



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:20 PM UTC

PDB ID : 2WIJ / pdb_00002wij
Title : NONAGED FORM OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY TABUN ANALOGUE TA5
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Deposited on : 2009-05-12
Resolution : 2.10 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
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

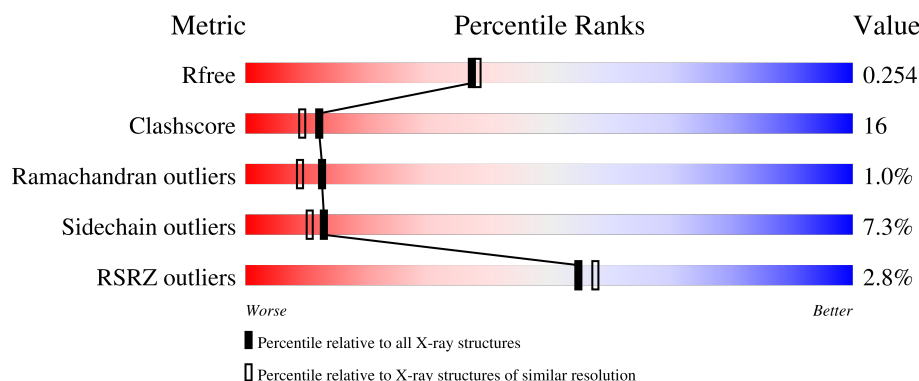
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	529	3% 73% 22% ..
2	B	3	67% 33%
2	D	3	33% 67%
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
7	CL	A	606	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4719 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.

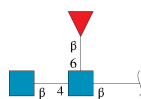
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	527	4214	2718	710	771	15	0	3	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.



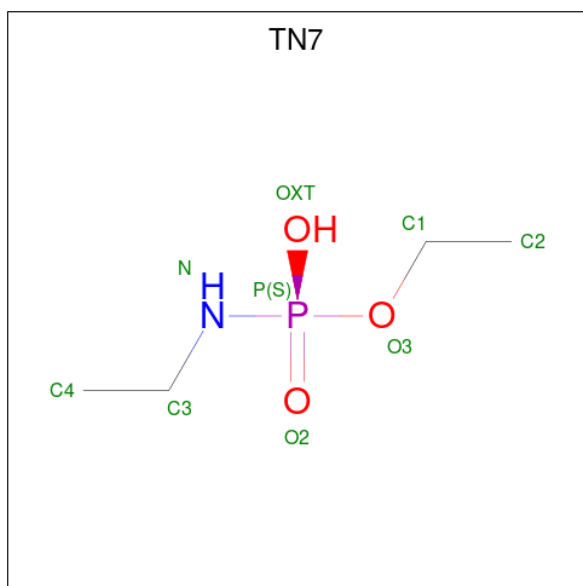
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	38	22	2	14	0	0	0
2	D	3	38	22	2	14	0	0	0

- 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
3	C	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is ethyl hydrogen ethylamidophosphate (CCD ID: TN7) (formula: $C_4H_{12}NO_3P$).



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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

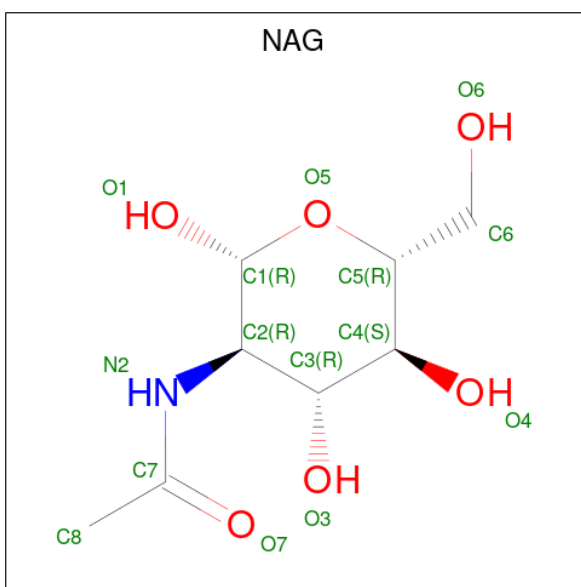


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

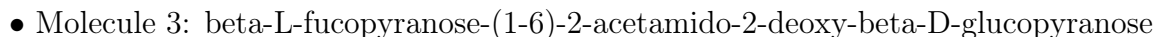
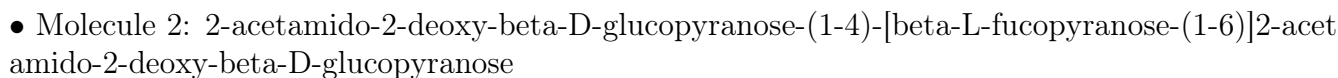


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	342	Total	O	0	0
			342	342		

- Molecule 1: CHOLINESTERASE



Chain C:



MAG1
FOL2

4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.02Å 155.02Å 127.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.05 – 2.10 55.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.05-2.10) 99.7 (55.05-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.200 , 0.253 0.200 , 0.254	Depositor DCC
R_{free} test set	1355 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4719	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, FUL, TN7, NA, NAG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	1/4342 (0.0%)	1.11	10/5895 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	PRO	CA-C	5.85	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	PHE	CA-C-N	8.06	129.92	119.84
1	A	358	PHE	C-N-CA	8.06	129.92	119.84
1	A	525	PHE	N-CA-C	5.89	118.59	111.40
1	A	99	ILE	CA-C-N	-5.86	114.72	120.52
1	A	99	ILE	C-N-CA	-5.86	114.72	120.52
1	A	23	GLY	N-CA-C	-5.45	102.16	111.27
1	A	454	ASP	N-CA-C	5.45	119.91	113.16
1	A	402	ALA	N-CA-C	-5.32	105.56	111.36
1	A	344	ILE	CA-C-N	-5.02	116.81	122.48
1	A	344	ILE	C-N-CA	-5.02	116.81	122.48

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	4214	0	4114	127	0
2	B	38	0	34	1	0
2	D	38	0	34	0	0
3	C	24	0	22	1	0
4	A	8	0	11	4	0
5	A	1	0	0	0	0
6	A	10	0	0	1	0
7	A	2	0	0	2	0
8	A	42	0	39	2	0
9	A	342	0	0	24	1
All	All	4719	0	4254	135	1

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 16.

All (135) 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:4:ILE:H	1:A:4:ILE:HD12	1.00	1.12
1:A:256:ASN:HB3	1:A:259:GLU:HG3	1.28	1.11
1:A:4:ILE:HD12	1:A:4:ILE:N	1.67	1.06
4:A:601:TN7:H31C	4:A:601:TN7:H23C	1.39	1.04
1:A:377:VAL:O	1:A:377:VAL:HG23	1.60	0.97
9:A:701:HOH:O	3:C:2:FUL:O3	1.83	0.91
1:A:518:GLN:HE21	1:A:518:GLN:H	1.09	0.90
1:A:4:ILE:H	1:A:4:ILE:CD1	1.82	0.88
1:A:42:ARG:HH22	1:A:269:PRO:HD3	1.38	0.87
1:A:380:GLN:HB2	7:A:606:CL:CL	2.15	0.82
1:A:42:ARG:NH2	1:A:269:PRO:HD3	1.95	0.80
1:A:253:SER:O	1:A:254:ARG:HD3	1.84	0.77
1:A:267:LYS:HE3	1:A:271:GLU:OE1	1.87	0.74
1:A:377:VAL:O	1:A:377:VAL:CG2	2.34	0.74
1:A:256:ASN:HB3	1:A:259:GLU:CG	2.15	0.74
4:A:601:TN7:H23C	4:A:601:TN7:C3	2.17	0.73
1:A:378:ASP:C	1:A:380:GLN:H	1.97	0.72
1:A:454:ASP:O	1:A:455:GLN:HB2	1.89	0.72
1:A:176[B]:GLN:HG3	1:A:180:LYS:HE3	1.72	0.72
1:A:378:ASP:O	1:A:380:GLN:N	2.25	0.69
1:A:255:GLU:H	1:A:255:GLU:CD	2.01	0.68
1:A:156:LEU:HD22	1:A:261:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:GLU:OE1	1:A:453:ARG:HG2	1.96	0.65
1:A:320:GLY:HA3	1:A:419:TYR:CE1	2.32	0.65
1:A:509:ARG:CZ	9:A:741:HOH:O	2.45	0.64
1:A:495:SER:O	1:A:496:THR:HG23	1.98	0.64
1:A:255:GLU:CD	1:A:255:GLU:N	2.55	0.64
1:A:494:LYS:HB2	9:A:705:HOH:O	1.97	0.64
1:A:304:ASP:HB3	9:A:1019:HOH:O	1.99	0.63
1:A:227:PHE:CD2	1:A:227:PHE:C	2.77	0.62
1:A:347:ARG:NH1	1:A:370:LEU:HD21	2.15	0.61
1:A:497:GLU:N	9:A:705:HOH:O	2.25	0.61
1:A:378:ASP:CG	1:A:379:ASP:H	2.09	0.60
1:A:495:SER:HA	9:A:702:HOH:O	2.01	0.60
1:A:495:SER:O	1:A:496:THR:CB	2.51	0.58
1:A:383:GLU:O	1:A:387:GLU:HG3	2.04	0.57
1:A:509:ARG:HD3	9:A:967:HOH:O	2.05	0.57
1:A:496:THR:N	9:A:702:HOH:O	1.98	0.56
1:A:518:GLN:HE21	1:A:518:GLN:N	1.91	0.56
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.40	0.56
1:A:48:SER:CB	9:A:966:HOH:O	2.54	0.55
1:A:381:ARG:NH2	1:A:383:GLU:OE1	2.40	0.55
1:A:54:ASP:HB2	9:A:716:HOH:O	2.05	0.54
1:A:428:LEU:CD1	1:A:430:TRP:HB2	2.37	0.54
1:A:495:SER:O	1:A:496:THR:OG1	2.25	0.54
1:A:51:LYS:N	9:A:710:HOH:O	2.35	0.54
1:A:256:ASN:CB	1:A:259:GLU:HG3	2.20	0.54
1:A:425:SER:O	9:A:703:HOH:O	2.19	0.54
1:A:526:PHE:N	1:A:527:PRO:CD	2.71	0.54
1:A:198:SER:HA	1:A:224:SER:O	2.08	0.53
1:A:495:SER:CA	9:A:702:HOH:O	2.57	0.53
1:A:280:VAL:HG13	1:A:282:TYR:O	2.08	0.53
1:A:50:THR:O	1:A:51:LYS:CB	2.56	0.53
1:A:178:VAL:HG13	1:A:182:ILE:HB	1.90	0.53
1:A:414:ASN:HB2	9:A:713:HOH:O	2.08	0.53
1:A:48:SER:HA	9:A:966:HOH:O	2.10	0.52
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.91	0.52
1:A:448:LEU:N	1:A:449:PRO:CD	2.72	0.52
1:A:76:PHE:O	1:A:80:GLU:HG3	2.10	0.52
1:A:48:SER:HB3	9:A:966:HOH:O	2.08	0.51
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.46	0.51
1:A:495:SER:O	1:A:496:THR:CG2	2.59	0.51
1:A:16:MET:HE2	1:A:18:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:MET:HE2	1:A:437:MET:HE3	1.92	0.51
1:A:388:ALA:O	1:A:392:VAL:HG23	2.11	0.50
1:A:172:GLN:O	1:A:176[A]:GLN:HG3	2.12	0.50
1:A:253:SER:O	1:A:254:ARG:CD	2.57	0.49
1:A:509:ARG:CD	9:A:967:HOH:O	2.59	0.49
1:A:50:THR:O	1:A:51:LYS:CG	2.60	0.49
1:A:156:LEU:CD2	1:A:261:ILE:HD11	2.42	0.48
1:A:176[B]:GLN:HE21	1:A:180:LYS:HG3	1.77	0.48
8:A:612:NAG:H61	9:A:939:HOH:O	2.13	0.48
1:A:214:HIS:HE1	9:A:970:HOH:O	1.95	0.48
1:A:310:GLY:HA3	1:A:412:TRP:CE2	2.49	0.48
1:A:381:ARG:HB2	1:A:384:ASN:OD1	2.14	0.48
1:A:377:VAL:N	1:A:378:ASP:HA	2.28	0.47
1:A:176[A]:GLN:NE2	9:A:722:HOH:O	2.47	0.47
1:A:428:LEU:CD2	1:A:440:TYR:CD2	2.97	0.47
1:A:53:SER:O	1:A:54:ASP:HB2	2.13	0.47
1:A:417:PHE:CE2	1:A:492:VAL:HG12	2.50	0.47
1:A:48:SER:CA	9:A:966:HOH:O	2.62	0.47
1:A:301:ASP:O	1:A:302:MET:C	2.57	0.46
1:A:24:THR:O	1:A:101:ALA:HB3	2.16	0.46
1:A:361:VAL:O	1:A:366:LYS:NZ	2.48	0.46
1:A:132:PHE:CE2	1:A:448:LEU:HD22	2.51	0.46
1:A:268:ASP:O	1:A:269:PRO:C	2.59	0.46
1:A:448:LEU:HB2	1:A:449:PRO:HD3	1.97	0.46
4:A:601:TN7:H31C	4:A:601:TN7:C2	2.26	0.46
1:A:454:ASP:O	1:A:455:GLN:CB	2.57	0.46
1:A:61:TYR:CD1	1:A:124:SER:HB3	2.51	0.45
1:A:156:LEU:HD12	1:A:156:LEU:HA	1.82	0.45
1:A:319:VAL:O	1:A:418:PHE:HA	2.16	0.45
1:A:49:LEU:HD12	1:A:50:THR:H	1.80	0.45
6:A:603:SO4:O4	9:A:704:HOH:O	2.20	0.45
1:A:312:PHE:CE1	1:A:314:LYS:HE3	2.52	0.45
1:A:383:GLU:CD	1:A:383:GLU:H	2.23	0.45
1:A:254:ARG:HB2	1:A:260:ILE:HG13	1.99	0.45
1:A:274:LEU:HD12	1:A:274:LEU:HA	1.93	0.45
1:A:110:LEU:HD11	1:A:475:ALA:CB	2.48	0.44
1:A:355:LYS:HE2	1:A:355:LYS:HB2	1.77	0.44
1:A:337:PHE:CE1	1:A:389:LEU:HD23	2.53	0.44
1:A:525:PHE:O	1:A:528:LYS:HB2	2.17	0.44
8:A:612:NAG:C6	9:A:939:HOH:O	2.65	0.44
1:A:96:ASN:O	1:A:142:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:NZ	9:A:728:HOH:O	2.50	0.43
1:A:338:SER:HB2	2:B:1:NAG:H62	1.99	0.43
1:A:422:GLU:HG3	1:A:504:ASN:HB3	2.01	0.43
1:A:304:ASP:OD1	1:A:304:ASP:N	2.47	0.43
1:A:453:ARG:HG2	1:A:453:ARG:H	1.62	0.43
1:A:495:SER:C	1:A:496:THR:HG23	2.43	0.43
1:A:247:ALA:O	1:A:248:LYS:C	2.61	0.43
1:A:320:GLY:HA3	1:A:419:TYR:CD1	2.53	0.43
1:A:209:LEU:HD13	1:A:306:LEU:HB2	2.00	0.43
1:A:378:ASP:OD1	1:A:379:ASP:OD1	2.37	0.43
1:A:428:LEU:HD11	1:A:437:MET:SD	2.59	0.43
1:A:50:THR:O	1:A:51:LYS:HB3	2.19	0.42
1:A:510:ILE:C	1:A:511:MET:HG2	2.39	0.42
1:A:506:GLU:HB2	1:A:507:SER:H	1.74	0.42
1:A:56:TRP:CD1	1:A:56:TRP:C	2.97	0.42
1:A:204:VAL:CG1	1:A:220:ALA:HB1	2.49	0.42
1:A:372[A]:HIS:CE1	1:A:518:GLN:HA	2.54	0.42
1:A:428:LEU:HD13	1:A:430:TRP:HB2	2.00	0.42
1:A:381:ARG:HH22	1:A:383:GLU:CG	2.32	0.42
1:A:278:PHE:C	1:A:280:VAL:H	2.28	0.42
1:A:428:LEU:HD13	1:A:430:TRP:H	1.84	0.41
1:A:381:ARG:HH22	1:A:383:GLU:HG2	1.86	0.41
1:A:516:ALA:O	1:A:520:ARG:HG3	2.20	0.41
1:A:525:PHE:CD1	1:A:525:PHE:C	2.95	0.41
1:A:378:ASP:CG	1:A:379:ASP:N	2.77	0.41
4:A:601:TN7:C3	4:A:601:TN7:C2	2.94	0.41
1:A:518:GLN:H	1:A:518:GLN:NE2	1.94	0.40
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.88	0.40
1:A:317:ILE:HD13	1:A:317:ILE:HG21	1.88	0.40
1:A:526:PHE:C	1:A:528:LYS:H	2.29	0.40
1:A:378:ASP:N	7:A:606:CL:CL	2.82	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:875:HOH:O	9:A:975:HOH:O[7_555]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	528/529 (100%)	497 (94%)	26 (5%)	5 (1%)	14 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP
1	A	496	THR
1	A	51	LYS
1	A	361	VAL
1	A	506	GLU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	454/454 (100%)	421 (93%)	33 (7%)	13 10

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

Mol	Chain	Res	Type
1	A	4	ILE
1	A	5	ILE
1	A	9	LYS
1	A	16	MET
1	A	38	LEU
1	A	50	THR

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Mol	Chain	Res	Type
1	A	53	SER
1	A	69	ILE
1	A	110	LEU
1	A	156	LEU
1	A	195	PHE
1	A	236	LEU
1	A	240	ARG
1	A	255	GLU
1	A	262	LYS
1	A	267	LYS
1	A	274	LEU
1	A	280	VAL
1	A	299	LEU
1	A	355	LYS
1	A	359	PRO
1	A	361	VAL
1	A	367	GLU
1	A	377	VAL
1	A	380	GLN
1	A	428	LEU
1	A	448	LEU
1	A	453	ARG
1	A	454	ASP
1	A	458	LYS
1	A	506	GLU
1	A	518	GLN
1	A	529	VAL

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	275	ASN
1	A	289	ASN
1	A	380	GLN
1	A	455	GLN
1	A	517	GLN
1	A	518	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	2,1	14,14,15	1.19	2 (14%)	17,19,21	1.72	3 (17%)
2	NAG	B	2	2	14,14,15	0.67	1 (7%)	17,19,21	1.08	2 (11%)
2	FUL	B	3	2	10,10,11	0.88	0	14,14,16	2.37	3 (21%)
3	NAG	C	1	3,1	14,14,15	0.66	0	17,19,21	1.41	3 (17%)
3	FUL	C	2	3	10,10,11	0.67	0	14,14,16	2.19	4 (28%)
2	NAG	D	1	2,1	14,14,15	0.52	0	17,19,21	1.36	2 (11%)
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	0.92	0
2	FUL	D	3	2	10,10,11	0.79	0	14,14,16	2.39	3 (21%)

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	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	4/6/23/26	0/1/1/1
3	FUL	C	2	3	-	-	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	FUL	D	3	2	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	-2.63	1.39	1.43
2	B	1	NAG	C2-N2	-2.03	1.42	1.46
2	B	2	NAG	O5-C1	-2.00	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	FUL	C1-C2-C3	-6.76	99.80	109.64
2	D	3	FUL	C1-C2-C3	-6.24	100.55	109.64
2	B	3	FUL	C1-C2-C3	-6.21	100.61	109.64
2	D	1	NAG	O5-C1-C2	-4.07	104.99	111.29
2	D	3	FUL	C3-C4-C5	3.61	115.30	109.81
2	B	1	NAG	O5-C1-C2	-3.55	105.80	111.29
2	D	3	FUL	C1-O5-C5	-3.52	104.65	112.97
2	B	3	FUL	O5-C1-C2	-3.42	102.63	110.79
2	B	1	NAG	C3-C4-C5	-3.40	104.07	110.23
3	C	1	NAG	C3-C4-C5	-3.21	104.41	110.23
2	B	1	NAG	C2-N2-C7	3.11	127.07	122.90
2	B	3	FUL	C3-C4-C5	2.61	113.78	109.81
3	C	1	NAG	O5-C5-C6	2.50	112.53	107.66
3	C	2	FUL	O5-C5-C6	2.48	112.79	107.40
3	C	1	NAG	O5-C1-C2	-2.28	107.77	111.29
3	C	2	FUL	C1-O5-C5	-2.21	107.76	112.97
2	B	2	NAG	C3-C4-C5	2.11	114.06	110.23
2	B	2	NAG	C1-O5-C5	-2.04	109.45	112.19
3	C	2	FUL	O2-C2-C1	2.04	113.90	109.22
2	D	1	NAG	O7-C7-C8	-2.01	118.48	122.05

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

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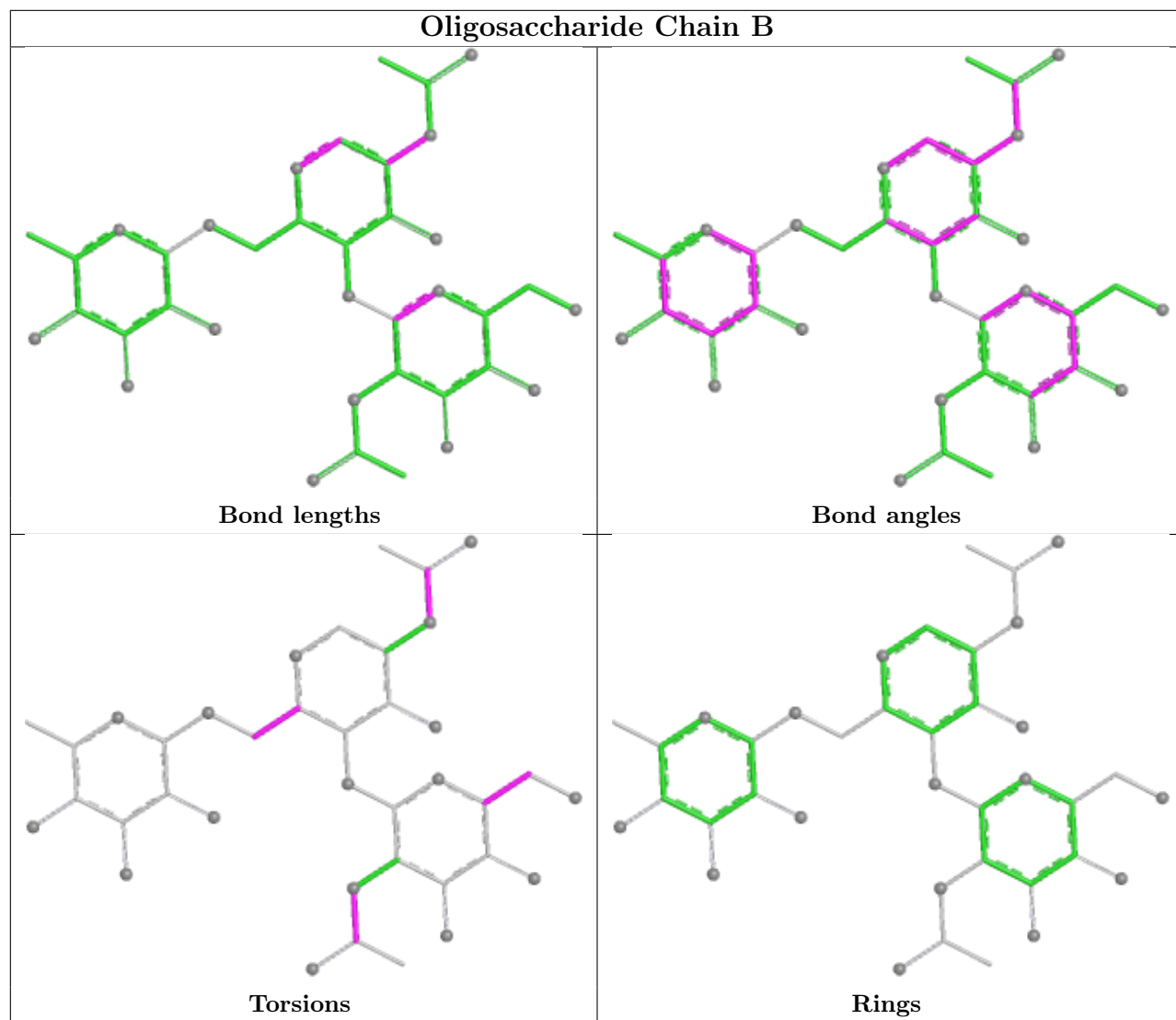
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

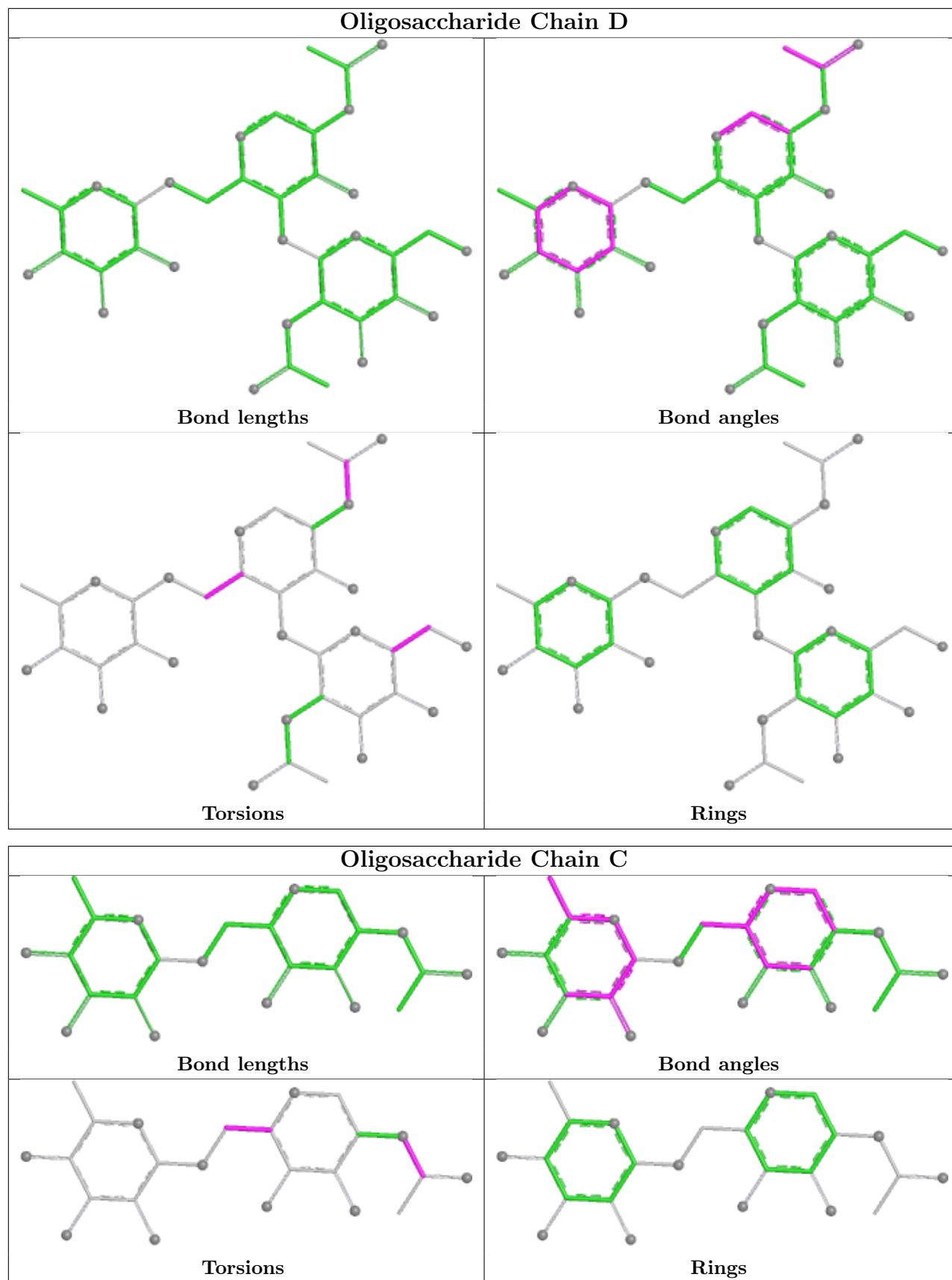
There are no ring outliers.

2 monomers are involved in 2 short contacts:

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





5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 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$
6	SO4	A	605	-	4,4,4	0.29	0	6,6,6	0.40	0
8	NAG	A	613	1	14,14,15	0.69	0	17,19,21	1.70	4 (23%)
6	SO4	A	603	-	4,4,4	0.18	0	6,6,6	0.23	0
4	TN7	A	601	1	4,7,8	0.66	0	2,7,10	0.11	0
8	NAG	A	614	1	14,14,15	0.55	0	17,19,21	1.16	1 (5%)
8	NAG	A	612	1	14,14,15	0.59	0	17,19,21	1.43	3 (17%)

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	613	1	-	0/6/23/26	0/1/1/1
4	TN7	A	601	1	-	0/1/6/8	-
8	NAG	A	612	1	-	4/6/23/26	0/1/1/1
8	NAG	A	614	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	A	613	NAG	C2-N2-C7	-4.11	117.39	122.90
8	A	612	NAG	O5-C1-C2	-2.69	107.12	111.29
8	A	612	NAG	C1-O5-C5	2.58	115.65	112.19
8	A	613	NAG	O5-C1-C2	-2.55	107.35	111.29
8	A	614	NAG	C4-C3-C2	2.55	114.75	111.02
8	A	613	NAG	O3-C3-C4	-2.53	104.42	110.38
8	A	612	NAG	C3-C4-C5	2.50	114.77	110.23
8	A	613	NAG	C4-C3-C2	2.30	114.38	111.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	614	NAG	C8-C7-N2-C2
8	A	614	NAG	O7-C7-N2-C2
8	A	612	NAG	O5-C5-C6-O6
8	A	612	NAG	C8-C7-N2-C2
8	A	612	NAG	O7-C7-N2-C2
8	A	612	NAG	C4-C5-C6-O6
8	A	614	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	SO4	1	0
4	A	601	TN7	4	0
8	A	612	NAG	2	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%)	0.13	15 (2%) 55 57	18, 31, 54, 69	11 (2%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	THR	5.6
1	A	377	VAL	4.5
1	A	22	GLY	3.6
1	A	54	ASP	3.5
1	A	525	PHE	3.3
1	A	4	ILE	2.9
1	A	282	TYR	2.8
1	A	380	GLN	2.6
1	A	50	THR	2.5
1	A	360	GLY	2.3
1	A	237	TYR	2.3
1	A	52	TRP	2.2
1	A	255	GLU	2.2
1	A	497	GLU	2.1
1	A	55	ILE	2.1

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

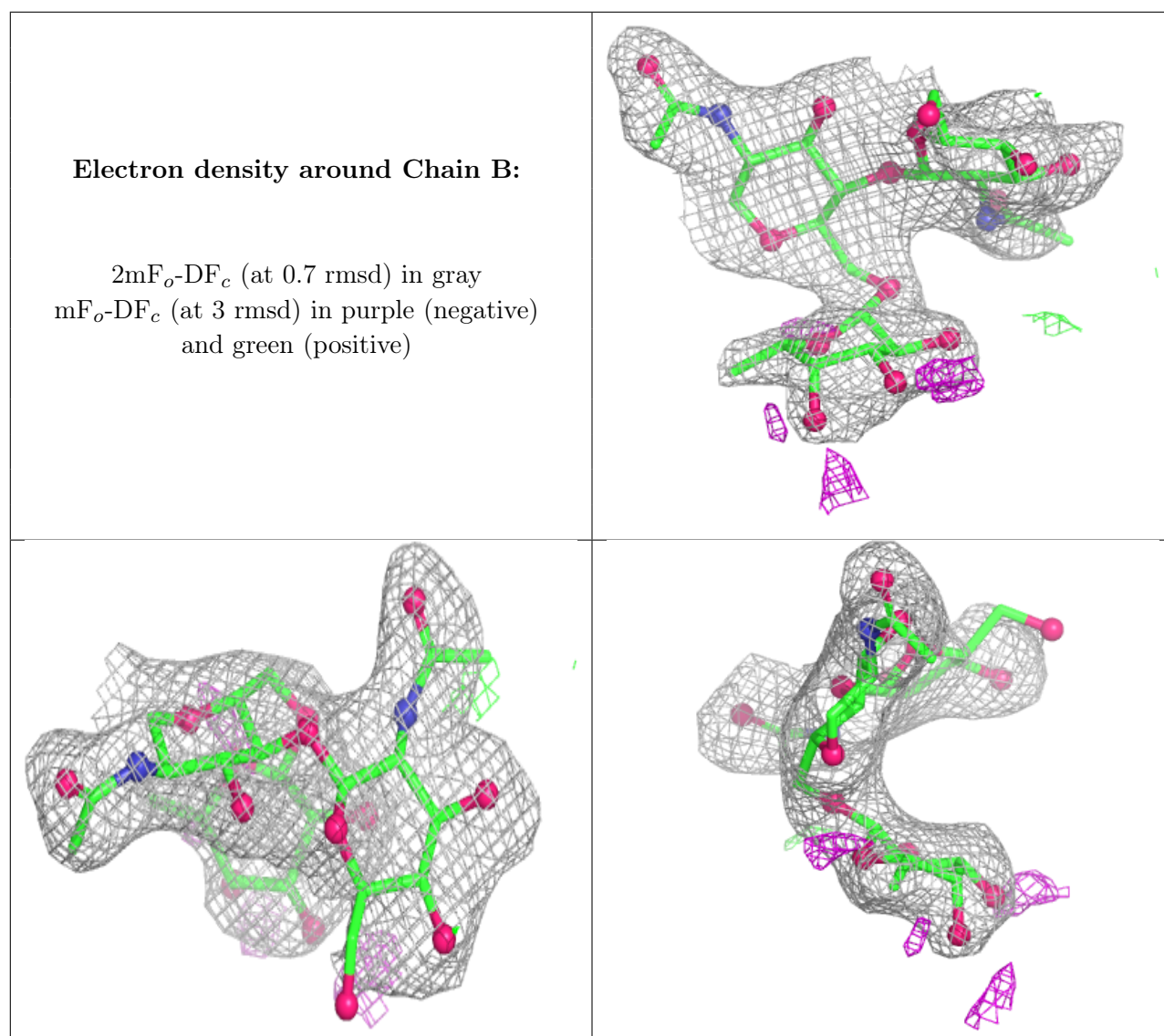
There are no non-standard protein/DNA/RNA residues in this entry.

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.

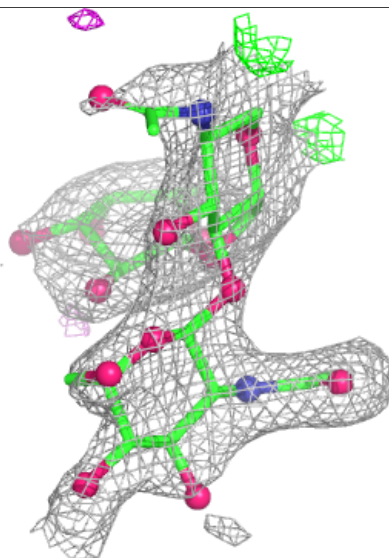
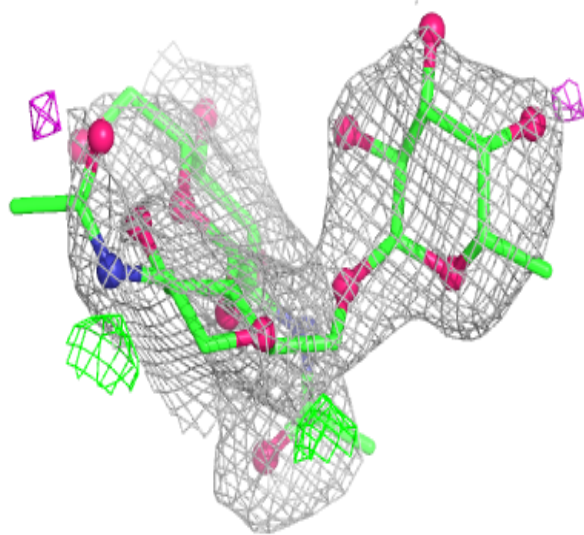
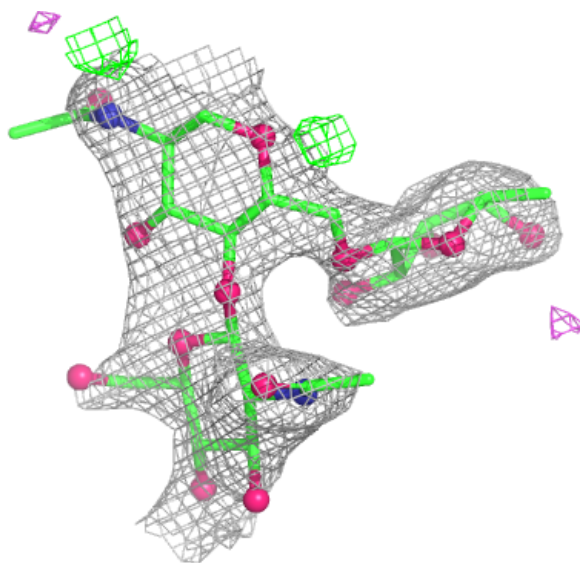
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUL	B	3	10/11	0.73	0.18	63,65,66,67	0
3	NAG	C	1	14/15	0.75	0.14	53,60,63,67	0
3	FUL	C	2	10/11	0.77	0.18	67,70,72,74	0
2	NAG	B	2	14/15	0.78	0.14	59,64,68,69	0
2	NAG	D	1	14/15	0.80	0.17	62,64,70,71	0
2	NAG	D	2	14/15	0.83	0.13	61,69,72,73	0
2	FUL	D	3	10/11	0.89	0.13	65,65,66,68	0
2	NAG	B	1	14/15	0.94	0.10	40,46,54,58	0

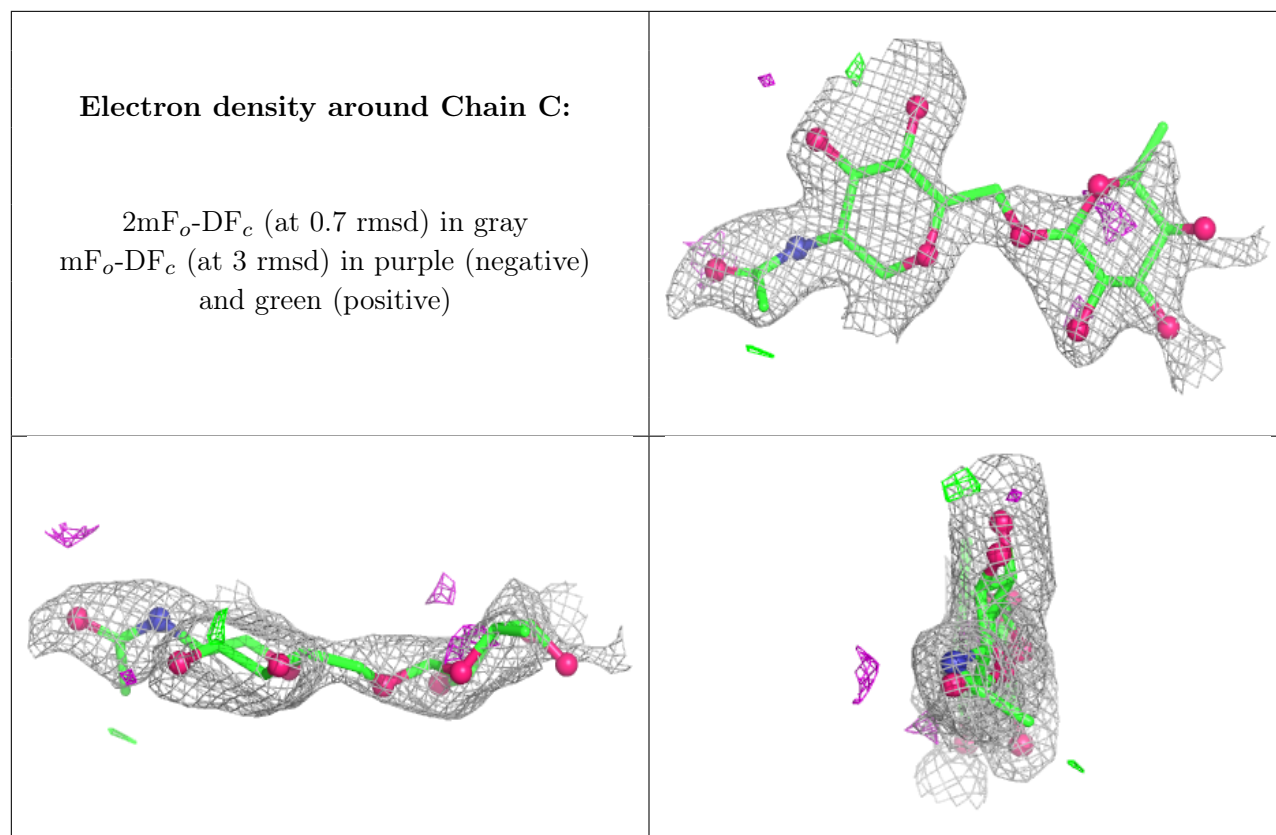
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain 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
8	NAG	A	612	14/15	0.66	0.14	65,70,70,73	0
8	NAG	A	614	14/15	0.72	0.14	81,86,87,87	0
8	NAG	A	613	14/15	0.84	0.12	54,65,69,69	0
5	NA	A	602	1/1	0.86	0.26	64,64,64,64	1
7	CL	A	606	1/1	0.91	0.15	72,72,72,72	0
7	CL	A	604	1/1	0.93	0.15	68,68,68,68	0
6	SO4	A	605	5/5	0.94	0.09	32,36,38,39	5
6	SO4	A	603	5/5	0.94	0.08	46,48,50,51	5
4	TN7	A	601	8/9	0.95	0.12	28,32,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.