wwPDB X-ray Structure Validation Summary Report (i)

Oct 11, 2023 – 02:30 AM EDT

PDB ID	:	6WJ1
Title	:	Crystal structure of Fab 54-4H03 bound to H1 influenza hemagglutinin
Authors	:	Wu, N.C.; Wilson, I.A.
Deposited on	:	2020-04-11
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

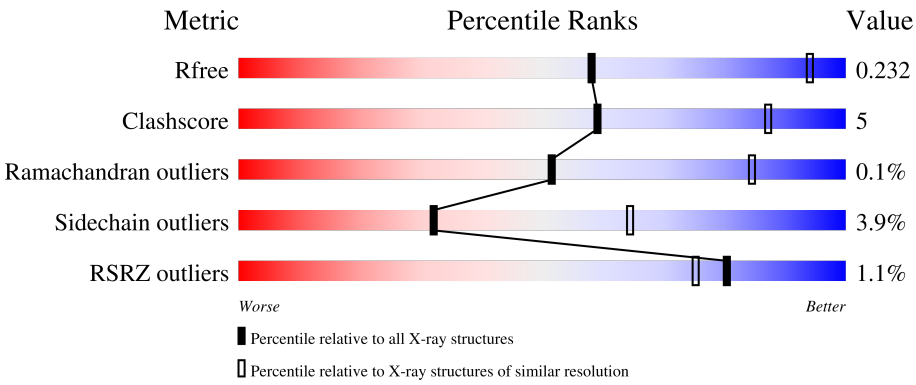
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	330	87% 11% • •
1	C	330	84% 14% •
1	E	330	82% 16% • •
2	B	175	89% 10% •
2	D	175	89% 9% •

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Mol	Chain	Length	Quality of chain
2	F	175	86% 11%
3	G	230	8% 83% 13%
3	H	230	% 80% 18%
3	J	230	% 76% 20%
4	I	216	3% 85% 14%
4	K	216	85% 14%
4	L	216	85% 13%
5	M	2	100%
5	O	2	100%
5	T	2	100%
6	N	5	60% 40%
7	P	4	25% 75%
8	Q	2	100%
9	R	4	50% 50%
10	S	3	100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 22401 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2529	1599	436	483	11	0	0	0
1	C	324	2530	1601	436	482	11	0	0	0
1	E	326	2544	1608	438	487	11	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ASP	-	expression tag	UNP A0A3S7XTA4
A	9	PRO	-	expression tag	UNP A0A3S7XTA4
A	10	GLY	-	expression tag	UNP A0A3S7XTA4
C	8	ASP	-	expression tag	UNP A0A3S7XTA4
C	9	PRO	-	expression tag	UNP A0A3S7XTA4
C	10	GLY	-	expression tag	UNP A0A3S7XTA4
E	8	ASP	-	expression tag	UNP A0A3S7XTA4
E	9	PRO	-	expression tag	UNP A0A3S7XTA4
E	10	GLY	-	expression tag	UNP A0A3S7XTA4

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	175	1406	881	238	281	6	0	0	0
2	D	171	1375	863	234	272	6	0	0	0
2	F	171	1375	863	234	272	6	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	GLY	GLU	conflict	UNP A0A3S5H8L7
B	77	ILE	VAL	conflict	UNP A0A3S5H8L7
B	175	SER	GLY	conflict	UNP A0A3S5H8L7
D	47	GLY	GLU	conflict	UNP A0A3S5H8L7
D	77	ILE	VAL	conflict	UNP A0A3S5H8L7
D	175	SER	GLY	conflict	UNP A0A3S5H8L7
F	47	GLY	GLU	conflict	UNP A0A3S5H8L7
F	77	ILE	VAL	conflict	UNP A0A3S5H8L7
F	175	SER	GLY	conflict	UNP A0A3S5H8L7

- Molecule 3 is a protein called Fab 54-4H03 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	228	1746	1106	296	339	5	0	1	0
3	J	228	1746	1106	296	339	5	0	1	0
3	G	228	1746	1106	296	339	5	0	1	0

- Molecule 4 is a protein called Fab 54-4H03 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	215	1652	1033	275	339	5	0	0	0
4	K	215	1652	1033	275	339	5	0	0	0
4	I	215	1652	1033	275	339	5	0	0	0

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	M	2	28	16	2	10	0	0	0
5	O	2	28	16	2	10	0	0	0

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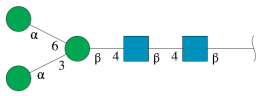
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	T	2	28	16	2	10	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
			Total	C	N	O			
6	N	5	61	34	2	25	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
			Total	C	N	O			
7	P	4	50	28	2	20	0	0	0

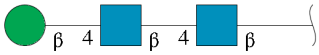
- Molecule 8 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 9 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.

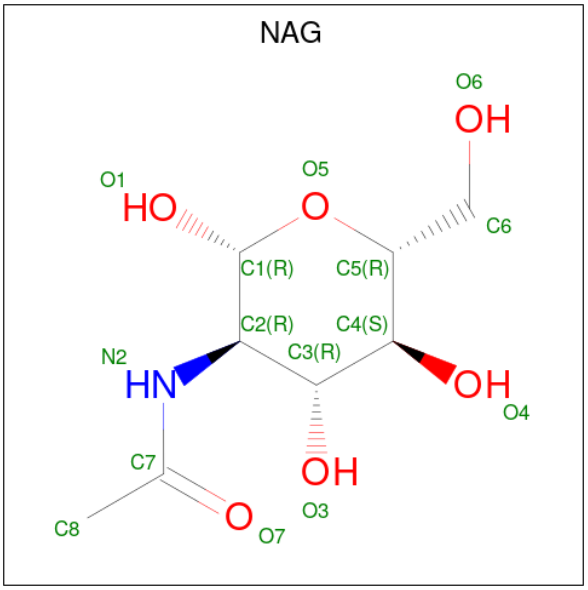
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	R	4	50	28	2	20	0	0	0

- Molecule 10 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
			Total	C	N	O			
10	S	3	39	22	2	15	0	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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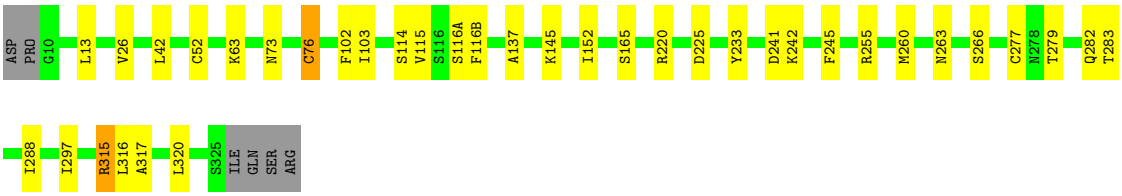
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	C	1	14	8	1	5	0	0
			Total	C	N	O		
11	C	1	14	8	1	5	0	0
			Total	C	N	O		
11	C	1	14	8	1	5	0	0
			Total	C	N	O		
11	E	1	14	8	1	5	0	0
			Total	C	N	O		
11	E	1	14	8	1	5	0	0
			Total	C	N	O		
11	E	1	14	8	1	5	0	0
			Total	C	N	O		
11	B	1	14	8	1	5	0	0
			Total	C	N	O		
11	D	1	14	8	1	5	0	0

3 Residue-property plots (i)

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

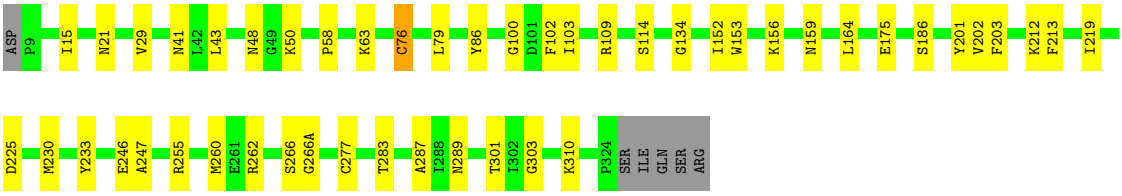
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



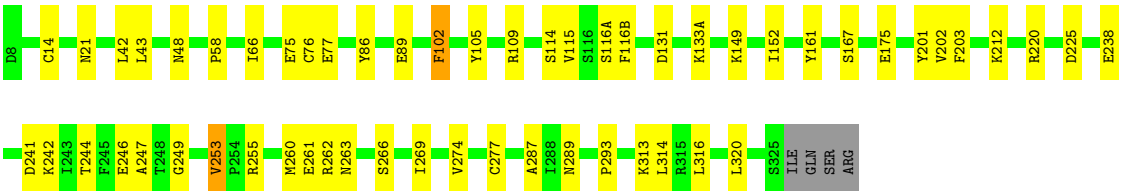
- Molecule 1: Hemagglutinin HA1 chain

Chain C:



- Molecule 1: Hemagglutinin HA1 chain

Chain E:



- Molecule 2: Hemagglutinin HA2 chain

Chain B:

• Molecule 2: Hemagglutinin HA2 chain

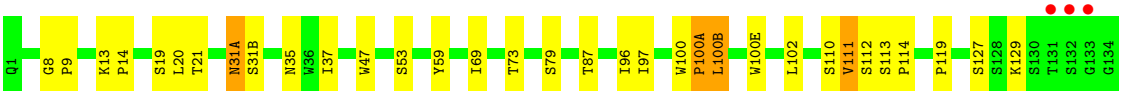
Chain D:

• Molecule 2: Hemagglutinin HA2 chain

Chain F:

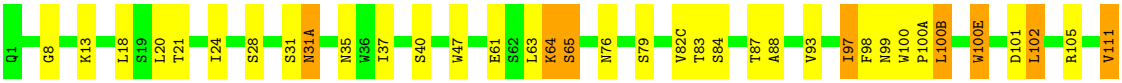
• Molecule 3: Fab 54-4H03 heavy chain

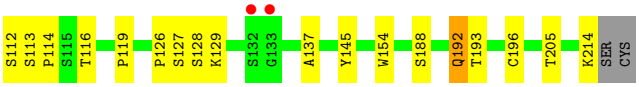
Chain H:



• Molecule 3: Fab 54-4H03 heavy chain

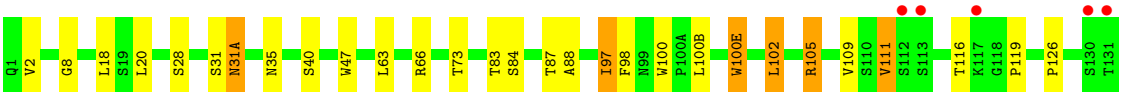
Chain J:

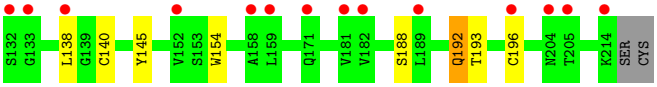




• Molecule 3: Fab 54-4H03 heavy chain

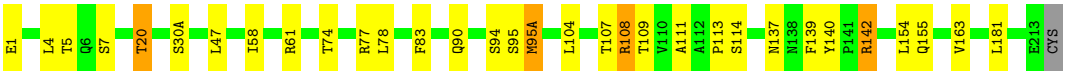
Chain G:





• Molecule 4: Fab 54-4H03 light chain

Chain L:

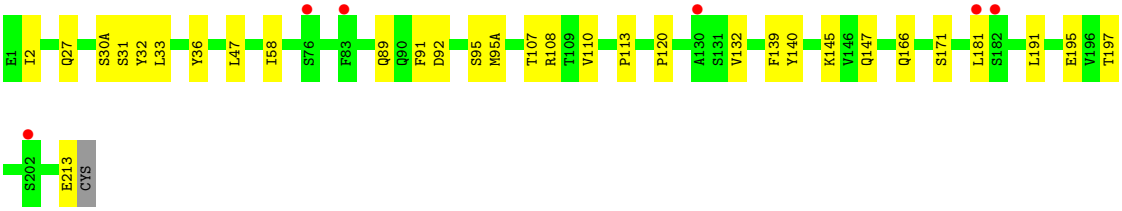


• Molecule 4: Fab 54-4H03 light chain

Chain K:

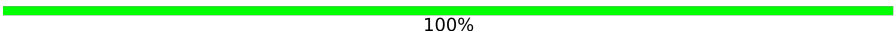
• Molecule 4: Fab 54-4H03 light chain

Chain I:



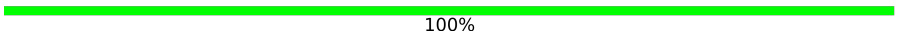
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



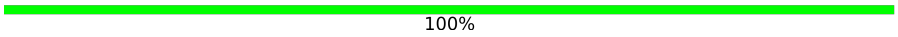
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



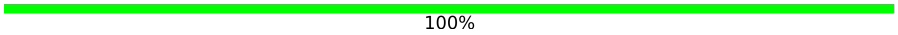
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

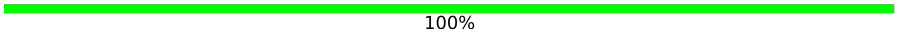
• Molecule 8: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 

• Molecule 9: 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 R:

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	231.54Å 259.21Å 165.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 3.50 47.22 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.22-3.50) 99.6 (47.22-3.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.179 , 0.232 0.179 , 0.232	Depositor DCC
R_{free} test set	3149 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	99.2	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22401	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN, 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	0/2593	0.45	0/3524
1	C	0.25	0/2595	0.46	0/3527
1	E	0.25	0/2609	0.45	0/3547
2	B	0.25	0/1434	0.41	0/1932
2	D	0.26	0/1403	0.41	0/1890
2	F	0.25	0/1403	0.42	0/1890
3	G	0.25	0/1794	0.47	0/2450
3	H	0.26	0/1794	0.48	0/2450
3	J	0.26	0/1794	0.48	0/2450
4	I	0.25	0/1687	0.44	0/2292
4	K	0.26	0/1687	0.45	0/2292
4	L	0.26	0/1687	0.47	0/2292
All	All	0.25	0/22480	0.45	0/30536

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	I	0	1
4	K	0	1
4	L	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	95	SER	Peptide
4	K	95	SER	Peptide
4	L	95(A)	MET	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2529	0	2474	18	0
1	C	2530	0	2475	27	0
1	E	2544	0	2485	32	0
2	B	1406	0	1325	11	0
2	D	1375	0	1299	13	0
2	F	1375	0	1299	11	0
3	G	1746	0	1714	20	0
3	H	1746	0	1714	25	0
3	J	1746	0	1714	31	0
4	I	1652	0	1595	13	0
4	K	1652	0	1595	15	0
4	L	1652	0	1595	14	0
5	M	28	0	25	0	0
5	O	28	0	25	0	0
5	T	28	0	25	0	0
6	N	61	0	52	0	0
7	P	50	0	41	1	0
8	Q	24	0	22	0	0
9	R	50	0	43	1	0
10	S	39	0	34	0	0
11	A	28	0	26	0	0
11	B	14	0	13	0	0
11	C	42	0	39	1	0
11	D	14	0	13	0	0
11	E	42	0	39	0	0
All	All	22401	0	21681	209	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 5.

The worst 5 of 209 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)
3:H:100:TRP:HA	3:H:100(B):LEU:H	1.47	0.79
4:I:107:THR:HG22	4:I:171:SER:HB3	1.72	0.72
3:G:119:PRO:HB3	3:G:145:TYR:HB3	1.72	0.71
1:C:310:LYS:HG2	2:D:89:LEU:HD11	1.73	0.70
3:G:28:SER:HB3	3:G:31:SER:HB2	1.75	0.69

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	322/330 (98%)	317 (98%)	5 (2%)	0	100	100
1	C	322/330 (98%)	318 (99%)	4 (1%)	0	100	100
1	E	324/330 (98%)	316 (98%)	8 (2%)	0	100	100
2	B	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
2	D	169/175 (97%)	164 (97%)	5 (3%)	0	100	100
2	F	169/175 (97%)	167 (99%)	2 (1%)	0	100	100
3	G	227/230 (99%)	215 (95%)	12 (5%)	0	100	100
3	H	227/230 (99%)	215 (95%)	10 (4%)	2 (1%)	17	56
3	J	227/230 (99%)	205 (90%)	21 (9%)	1 (0%)	34	72
4	I	213/216 (99%)	202 (95%)	11 (5%)	0	100	100
4	K	213/216 (99%)	201 (94%)	12 (6%)	0	100	100
4	L	213/216 (99%)	203 (95%)	9 (4%)	1 (0%)	29	68
All	All	2799/2853 (98%)	2688 (96%)	107 (4%)	4 (0%)	51	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	100(A)	PRO
4	L	95(A)	MET
3	H	53	SER
3	J	64	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/290 (98%)	277 (98%)	7 (2%)	47	75
1	C	284/290 (98%)	277 (98%)	7 (2%)	47	75
1	E	286/290 (99%)	276 (96%)	10 (4%)	36	67
2	B	150/150 (100%)	145 (97%)	5 (3%)	38	68
2	D	146/150 (97%)	144 (99%)	2 (1%)	67	85
2	F	146/150 (97%)	140 (96%)	6 (4%)	30	63
3	G	202/203 (100%)	191 (95%)	11 (5%)	22	55
3	H	202/203 (100%)	189 (94%)	13 (6%)	17	50
3	J	202/203 (100%)	189 (94%)	13 (6%)	17	50
4	I	187/188 (100%)	180 (96%)	7 (4%)	34	65
4	K	187/188 (100%)	180 (96%)	7 (4%)	34	65
4	L	187/188 (100%)	178 (95%)	9 (5%)	25	60
All	All	2463/2493 (99%)	2366 (96%)	97 (4%)	32	64

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	155	GLN
3	J	193	THR
3	J	13	LYS
3	J	100(E)	TRP
4	K	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	41	ASN
2	B	42	GLN
2	F	42	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	$\#\|Z\| > 2$
5	NAG	M	1	5,1	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	M	2	5	14,14,15	0.23	0	17,19,21	0.53	0
6	NAG	N	1	6,1	14,14,15	0.23	0	17,19,21	0.52	0
6	NAG	N	2	6	14,14,15	0.18	0	17,19,21	0.43	0
6	BMA	N	3	6	11,11,12	0.65	0	15,15,17	0.80	0
6	MAN	N	4	6	11,11,12	0.77	0	15,15,17	1.11	2 (13%)
6	MAN	N	5	6	11,11,12	0.76	0	15,15,17	1.15	3 (20%)
5	NAG	O	1	5,1	14,14,15	0.19	0	17,19,21	0.56	0
5	NAG	O	2	5	14,14,15	0.25	0	17,19,21	0.40	0
7	NAG	P	1	7,1	14,14,15	0.31	0	17,19,21	0.50	0
7	NAG	P	2	7	14,14,15	0.23	0	17,19,21	0.41	0
7	BMA	P	3	7	11,11,12	0.63	0	15,15,17	0.80	0
7	MAN	P	4	7	11,11,12	0.69	0	15,15,17	1.05	2 (13%)
8	NAG	Q	1	8,1	14,14,15	0.34	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FUC	Q	2	8	10,10,11	0.82	0	14,14,16	0.80	0
9	NAG	R	1	9,1	14,14,15	0.22	0	17,19,21	0.54	0
9	NAG	R	2	9	14,14,15	0.23	0	17,19,21	0.40	0
9	BMA	R	3	9	11,11,12	0.67	0	15,15,17	0.74	0
9	MAN	R	4	9	11,11,12	0.88	0	15,15,17	1.39	2 (13%)
10	NAG	S	1	10,1	14,14,15	0.39	0	17,19,21	0.52	0
10	NAG	S	2	10	14,14,15	0.28	0	17,19,21	0.39	0
10	BMA	S	3	10	11,11,12	0.65	0	15,15,17	0.88	0
5	NAG	T	1	2,5	14,14,15	0.33	0	17,19,21	0.44	0
5	NAG	T	2	5	14,14,15	0.30	0	17,19,21	0.58	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
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	2/2/19/22	0/1/1/1
6	MAN	N	5	6	-	2/2/19/22	0/1/1/1
5	NAG	O	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
7	NAG	P	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1
8	NAG	Q	1	8,1	-	0/6/23/26	0/1/1/1
8	FUC	Q	2	8	-	-	0/1/1/1
9	NAG	R	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	2/6/23/26	0/1/1/1
9	BMA	R	3	9	-	0/2/19/22	0/1/1/1
9	MAN	R	4	9	-	0/2/19/22	1/1/1/1
10	NAG	S	1	10,1	-	2/6/23/26	0/1/1/1
10	NAG	S	2	10	-	2/6/23/26	0/1/1/1
10	BMA	S	3	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	T	1	2,5	-	3/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	4	MAN	C1-O5-C5	3.95	117.55	112.19
7	P	4	MAN	C1-O5-C5	2.46	115.53	112.19
7	P	4	MAN	O2-C2-C3	-2.32	105.50	110.14
6	N	5	MAN	C1-O5-C5	2.29	115.30	112.19
9	R	4	MAN	O2-C2-C3	-2.20	105.73	110.14

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	2	NAG	O5-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

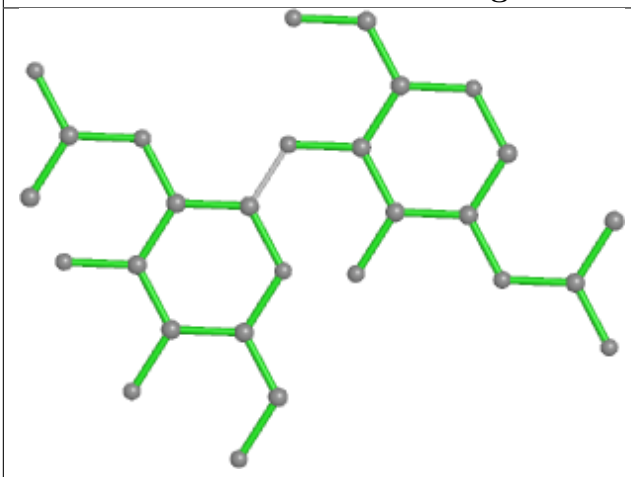
Mol	Chain	Res	Type	Atoms
9	R	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

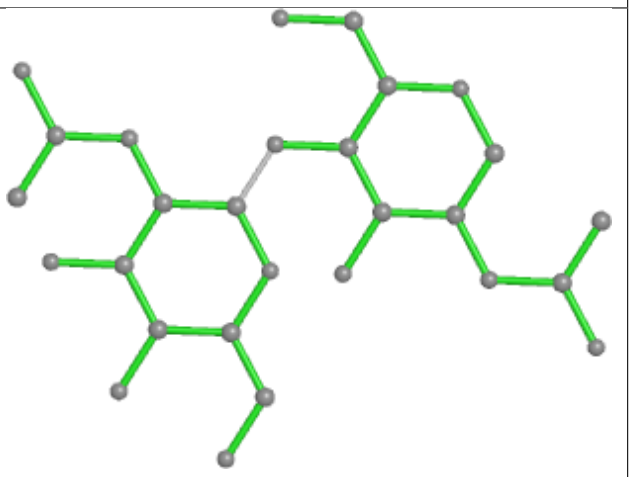
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	2	NAG	1	0
7	P	3	BMA	1	0
9	R	1	NAG	1	0

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

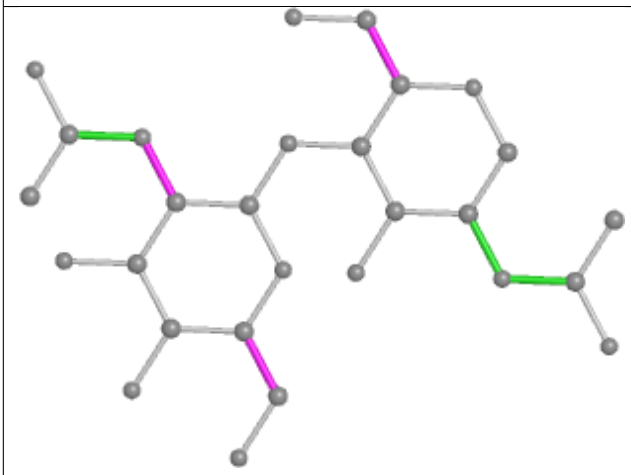
Oligosaccharide Chain M



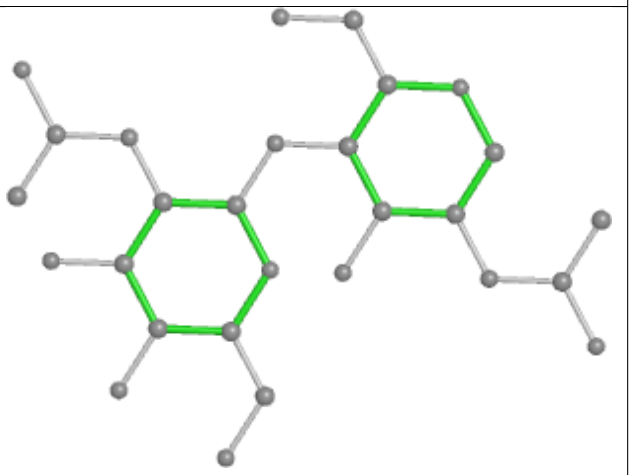
Bond lengths



Bond angles

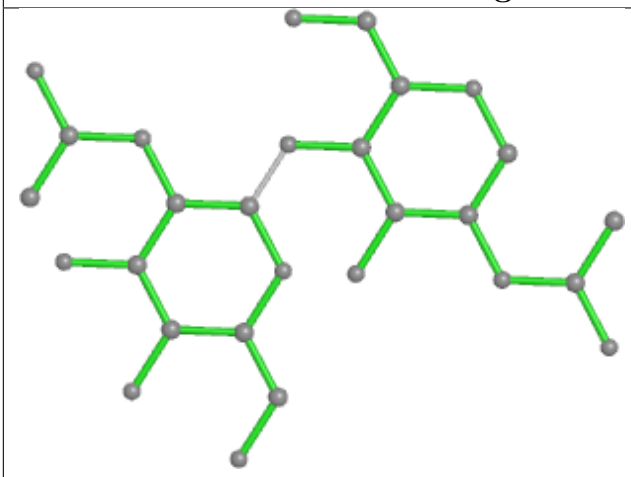


Torsions

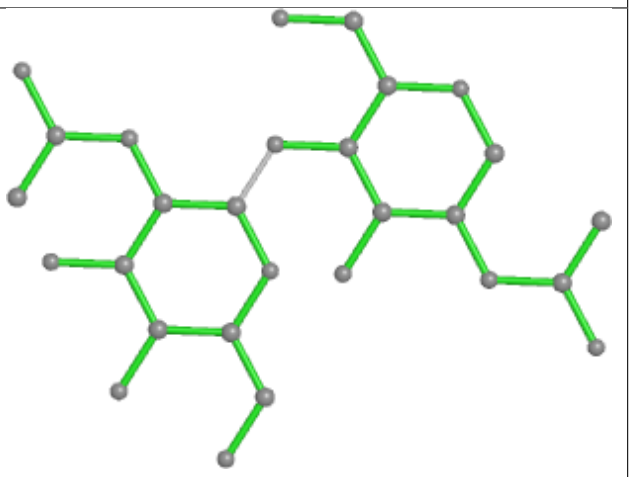


Rings

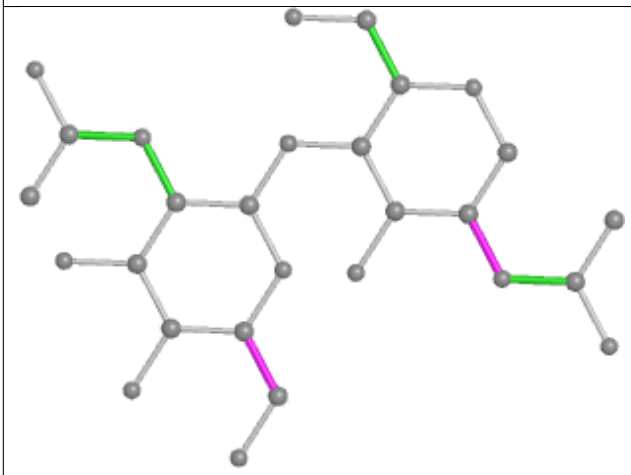
Oligosaccharide Chain O



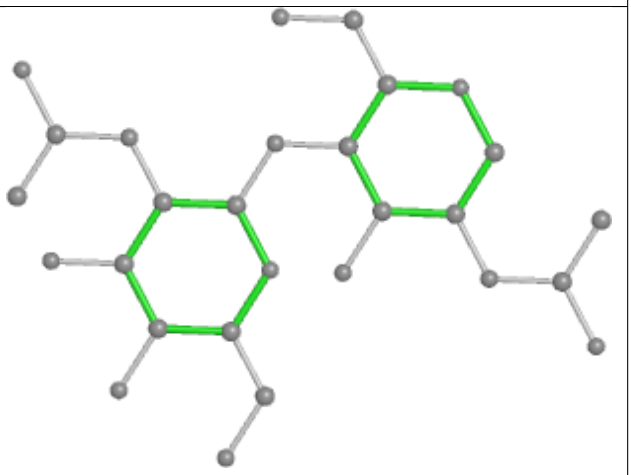
Bond lengths



Bond angles

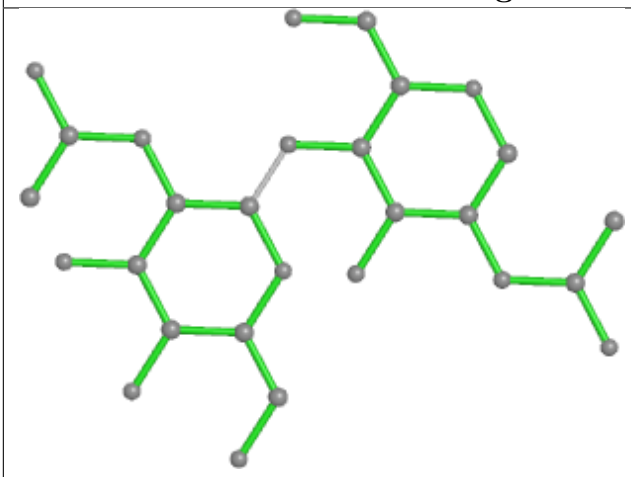


Torsions

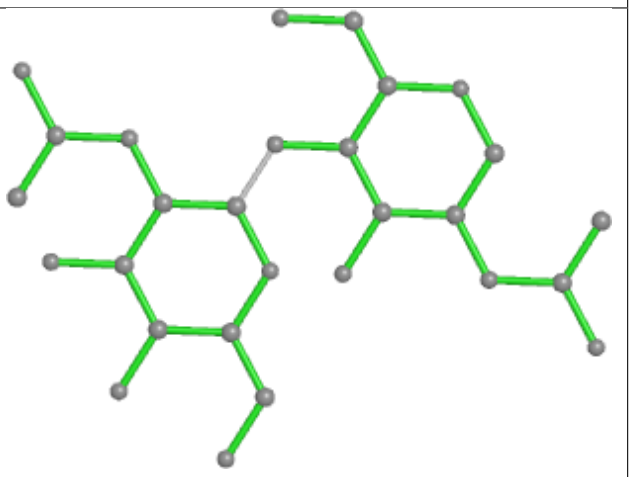


Rings

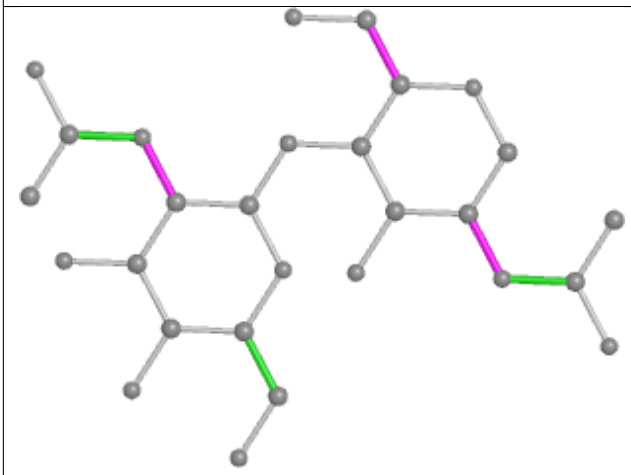
Oligosaccharide Chain T



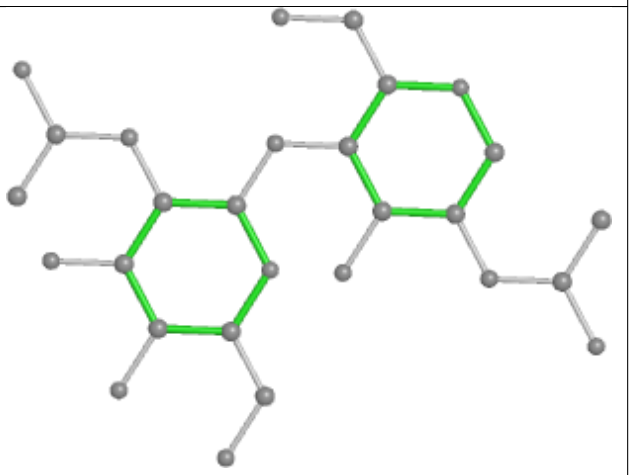
Bond lengths



Bond angles

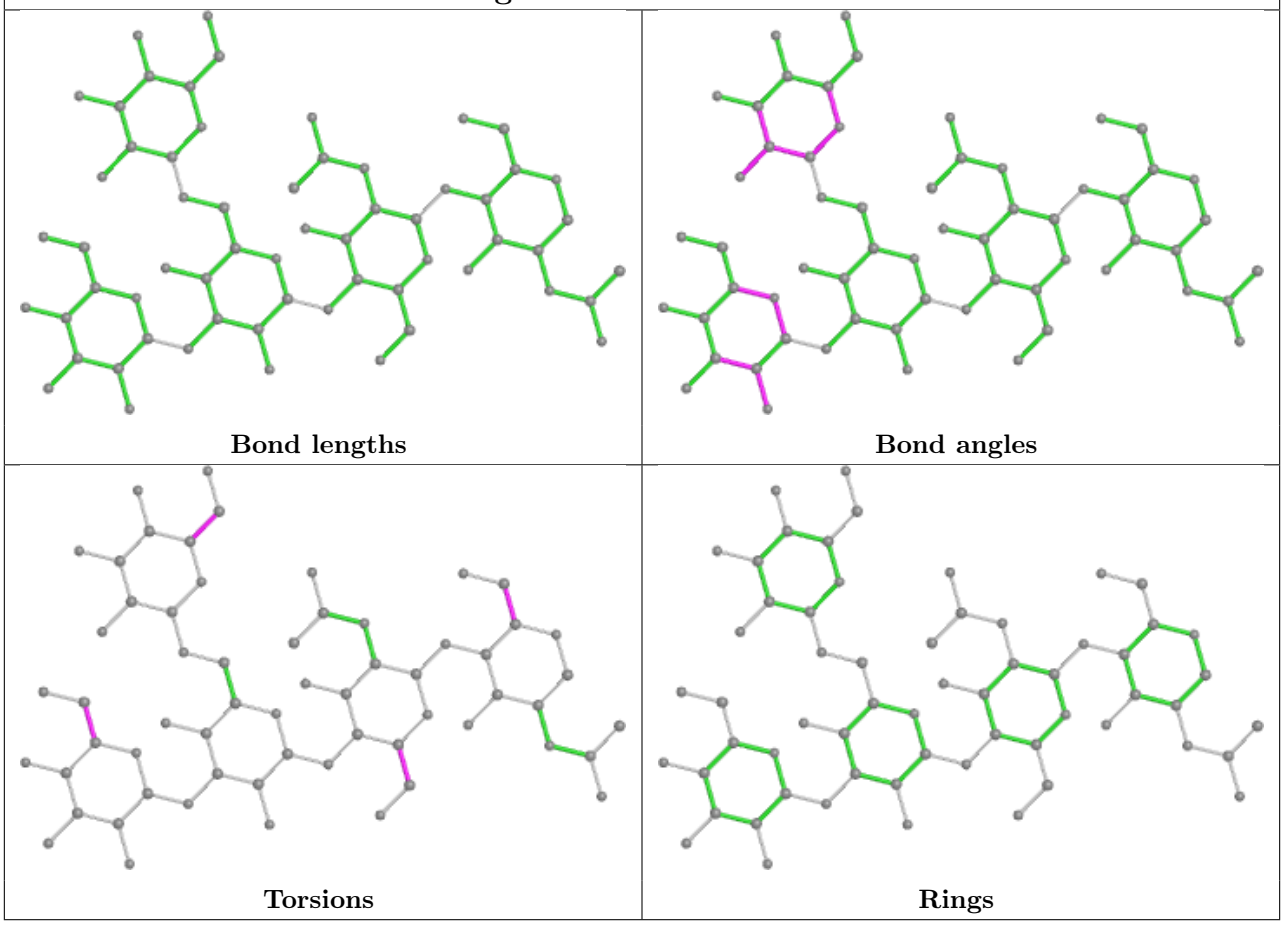


Torsions

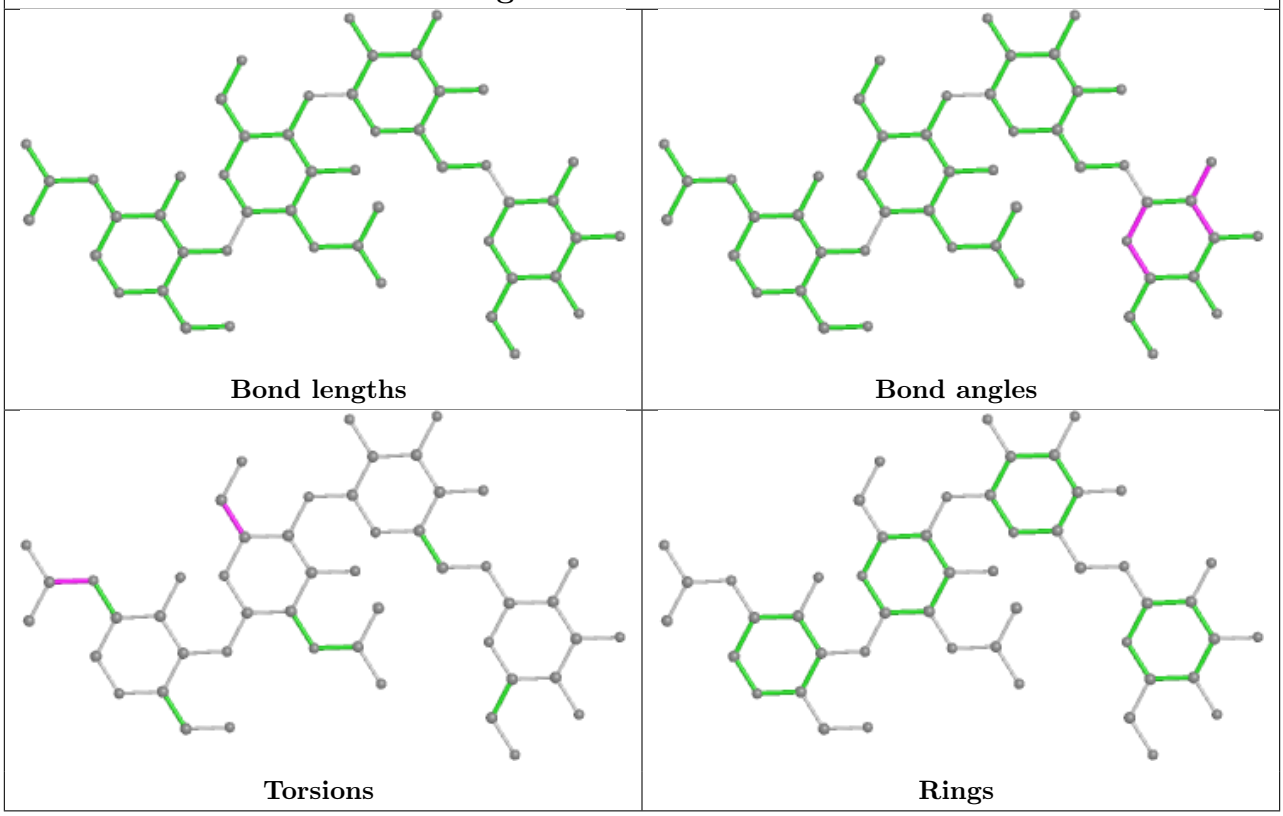


Rings

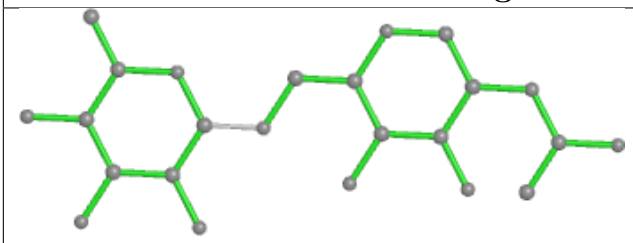
Oligosaccharide Chain N



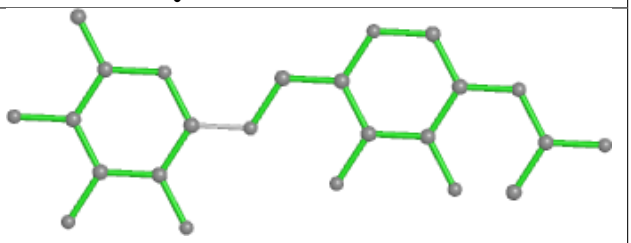
Oligosaccharide Chain P



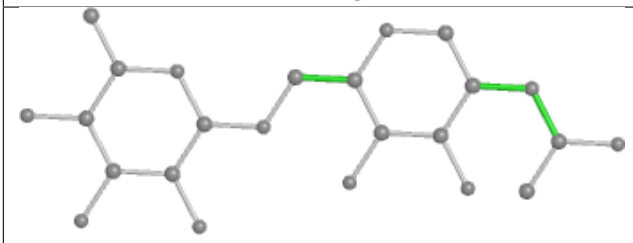
Oligosaccharide Chain Q



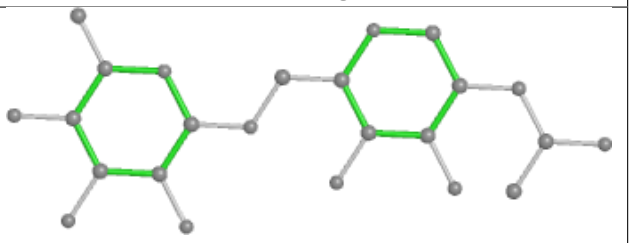
Bond lengths



Bond angles

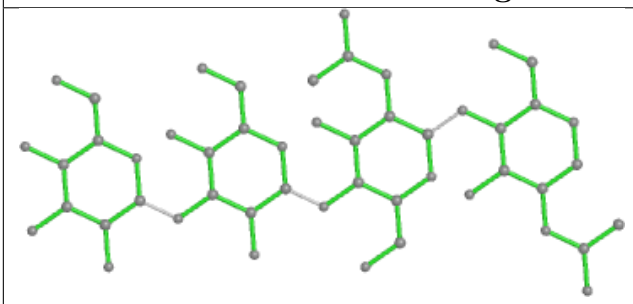


Torsions

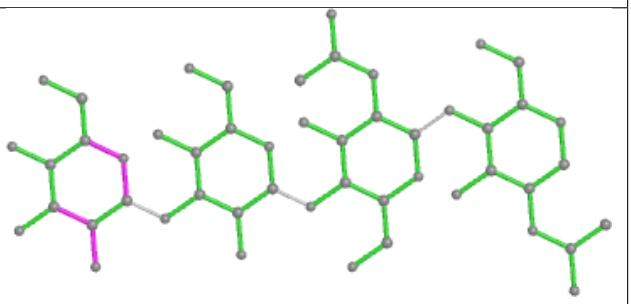


Rings

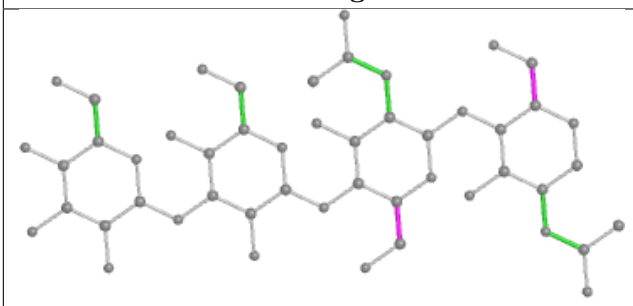
Oligosaccharide Chain R



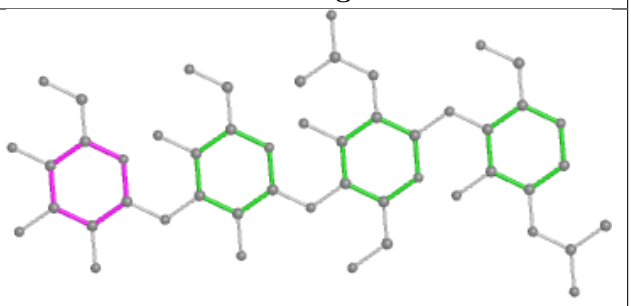
Bond lengths



Bond angles

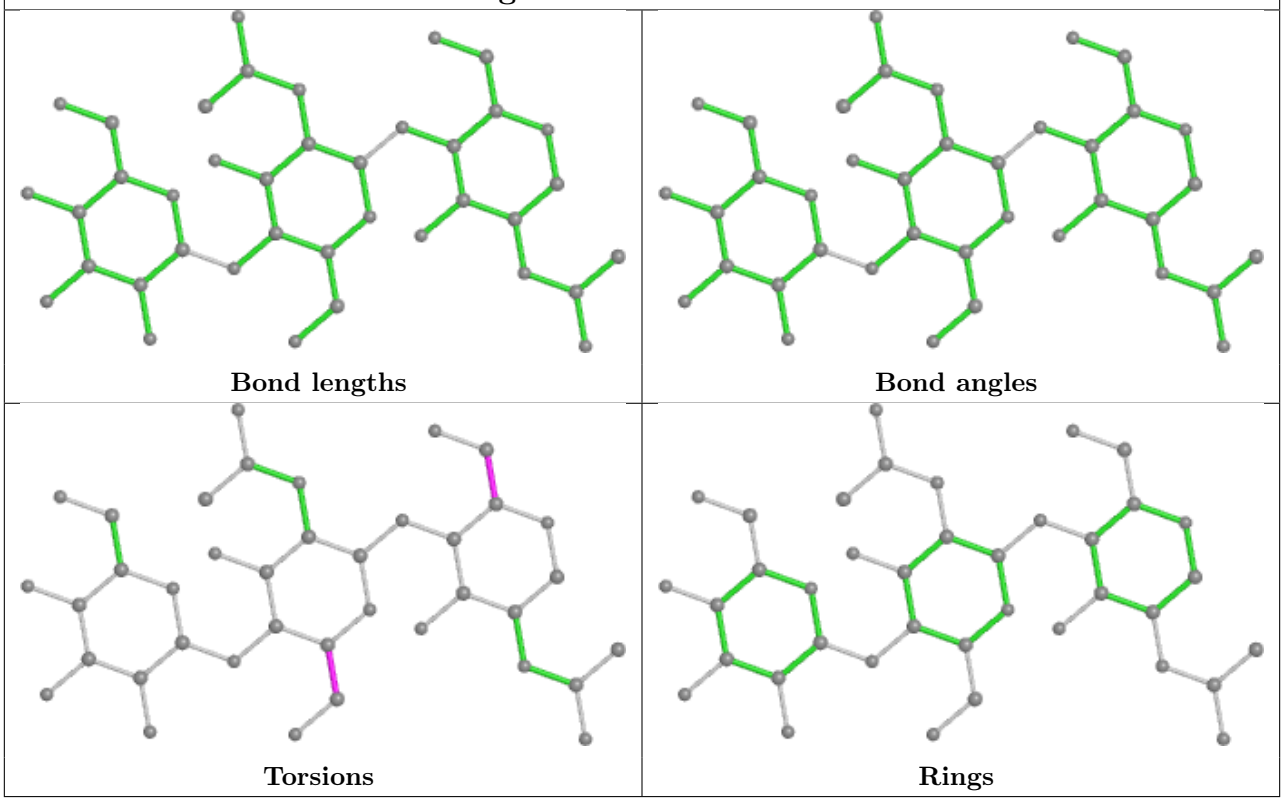


Torsions



Rings

Oligosaccharide Chain S



5.6 Ligand geometry (i)

10 ligands 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	$\#\|Z\| > 2$
11	NAG	C	408	1	14,14,15	0.40	0	17,19,21	0.53	0
11	NAG	E	410	1	14,14,15	0.45	0	17,19,21	0.43	0
11	NAG	B	201	2	14,14,15	0.31	0	17,19,21	0.53	0
11	NAG	C	409	1	14,14,15	0.38	0	17,19,21	0.58	0
11	NAG	E	409	1	14,14,15	0.38	0	17,19,21	0.55	0
11	NAG	A	411	1	14,14,15	0.37	0	17,19,21	0.43	0
11	NAG	D	201	2	14,14,15	0.32	0	17,19,21	0.59	0
11	NAG	E	401	1	14,14,15	0.34	0	17,19,21	0.38	0
11	NAG	A	410	1	14,14,15	0.40	0	17,19,21	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	C	401	1	14,14,15	0.61	1 (7%)	17,19,21	0.63	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
11	NAG	C	408	1	-	0/6/23/26	0/1/1/1
11	NAG	E	410	1	-	0/6/23/26	0/1/1/1
11	NAG	B	201	2	-	2/6/23/26	0/1/1/1
11	NAG	C	409	1	-	2/6/23/26	0/1/1/1
11	NAG	E	409	1	-	1/6/23/26	0/1/1/1
11	NAG	A	411	1	-	2/6/23/26	0/1/1/1
11	NAG	D	201	2	-	3/6/23/26	0/1/1/1
11	NAG	E	401	1	-	2/6/23/26	0/1/1/1
11	NAG	A	410	1	-	1/6/23/26	0/1/1/1
11	NAG	C	401	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	401	NAG	C1-C2	2.00	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	409	NAG	O5-C5-C6-O6
11	C	401	NAG	O5-C5-C6-O6
11	E	401	NAG	O5-C5-C6-O6
11	A	410	NAG	O5-C5-C6-O6
11	E	409	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	401	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	324/330 (98%)	-0.43	0	100	100	77, 124, 180, 202	0
1	C	324/330 (98%)	-0.43	0	100	100	69, 113, 159, 233	0
1	E	326/330 (98%)	-0.37	0	100	100	60, 132, 188, 217	0
2	B	175/175 (100%)	-0.37	0	100	100	62, 106, 170, 211	0
2	D	171/175 (97%)	-0.42	0	100	100	52, 93, 148, 185	0
2	F	171/175 (97%)	-0.50	0	100	100	60, 93, 145, 179	0
3	G	228/230 (99%)	0.41	19 (8%)	11	12	116, 203, 279, 386	0
3	H	228/230 (99%)	-0.46	3 (1%)	77	71	64, 98, 165, 255	0
3	J	228/230 (99%)	-0.42	2 (0%)	84	79	52, 104, 185, 254	0
4	I	215/216 (99%)	0.09	6 (2%)	53	47	108, 195, 263, 299	0
4	K	215/216 (99%)	-0.58	0	100	100	55, 89, 132, 179	0
4	L	215/216 (99%)	-0.49	0	100	100	55, 78, 120, 160	0
All	All	2820/2853 (98%)	-0.33	30 (1%)	80	75	52, 114, 228, 386	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	181	LEU	7.2
3	G	113	SER	4.8
3	G	112	SER	4.4
3	G	138	LEU	4.3
3	G	132	SER	4.1

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)

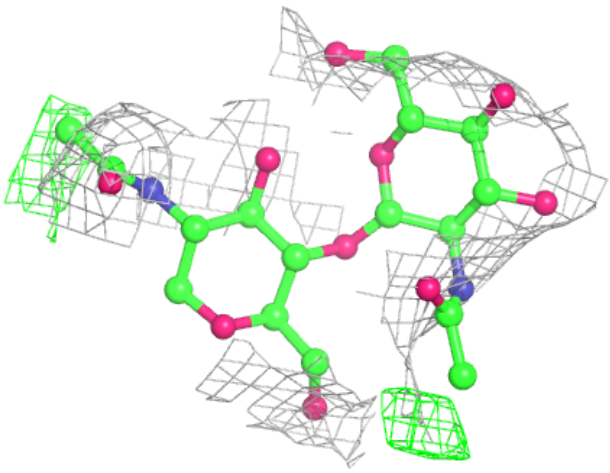
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

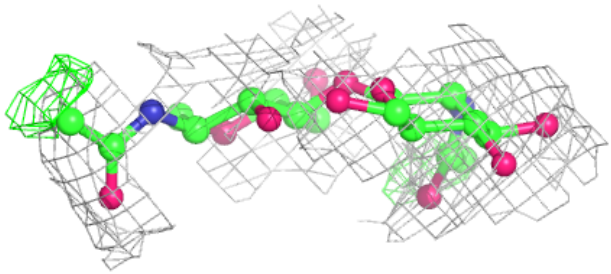
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	BMA	S	3	11/12	0.59	0.36	204,216,221,222	0
6	MAN	N	5	11/12	0.62	0.30	207,218,220,222	0
5	NAG	T	2	14/15	0.70	0.33	140,177,191,196	0
10	NAG	S	2	14/15	0.73	0.38	181,197,213,221	0
5	NAG	O	2	14/15	0.77	0.30	171,200,203,204	0
5	NAG	M	2	14/15	0.79	0.29	175,195,216,219	0
9	MAN	R	4	11/12	0.79	0.19	195,199,205,207	0
5	NAG	O	1	14/15	0.80	0.20	156,174,189,202	0
5	NAG	T	1	14/15	0.81	0.22	129,163,171,180	0
6	BMA	N	3	11/12	0.82	0.12	171,189,206,215	0
9	BMA	R	3	11/12	0.83	0.13	185,193,199,204	0
9	NAG	R	2	14/15	0.85	0.17	153,171,181,187	0
7	MAN	P	4	11/12	0.86	0.21	172,179,190,190	0
10	NAG	S	1	14/15	0.88	0.17	128,144,168,182	0
8	FUC	Q	2	10/11	0.88	0.13	186,198,201,203	0
7	BMA	P	3	11/12	0.88	0.15	156,166,172,176	0
8	NAG	Q	1	14/15	0.91	0.11	143,162,179,185	0
6	NAG	N	2	14/15	0.91	0.11	163,164,168,175	0
5	NAG	M	1	14/15	0.91	0.15	139,160,173,187	0
6	MAN	N	4	11/12	0.91	0.14	180,186,188,189	0
6	NAG	N	1	14/15	0.93	0.13	141,158,165,171	0
7	NAG	P	1	14/15	0.93	0.12	69,88,106,110	0
9	NAG	R	1	14/15	0.94	0.12	106,120,132,141	0
7	NAG	P	2	14/15	0.95	0.12	112,121,133,141	0

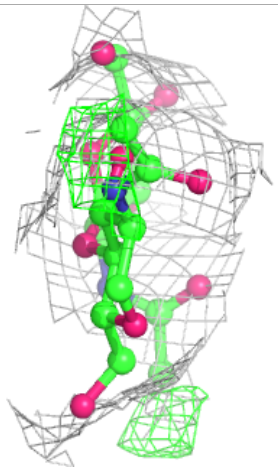
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

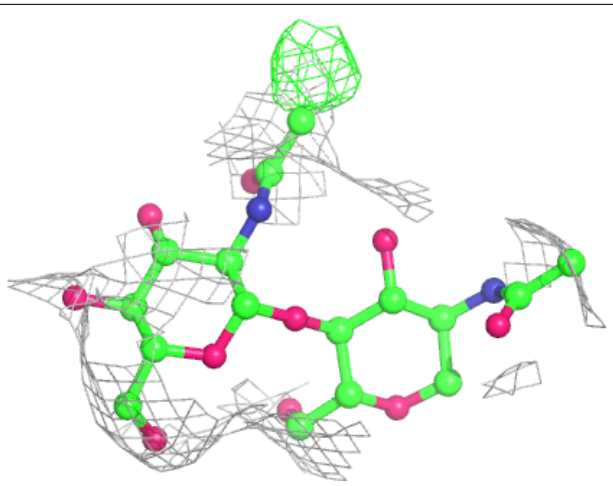


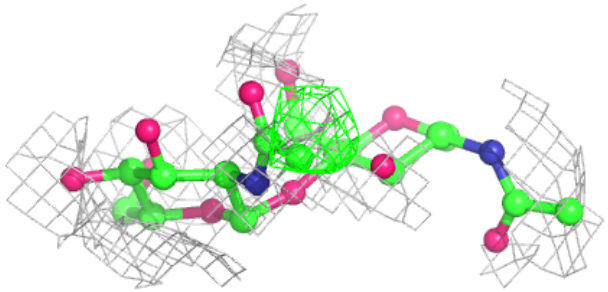


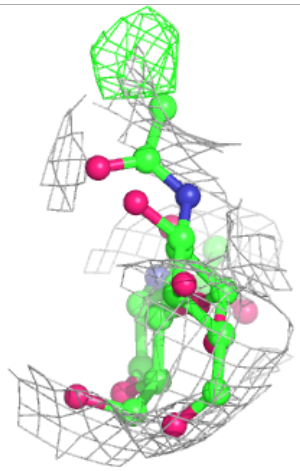


Electron density around Chain O:

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

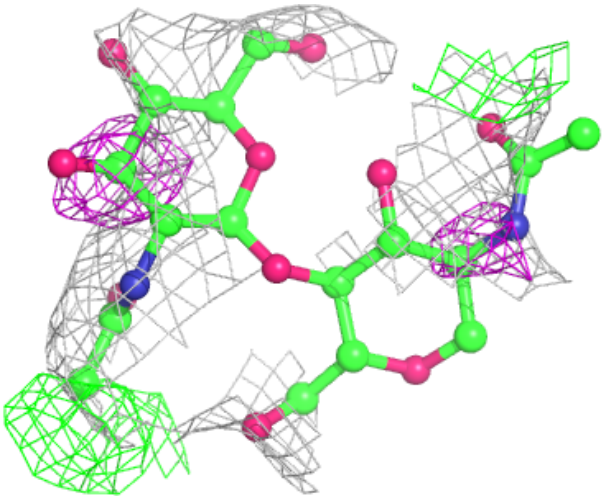


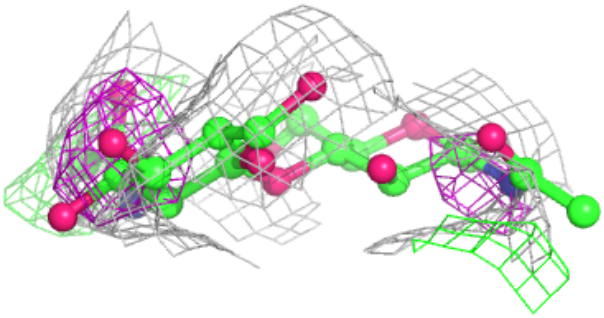


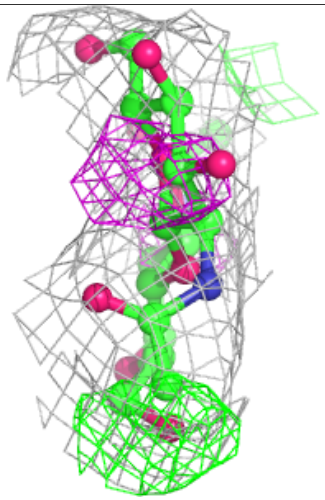


Electron density around Chain T:

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

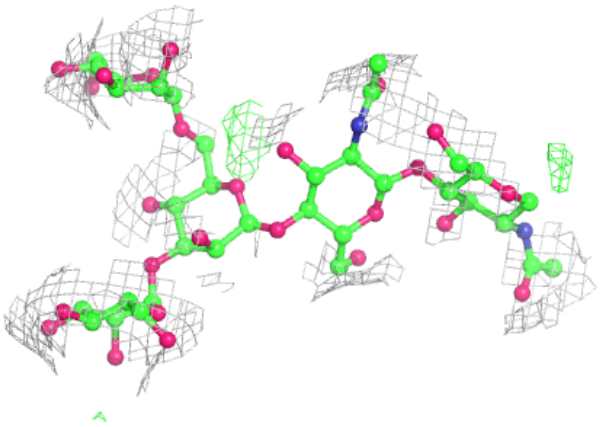


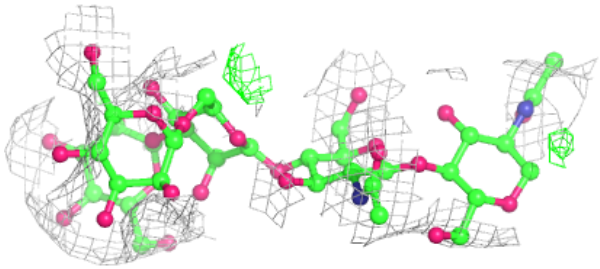


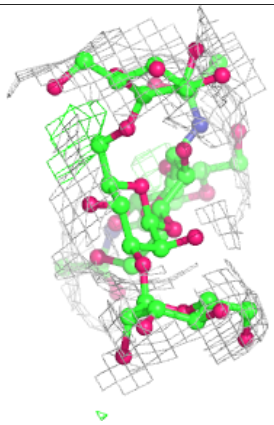


Electron density around Chain N:

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

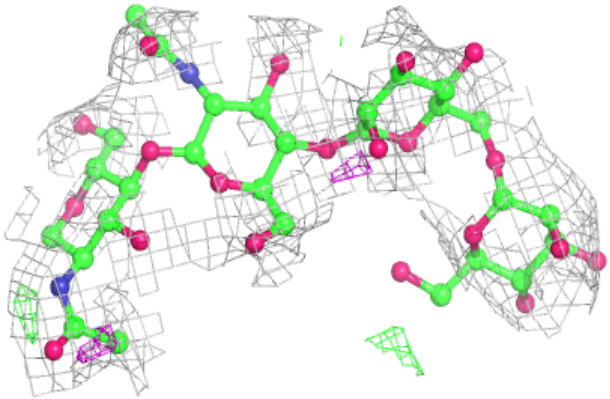


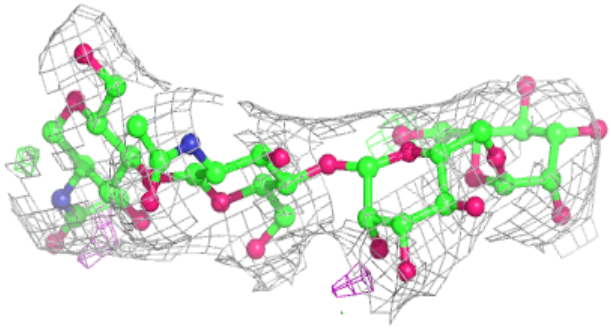


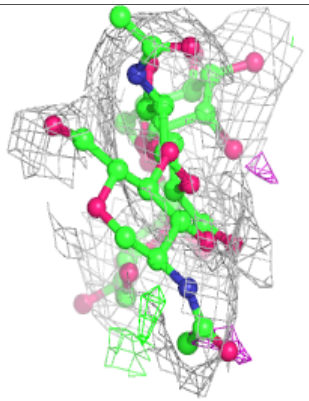


Electron density around Chain P:

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

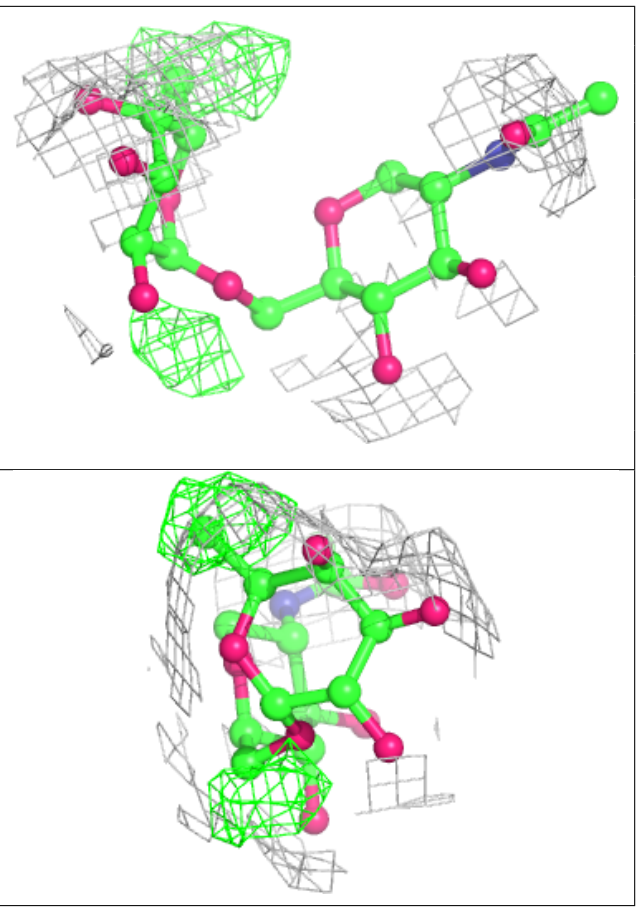






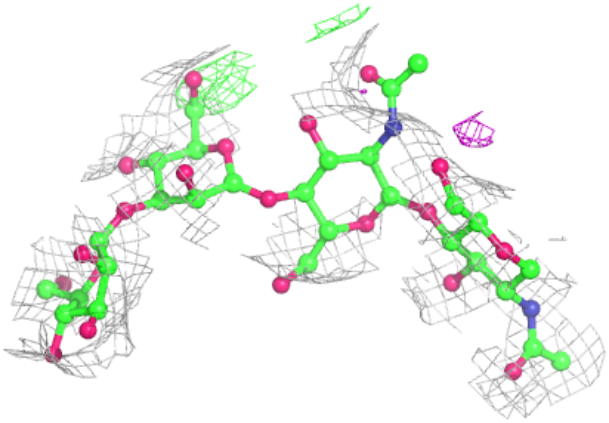
Electron density around Chain Q:

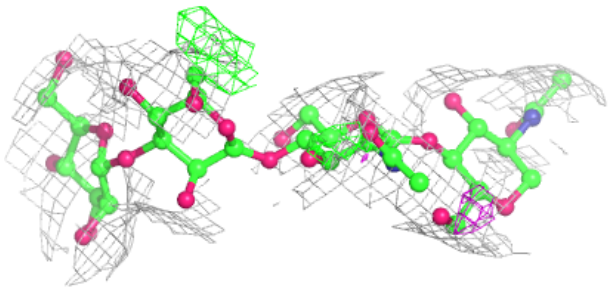
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

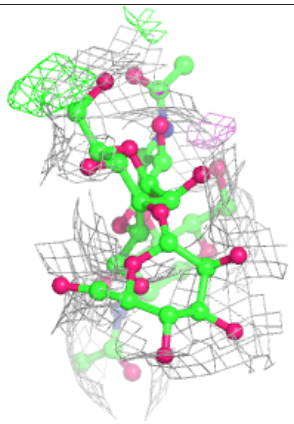


Electron density around Chain R:

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

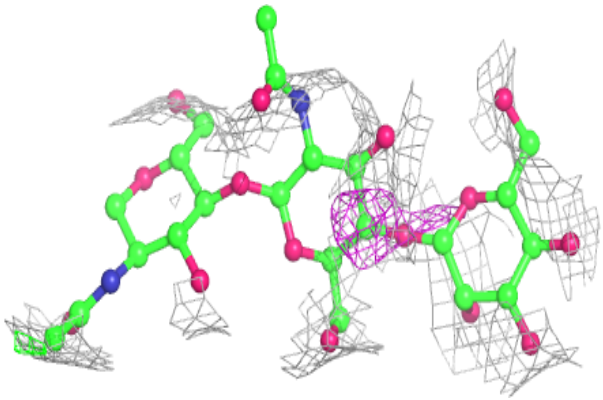


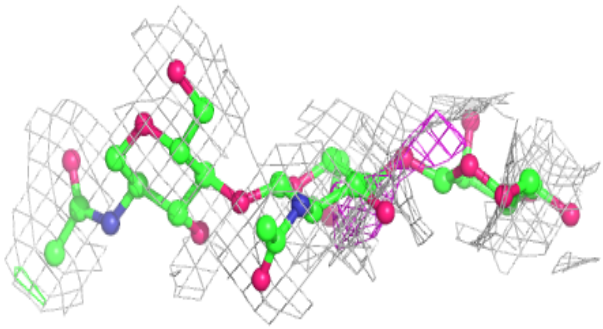


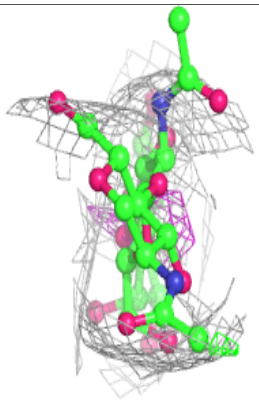


Electron density around Chain S:

$2mF_o$-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
11	NAG	A	411	14/15	0.78	0.19	130,143,152,152	0
11	NAG	E	409	14/15	0.79	0.27	160,173,182,182	0
11	NAG	E	410	14/15	0.79	0.25	137,153,161,162	0
11	NAG	A	410	14/15	0.83	0.21	174,182,199,202	0
11	NAG	C	401	14/15	0.84	0.20	145,168,170,172	0
11	NAG	D	201	14/15	0.84	0.17	115,138,144,145	0
11	NAG	E	401	14/15	0.86	0.14	132,157,167,171	0
11	NAG	B	201	14/15	0.86	0.22	142,158,178,184	0
11	NAG	C	408	14/15	0.86	0.20	119,135,141,142	0
11	NAG	C	409	14/15	0.87	0.16	148,156,170,173	0

6.5 Other polymers (i)

There are no such residues in this entry.