



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:11 AM UTC

PDB ID : 7S6N / pdb_00007s6n
Title : N-acetylglucosamine-1-phosphotransferase (GNPT) alpha and beta subunits (GNPTAB) catalytic domain, from zebrafish
Authors : Gorelik, A.; Illes, K.; Nagar, B.
Deposited on : 2021-09-14
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 ⓘ 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

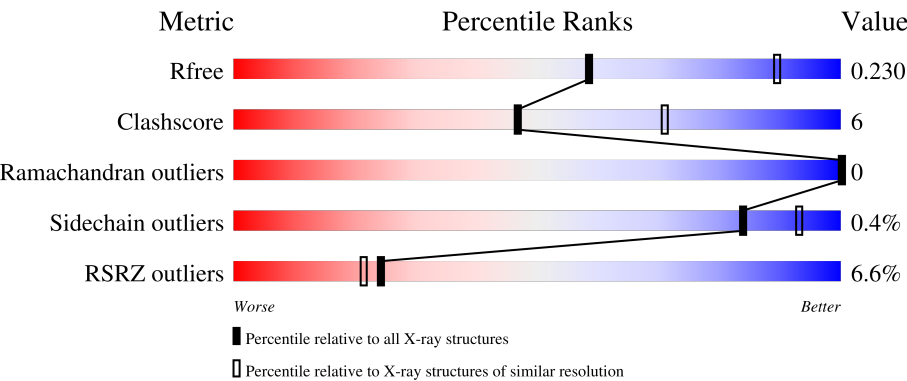
1 Overall quality at a glance i

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	495	5% 75% 10% 15%
1	B	495	6% 79% 11% 10%
2	C	4	50% 50%
3	D	2	50% 50%
4	E	3	100%

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Mol	Chain	Length	Quality of chain
5	F	3	 100%

2 Entry composition [i](#)

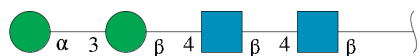
There are 8 unique types of molecules in this entry. The entry contains 14891 atoms, of which 7115 are hydrogens and 0 are deuteriums.

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 N-acetylglucosamine-1-phosphotransferase (GNPT) alpha (GNPTAB) catalytic domain,N-acetylglucosamine-1-phosphotransferase subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	H	N	O	S	0	0	0
			6873	2222	3394	600	641	16			
1	B	446	Total	C	H	N	O	S	0	0	0
			7287	2359	3591	640	680	17			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	H	N	O	0	0	0
			80	28	30	2	20			

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



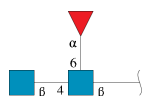
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	2	Total	C	H	N	O	0	0	0
			39	14	15	1	9			

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



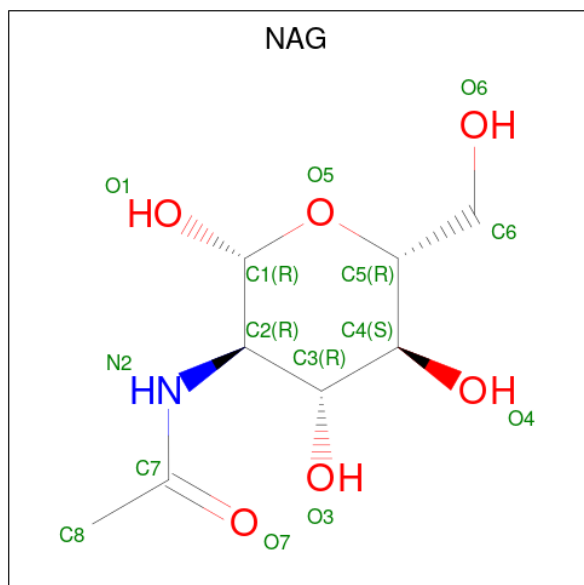
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	3	Total	C	H	N	O	0	0	0
			61	22	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	3	Total	C	H	N	O	0	0	0
			61	22	23	2	14			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			22	8	8	1	5		
6	A	1	Total	C	H	N	O	0	0
			22	8	8	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			22	8	8	1	5		
6	B	1	Total	C	H	N	O	0	0
			22	8	8	1	5		
6	B	1	Total	C	H	N	O	0	0
			22	8	8	1	5		

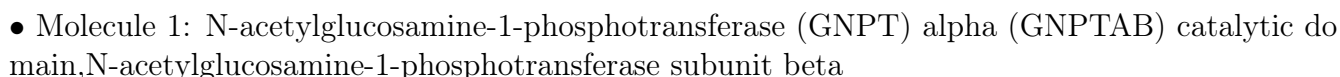
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	216	Total	O	0	0
			216	216		
8	B	162	Total	O	0	0
			162	162		

- Molecule 1: N-acetylglucosamine-1-phosphotransferase (GNPT) alpha (GNPTAB) catalytic domain, N-acetylglucosamine-1-phosphotransferase subunit beta



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

Chain C:  50% 50%

MAG1
MAG2
BMA3
MAN4

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

Chain D:  50% 50%

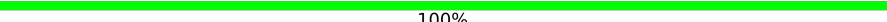
MAG1
FUC2

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

Chain E:  100%

MAG1
MAG2
BMA3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2
FUC3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.18Å 86.61Å 106.98Å 90.00° 112.17° 90.00°	Depositor
Resolution (Å)	48.42 – 2.70 48.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	71.5 (48.42-2.70) 84.5 (48.42-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.183 , 0.231 0.184 , 0.230	Depositor DCC
R_{free} test set	1948 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14891	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: CA, MAN, BMA, NAG, FUC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/3572	0.37	0/4842
1	B	0.22	0/3796	0.34	0/5149
All	All	0.23	0/7368	0.35	0/9991

There are no bond length outliers.

There are no bond angle outliers.

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	3479	3394	3394	52	0
1	B	3696	3591	3591	48	0
2	C	50	30	43	0	0
3	D	24	15	22	0	0
4	E	39	22	34	0	0
5	F	38	23	34	0	0
6	A	42	24	39	4	0
6	B	28	16	26	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	216	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	162	0	0	1	0
All	All	7776	7115	7183	83	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 6.

All (83) 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:371:GLU:HB3	1:A:403:MET:HE1	1.68	0.73
1:A:76:LEU:HD13	1:A:228:PRO:HB2	1.72	0.72
1:A:452:HIS:ND1	6:A:603:NAG:H82	2.07	0.70
1:A:449:ASN:HB3	1:A:452:HIS:HB3	1.79	0.64
1:A:57:LEU:HD22	1:B:57:LEU:HD22	1.82	0.61
1:A:57:LEU:HD11	1:B:71:GLN:HE22	1.64	0.61
1:A:350:ILE:HD11	1:A:406:VAL:HG21	1.83	0.60
1:B:54:TYR:CD1	1:B:54:TYR:N	2.69	0.60
1:A:251:PHE:HB3	1:A:312:GLN:HE22	1.68	0.59
1:B:54:TYR:N	1:B:54:TYR:HD1	2.01	0.58
1:A:57:LEU:HD11	1:B:57:LEU:HD21	1.85	0.58
1:A:253:ASP:OD1	1:A:256:ARG:NH2	2.36	0.58
1:B:76:LEU:HD13	1:B:228:PRO:HB2	1.85	0.58
1:A:372:GLN:HB2	6:A:601:NAG:H82	1.84	0.58
1:A:57:LEU:HD21	1:B:57:LEU:CD1	2.34	0.58
1:B:448:THR:HG21	1:B:478:HIS:HB3	1.85	0.58
1:A:78:MET:HE1	1:B:61:TYR:HA	1.86	0.57
1:B:448:THR:O	1:B:448:THR:HG22	2.05	0.57
1:B:254:SER:OG	1:B:310:ASP:O	2.22	0.56
1:A:57:LEU:HD21	1:B:57:LEU:HD11	1.88	0.55
1:B:350:ILE:HD11	1:B:406:VAL:HG21	1.89	0.54
1:A:448:THR:HG22	1:A:448:THR:O	2.08	0.53
1:A:373:MET:HG3	6:A:601:NAG:H81	1.91	0.53
1:A:426:LYS:O	1:A:428:GLN:HG3	2.09	0.53
1:A:57:LEU:CD1	1:B:71:GLN:HE22	2.24	0.51
1:B:162:ASN:OD1	1:B:164:GLN:HG3	2.10	0.51
1:A:54:TYR:CD1	1:A:54:TYR:N	2.79	0.51
1:B:499:PRO:HG3	1:B:506:ARG:HH21	1.76	0.51
1:A:460:ILE:HG21	1:A:468:ILE:HD13	1.93	0.50
1:A:370:LEU:HA	1:A:373:MET:HE3	1.93	0.49
1:A:448:THR:HG21	1:A:478:HIS:CG	2.48	0.49
1:A:57:LEU:HD11	1:B:71:GLN:NE2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLU:CB	1:A:403:MET:HE1	2.38	0.49
1:A:245:PRO:HG3	1:A:273:VAL:HG23	1.95	0.49
1:A:57:LEU:C	1:A:57:LEU:HD23	2.38	0.49
1:B:511:ARG:HG3	1:B:512:PHE:CD2	2.49	0.48
1:A:57:LEU:CD1	1:B:57:LEU:HD21	2.43	0.48
1:A:340:ASP:OD2	8:A:701:HOH:O	2.20	0.48
1:B:289:LEU:HD13	1:B:320:PHE:HB2	1.96	0.48
1:A:152:PRO:HB2	1:B:70:PHE:CZ	2.49	0.48
1:A:246:VAL:HG12	1:A:248:ASN:H	1.79	0.47
1:B:229:ASP:HA	1:B:232:TYR:O	2.15	0.47
1:B:86:TRP:CH2	1:B:88:ASN:HB2	2.49	0.47
1:A:57:LEU:CD2	1:B:57:LEU:HD13	2.45	0.47
1:B:213:PHE:O	1:B:280:MET:HA	2.15	0.46
1:A:312:GLN:HB2	1:A:315:PHE:HB3	1.96	0.46
1:A:303:HIS:CE1	1:A:307:HIS:CD2	3.04	0.46
1:B:509:ARG:NH1	1:B:513:LEU:HD21	2.31	0.46
1:A:261:LEU:HD11	1:A:296:GLU:HG2	1.97	0.46
1:A:57:LEU:CD2	1:B:57:LEU:CD1	2.94	0.45
1:A:457:LEU:O	1:A:461:ARG:HG3	2.16	0.45
1:A:442:ALA:HB2	1:A:465:ARG:HG2	1.99	0.45
1:B:415:LYS:N	1:B:416:PRO:HD2	2.31	0.45
1:B:57:LEU:C	1:B:57:LEU:HD23	2.41	0.45
1:A:160:VAL:HA	1:A:179:VAL:O	2.18	0.44
1:A:281:ILE:HG13	1:A:313:PHE:CZ	2.53	0.44
1:A:462:LYS:HD2	1:B:360:LEU:HG	2.00	0.44
1:B:356:ARG:HB3	1:B:425:PHE:HZ	1.82	0.44
1:A:448:THR:HA	1:A:484:VAL:HG21	1.99	0.44
1:B:62:ARG:NH1	8:B:710:HOH:O	2.51	0.44
6:A:603:NAG:O7	6:A:603:NAG:O3	2.32	0.44
1:B:289:LEU:HD22	1:B:317:TYR:HA	2.00	0.44
1:B:296:GLU:OE1	1:B:296:GLU:N	2.50	0.44
1:A:251:PHE:HB3	1:A:312:GLN:NE2	2.32	0.43
1:A:341:HIS:CD2	1:B:498:LEU:HD11	2.52	0.43
1:A:462:LYS:HB2	1:B:355:THR:HB	2.00	0.43
1:B:352:THR:O	1:B:356:ARG:HG2	2.19	0.43
1:B:506:ARG:HD2	1:B:506:ARG:H	1.84	0.43
1:B:334:PHE:CE2	1:B:345:LEU:HG	2.54	0.42
1:A:307:HIS:CD2	1:A:309:GLU:H	2.38	0.42
1:B:239:LYS:HB3	1:B:436:MET:HG3	2.02	0.42
1:B:153:TRP:CD1	1:B:153:TRP:H	2.35	0.42
1:B:307:HIS:CD2	1:B:309:GLU:H	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:CD1	1:A:191:LEU:HD21	2.55	0.42
1:B:243:THR:HG22	1:B:438:GLU:CD	2.44	0.42
1:A:239:LYS:HB3	1:A:436:MET:HG3	2.02	0.41
1:A:57:LEU:CD1	1:B:57:LEU:CD2	2.99	0.41
1:A:185:PHE:HB2	1:A:191:LEU:HD11	2.03	0.41
1:A:498:LEU:HD11	1:B:341:HIS:HD2	1.85	0.41
1:A:54:TYR:N	1:A:54:TYR:HD1	2.18	0.40
1:A:57:LEU:CD2	1:B:57:LEU:CD2	2.99	0.40
1:B:322:MET:HG2	1:B:433:PHE:CG	2.56	0.40
1:B:246:VAL:HG12	1:B:248:ASN:H	1.85	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	416/495 (84%)	406 (98%)	10 (2%)	0	100	100
1	B	440/495 (89%)	432 (98%)	8 (2%)	0	100	100
All	All	856/990 (86%)	838 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/465 (85%)	395 (100%)	1 (0%)	86	94
1	B	419/465 (90%)	417 (100%)	2 (0%)	81	92
All	All	815/930 (88%)	812 (100%)	3 (0%)	84	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	TYR
1	B	54	TYR
1	B	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	186	GLN
1	A	217	ASN
1	A	276	HIS
1	A	307	HIS
1	A	422	HIS
1	A	471	ASN
1	A	473	ASN
1	B	276	HIS
1	B	307	HIS
1	B	341	HIS

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 ⓘ

12 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	C	1	1,2	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	C	2	2	14,14,15	0.30	0	17,19,21	0.71	1 (5%)
2	BMA	C	3	2	11,11,12	0.64	0	15,15,17	0.97	0
2	MAN	C	4	2	11,11,12	0.73	0	15,15,17	0.95	2 (13%)
3	NAG	D	1	1,3	14,14,15	0.61	1 (7%)	17,19,21	0.45	0
3	FUC	D	2	3	10,10,11	0.59	0	14,14,16	0.82	0
4	NAG	E	1	1,4	14,14,15	0.49	0	17,19,21	0.55	0
4	NAG	E	2	4	14,14,15	0.44	0	17,19,21	0.41	0
4	BMA	E	3	4	11,11,12	0.64	0	15,15,17	0.75	0
5	NAG	F	1	1,5	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	F	2	5	14,14,15	0.23	0	17,19,21	0.41	0
5	FUC	F	3	5	10,10,11	0.65	0	14,14,16	0.76	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	1/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	FUC	F	3	5	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	NAG	C1-C2	2.09	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	2.44	115.46	112.19
2	C	4	MAN	C1-O5-C5	2.28	115.24	112.19
2	C	4	MAN	O2-C2-C3	-2.11	105.78	110.15

There are no chirality outliers.

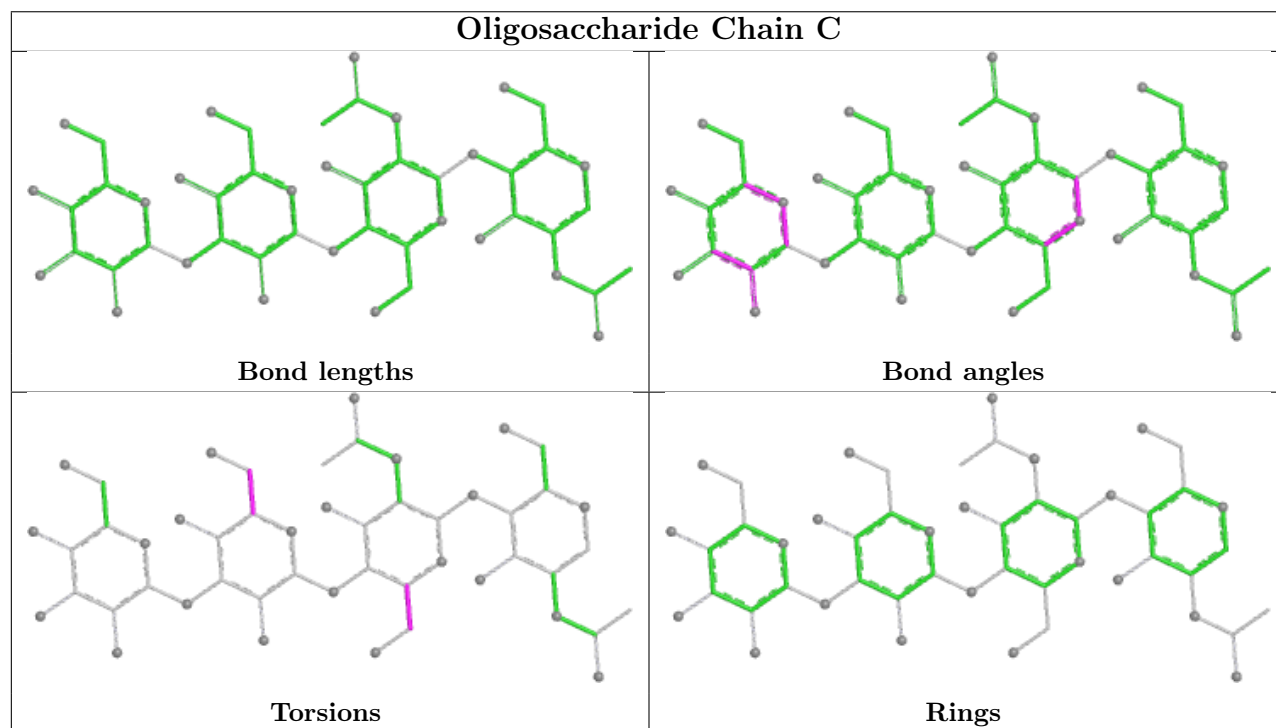
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	3	BMA	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6

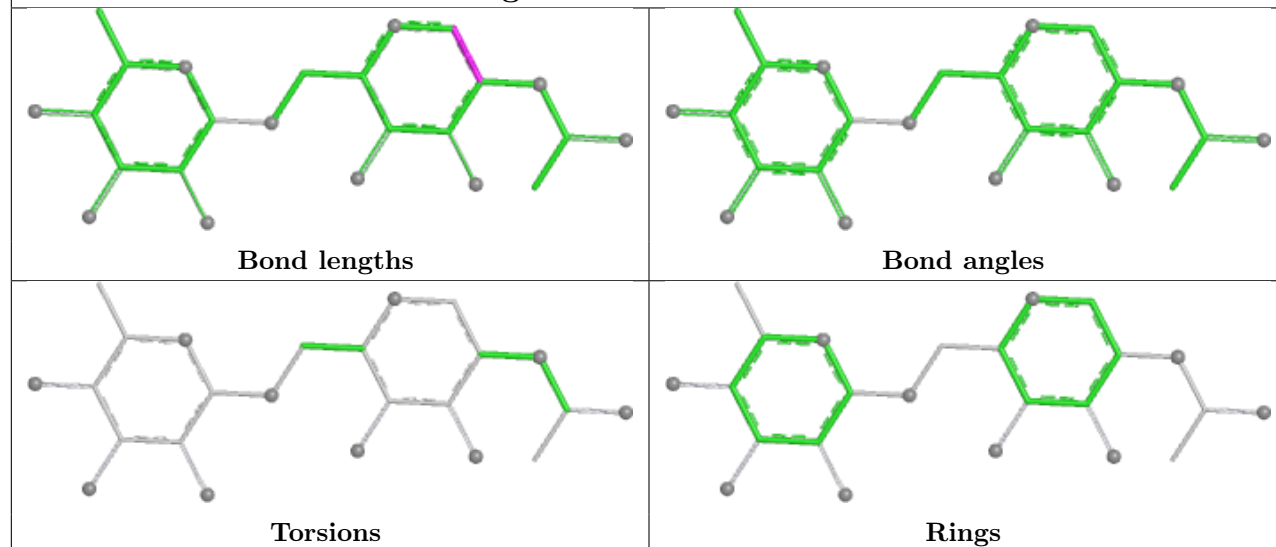
There are no ring outliers.

No monomer is involved in short contacts.

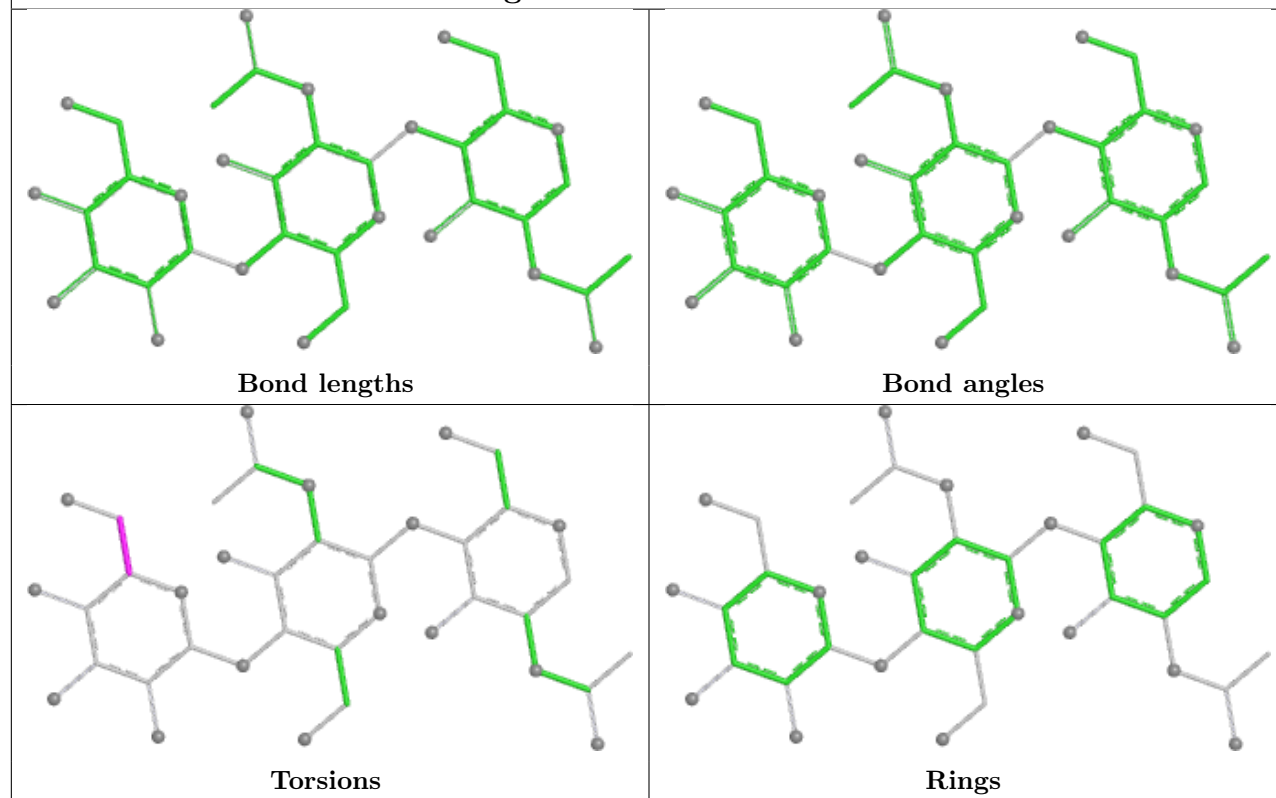
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

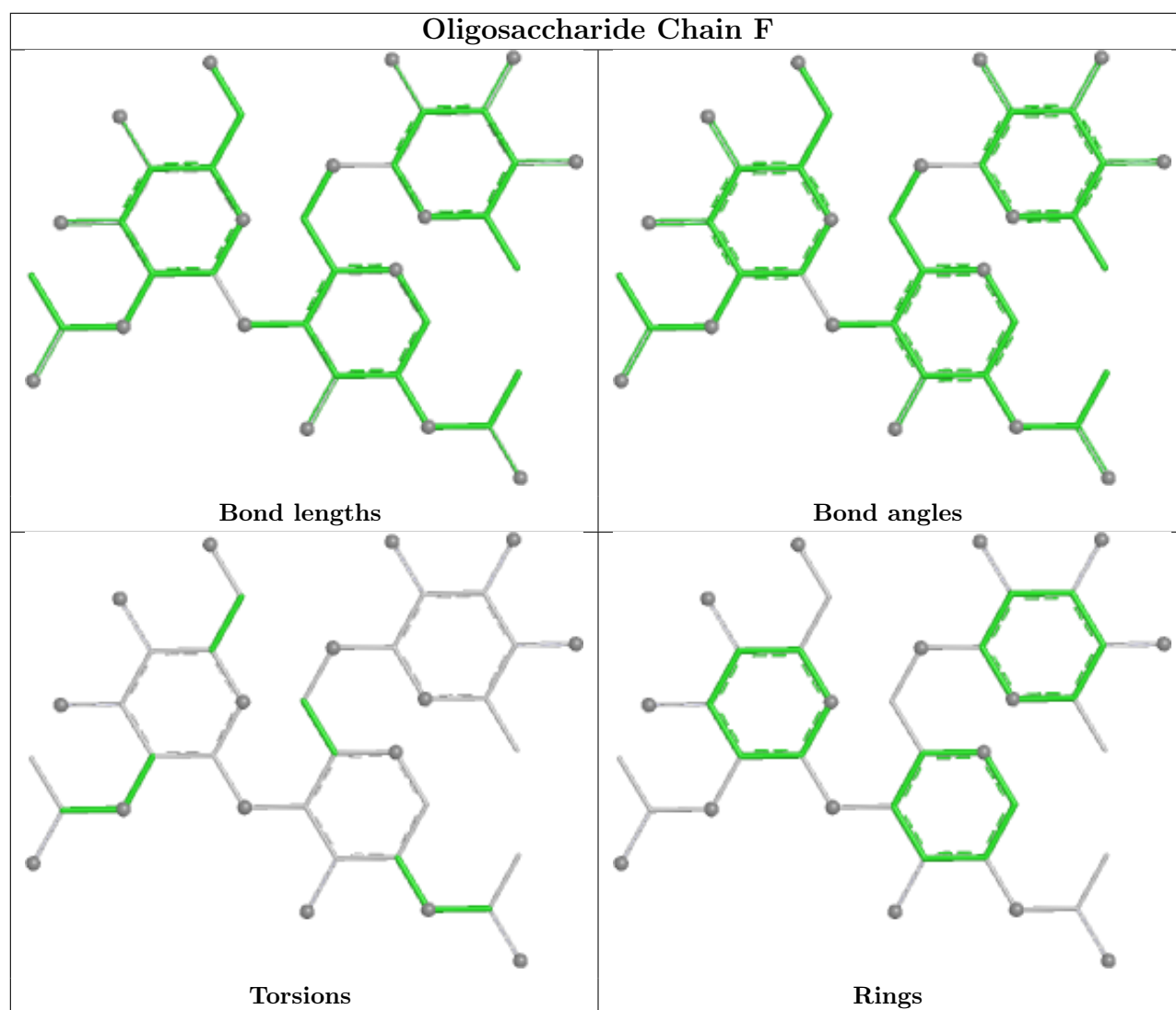


Oligosaccharide Chain D



Oligosaccharide Chain E





5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - 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	$\# Z > 2$
6	NAG	B	601	1	14,14,15	0.27	0	17,19,21	0.33	0
6	NAG	A	602	1	14,14,15	0.41	0	17,19,21	0.41	0
6	NAG	A	603	1	14,14,15	0.43	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	602	1	14,14,15	0.38	0	17,19,21	0.40	0
6	NAG	A	601	1	14,14,15	0.91	1 (7%)	17,19,21	0.62	1 (5%)

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
6	NAG	B	601	1	-	0/6/23/26	0/1/1/1
6	NAG	A	602	1	-	2/6/23/26	0/1/1/1
6	NAG	A	603	1	-	4/6/23/26	0/1/1/1
6	NAG	B	602	1	-	0/6/23/26	0/1/1/1
6	NAG	A	601	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)
6	A	601	NAG	O5-C1	3.24	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	NAG	C1-O5-C5	2.14	115.06	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	603	NAG	O5-C5-C6-O6
6	A	602	NAG	O5-C5-C6-O6
6	A	603	NAG	C1-C2-N2-C7
6	A	603	NAG	C3-C2-N2-C7
6	A	603	NAG	C4-C5-C6-O6
6	A	602	NAG	C4-C5-C6-O6
6	A	601	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	NAG	2	0
6	A	601	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	422/495 (85%)	-0.02	25 (5%) 28 25	13, 39, 104, 145	0
1	B	446/495 (90%)	0.23	32 (7%) 21 18	19, 50, 99, 137	0
All	All	868/990 (87%)	0.11	57 (6%) 24 21	13, 46, 101, 145	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	PHE	7.6
1	A	393	PRO	7.1
1	B	54	TYR	4.9
1	A	250	THR	4.7
1	B	101	LEU	4.4
1	B	426	LYS	4.2
1	A	506	ARG	4.2
1	A	52	ASP	4.1
1	B	393	PRO	4.1
1	A	55	HIS	4.1
1	A	54	TYR	3.8
1	A	251	PHE	3.7
1	A	476	HIS	3.7
1	A	246	VAL	3.6
1	B	247	PRO	3.5
1	A	58	PHE	3.5
1	B	43	SER	3.5
1	B	387	HIS	3.4
1	A	247	PRO	3.3
1	B	53	GLN	3.1
1	B	42	GLY	3.1
1	A	387	HIS	3.0
1	B	479	LYS	3.0
1	B	523	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	49	TRP	2.9
1	A	53	GLN	2.9
1	B	55	HIS	2.9
1	A	394	THR	2.9
1	B	249	ASP	2.8
1	B	99	THR	2.8
1	B	52	ASP	2.7
1	B	395	GLN	2.7
1	B	98	VAL	2.7
1	B	383	SER	2.6
1	B	427	ASP	2.6
1	A	105	LYS	2.6
1	A	56	VAL	2.5
1	A	426	LYS	2.5
1	A	249	ASP	2.4
1	B	392	SER	2.3
1	A	245	PRO	2.3
1	A	382	PRO	2.3
1	B	524	TYR	2.2
1	A	385	LEU	2.2
1	B	521	TRP	2.2
1	B	51	ARG	2.2
1	B	506	ARG	2.2
1	B	522	ARG	2.2
1	B	384	ASN	2.2
1	A	57	LEU	2.2
1	B	385	LEU	2.2
1	B	482	GLY	2.1
1	B	381	LEU	2.0
1	A	62	ARG	2.0
1	A	306	ARG	2.0
1	B	481	ALA	2.0
1	B	525	ARG	2.0

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

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

6.3 Carbohydrates

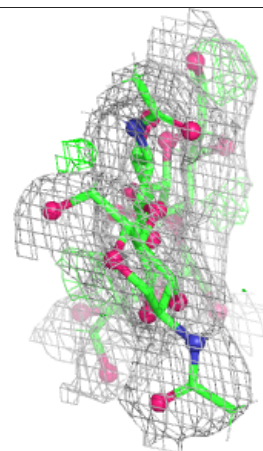
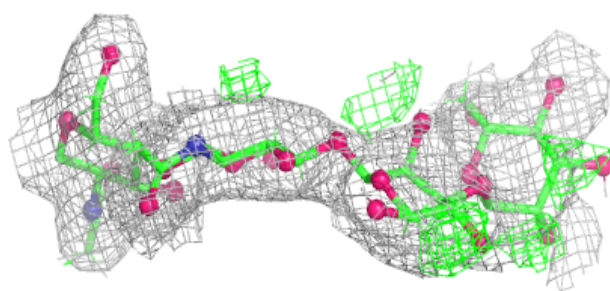
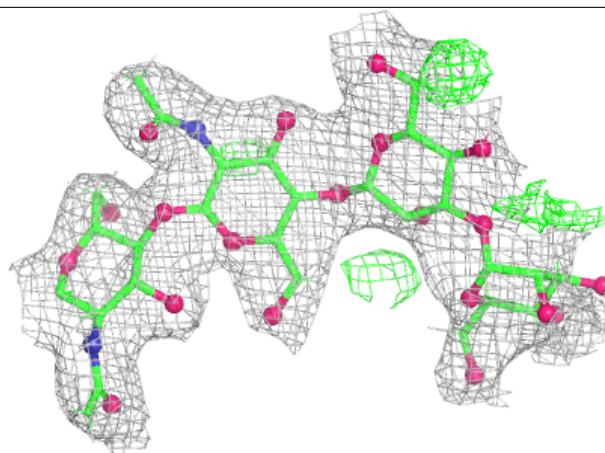
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	F	2	14/15	0.67	0.16	80,107,129,150	0
4	BMA	E	3	11/12	0.71	0.12	69,85,102,107	0
2	BMA	C	3	11/12	0.79	0.14	52,72,90,98	0
5	NAG	F	1	14/15	0.82	0.13	63,93,103,116	0
3	NAG	D	1	14/15	0.82	0.14	51,72,90,93	0
4	NAG	E	2	14/15	0.83	0.12	55,86,100,108	0
5	FUC	F	3	10/11	0.83	0.18	76,91,108,123	0
2	MAN	C	4	11/12	0.84	0.16	54,80,110,113	0
3	FUC	D	2	10/11	0.87	0.17	63,73,82,85	0
2	NAG	C	2	14/15	0.88	0.12	47,57,62,81	0
4	NAG	E	1	14/15	0.89	0.12	37,57,70,74	0
2	NAG	C	1	14/15	0.95	0.09	20,34,50,52	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.

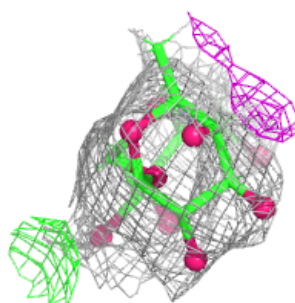
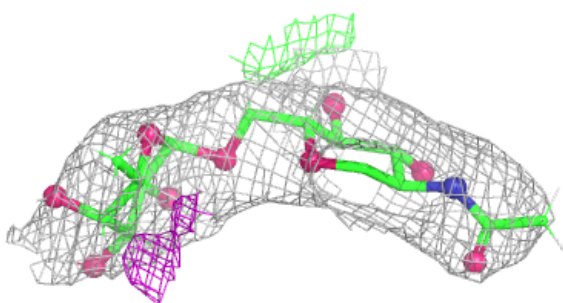
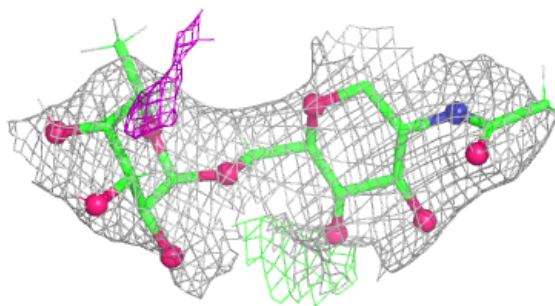
Electron density around Chain C:

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

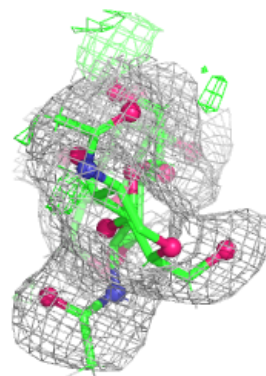
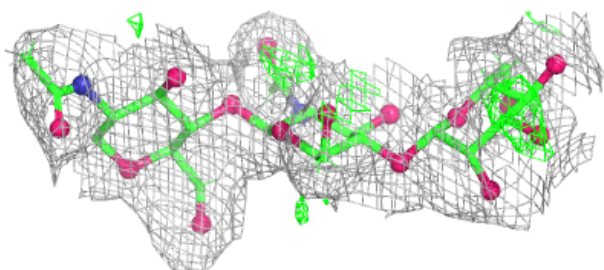
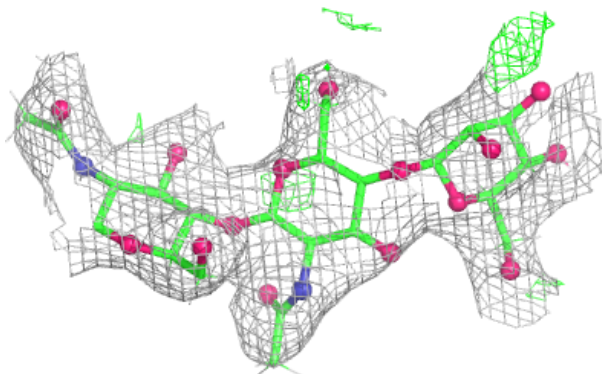


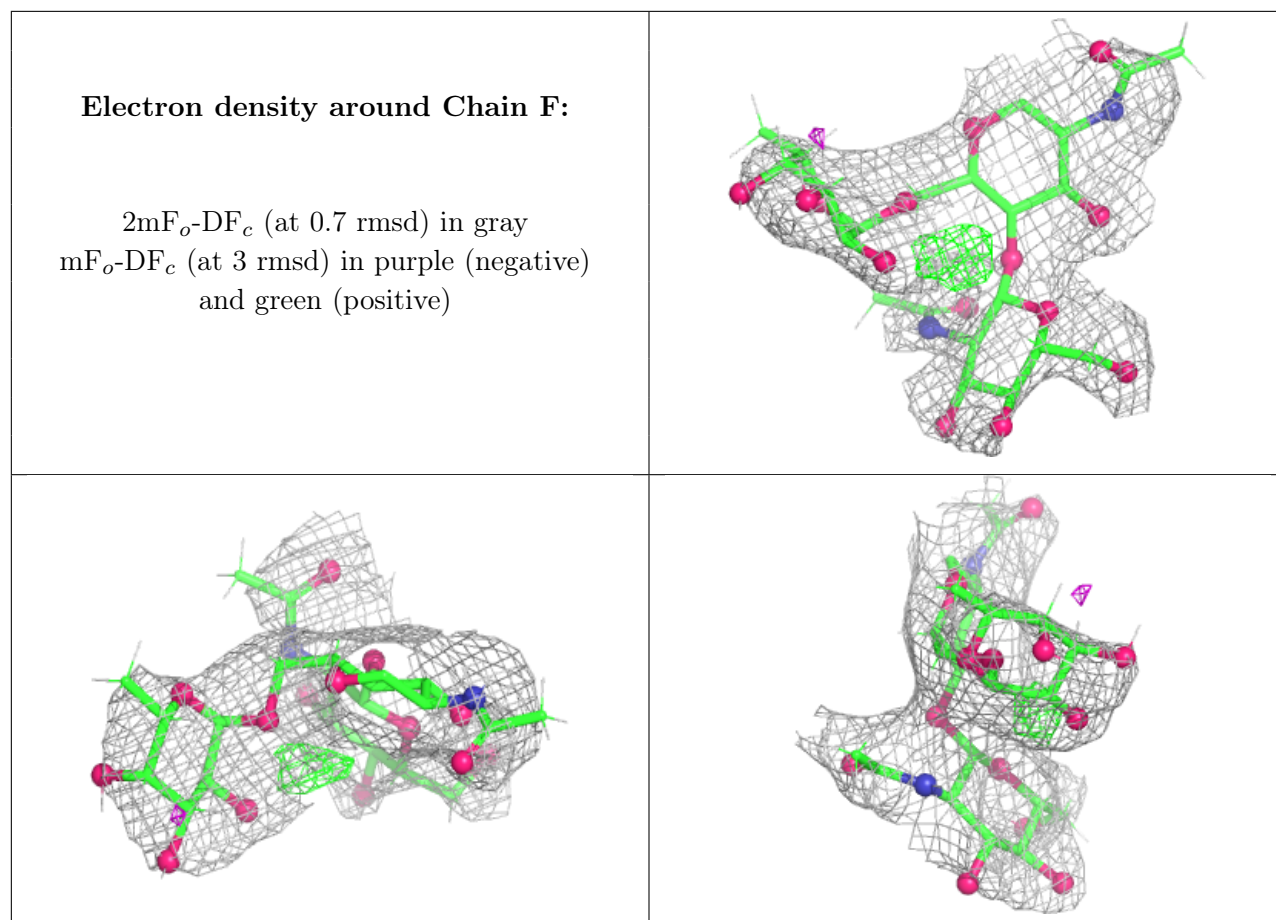
Electron density around Chain D:

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

**Electron density around Chain E:**

$2mF_o-DF_c$ (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
6	NAG	A	603	14/15	0.61	0.19	72,96,119,124	0
6	NAG	B	601	14/15	0.67	0.18	76,95,113,124	0
6	NAG	A	602	14/15	0.70	0.17	67,94,118,119	0
6	NAG	A	601	14/15	0.72	0.17	58,78,108,113	0
6	NAG	B	602	14/15	0.74	0.19	77,103,130,138	0
7	CA	A	604	1/1	0.99	0.03	40,40,40,40	0
7	CA	B	603	1/1	0.99	0.01	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.