:GLU:N	1:A:255:GLU:CD	2.64	0.51
1:A:208:LEU:O	1:A:214[B]:HIS:CE1	2.64	0.50
1:A:378:ASP:CG	1:A:379:ASP:H	2.14	0.50
1:A:414:ASN:HB2	9:A:734:HOH:O	2.12	0.50
1:A:40:ARG:NH1	9:A:711:HOH:O	2.33	0.50
1:A:110:LEU:HD21	1:A:475:ALA:HB2	1.94	0.50
1:A:383:GLU:O	1:A:387:GLU:CG	2.60	0.49
1:A:406:THR:HG22	1:A:493:PHE:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:TRP:CD1	1:A:52:TRP:O	2.66	0.48
1:A:339:LYS:O	1:A:431:PRO:HG3	2.13	0.48
1:A:40:ARG:HB2	9:A:946:HOH:O	2.13	0.48
1:A:231:TRP:CE3	6:A:603:TN6:H21C	2.48	0.48
8:A:613:NAG:H83	9:A:956:HOH:O	2.14	0.48
1:A:352:GLU:HA	1:A:355:LYS:HE3	1.95	0.48
1:A:253:SER:O	1:A:254:ARG:HD3	2.13	0.47
1:A:26:THR:HB	1:A:99:ILE:HG12	1.95	0.47
1:A:448:LEU:N	1:A:449:PRO:CD	2.77	0.47
1:A:50:THR:O	1:A:51:LYS:CG	2.60	0.47
1:A:377:VAL:N	1:A:378:ASP:HA	2.29	0.47
1:A:355:LYS:HD3	9:A:881:HOH:O	2.15	0.47
1:A:378:ASP:O	1:A:380:GLN:N	2.48	0.47
1:A:496:THR:OG1	9:A:703:HOH:O	2.20	0.47
1:A:347:ARG:HB2	1:A:385:TYR:CZ	2.50	0.46
1:A:495:SER:O	1:A:496:THR:CB	2.64	0.46
1:A:424:ARG:CZ	1:A:428:LEU:HD12	2.46	0.46
1:A:205:SER:O	1:A:208:LEU:HB2	2.15	0.46
1:A:267:LYS:HA	1:A:267:LYS:HD2	1.60	0.46
1:A:38:LEU:HD23	1:A:90:GLU:HB2	1.97	0.45
1:A:67:GLN:O	1:A:69:ILE:HD12	2.16	0.45
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.75	0.45
1:A:227:PHE:CD2	1:A:227:PHE:C	2.89	0.45
1:A:519:CYS:O	1:A:523:THR:HB	2.16	0.45
1:A:282:TYR:CD1	1:A:282:TYR:C	2.83	0.45
1:A:333:GLY:O	1:A:356:ILE:HG13	2.17	0.45
1:A:363:GLU:O	1:A:367:GLU:HG3	2.17	0.45
1:A:159:ASN:HA	1:A:160:PRO:HD3	1.89	0.44
1:A:320:GLY:CA	1:A:419:TYR:CE1	2.86	0.44
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.80	0.44
8:A:613:NAG:H83	8:A:613:NAG:H2	1.78	0.44
1:A:311:GLN:NE2	9:A:723:HOH:O	2.44	0.43
1:A:462:ILE:HD12	1:A:462:ILE:HG23	1.80	0.43
1:A:38:LEU:CD2	1:A:90:GLU:HB2	2.48	0.43
1:A:323:LYS:HB3	1:A:436:VAL:HB	1.99	0.43
1:A:106:ASN:HB2	3:C:1:NAG:H83	1.99	0.43
1:A:240:ARG:O	1:A:241:ASN:C	2.54	0.43
1:A:46:PRO:HB2	1:A:173:LEU:HD23	2.01	0.43
1:A:274:LEU:O	1:A:278:PHE:HE2	1.97	0.43
1:A:281:PRO:HG3	2:D:1:NAG:H83	2.00	0.43
1:A:231:TRP:CD2	6:A:603:TN6:H21C	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:THR:O	1:A:508:THR:HB	2.18	0.43
1:A:210:SER:HA	1:A:211:PRO:HD2	1.70	0.43
1:A:457:THR:OG1	1:A:460:GLU:HG3	2.19	0.42
1:A:44:LYS:HB3	1:A:44:LYS:HE3	1.93	0.42
1:A:209:LEU:HD23	1:A:209:LEU:HA	1.80	0.42
1:A:341:ASN:OD1	1:A:341:ASN:C	2.57	0.42
1:A:200:GLY:O	1:A:203:SER:HB2	2.20	0.42
1:A:266:ASN:HB3	9:A:998:HOH:O	2.19	0.42
1:A:33:TYR:OH	1:A:170:ASP:HB3	2.20	0.42
1:A:159:ASN:OD1	1:A:159:ASN:C	2.58	0.42
1:A:157:PRO:HD2	1:A:240:ARG:CD	2.49	0.42
1:A:501:LEU:HD12	1:A:510:ILE:HD13	2.02	0.42
1:A:169:PHE:CE1	1:A:298:PHE:HB2	2.55	0.41
1:A:56:TRP:CD1	1:A:56:TRP:C	2.93	0.41
1:A:137:GLU:OE2	1:A:465:ARG:NH2	2.51	0.41
1:A:253:SER:C	1:A:254:ARG:HD3	2.41	0.41
1:A:299:LEU:HA	1:A:299:LEU:HD23	1.68	0.41
1:A:328:ALA:HA	1:A:434:MET:HE3	1.97	0.41
1:A:506:GLU:H	1:A:506:GLU:HG3	1.66	0.41
1:A:358:PHE:N	1:A:359:PRO:CD	2.84	0.41
1:A:452:ARG:O	1:A:453:ARG:C	2.58	0.41
1:A:214[A]:HIS:NE2	9:A:713:HOH:O	2.37	0.41
1:A:268:ASP:O	1:A:269:PRO:C	2.59	0.40
1:A:73:PHE:O	1:A:76:PHE:HB3	2.21	0.40
1:A:310:GLY:HA3	1:A:412:TRP:CE2	2.56	0.40
1:A:169:PHE:CZ	1:A:298:PHE:HB2	2.57	0.40
1:A:255:GLU:CD	1:A:255:GLU:H	2.25	0.40
1:A:165:ASN:OD1	1:A:292:PRO:HA	2.22	0.40
1:A:312:PHE:CD1	1:A:409:PHE:CE1	3.10	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%)	489 (93%)	33 (6%)	5 (1%)	17 14

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 (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	453/454 (100%)	421 (93%)	32 (7%)	14 13

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	38	LEU
1	A	53	SER
1	A	69	ILE
1	A	99	ILE
1	A	105	LYS
1	A	144	MET
1	A	154	LEU
1	A	156	LEU
1	A	195	PHE
1	A	255	GLU
1	A	258	THR
1	A	259	GLU
1	A	268	ASP
1	A	278	PHE

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Mol	Chain	Res	Type
1	A	282	TYR
1	A	286	LEU
1	A	287	SER
1	A	361	VAL
1	A	363	GLU
1	A	375	ASP
1	A	377	VAL
1	A	380	GLN
1	A	387	GLU
1	A	428	LEU
1	A	454	ASP
1	A	455	GLN
1	A	486	ASN
1	A	506	GLU
1	A	511	MET
1	A	518	GLN

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 (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	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	1,3	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	1,2	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	1,2	-	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	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	-	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

All (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
2	D	2	NAG	C1-O5-C5	4.70	118.56	112.19
2	B	2	NAG	C1-O5-C5	-4.61	105.95	112.19
3	C	2	FUL	C1-C2-C3	-4.47	104.17	109.67
3	C	1	NAG	O5-C5-C6	4.36	114.05	107.20
2	B	3	FUL	C1-O5-C5	-4.27	103.11	112.78
3	C	2	FUL	C1-O5-C5	-4.25	103.14	112.78
3	C	1	NAG	C8-C7-N2	4.25	123.29	116.10
3	C	1	NAG	C3-C4-C5	-4.06	103.00	110.24
3	C	2	FUL	C3-C4-C5	4.02	116.04	109.77
2	B	1	NAG	O5-C1-C2	-3.96	105.04	111.29
2	D	1	NAG	C1-C2-N2	3.92	117.18	110.49
2	D	3	FUL	O5-C1-C2	-3.92	104.73	110.77
2	B	3	FUL	O2-C2-C1	3.84	117.01	109.15
3	C	1	NAG	O4-C4-C5	3.56	118.14	109.30
2	B	2	NAG	O5-C5-C6	3.49	112.68	107.20
3	C	2	FUL	C2-C3-C4	-3.30	105.18	110.89
3	C	1	NAG	C2-N2-C7	3.19	127.44	122.90
2	B	3	FUL	O5-C1-C2	-3.17	105.87	110.77
2	B	3	FUL	C6-C5-C4	3.03	118.67	113.07
2	D	2	NAG	C2-N2-C7	2.68	126.72	122.90
3	C	1	NAG	C6-C5-C4	2.62	119.15	113.00
2	B	1	NAG	C2-N2-C7	2.55	126.53	122.90
2	D	3	FUL	O2-C2-C3	2.49	115.12	110.14
2	D	3	FUL	C3-C4-C5	2.45	113.59	109.77
3	C	1	NAG	O7-C7-C8	-2.42	117.57	122.06
2	B	1	NAG	C3-C4-C5	-2.38	105.99	110.24
3	C	2	FUL	O5-C1-C2	-2.34	107.17	110.77
2	D	1	NAG	O7-C7-C8	-2.31	117.76	122.06
2	B	2	NAG	C2-N2-C7	2.31	126.19	122.90
2	D	2	NAG	O3-C3-C2	2.26	114.15	109.47
3	C	1	NAG	O5-C1-C2	-2.26	107.72	111.29
3	C	2	FUL	O2-C2-C3	2.24	114.63	110.14
2	B	1	NAG	C1-C2-N2	2.16	114.17	110.49
2	B	2	NAG	O6-C6-C5	-2.15	103.91	111.29
3	C	2	FUL	O3-C3-C2	2.13	114.07	109.99
2	D	2	NAG	C6-C5-C4	-2.11	108.06	113.00
2	D	3	FUL	O2-C2-C1	2.10	113.44	109.15
2	B	1	NAG	O5-C5-C6	2.04	110.40	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C4-C3-C2	2.01	113.97	111.02

There are no chirality outliers.

All (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
2	D	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	B	1	NAG	C3-C2-N2-C7
2	B	1	NAG	C1-C2-N2-C7

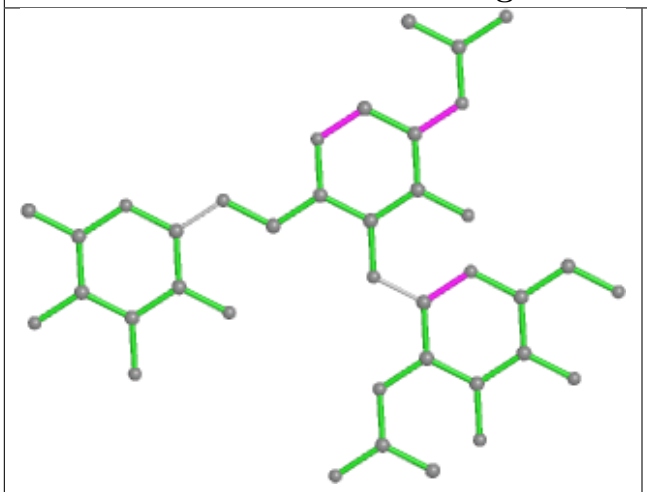
There are no ring outliers.

3 monomers are involved in 3 short contacts:

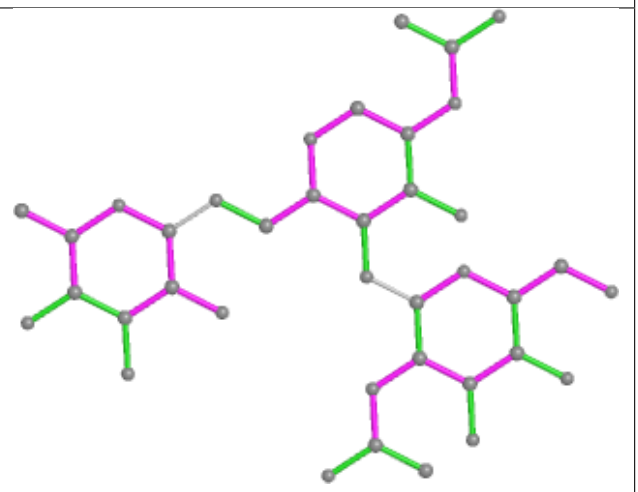
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	FUL	1	0
3	C	1	NAG	1	0
2	D	1	NAG	1	0

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

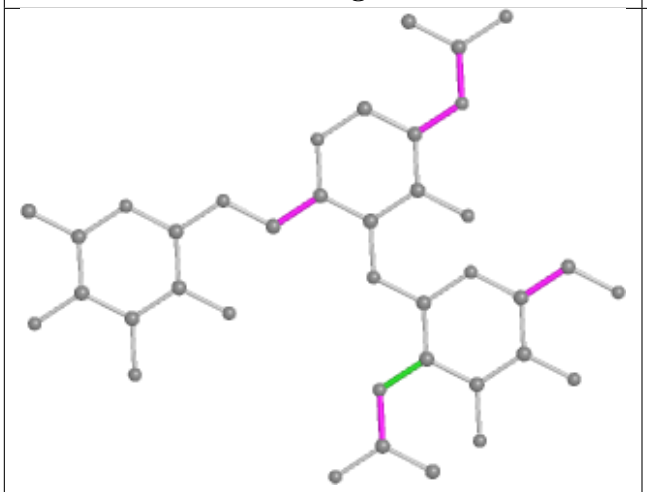
Oligosaccharide Chain B



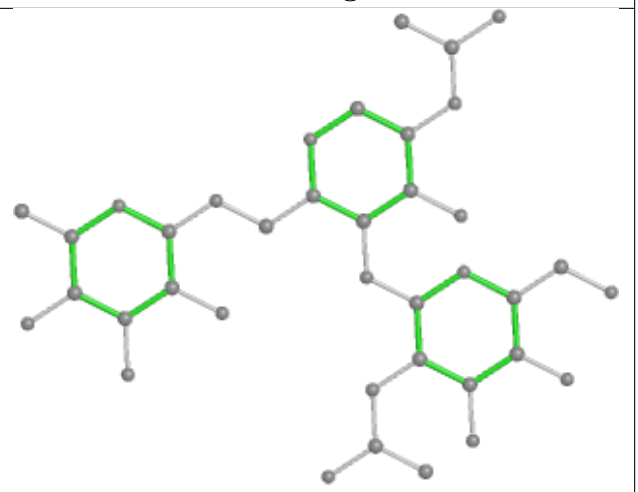
Bond lengths



Bond angles

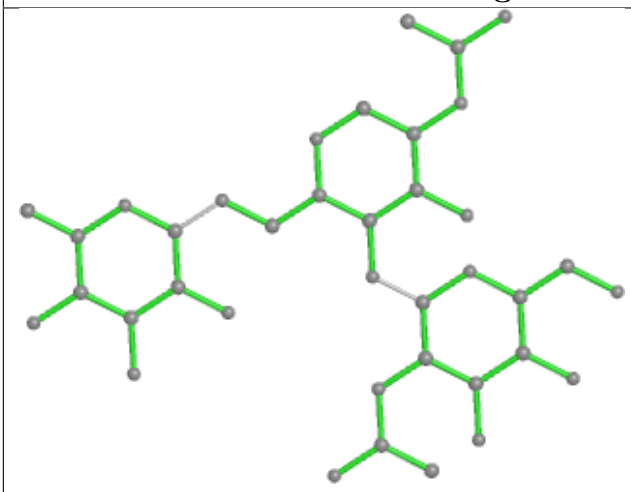


Torsions

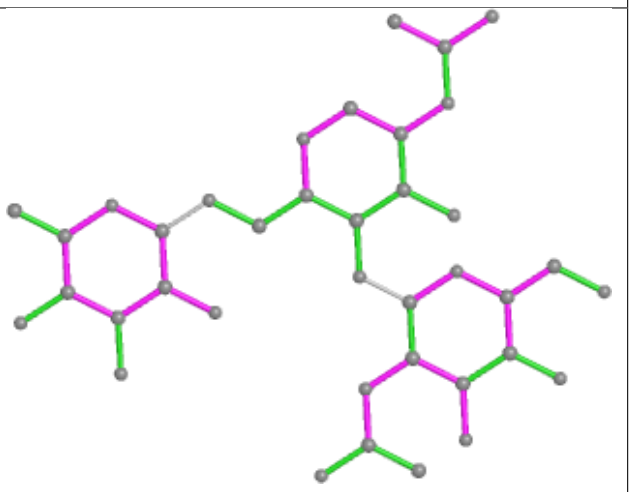


Rings

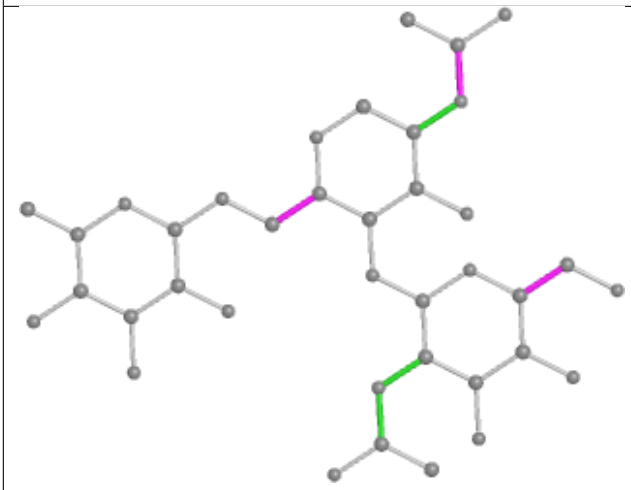
Oligosaccharide Chain D



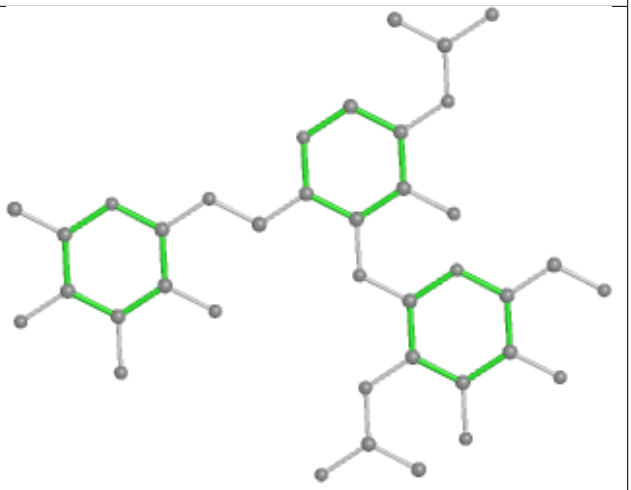
Bond lengths



Bond angles

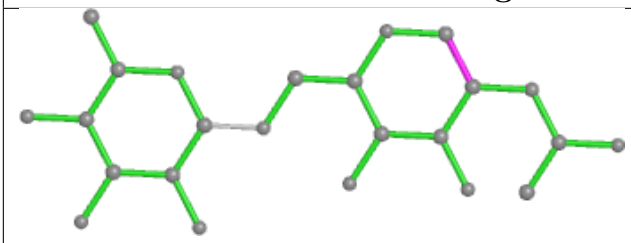


Torsions

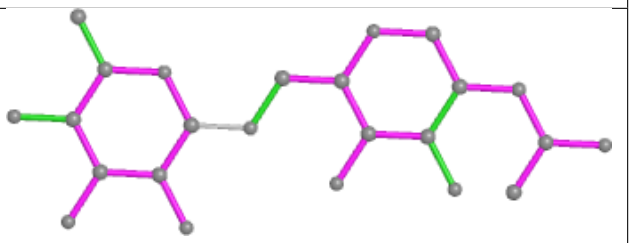


Rings

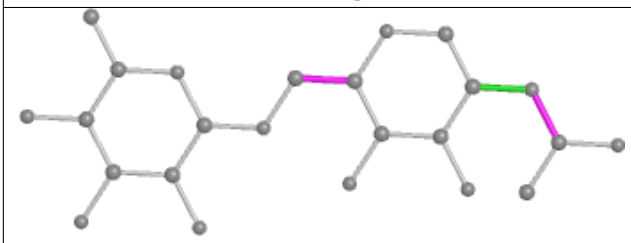
Oligosaccharide Chain C



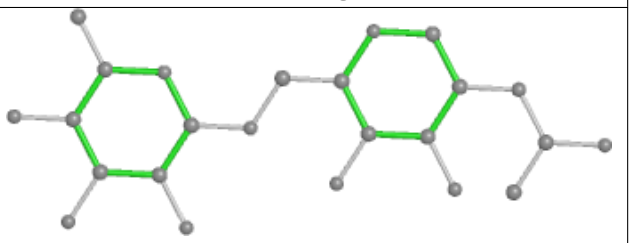
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 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	614	1	14,14,15	0.86	0	17,19,21	1.92	2 (11%)
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
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%)
8	NAG	A	613	1	14,14,15	0.58	0	17,19,21	1.96	5 (29%)

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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
8	A	613	NAG	O5-C1-C2	-3.52	105.73	111.29
8	A	613	NAG	C3-C4-C5	3.50	116.48	110.24
8	A	615	NAG	O5-C1-C2	-3.48	105.80	111.29
8	A	613	NAG	C4-C3-C2	2.92	115.29	111.02
8	A	614	NAG	C4-C3-C2	2.55	114.76	111.02
8	A	613	NAG	O5-C5-C6	2.40	110.97	107.20

There are no chirality outliers.

All (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
8	A	614	NAG	O5-C5-C6-O6
8	A	614	NAG	C4-C5-C6-O6
8	A	615	NAG	O5-C5-C6-O6
8	A	613	NAG	C4-C5-C6-O6
6	A	603	TN6	C4-C3-N-C1

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	TN6	3	0
8	A	615	NAG	1	0
8	A	613	NAG	4	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%)	0.14	26 (4%) 29 32	17, 34, 58, 76	9 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	5.4
1	A	379	ASP	5.0
1	A	50	THR	5.0
1	A	3	ASP	4.3
1	A	282	TYR	4.3
1	A	380	GLN	4.0
1	A	255	GLU	3.9
1	A	453	ARG	3.8
1	A	256	ASN	3.6
1	A	55	ILE	3.1
1	A	51	LYS	3.0
1	A	455	GLN	2.9
1	A	342	ASN	2.8
1	A	377	VAL	2.6
1	A	259	GLU	2.5
1	A	40	ARG	2.4
1	A	376	TRP	2.4
1	A	260	ILE	2.4
1	A	266	ASN	2.4
1	A	254	ARG	2.3
1	A	240	ARG	2.3
1	A	257	GLU	2.2
1	A	278	PHE	2.1
1	A	253	SER	2.1
1	A	54	ASP	2.0
1	A	251	GLY	2.0

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)

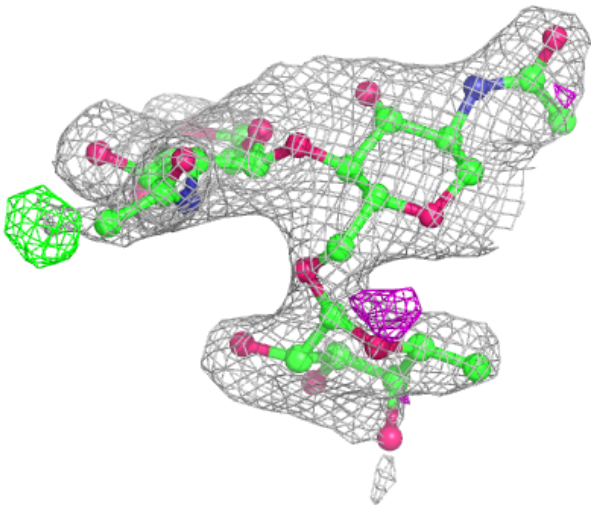
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

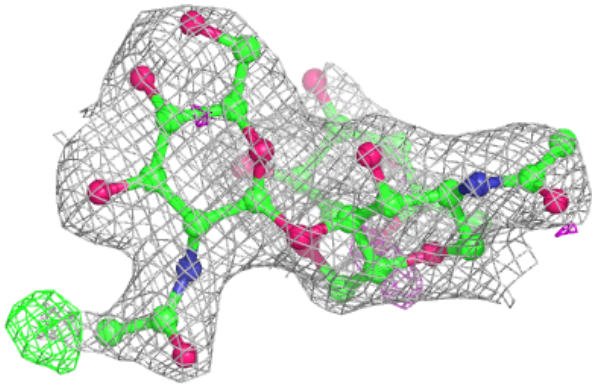
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUL	C	2	10/11	0.71	0.31	40,46,47,49	10
2	FUL	B	3	10/11	0.74	0.30	65,69,73,73	0
2	NAG	D	2	14/15	0.76	0.39	65,76,78,78	0
2	FUL	D	3	10/11	0.77	0.29	71,73,75,77	0
2	NAG	B	2	14/15	0.78	0.22	62,67,70,70	0
3	NAG	C	1	14/15	0.80	0.24	54,59,61,64	0
2	NAG	D	1	14/15	0.87	0.25	67,72,79,79	0
2	NAG	B	1	14/15	0.95	0.17	46,52,58,64	0

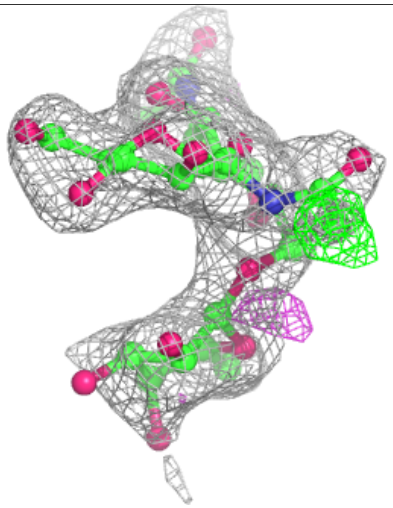
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

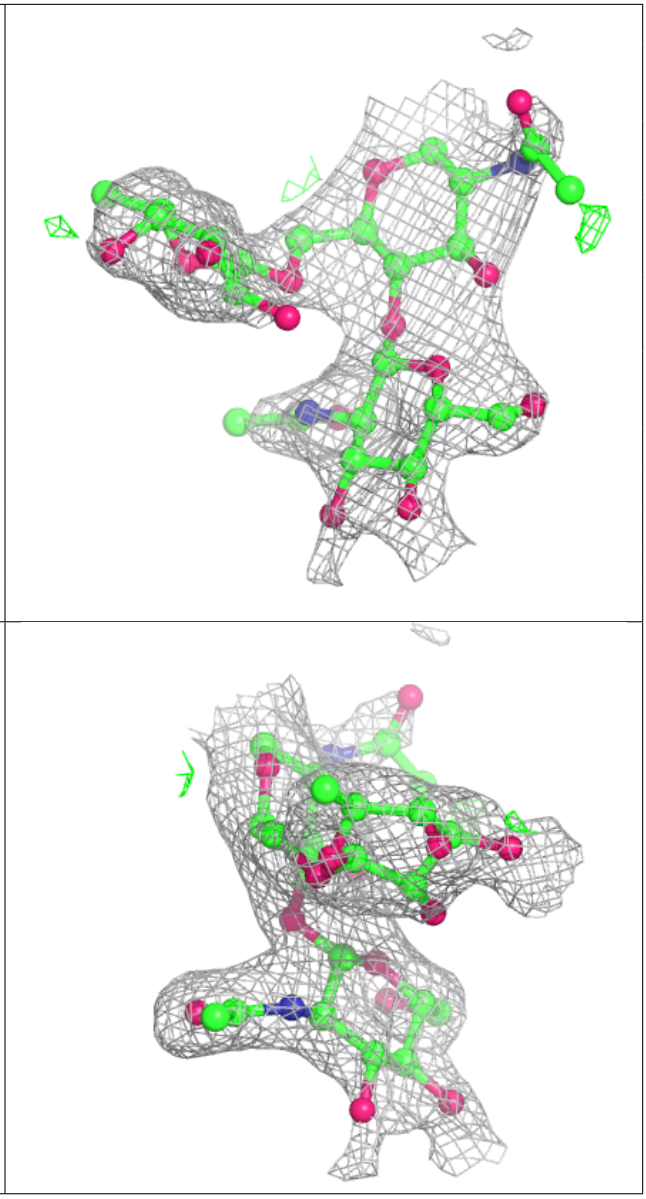


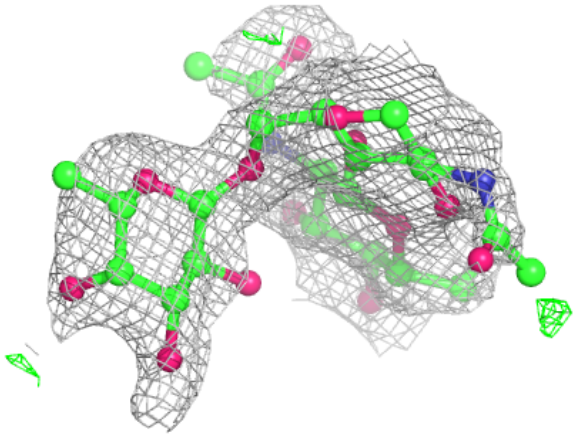




Electron density around Chain D:

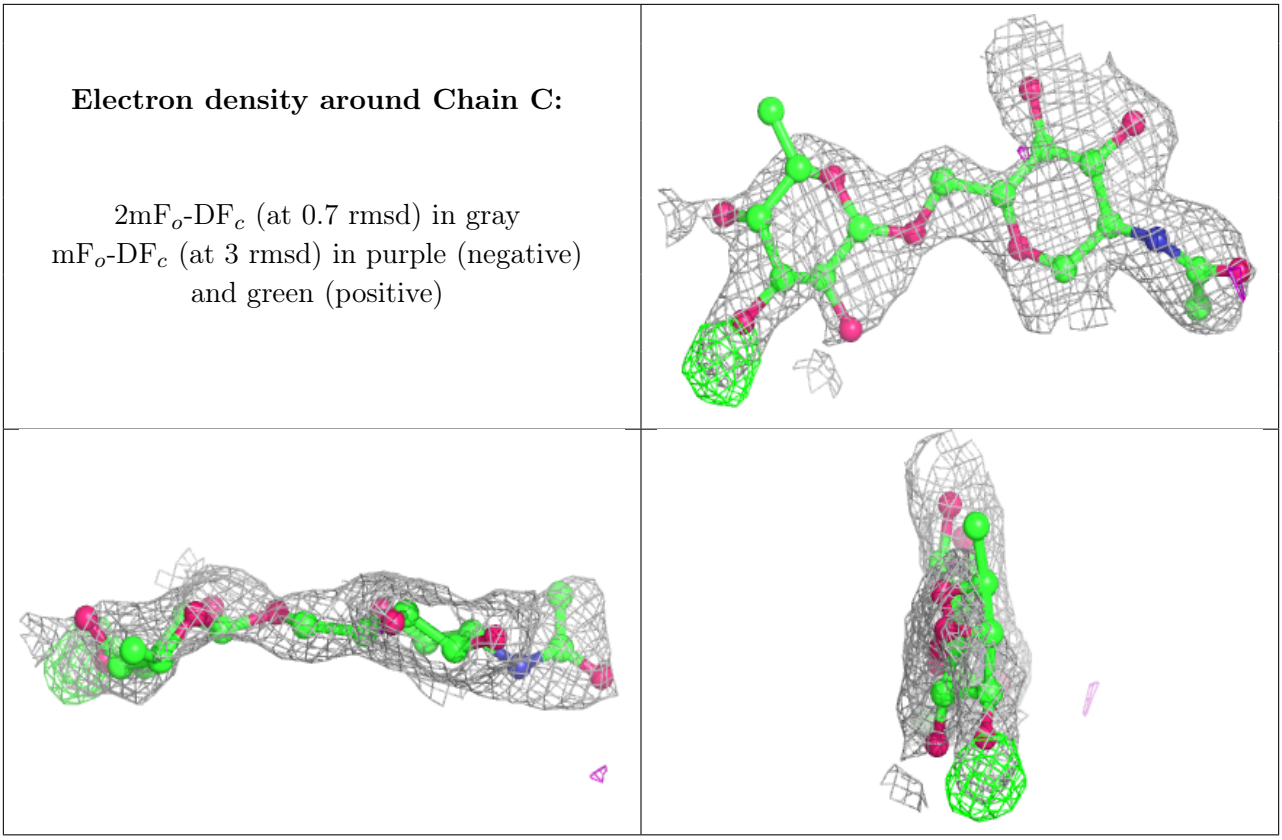
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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	NAG	A	613	14/15	0.58	0.36	73,77,79,82	0
8	NAG	A	614	14/15	0.69	0.22	45,60,64,66	0
8	NAG	A	615	14/15	0.82	0.51	82,85,88,88	0
5	CL	A	606	1/1	0.92	0.12	62,62,62,62	0
5	CL	A	602	1/1	0.94	0.18	58,58,58,58	0
5	CL	A	604	1/1	0.94	0.16	71,71,71,71	0
7	SO4	A	605	5/5	0.96	0.10	52,52,57,58	5
7	SO4	A	607	5/5	0.97	0.20	40,42,43,45	5
6	TN6	A	603	8/9	0.98	0.15	24,27,28,29	0
4	NA	A	601	1/1	0.99	0.24	41,41,41,41	1

6.5 Other polymers (i)

There are no such residues in this entry.