Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 02:13 PM EDT

PDB ID	:	6WWX
Title	:	Crystal structure of truncated bacteriophage hyaluronan lyase HylP in complex with unsaturated hyaluronan tetra-saccharides
Authors	:	Deivanayagam, C.; Schormann, N.
Deposited on	:	2020-05-09
Resolution	:	2.20 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:

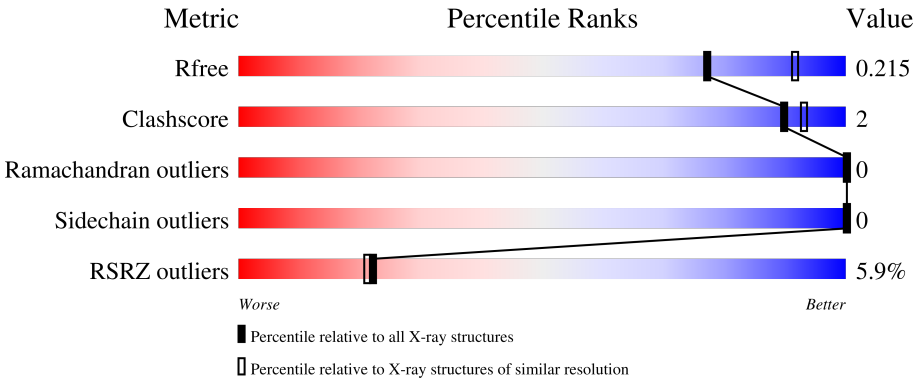
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	293	7%, 90%, 7%
1	B	293	4%, 91%, 8%
1	C	293	5%, 88%, 7%
2	D	4	50%, 25%, 25%
2	E	4	50%, 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	4	50% 50%
2	G	4	100%
2	H	4	100%
2	I	4	75% 25%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6771 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 Hyaluronoglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2044	1266	360	411	7			
1	B	271	Total	C	N	O	S	0	0	0
			2028	1257	358	406	7			
1	C	272	Total	C	N	O	S	0	0	0
			2030	1258	357	408	7			

There are 24 discrepancies between the modelled and reference sequences:

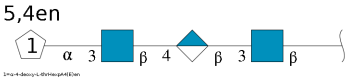
Chain	Residue	Modelled	Actual	Comment	Reference
A	372	LEU	-	expression tag	UNP P15316
A	373	GLU	-	expression tag	UNP P15316
A	374	HIS	-	expression tag	UNP P15316
A	375	HIS	-	expression tag	UNP P15316
A	376	HIS	-	expression tag	UNP P15316
A	377	HIS	-	expression tag	UNP P15316
A	378	HIS	-	expression tag	UNP P15316
A	379	HIS	-	expression tag	UNP P15316
B	372	LEU	-	expression tag	UNP P15316
B	373	GLU	-	expression tag	UNP P15316
B	374	HIS	-	expression tag	UNP P15316
B	375	HIS	-	expression tag	UNP P15316
B	376	HIS	-	expression tag	UNP P15316
B	377	HIS	-	expression tag	UNP P15316
B	378	HIS	-	expression tag	UNP P15316
B	379	HIS	-	expression tag	UNP P15316
C	372	LEU	-	expression tag	UNP P15316
C	373	GLU	-	expression tag	UNP P15316
C	374	HIS	-	expression tag	UNP P15316
C	375	HIS	-	expression tag	UNP P15316
C	376	HIS	-	expression tag	UNP P15316
C	377	HIS	-	expression tag	UNP P15316
C	378	HIS	-	expression tag	UNP P15316

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	379	HIS	-	expression tag	UNP P15316

- Molecule 2 is an oligosaccharide called 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	E	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	F	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	G	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	H	4	Total	C	N	O	0	0	0
			52	28	2	22			
2	I	4	Total	C	N	O	0	0	0
			52	28	2	22			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ni	0	0
			1	1		

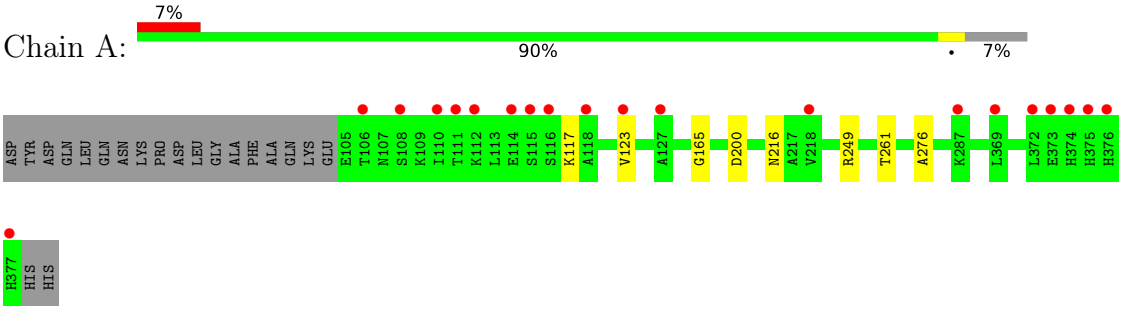
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	111	Total	O	0	0
			111	111		
4	C	122	Total	O	0	0
			122	122		

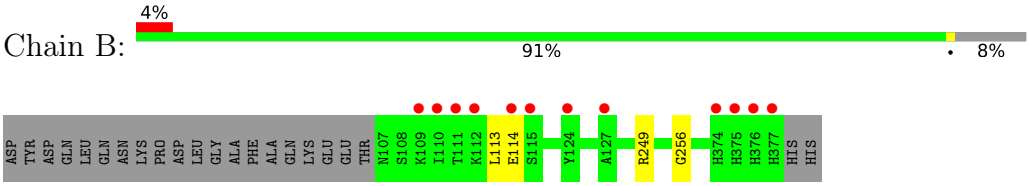
3 Residue-property plots (i)

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.

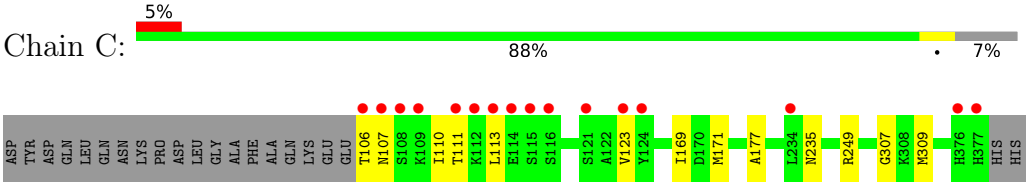
• Molecule 1: Hyaluronoglucosaminidase



• Molecule 1: Hyaluronoglucosaminidase



• Molecule 1: Hyaluronoglucosaminidase



• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

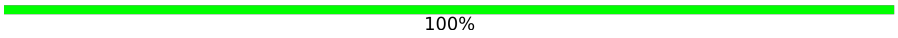
Chain E:

• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

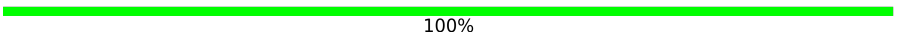
• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 2: 4-deoxy-alpha-L-threo-hex-4-enopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-glucopyranuronic acid-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.53Å 86.82Å 168.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.68 – 2.20 37.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.68-2.20) 99.6 (37.93-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.182 , 0.210 0.190 , 0.215	Depositor DCC
R_{free} test set	2595 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6771	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BDP, GCD, NAG, NI

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	0.46	0/2071	0.68	2/2781 (0.1%)
1	B	0.46	0/2055	0.69	2/2759 (0.1%)
1	C	0.47	0/2056	0.69	1/2761 (0.0%)
All	All	0.46	0/6182	0.69	5/8301 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	249	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	249	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	249	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	249	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	200	ASP	CB-CG-OD2	5.30	123.07	118.30

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	2044	0	2071	8	0
1	B	2028	0	2058	4	0
1	C	2030	0	2060	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	52	0	37	6	0
2	E	52	0	37	0	0
2	F	52	0	37	0	0
2	G	52	0	37	0	0
2	H	52	0	37	0	0
2	I	52	0	37	0	0
3	B	1	0	0	0	0
4	A	123	0	0	0	0
4	B	111	0	0	0	0
4	C	122	0	0	0	0
All	All	6771	0	6411	23	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 2.

All (23) 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:261:THR:OG1	2:D:1:NAG:H81	1.53	1.08
1:B:113:LEU:HD23	1:C:113:LEU:HD23	1.59	0.83
1:C:107:ASN:HA	1:C:110:ILE:CG2	2.17	0.75
1:A:261:THR:OG1	2:D:1:NAG:C8	2.35	0.69
1:C:169:ILE:HG22	1:C:171:MET:HE3	1.76	0.67
1:A:261:THR:CB	2:D:1:NAG:H81	2.25	0.67
1:A:216:ASN:HD22	2:D:3:NAG:H81	1.61	0.65
1:C:107:ASN:HA	1:C:110:ILE:HG22	1.79	0.64
1:C:110:ILE:HG23	1:C:111:THR:H	1.72	0.55
1:A:117:LYS:HE2	1:B:114:GLU:HA	1.88	0.55
1:C:307:GLY:O	1:C:309:MET:CE	2.58	0.51
1:A:123:VAL:HG11	1:C:123:VAL:HG21	1.96	0.47
1:C:169:ILE:HG22	1:C:171:MET:CE	2.42	0.47
1:A:276:ALA:O	1:B:256:GLY:HA2	2.16	0.45
1:C:235:ASN:HD22	2:D:3:NAG:H83	1.83	0.44
1:A:165:GLY:HA2	1:C:177:ALA:O	2.17	0.44
1:C:110:ILE:HG23	1:C:111:THR:N	2.31	0.44
1:C:235:ASN:ND2	2:D:3:NAG:H83	2.32	0.43
1:B:113:LEU:CD2	1:C:113:LEU:HD23	2.41	0.43
1:C:107:ASN:CA	1:C:110:ILE:HG22	2.49	0.43
1:C:107:ASN:O	1:C:110:ILE:HG23	2.19	0.42
1:C:107:ASN:HA	1:C:110:ILE:HG21	1.99	0.42
1:C:106:THR:O	1:C:110:ILE:HG22	2.19	0.42

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	271/293 (92%)	267 (98%)	4 (2%)	0	100	100
1	B	269/293 (92%)	264 (98%)	5 (2%)	0	100	100
1	C	270/293 (92%)	266 (98%)	4 (2%)	0	100	100
All	All	810/879 (92%)	797 (98%)	13 (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	223/240 (93%)	223 (100%)	0	100	100
1	B	221/240 (92%)	221 (100%)	0	100	100
1	C	221/240 (92%)	221 (100%)	0	100	100
All	All	665/720 (92%)	665 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

24 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	D	1	2	15,15,15	0.23	0	21,21,21	0.43	0
2	BDP	D	2	2	12,12,13	0.25	0	14,17,19	0.36	0
2	NAG	D	3	2	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
2	GCD	D	4	2	10,11,12	0.19	0	13,15,17	0.36	0
2	NAG	E	1	2	15,15,15	0.21	0	21,21,21	0.91	1 (4%)
2	BDP	E	2	2	12,12,13	1.18	2 (16%)	14,17,19	0.95	1 (7%)
2	NAG	E	3	2	14,14,15	0.23	0	17,19,21	0.86	0
2	GCD	E	4	2	10,11,12	0.29	0	13,15,17	0.59	0
2	NAG	F	1	2	15,15,15	0.19	0	21,21,21	0.53	0
2	BDP	F	2	2	12,12,13	1.18	2 (16%)	14,17,19	1.01	2 (14%)
2	NAG	F	3	2	14,14,15	0.22	0	17,19,21	0.60	0
2	GCD	F	4	2	10,11,12	0.34	0	13,15,17	1.98	2 (15%)
2	NAG	G	1	2	15,15,15	0.13	0	21,21,21	0.38	0
2	BDP	G	2	2	12,12,13	0.30	0	14,17,19	0.53	0
2	NAG	G	3	2	14,14,15	0.25	0	17,19,21	0.53	0
2	GCD	G	4	2	10,11,12	0.26	0	13,15,17	0.42	0
2	NAG	H	1	2	15,15,15	0.16	0	21,21,21	0.54	0
2	BDP	H	2	2	12,12,13	0.26	0	14,17,19	0.43	0
2	NAG	H	3	2	14,14,15	0.24	0	17,19,21	0.53	0
2	GCD	H	4	2	10,11,12	0.24	0	13,15,17	0.42	0
2	NAG	I	1	2	15,15,15	0.14	0	21,21,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BDP	I	2	2	12,12,13	0.21	0	14,17,19	0.33	0
2	NAG	I	3	2	14,14,15	0.23	0	17,19,21	0.70	0
2	GCD	I	4	2	10,11,12	1.23	2 (20%)	13,15,17	2.62	3 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2	-	3/6/26/26	0/1/1/1
2	BDP	D	2	2	-	0/4/21/24	0/1/1/1
2	NAG	D	3	2	-	2/6/23/26	0/1/1/1
2	GCD	D	4	2	-	0/4/17/20	0/1/1/1
2	NAG	E	1	2	-	1/6/26/26	0/1/1/1
2	BDP	E	2	2	-	0/4/21/24	0/1/1/1
2	NAG	E	3	2	-	0/6/23/26	0/1/1/1
2	GCD	E	4	2	-	0/4/17/20	0/1/1/1
2	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	BDP	F	2	2	-	0/4/21/24	0/1/1/1
2	NAG	F	3	2	-	0/6/23/26	0/1/1/1
2	GCD	F	4	2	-	0/4/17/20	0/1/1/1
2	NAG	G	1	2	-	0/6/26/26	0/1/1/1
2	BDP	G	2	2	-	3/4/21/24	0/1/1/1
2	NAG	G	3	2	-	0/6/23/26	0/1/1/1
2	GCD	G	4	2	-	0/4/17/20	0/1/1/1
2	NAG	H	1	2	-	0/6/26/26	0/1/1/1
2	BDP	H	2	2	-	0/4/21/24	0/1/1/1
2	NAG	H	3	2	-	0/6/23/26	0/1/1/1
2	GCD	H	4	2	-	0/4/17/20	0/1/1/1
2	NAG	I	1	2	-	0/6/26/26	0/1/1/1
2	BDP	I	2	2	-	0/4/21/24	0/1/1/1
2	NAG	I	3	2	-	0/6/23/26	0/1/1/1
2	GCD	I	4	2	-	0/4/17/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	BDP	O6A-C6	3.06	1.31	1.22
2	F	2	BDP	O6A-C6	2.96	1.31	1.22
2	I	4	GCD	O6A-C6	2.70	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	BDP	O6B-C6	-2.68	1.21	1.30
2	I	4	GCD	O6B-C6	-2.67	1.22	1.30
2	E	2	BDP	O6B-C6	-2.55	1.22	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	4	GCD	C2-C3-C4	-7.39	102.22	112.32
2	F	4	GCD	C2-C3-C4	-6.16	103.90	112.32
2	I	4	GCD	O6B-C6-C5	3.00	121.68	114.20
2	I	4	GCD	C3-C4-C5	-2.85	116.79	121.60
2	D	3	NAG	C2-N2-C7	2.78	126.87	122.90
2	F	2	BDP	O6B-C6-C5	2.61	123.22	113.65
2	F	2	BDP	O6A-C6-C5	-2.36	112.15	120.81
2	E	2	BDP	O6B-C6-C5	2.27	121.97	113.65
2	E	1	NAG	O5-C5-C4	2.08	113.46	109.69
2	F	4	GCD	C3-C4-C5	-2.06	118.12	121.60

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	3	NAG	C8-C7-N2-C2
2	D	3	NAG	O7-C7-N2-C2
2	E	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	G	2	BDP	O5-C5-C6-O6A
2	G	2	BDP	O5-C5-C6-O6B
2	G	2	BDP	C4-C5-C6-O6B

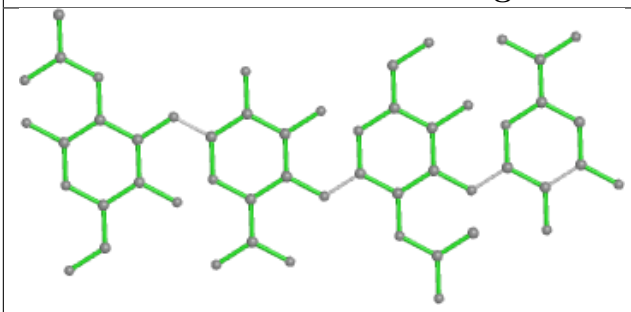
There are no ring outliers.

2 monomers are involved in 6 short contacts:

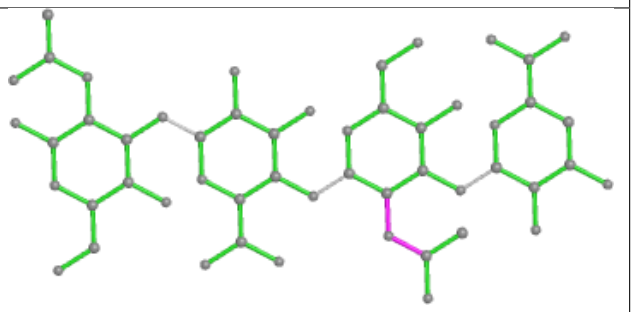
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	3	0
2	D	3	NAG	3	0

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

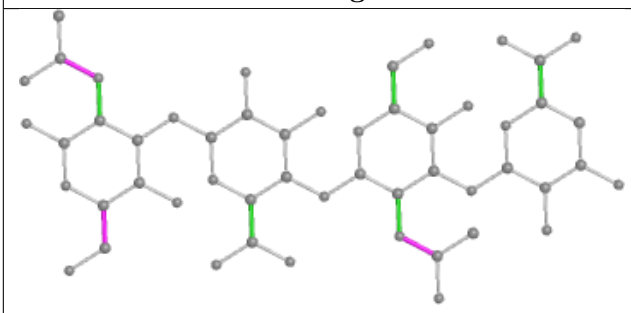
Oligosaccharide Chain D



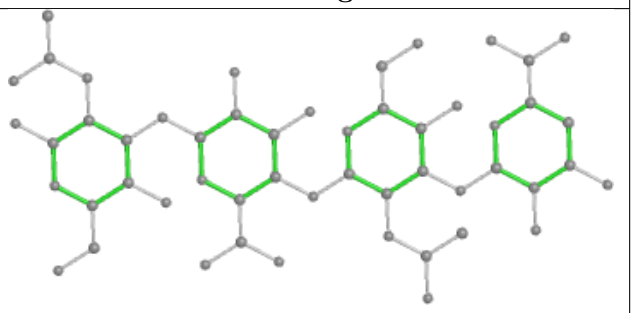
Bond lengths



Bond angles

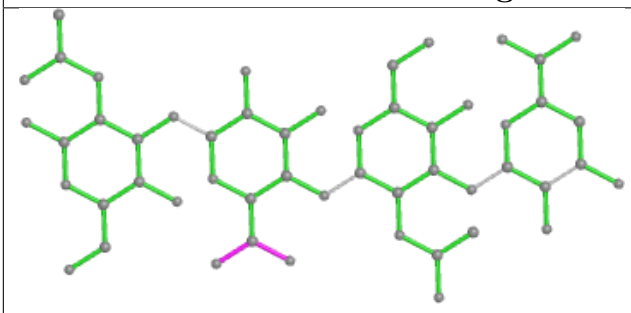


Torsions

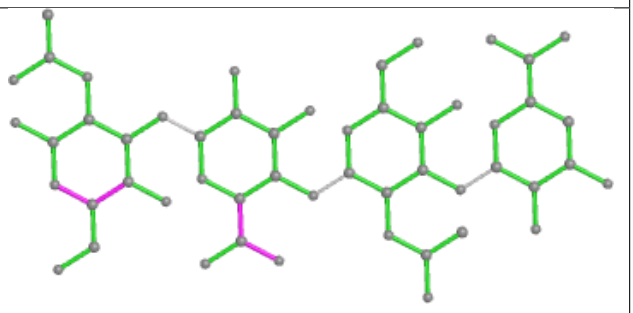


Rings

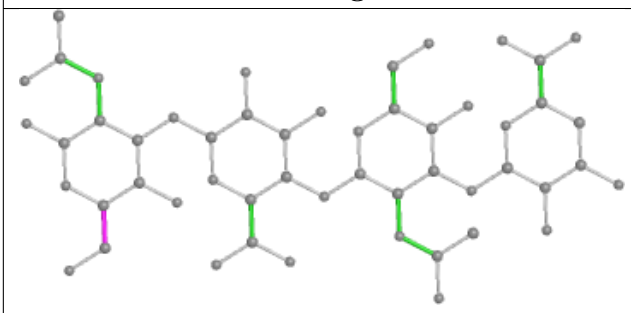
Oligosaccharide Chain E



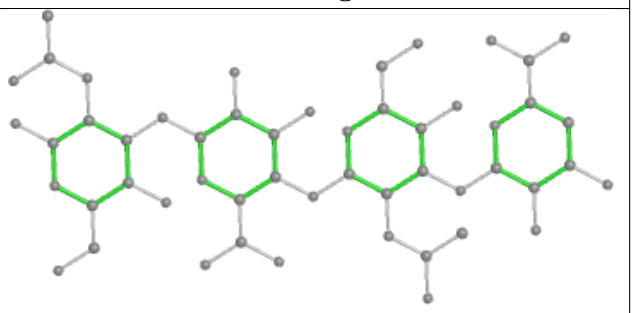
Bond lengths



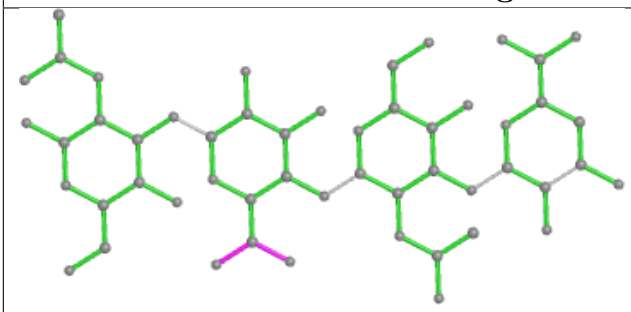
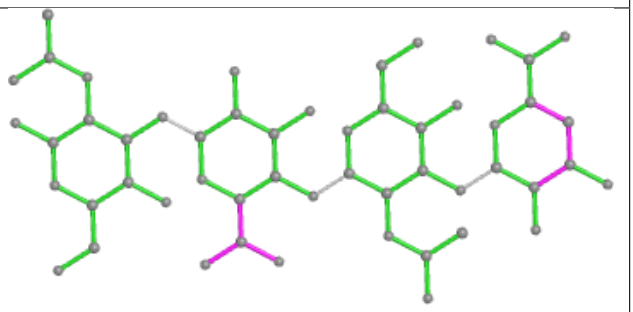
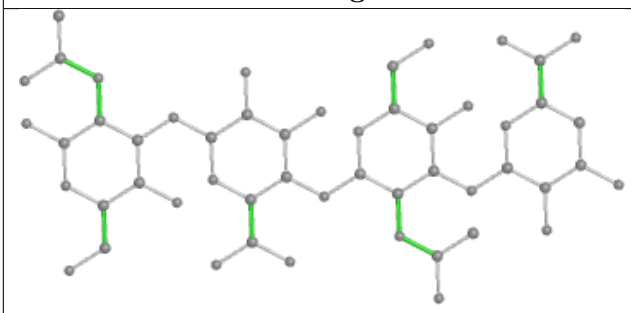
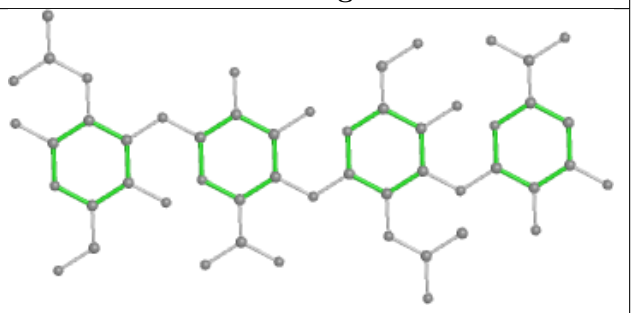
Bond angles

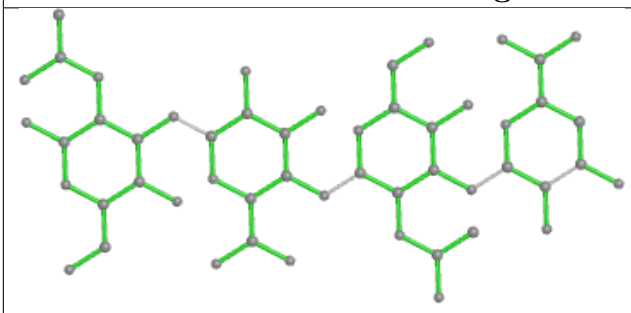
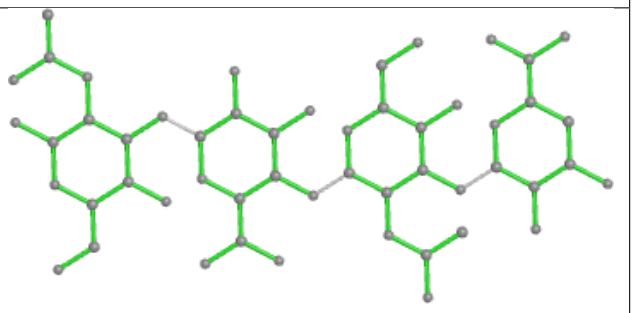
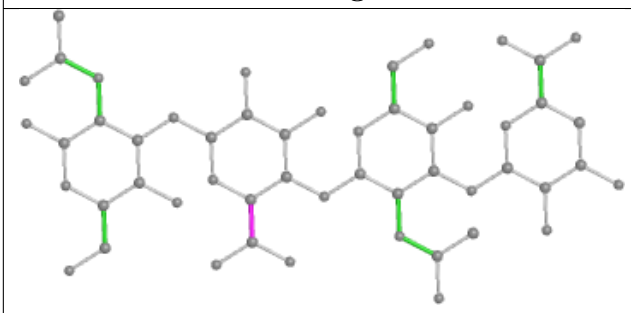
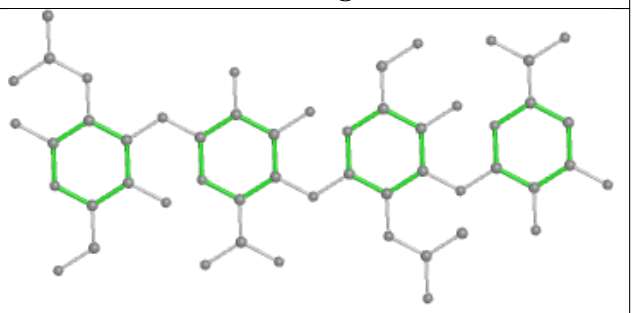


Torsions

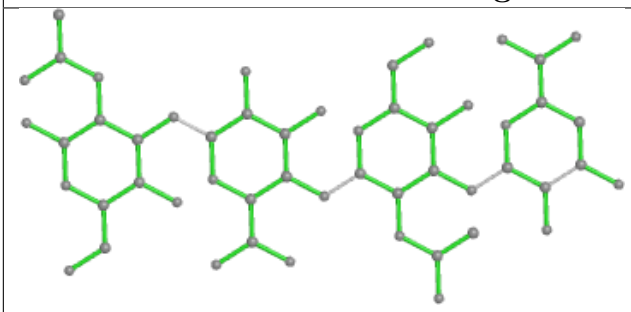


Rings

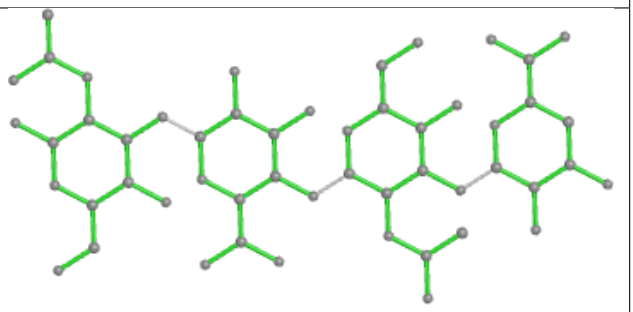
Oligosaccharide Chain F	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

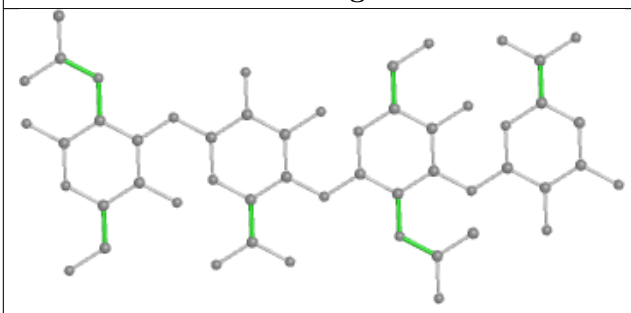
Oligosaccharide Chain H



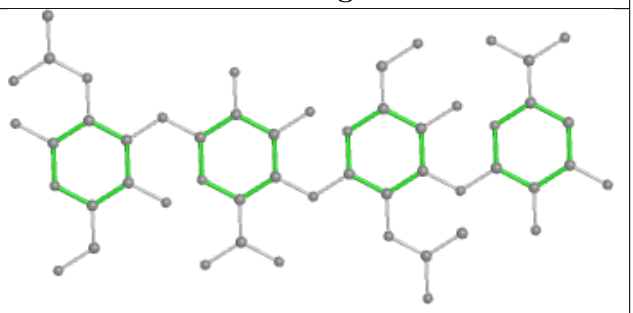
Bond lengths



Bond angles

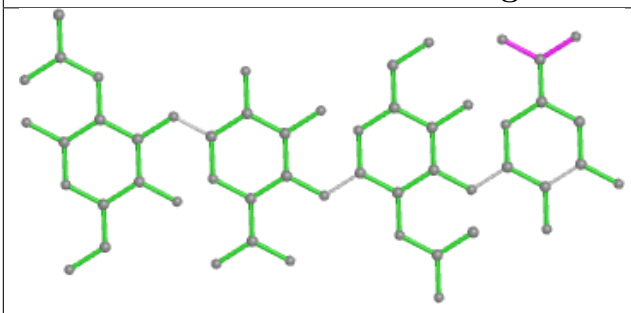


Torsions

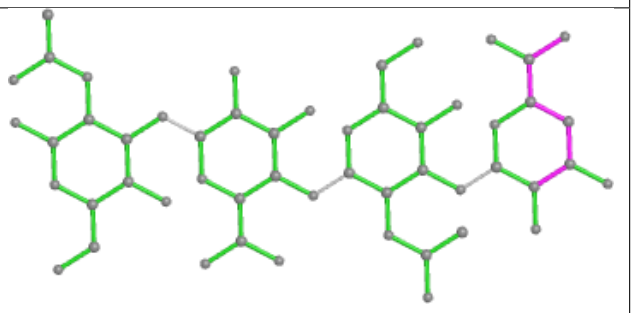


Rings

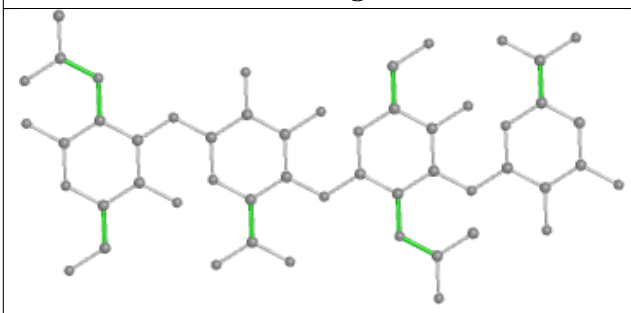
Oligosaccharide Chain I



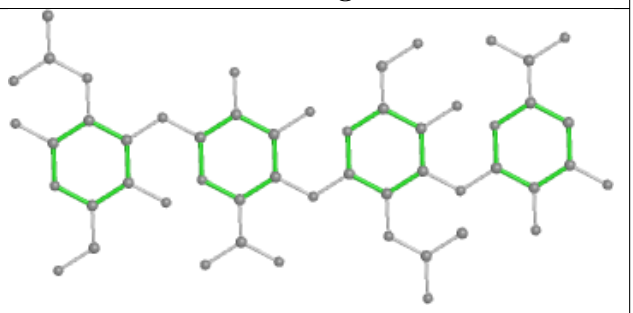
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	273/293 (93%)	0.02	20 (7%)	15	14	25, 39, 80, 105	0
1	B	271/293 (92%)	-0.02	12 (4%)	34	32	25, 38, 80, 112	0
1	C	272/293 (92%)	-0.01	16 (5%)	22	21	25, 39, 84, 109	0
All	All	816/879 (92%)	-0.00	48 (5%)	22	21	25, 38, 84, 112	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	377	HIS	6.7
1	A	376	HIS	6.3
1	C	376	HIS	5.5
1	B	110	ILE	4.7
1	B	377	HIS	4.6
1	A	372	LEU	4.6
1	B	376	HIS	4.5
1	C	111	THR	4.4
1	B	112	LYS	4.4
1	C	106	THR	4.2
1	C	113	LEU	3.7
1	C	109	LYS	3.7
1	A	112	LYS	3.4
1	B	111	THR	3.3
1	B	124	TYR	3.3
1	C	107	ASN	3.2
1	B	374	HIS	3.1
1	A	374	HIS	3.1
1	A	115	SER	3.1
1	C	115	SER	3.0
1	C	116	SER	2.9
1	A	375	HIS	2.9
1	C	123	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	127	ALA	2.8
1	A	123	VAL	2.7
1	A	106	THR	2.7
1	A	116	SER	2.7
1	C	108	SER	2.7
1	C	114	GLU	2.6
1	B	115	SER	2.6
1	B	375	HIS	2.6
1	A	287	LYS	2.6
1	A	369	LEU	2.5
1	A	108	SER	2.5
1	B	114	GLU	2.5
1	A	118	ALA	2.4
1	A	377	HIS	2.4
1	A	110	ILE	2.3
1	C	121	SER	2.2
1	B	109	LYS	2.2
1	C	112	LYS	2.2
1	A	114	GLU	2.2
1	A	373	GLU	2.2
1	A	111	THR	2.2
1	A	218	VAL	2.2
1	C	124	TYR	2.2
1	A	127	ALA	2.1
1	C	234	LEU	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GCD	I	4	11/12	0.81	0.23	51,58,64,64	0
2	GCD	D	4	11/12	0.82	0.19	59,65,66,69	0
2	BDP	E	2	12/13	0.83	0.17	56,63,65,65	0

Continued on next page...

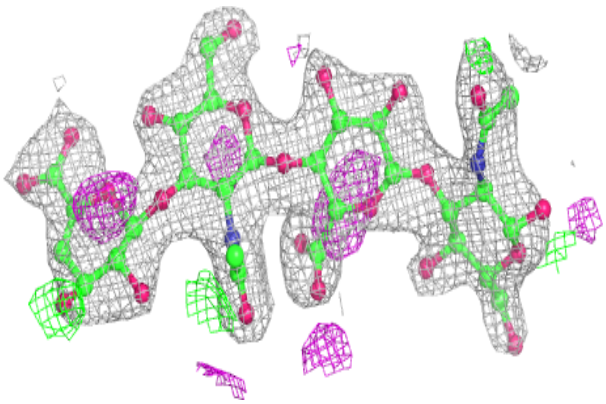
Continued from previous page...

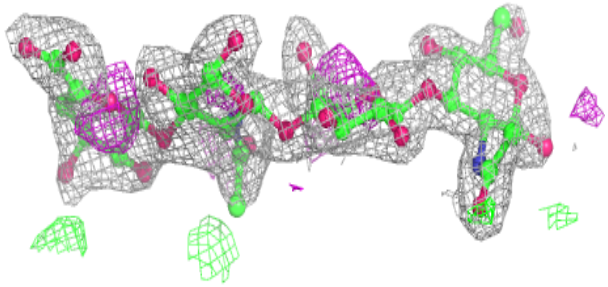
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GCD	F	4	11/12	0.84	0.25	57,64,68,69	0
2	NAG	G	1	15/15	0.85	0.19	52,56,63,66	0
2	BDP	D	2	12/13	0.86	0.16	50,55,56,56	0
2	NAG	D	1	15/15	0.86	0.18	57,63,67,69	0
2	GCD	E	4	11/12	0.88	0.20	69,75,76,77	0
2	NAG	E	1	15/15	0.89	0.15	68,71,77,78	0
2	NAG	D	3	14/15	0.89	0.13	47,53,54,57	0
2	GCD	G	4	11/12	0.91	0.14	51,52,54,56	0
2	NAG	I	1	15/15	0.91	0.12	44,51,55,63	0
2	NAG	E	3	14/15	0.91	0.13	44,56,61,61	0
2	BDP	G	2	12/13	0.92	0.17	45,50,53,54	0
2	NAG	F	1	15/15	0.92	0.12	45,50,52,56	0
2	BDP	F	2	12/13	0.93	0.09	40,43,44,45	0
2	NAG	H	1	15/15	0.93	0.11	41,43,48,53	0
2	BDP	H	2	12/13	0.94	0.11	37,40,43,43	0
2	GCD	H	4	11/12	0.94	0.10	41,41,45,46	0
2	NAG	F	3	14/15	0.94	0.11	31,41,46,48	0
2	NAG	G	3	14/15	0.94	0.16	43,44,46,48	0
2	NAG	I	3	14/15	0.95	0.11	31,38,45,46	0
2	NAG	H	3	14/15	0.95	0.10	35,37,37,39	0
2	BDP	I	2	12/13	0.96	0.08	39,41,43,44	0

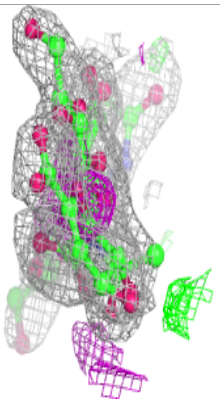
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

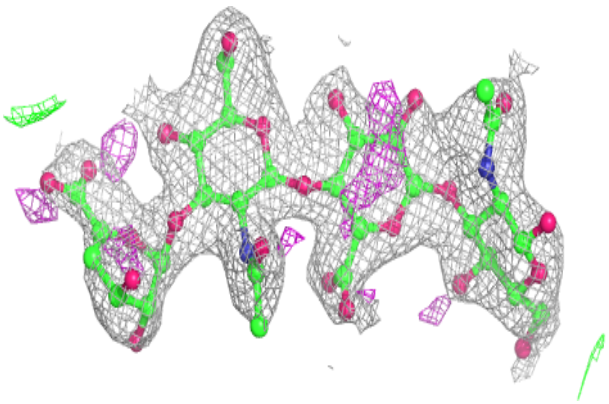


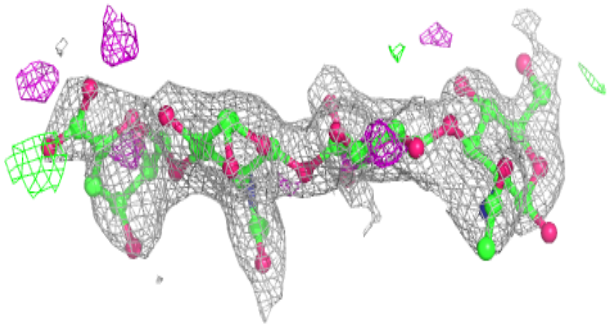


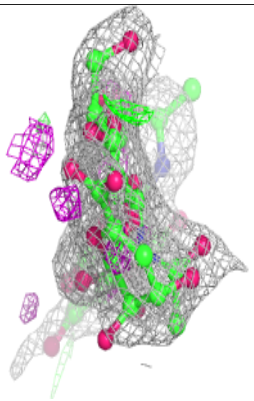


Electron density around Chain E:

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

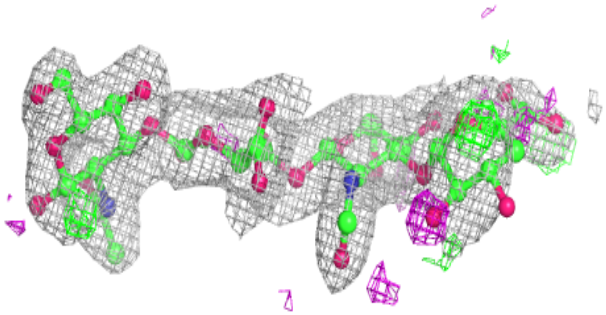


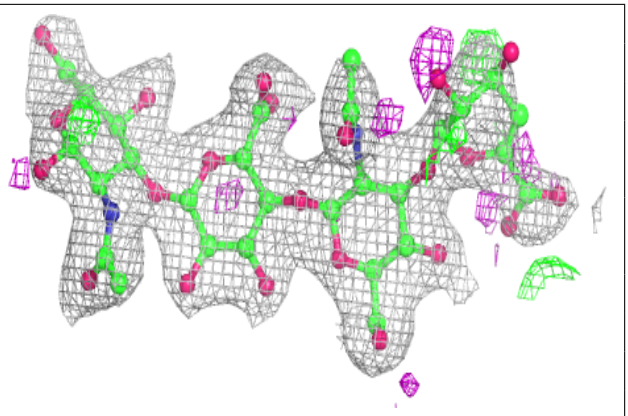


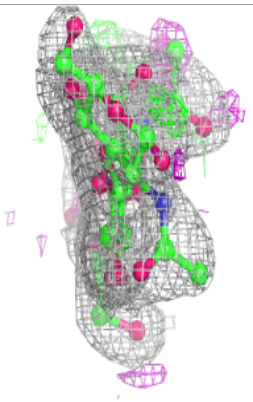


Electron density around Chain F:

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

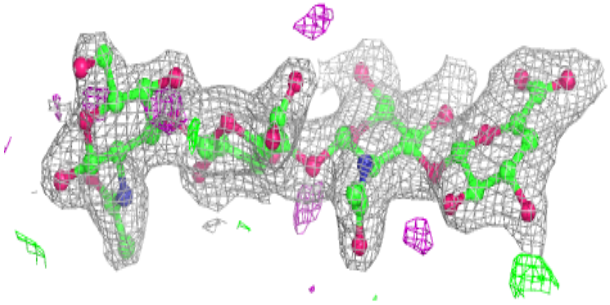


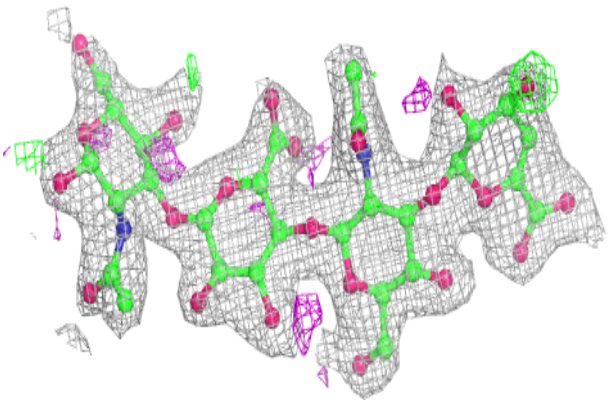


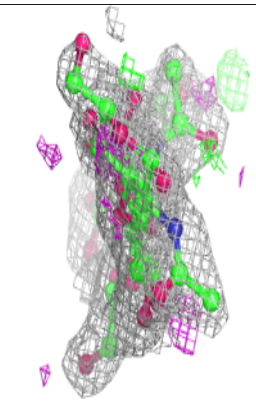


Electron density around Chain G:

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

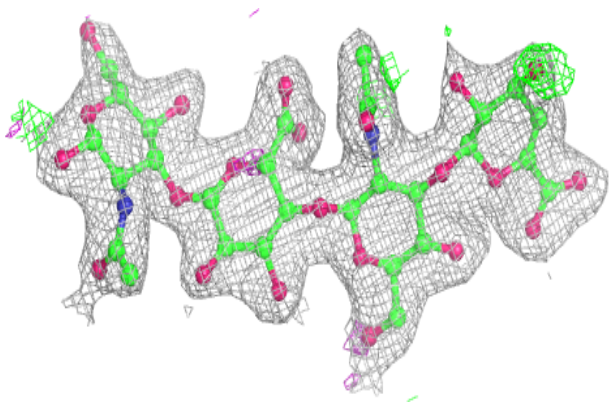


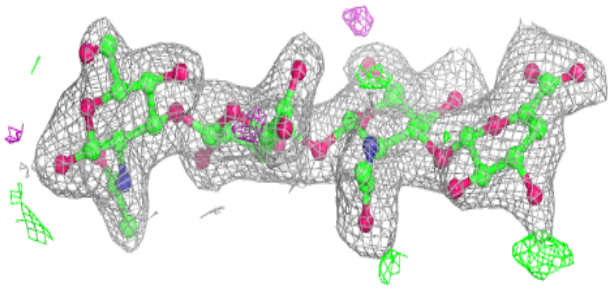


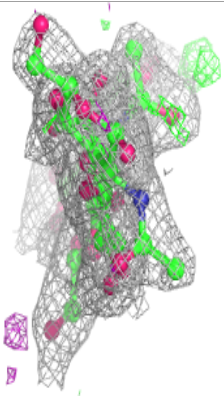


Electron density around Chain H:

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

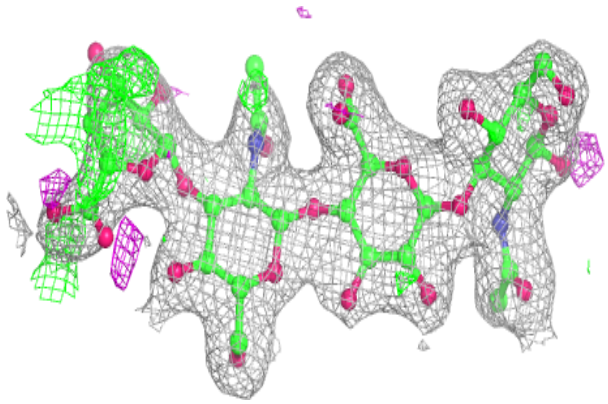


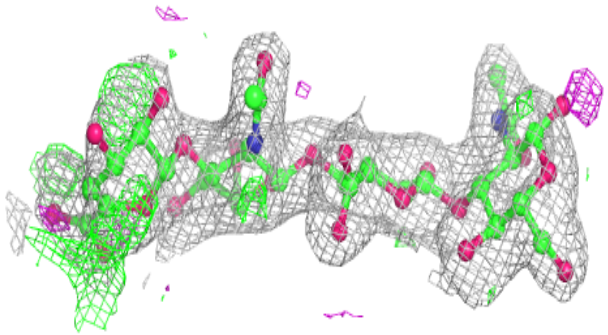


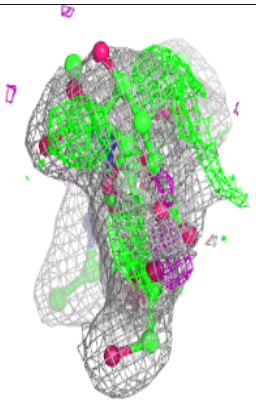


Electron density around Chain I:

$2mF_o$-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)

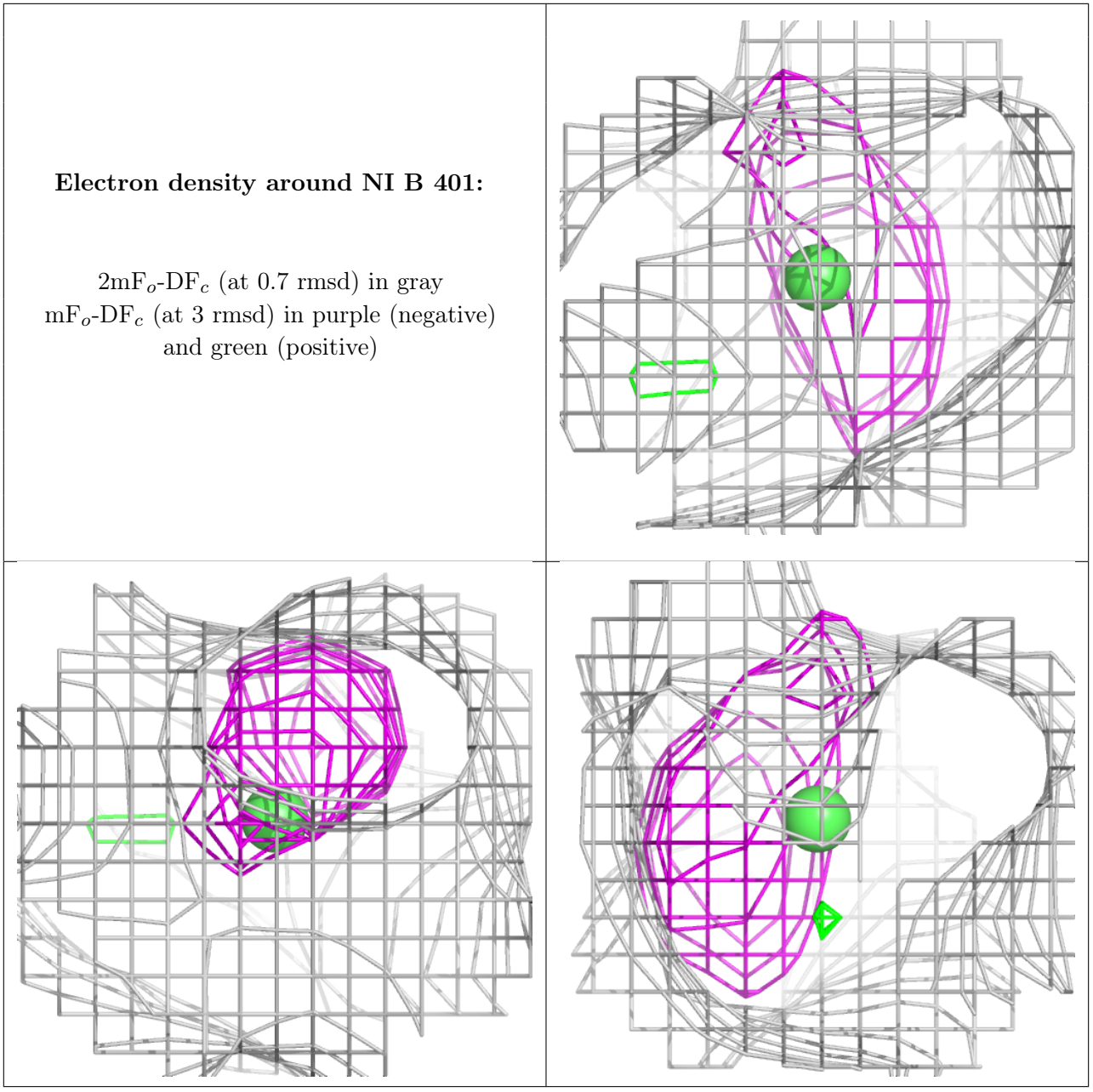
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NI	B	401	1/1	0.54	0.07	77,77,77,77	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NI B 401:

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



6.5 Other polymers

There are no such residues in this entry.