wwPDB X-ray Structure Validation Summary Report (i)

Feb 21, 2023 – 12:37 am GMT

PDB ID	:	4UM9
Title	:	Crystal structure of alpha V beta 6 with peptide
Authors	:	Dong, X.; Springer, T.A.
Deposited on	:	2014-05-15
Resolution	:	2.50 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:

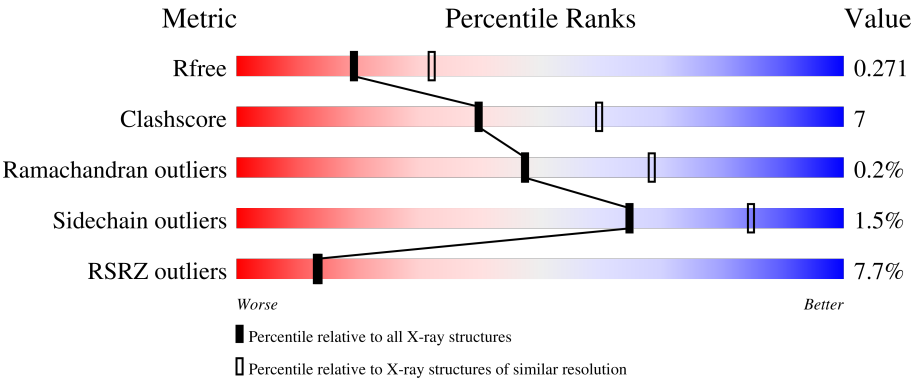
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	604	2% 82% 16% ·
1	C	604	4% 82% 15% ··
2	B	483	11% 74% 18% · 7%
3	D	483	14% 73% 20% 6%
4	E	13	8% 69% 15% 15%

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Mol	Chain	Length	Quality of chain
4	F	13	8% 85% 15%
5	G	2	100%
5	J	2	100%
5	K	2	50% 50%
5	L	2	100%
5	M	2	100%
5	P	2	100%
6	H	4	75% 25%
7	I	6	33% 67%
7	N	6	33% 33% 33%
8	O	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	NAG	B	507	-	-	-	X
12	NAG	D	2004	-	-	-	X
7	MAN	N	5	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 17049 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 Integrin alpha-V heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4601	2917	781	882	21			
1	C	589	Total	C	N	O	S	0	0	0
			4566	2897	774	874	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	CYS	MET	conflict	UNP P06756
A	596	THR	-	expression tag	UNP P06756
A	597	GLY	-	expression tag	UNP P06756
A	598	GLY	-	expression tag	UNP P06756
A	599	LEU	-	expression tag	UNP P06756
A	600	GLU	-	expression tag	UNP P06756
A	601	VAL	-	expression tag	UNP P06756
A	602	LEU	-	expression tag	UNP P06756
A	603	PHE	-	expression tag	UNP P06756
A	604	GLN	-	expression tag	UNP P06756
C	400	CYS	MET	conflict	UNP P06756
C	596	THR	-	expression tag	UNP P06756
C	597	GLY	-	expression tag	UNP P06756
C	598	GLY	-	expression tag	UNP P06756
C	599	LEU	-	expression tag	UNP P06756
C	600	GLU	-	expression tag	UNP P06756
C	601	VAL	-	expression tag	UNP P06756
C	602	LEU	-	expression tag	UNP P06756
C	603	PHE	-	expression tag	UNP P06756
C	604	GLN	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	448	Total	C	N	O	S	0	0	0
			3433	2155	586	662	30			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	270	CYS	ILE	conflict	UNP P18564
B	452	ASN	HIS	conflict	UNP P18564
B	475	SER	-	expression tag	UNP P18564
B	476	ARG	-	expression tag	UNP P18564
B	477	GLY	-	expression tag	UNP P18564
B	478	LEU	-	expression tag	UNP P18564
B	479	GLN	-	expression tag	UNP P18564
B	480	THR	-	expression tag	UNP P18564
B	481	LEU	-	expression tag	UNP P18564
B	482	PHE	-	expression tag	UNP P18564
B	483	GLN	-	expression tag	UNP P18564

- Molecule 3 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	455	Total	C	N	O	S	0	0	0
			3485	2185	593	677	30			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	GLN	conflict	UNP P18564
D	270	CYS	ILE	conflict	UNP P18564
D	452	ASN	HIS	conflict	UNP P18564
D	475	SER	-	expression tag	UNP P18564
D	476	ARG	-	expression tag	UNP P18564
D	477	GLY	-	expression tag	UNP P18564
D	478	LEU	-	expression tag	UNP P18564
D	479	GLN	-	expression tag	UNP P18564
D	480	THR	-	expression tag	UNP P18564
D	481	LEU	-	expression tag	UNP P18564
D	482	PHE	-	expression tag	UNP P18564
D	483	GLN	-	expression tag	UNP P18564

- Molecule 4 is a protein called Latency-associated peptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	E	11	Total C N O 77 46 19 12	0	0	1
4	F	13	Total C N O 89 53 22 14	0	0	2

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	238	ACE	-	expression tag	UNP P10600
E	250	NH2	-	expression tag	UNP P10600
F	238	ACE	-	expression tag	UNP P10600
F	250	NH2	-	expression tag	UNP P10600

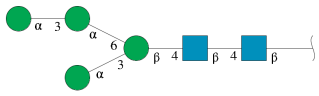
- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	G	2	Total C N O 28 16 2 10	0	0	0
5	J	2	Total C N O 28 16 2 10	0	0	0
5	K	2	Total C N O 28 16 2 10	0	0	0
5	L	2	Total C N O 28 16 2 10	0	0	0
5	M	2	Total C N O 28 16 2 10	0	0	0
5	P	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 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.

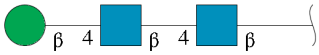
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	H	4	Total C N O 50 28 2 20	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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.



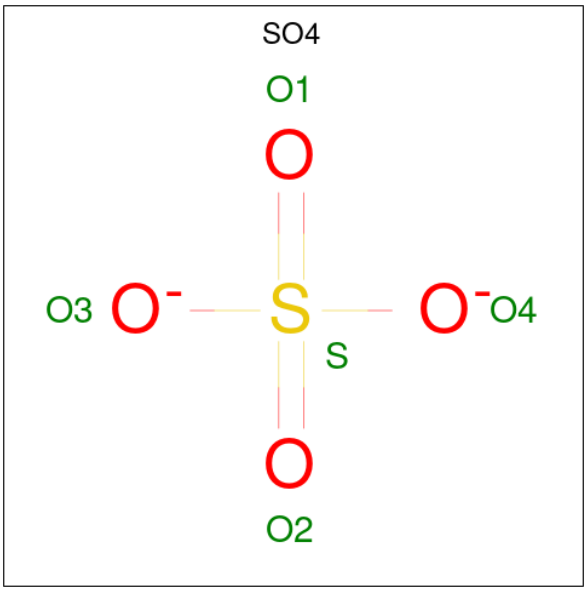
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	I	6	Total C N O 72 40 2 30	0	0	0
7	N	6	Total C N O 72 40 2 30	0	0	0

- Molecule 8 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
8	O	3	Total C N O 39 22 2 15	0	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0

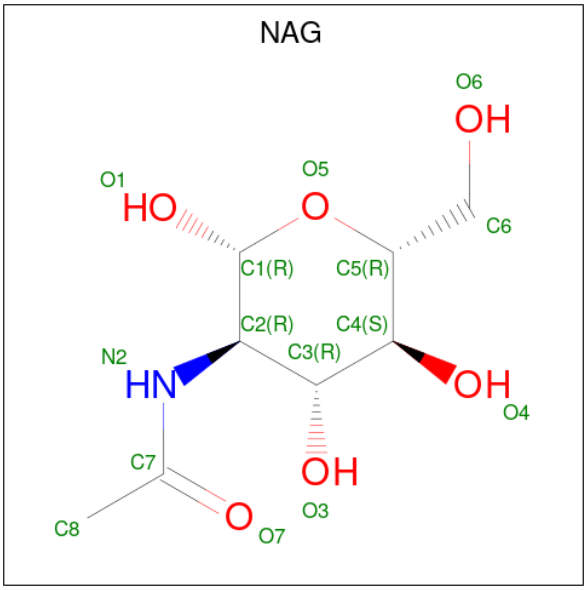
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	4	Total Ca 4 4	0	0
10	B	2	Total Ca 2 2	0	0
10	C	4	Total Ca 4 4	0	0
10	D	2	Total Ca 2 2	0	0

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

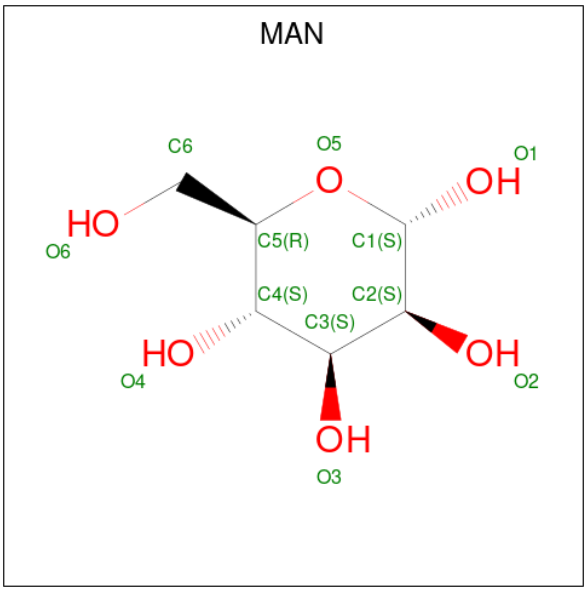
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total Mg 1 1	0	0
11	D	1	Total Mg 1 1	0	0

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 13 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 11 6 5	0	0

- Molecule 14 is water.

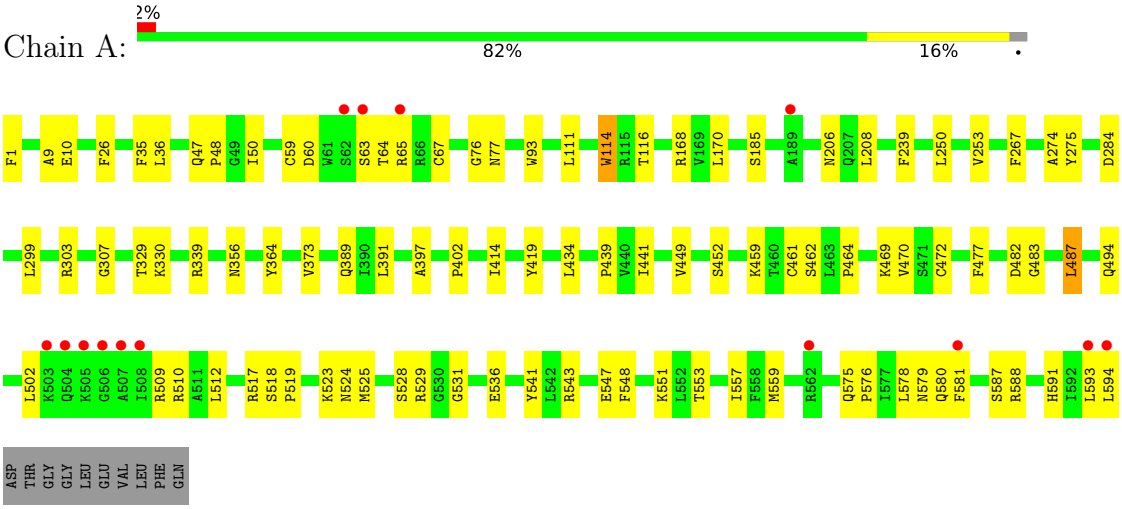
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	85	Total O 85 85	0	0
14	B	65	Total O 65 65	0	0
14	C	52	Total O 52 52	0	0
14	D	25	Total O 25 25	0	0
14	E	3	Total O 3 3	0	0

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.

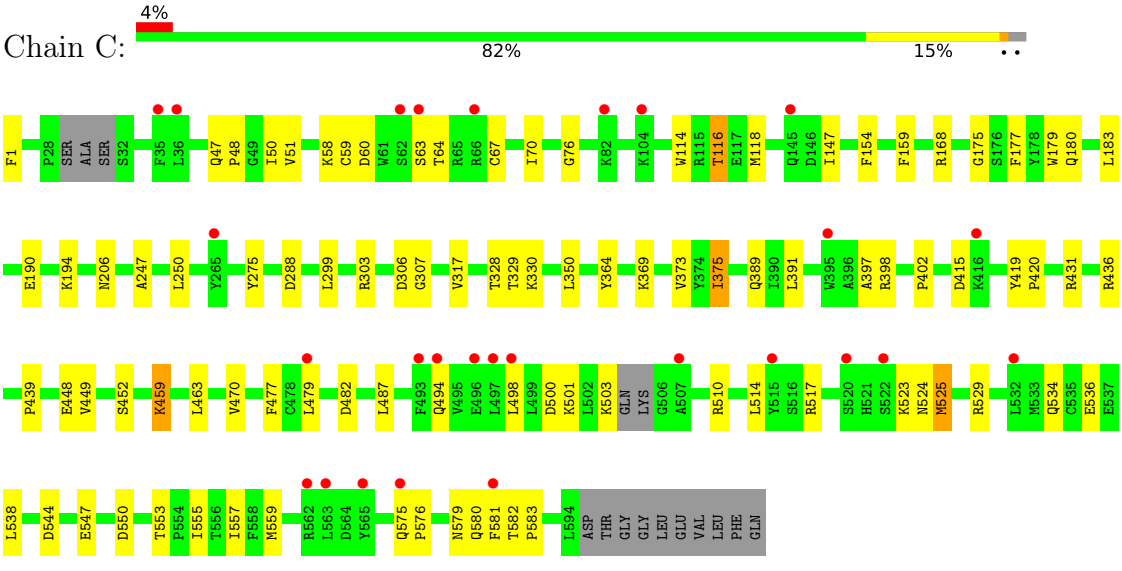
• Molecule 1: Integrin alpha-V heavy chain

Chain A:



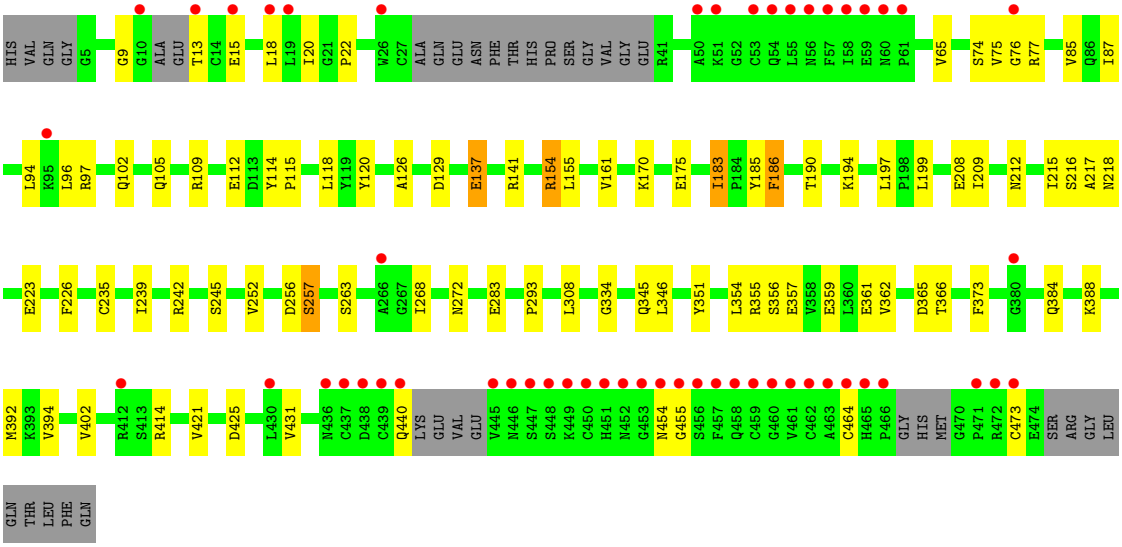
• Molecule 1: Integrin alpha-V heavy chain

Chain C:

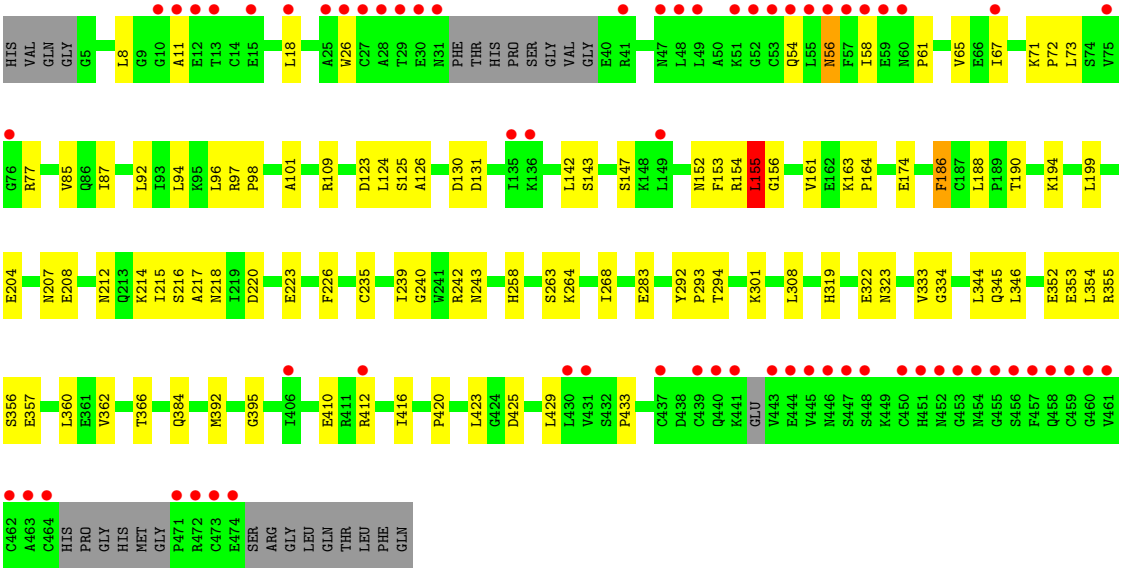


• Molecule 2: Integrin beta-6

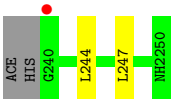
Chain B:



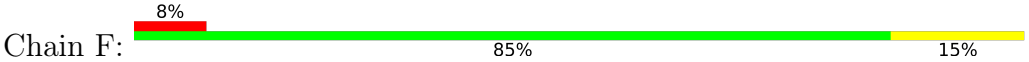
• Molecule 3: Integrin beta-6

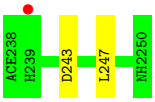


• Molecule 4: Latency-associated peptide



• Molecule 4: Latency-associated peptide





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

Chain G:

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

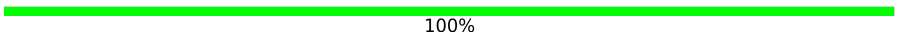
Chain J:

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

Chain K:

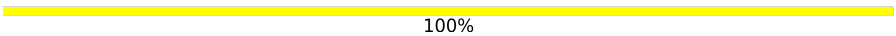
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



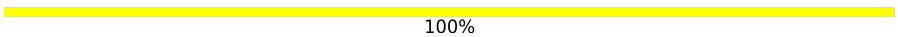
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain P:

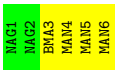


• Molecule 6: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

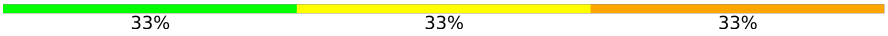
• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[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 N:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	185.02Å 168.09Å 101.80Å 90.00° 98.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-2.50) 94.4 (48.39-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.222 , 0.266 0.226 , 0.271	Depositor DCC
R_{free} test set	1416 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17049	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: NAG, MAN, BMA, MG, NH2, SO4, CA, ACE

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	0.31	0/4705	0.63	2/6370 (0.0%)
1	C	0.32	0/4668	0.65	2/6318 (0.0%)
2	B	0.30	0/3493	0.61	5/4728 (0.1%)
3	D	0.30	0/3544	0.58	3/4797 (0.1%)
4	E	0.21	0/75	0.32	0/95
4	F	0.20	0/87	0.35	0/112
All	All	0.31	0/16572	0.62	12/22420 (0.1%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	186	PHE	CB-CG-CD1	-7.15	115.80	120.80
3	D	186	PHE	CB-CG-CD2	6.99	125.69	120.80
1	A	502	LEU	CA-CB-CG	6.14	129.42	115.30
1	C	116	THR	N-CA-C	-5.88	95.13	111.00
2	B	186	PHE	CB-CG-CD1	-5.87	116.69	120.80

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	4601	0	4452	57	1
1	C	4566	0	4414	56	1
2	B	3433	0	3381	63	0
3	D	3485	0	3431	63	0
4	E	77	0	86	2	0
4	F	89	0	94	2	0
5	G	28	0	25	0	0
5	J	28	0	25	0	0
5	K	28	0	25	0	0
5	L	28	0	25	0	0
5	M	28	0	25	1	0
5	P	28	0	25	1	0
6	H	50	0	43	0	0
7	I	72	0	61	0	0
7	N	72	0	61	1	0
8	O	39	0	34	2	0
9	A	15	0	0	1	0
9	B	5	0	0	0	0
9	C	10	0	0	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
10	C	4	0	0	0	0
10	D	2	0	0	0	0
11	B	1	0	0	0	0
11	D	1	0	0	0	0
12	B	42	0	39	0	0
12	C	28	0	26	0	0
12	D	42	0	39	0	0
13	C	11	0	10	1	0
14	A	85	0	0	0	0
14	B	65	0	0	2	0
14	C	52	0	0	3	0
14	D	25	0	0	4	0
14	E	3	0	0	0	0
All	All	17049	0	16321	241	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 241 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:509:ARG:O	1:A:543:ARG:NH1	2.03	0.91
1:A:494:GLN:NE2	1:A:524:ASN:OD1	2.11	0.84
1:A:10:GLU:H	1:A:65:ARG:HH11	1.35	0.75
3:D:154:ARG:NH2	3:D:240:GLY:O	2.20	0.75
2:B:208:GLU:O	2:B:212:ASN:ND2	2.19	0.74

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:SER:OG	1:C:452:SER:OG[4_555]	2.19	0.01

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	592/604 (98%)	567 (96%)	24 (4%)	1 (0%)	47 68
1	C	583/604 (96%)	564 (97%)	18 (3%)	1 (0%)	47 68
2	B	438/483 (91%)	418 (95%)	20 (5%)	0	100 100
3	D	447/483 (92%)	424 (95%)	21 (5%)	2 (0%)	34 54
4	E	9/13 (69%)	9 (100%)	0	0	100 100
4	F	11/13 (85%)	11 (100%)	0	0	100 100
All	All	2080/2200 (94%)	1993 (96%)	83 (4%)	4 (0%)	47 68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593	LEU
1	C	459	LYS
3	D	8	LEU
3	D	77	ARG

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	487/495 (98%)	480 (99%)	7 (1%)	67 86
1	C	483/495 (98%)	473 (98%)	10 (2%)	53 78
2	B	393/421 (93%)	390 (99%)	3 (1%)	81 93
3	D	398/421 (94%)	392 (98%)	6 (2%)	65 85
4	E	7/8 (88%)	7 (100%)	0	100 100
4	F	8/8 (100%)	8 (100%)	0	100 100
All	All	1776/1848 (96%)	1750 (98%)	26 (2%)	65 85

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	275	TYR
1	C	514	LEU
3	D	384	GLN
1	C	479	LEU
1	C	525	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	GLN
1	C	327	GLN
1	C	494	GLN
1	C	534	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)

31 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	G	1	1,5	14,14,15	0.28	0	17,19,21	0.49	0
5	NAG	G	2	5	14,14,15	0.30	0	17,19,21	0.54	0
6	NAG	H	1	1,6	14,14,15	0.21	0	17,19,21	0.39	0
6	NAG	H	2	6	14,14,15	0.19	0	17,19,21	0.43	0
6	BMA	H	3	6	11,11,12	0.74	0	15,15,17	0.95	0
6	MAN	H	4	6	11,11,12	0.70	0	15,15,17	1.02	2 (13%)
7	NAG	I	1	7,1	14,14,15	0.52	0	17,19,21	0.41	0
7	NAG	I	2	7	14,14,15	0.41	0	17,19,21	0.41	0
7	BMA	I	3	7	11,11,12	0.90	1 (9%)	15,15,17	0.76	0
7	MAN	I	4	7	11,11,12	0.81	1 (9%)	15,15,17	0.91	1 (6%)
7	MAN	I	5	7	11,11,12	0.71	0	15,15,17	1.05	2 (13%)
7	MAN	I	6	7	11,11,12	0.75	1 (9%)	15,15,17	0.94	2 (13%)
5	NAG	J	1	1,5	14,14,15	0.71	0	17,19,21	0.47	0
5	NAG	J	2	5	14,14,15	0.30	0	17,19,21	0.46	0
5	NAG	K	1	1,5	14,14,15	0.53	0	17,19,21	0.66	1 (5%)
5	NAG	K	2	5	14,14,15	0.32	0	17,19,21	0.40	0
5	NAG	L	1	1,5	14,14,15	0.34	0	17,19,21	0.41	0
5	NAG	L	2	5	14,14,15	0.32	0	17,19,21	0.45	0
5	NAG	M	1	1,5	14,14,15	0.20	0	17,19,21	0.49	0
5	NAG	M	2	5	14,14,15	0.22	0	17,19,21	0.48	0
7	NAG	N	1	7,1	14,14,15	0.50	0	17,19,21	0.50	0
7	NAG	N	2	7	14,14,15	0.27	0	17,19,21	0.40	0
7	BMA	N	3	7	11,11,12	0.81	1 (9%)	15,15,17	0.80	1 (6%)
7	MAN	N	4	7	11,11,12	0.66	0	15,15,17	1.07	2 (13%)
7	MAN	N	5	7	11,11,12	0.71	0	15,15,17	1.06	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	N	6	7	11,11,12	0.70	0	15,15,17	0.96	2 (13%)
8	NAG	O	1	8,1	14,14,15	0.74	1 (7%)	17,19,21	0.44	0
8	NAG	O	2	8	14,14,15	0.75	1 (7%)	17,19,21	0.98	1 (5%)
8	BMA	O	3	8	11,11,12	0.98	1 (9%)	15,15,17	2.60	5 (33%)
5	NAG	P	1	1,5	14,14,15	0.46	0	17,19,21	0.41	0
5	NAG	P	2	5	14,14,15	0.45	0	17,19,21	0.51	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	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
6	NAG	H	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	4/6/23/26	0/1/1/1
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1
6	MAN	H	4	6	-	0/2/19/22	0/1/1/1
7	NAG	I	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	1/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	MAN	I	5	7	-	0/2/19/22	0/1/1/1
7	MAN	I	6	7	-	1/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	1/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	0/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	0/6/23/26	0/1/1/1
7	BMA	N	3	7	-	1/2/19/22	0/1/1/1
7	MAN	N	4	7	-	0/2/19/22	0/1/1/1
7	MAN	N	5	7	-	1/2/19/22	0/1/1/1
7	MAN	N	6	7	-	1/2/19/22	0/1/1/1
8	NAG	O	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1
5	NAG	P	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	O	2	NAG	O5-C1	-2.66	1.39	1.43
7	I	3	BMA	O5-C1	-2.55	1.39	1.43
8	O	1	NAG	O5-C1	-2.51	1.39	1.43
8	O	3	BMA	C1-C2	2.43	1.57	1.52
7	I	4	MAN	O5-C1	-2.26	1.40	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	3	BMA	C1-C2-C3	-6.36	101.85	109.67
8	O	3	BMA	O3-C3-C2	5.56	120.63	109.99
8	O	3	BMA	C3-C4-C5	-3.21	104.52	110.24
8	O	2	NAG	O4-C4-C3	-2.87	103.72	110.35
7	I	5	MAN	C1-O5-C5	2.63	115.75	112.19

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	2	NAG	O5-C5-C6-O6
6	H	2	NAG	C8-C7-N2-C2
6	H	2	NAG	O7-C7-N2-C2
5	G	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	O	3	BMA	1	0
5	M	2	NAG	1	0
7	N	4	MAN	1	0
5	P	2	NAG	1	0
7	N	3	BMA	1	0

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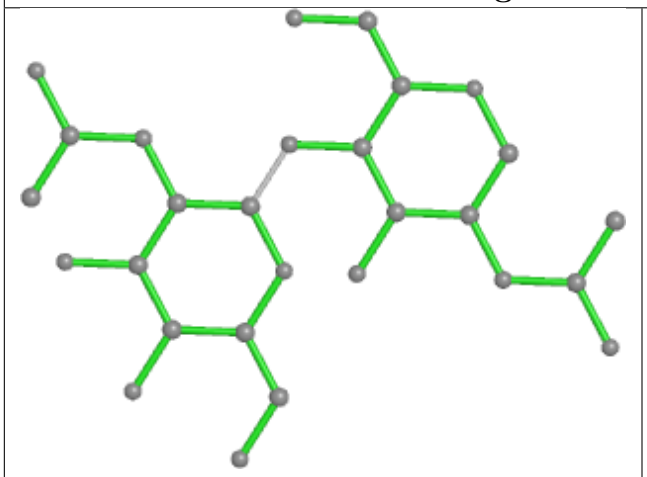
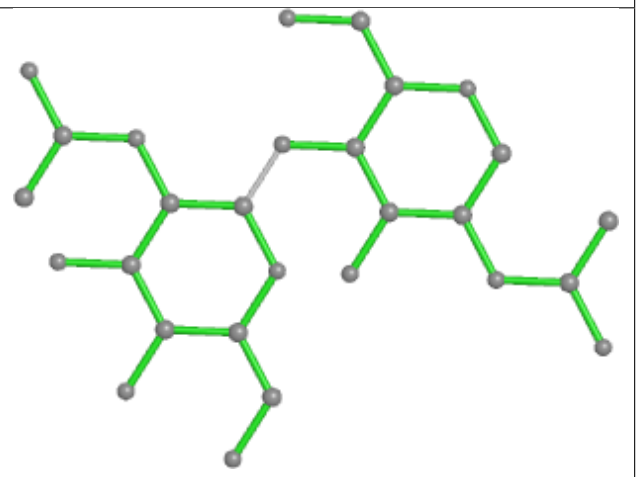
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	O	1	NAG	1	0
5	P	1	NAG	1	0
5	M	1	NAG	1	0
8	O	2	NAG	2	0

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

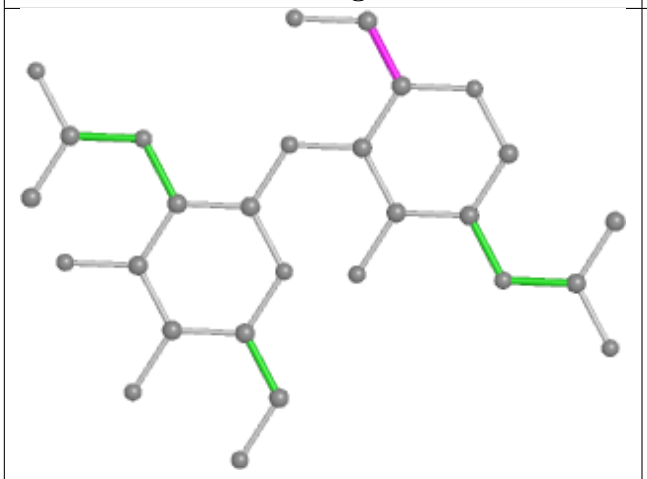
Oligosaccharide Chain G



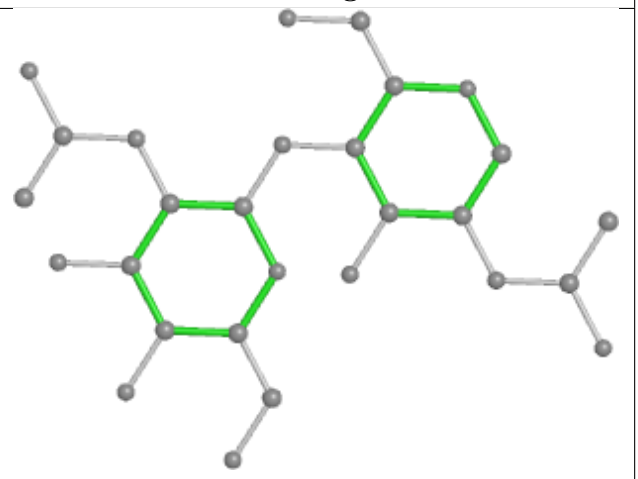
Bond lengths



Bond angles

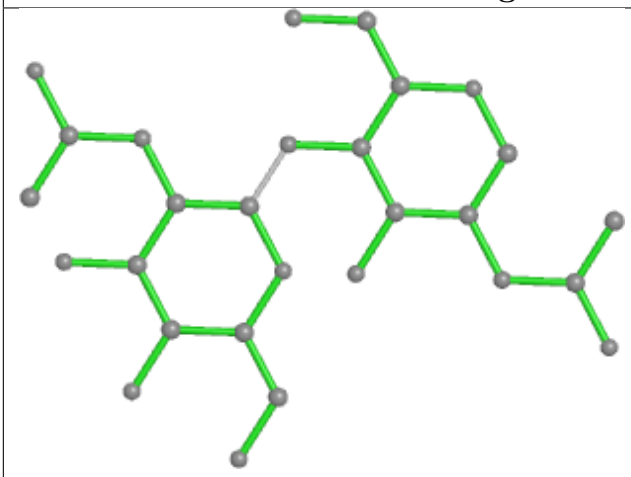


Torsions

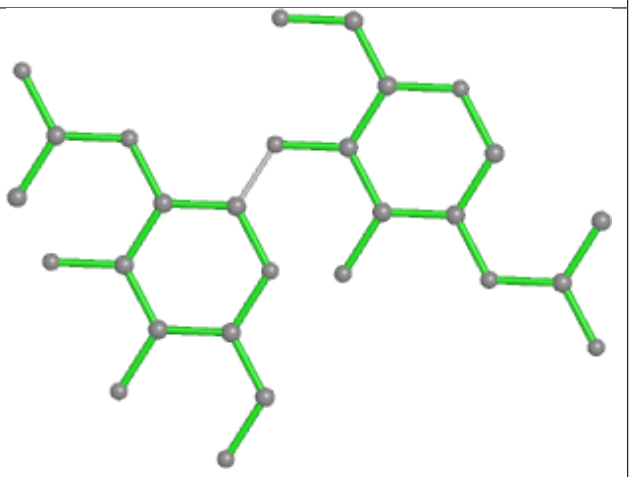


Rings

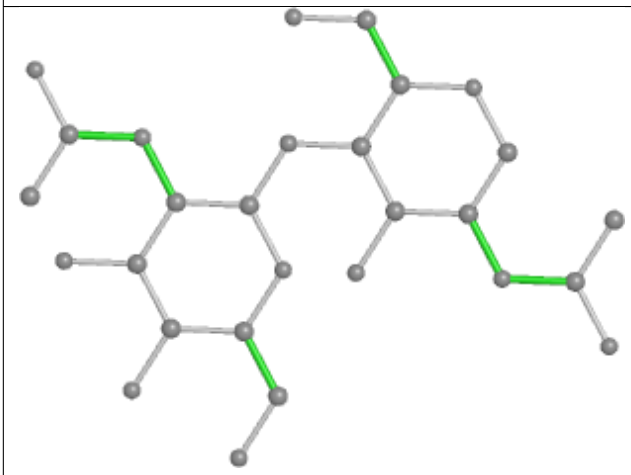
Oligosaccharide Chain J



Bond lengths



Bond angles



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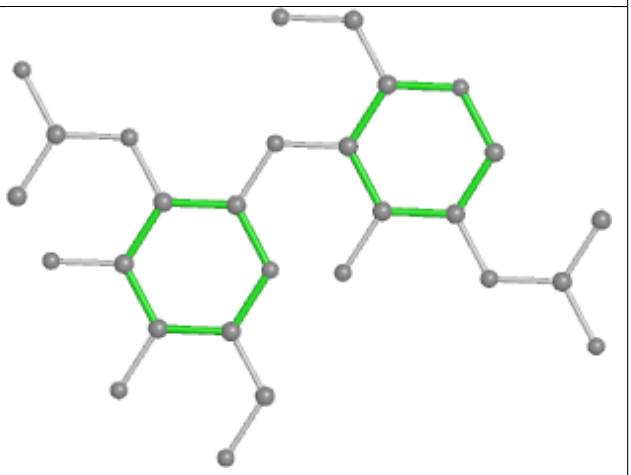
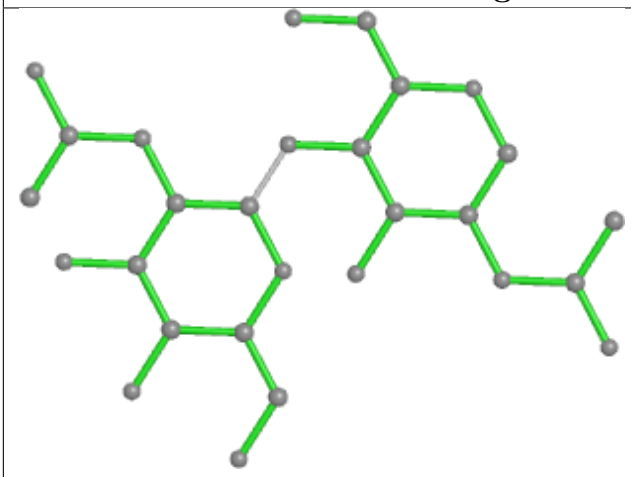
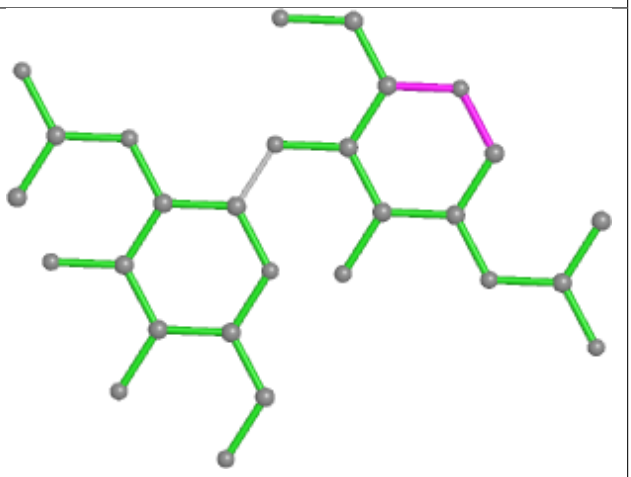


Rings

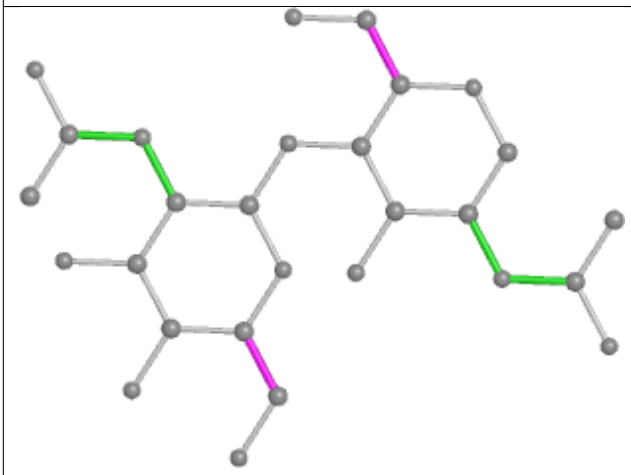
Oligosaccharide Chain K



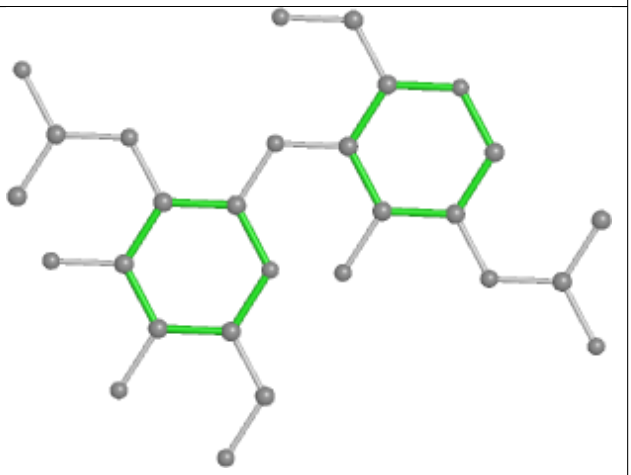
Bond lengths



Bond angles

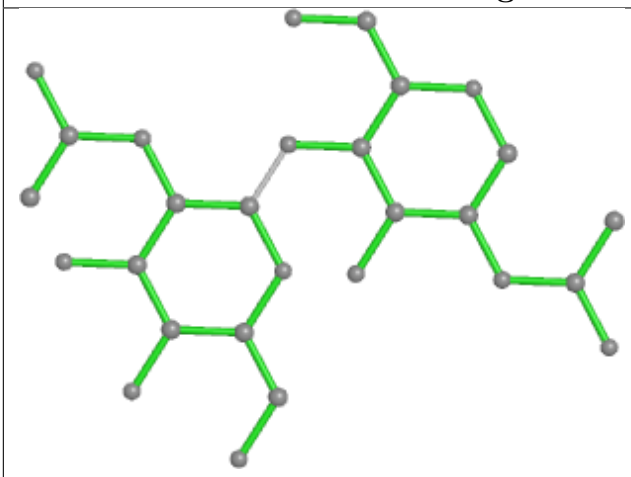


Torsions

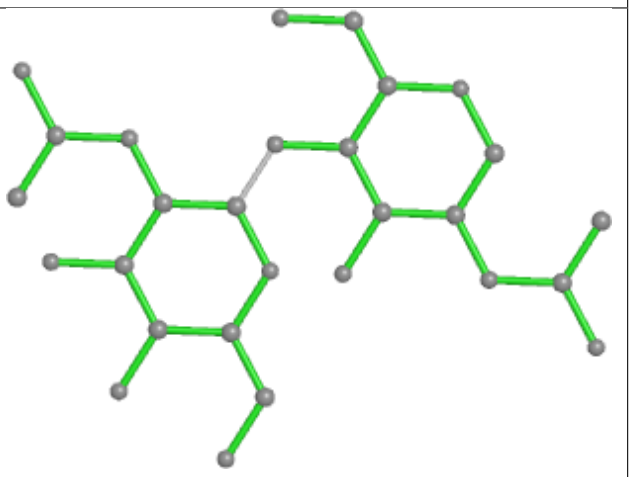


Rings

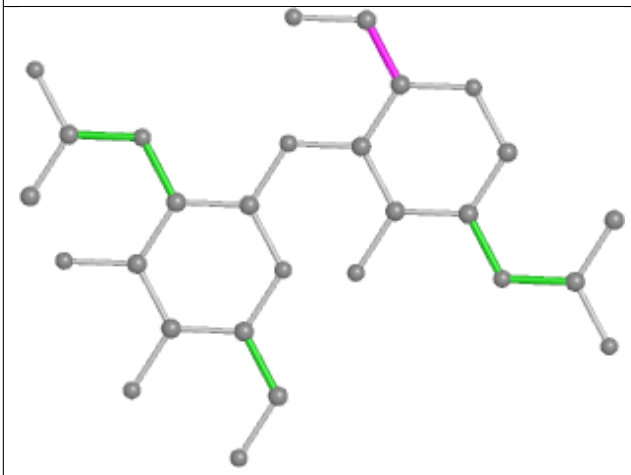
Oligosaccharide Chain L



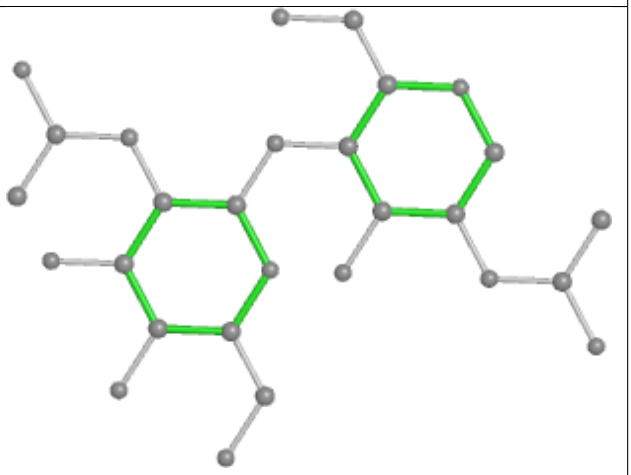
Bond lengths



Bond angles

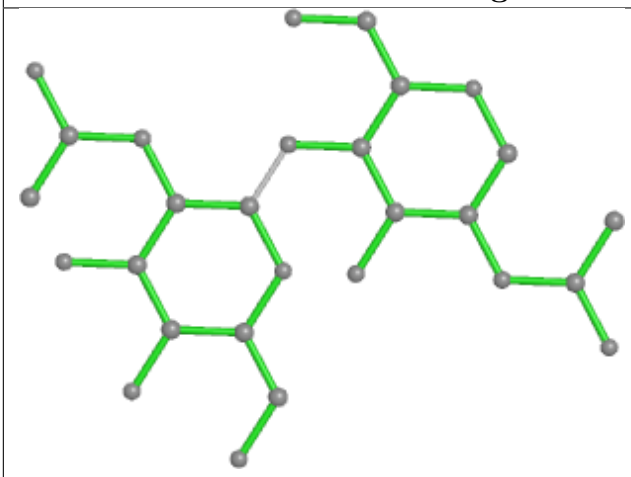


Torsions

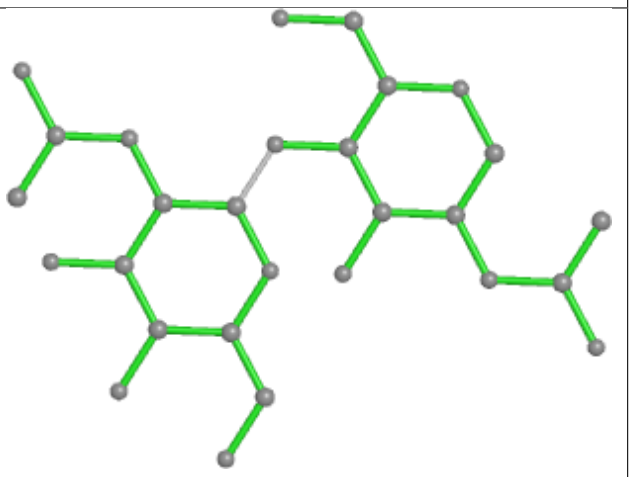


Rings

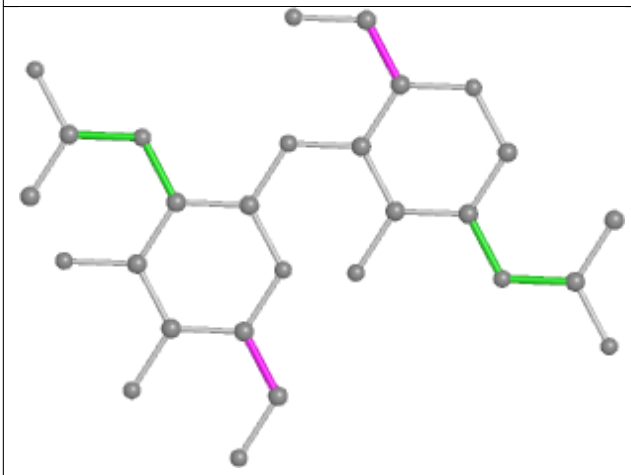
Oligosaccharide Chain M



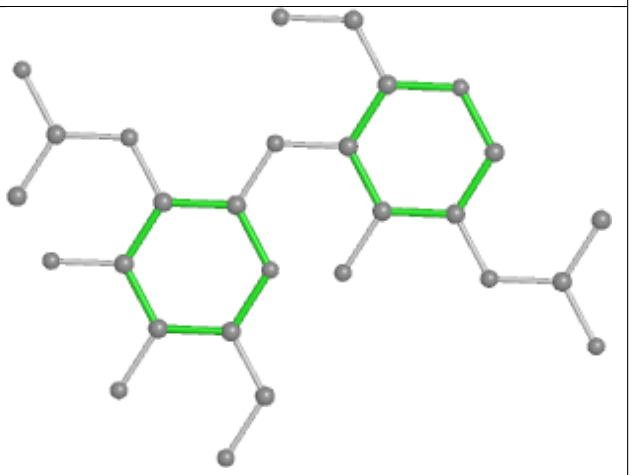
Bond lengths



Bond angles

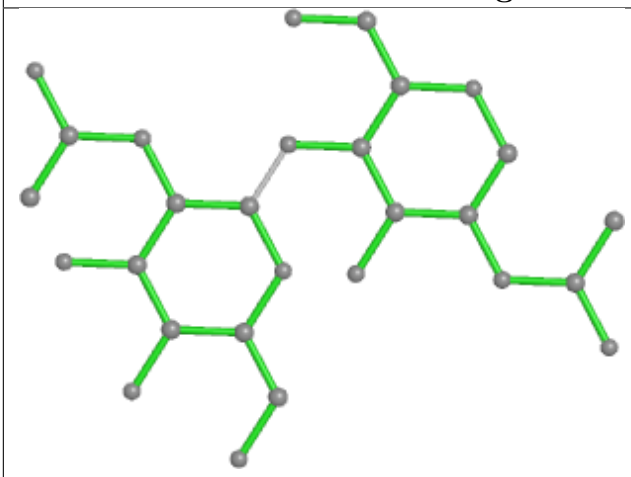


Torsions

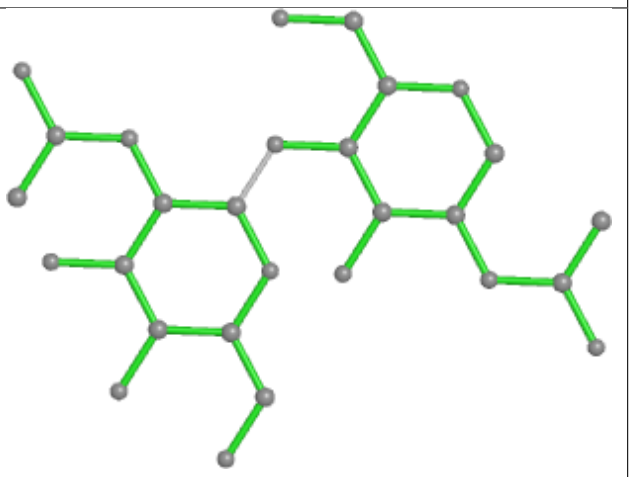


Rings

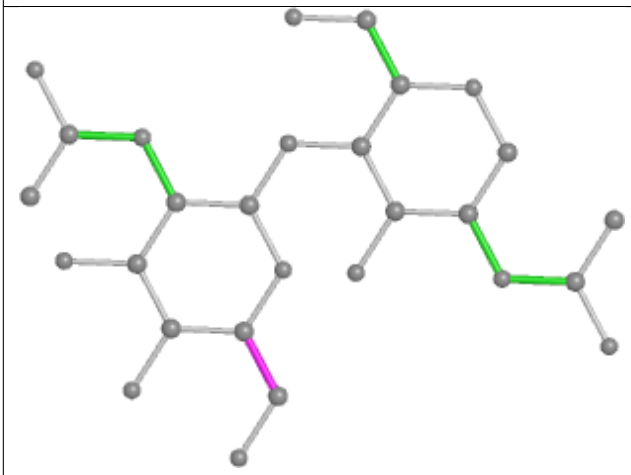
Oligosaccharide Chain P



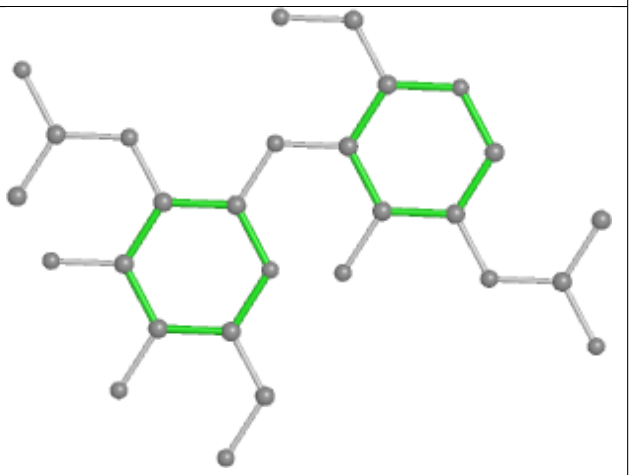
Bond lengths



Bond angles

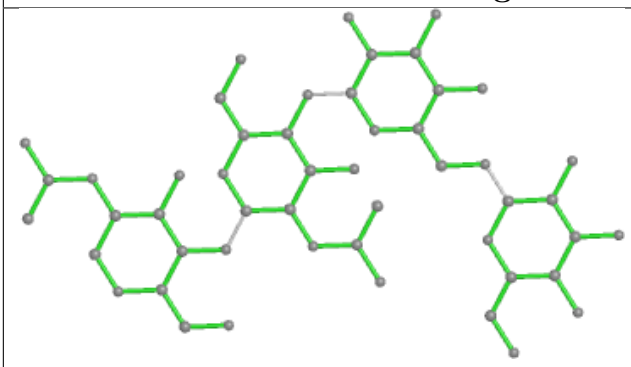


Torsions

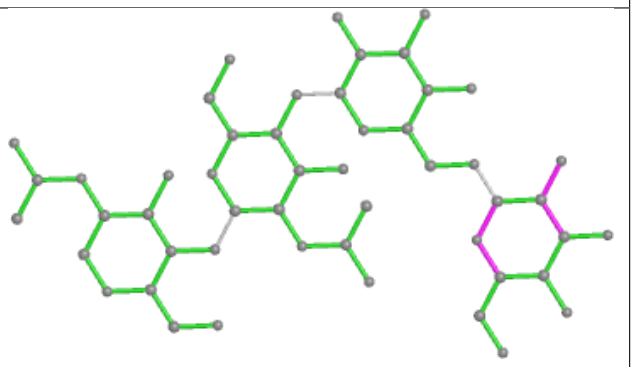


Rings

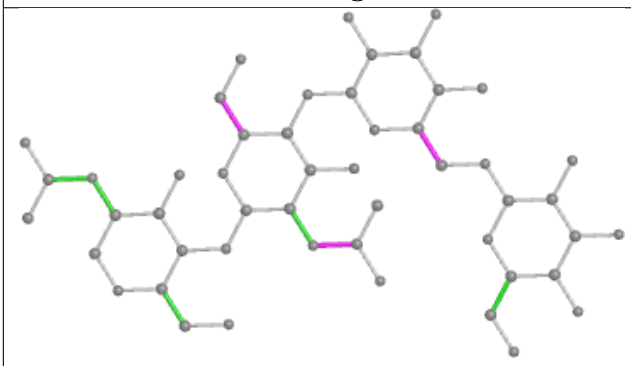
Oligosaccharide Chain H



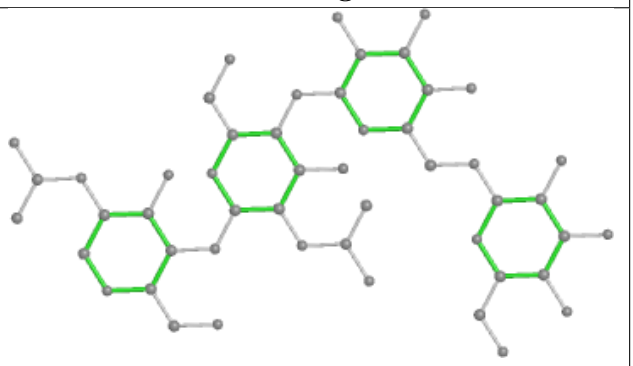
Bond lengths



Bond angles

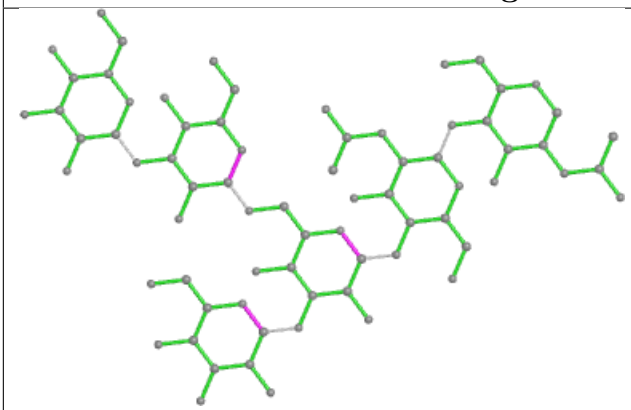


Torsions

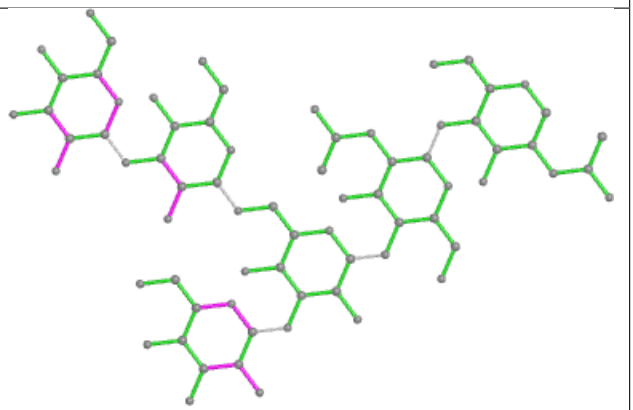


Rings

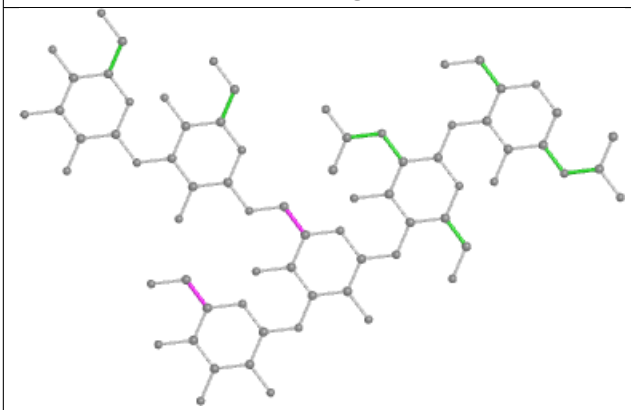
Oligosaccharide Chain I



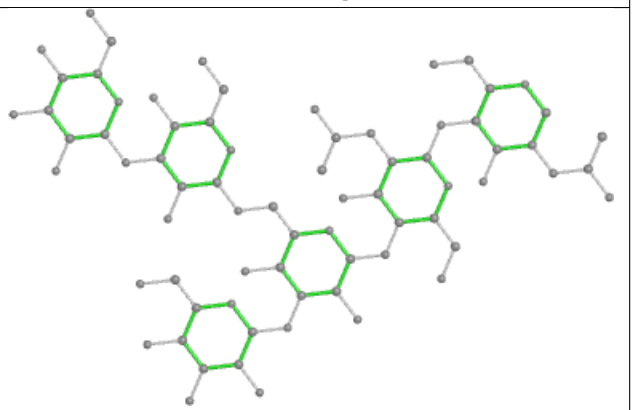
Bond lengths



Bond angles

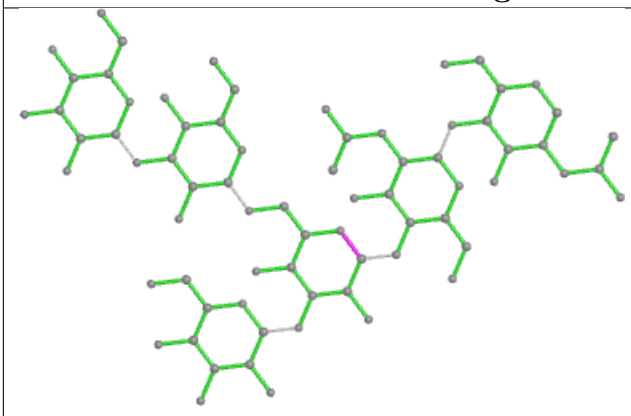


Torsions

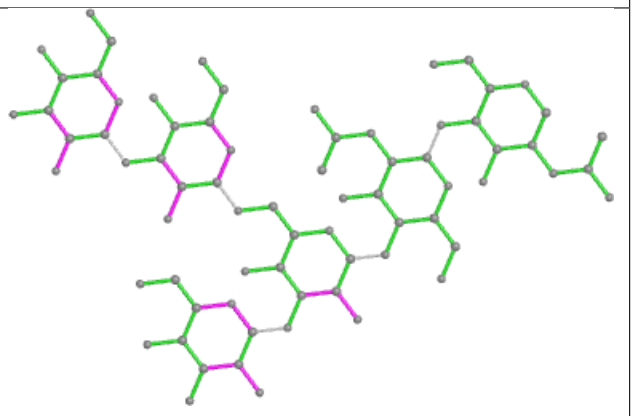


Rings

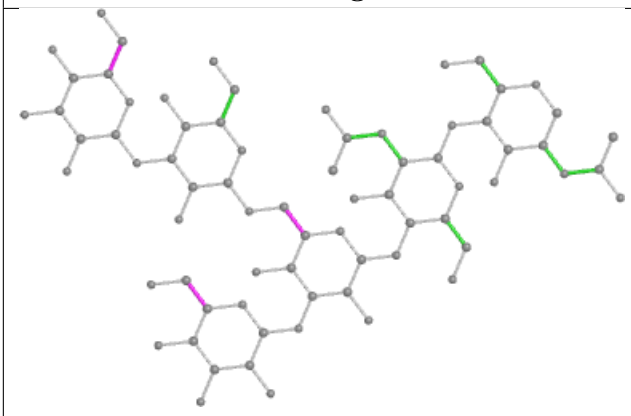
Oligosaccharide Chain N



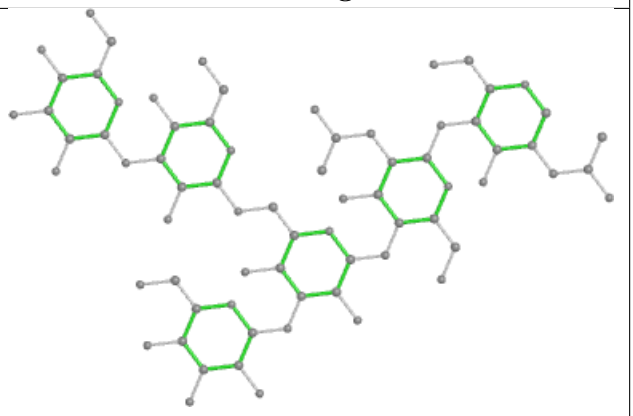
Bond lengths



Bond angles

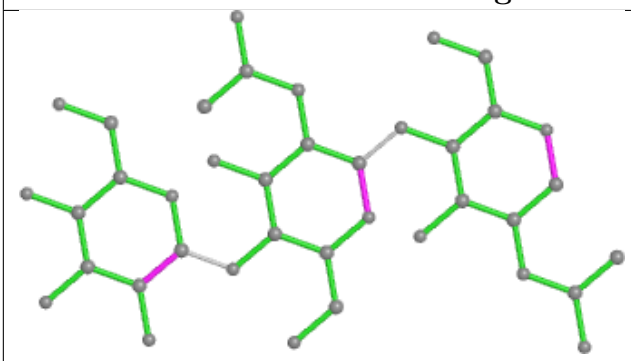


Torsions

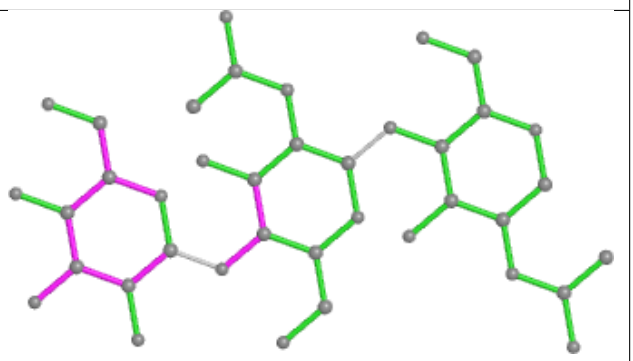


Rings

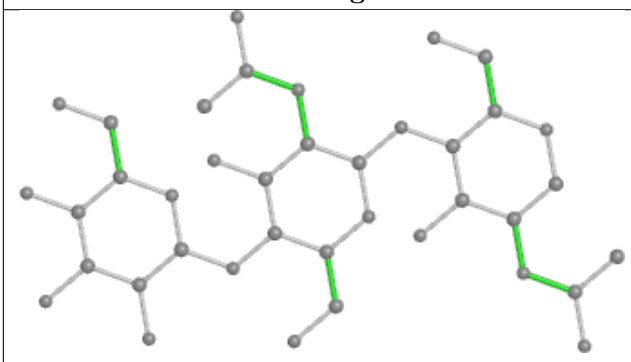
Oligosaccharide Chain O



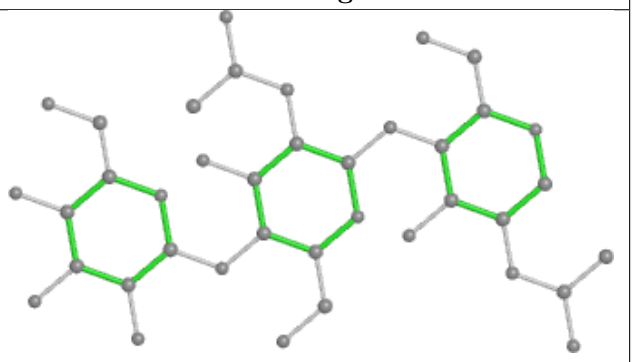
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 14 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
9	SO4	A	701	-	4,4,4	0.15	0	6,6,6	0.11	0
12	NAG	C	709	1	14,14,15	0.43	0	17,19,21	0.42	0
9	SO4	A	703	-	4,4,4	0.14	0	6,6,6	0.13	0
9	SO4	C	701	-	4,4,4	0.14	0	6,6,6	0.11	0
9	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.05	0
12	NAG	C	707	1	14,14,15	0.19	0	17,19,21	0.36	0
12	NAG	B	507	2	14,14,15	0.63	1 (7%)	17,19,21	0.55	0
12	NAG	B	506	2	14,14,15	0.34	0	17,19,21	0.50	0
12	NAG	D	2005	3	14,14,15	0.37	0	17,19,21	0.44	0
9	SO4	A	702	-	4,4,4	0.14	0	6,6,6	0.09	0
12	NAG	D	2004	3	14,14,15	0.33	0	17,19,21	0.57	0
13	MAN	C	708	-	11,11,12	1.52	3 (27%)	15,15,17	1.88	4 (26%)
12	NAG	D	2006	3	14,14,15	0.43	0	17,19,21	0.51	0
12	NAG	B	505	2	14,14,15	0.27	0	17,19,21	0.36	0
9	SO4	C	702	-	4,4,4	0.14	0	6,6,6	0.05	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
12	NAG	C	709	1	-	2/6/23/26	0/1/1/1
12	NAG	C	707	1	-	1/6/23/26	0/1/1/1
12	NAG	B	507	2	-	4/6/23/26	0/1/1/1
12	NAG	B	506	2	-	0/6/23/26	0/1/1/1
12	NAG	D	2005	3	-	3/6/23/26	0/1/1/1
12	NAG	D	2004	3	-	0/6/23/26	0/1/1/1
13	MAN	C	708	-	-	0/2/19/22	0/1/1/1
12	NAG	D	2006	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	B	505	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	708	MAN	O5-C1	-2.81	1.39	1.43
13	C	708	MAN	C1-C2	-2.74	1.45	1.52
13	C	708	MAN	O5-C5	2.19	1.47	1.43
12	B	507	NAG	C1-C2	2.14	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	708	MAN	C1-C2-C3	-4.76	103.81	109.67
13	C	708	MAN	O5-C1-C2	3.21	115.73	110.77
13	C	708	MAN	O2-C2-C3	-3.09	103.95	110.14
13	C	708	MAN	O5-C5-C6	2.03	110.39	107.20

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	2005	NAG	O5-C5-C6-O6
12	B	507	NAG	O5-C5-C6-O6
12	D	2006	NAG	O5-C5-C6-O6
12	B	507	NAG	C4-C5-C6-O6
12	D	2005	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	703	SO4	1	0
13	C	708	MAN	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

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	594/604 (98%)	0.20	14 (2%) 59 62	34, 60, 103, 176	0
1	C	589/604 (97%)	0.30	27 (4%) 32 34	41, 71, 110, 204	0
2	B	448/483 (92%)	0.66	53 (11%) 4 4	25, 61, 148, 228	0
3	D	455/483 (94%)	0.83	66 (14%) 2 2	29, 66, 174, 227	0
4	E	10/13 (76%)	0.56	1 (10%) 7 6	57, 61, 107, 111	0
4	F	11/13 (84%)	0.50	1 (9%) 9 9	53, 67, 103, 157	0
All	All	2107/2200 (95%)	0.47	162 (7%) 13 13	25, 65, 141, 228	0

The worst 5 of 162 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	473	CYS	13.2
3	D	452	ASN	10.9
3	D	458	GLN	9.2
2	B	462	CYS	8.7
3	D	448	SER	8.2

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

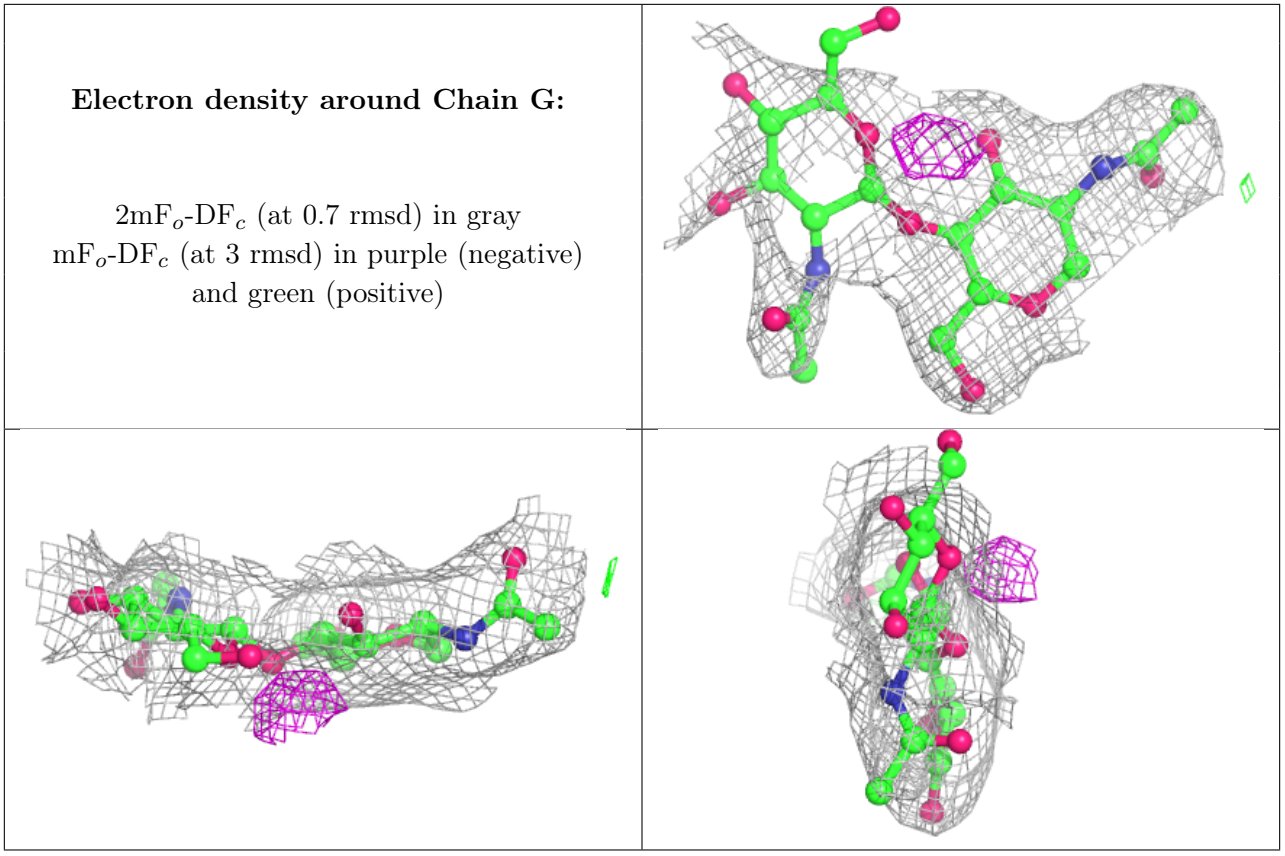
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	NAG	P	2	14/15	0.58	0.38	174,184,193,200	0
6	BMA	H	3	11/12	0.58	0.28	142,152,156,157	0
7	MAN	N	5	11/12	0.65	0.40	155,163,173,177	0
8	BMA	O	3	11/12	0.70	0.21	113,119,152,154	0
5	NAG	K	2	14/15	0.77	0.32	133,157,165,169	0
5	NAG	M	2	14/15	0.79	0.27	76,126,134,141	0
7	MAN	I	5	11/12	0.79	0.40	153,161,166,166	0
5	NAG	K	1	14/15	0.81	0.27	119,129,160,162	0
8	NAG	O	2	14/15	0.81	0.19	106,123,142,150	0
5	NAG	L	2	14/15	0.81	0.32	166,175,183,187	0
7	MAN	N	6	11/12	0.82	0.41	120,148,159,168	0
5	NAG	G	2	14/15	0.82	0.30	110,137,151,156	0
5	NAG	J	2	14/15	0.82	0.18	94,125,134,134	0
7	MAN	I	6	11/12	0.84	0.39	100,135,158,161	0
7	BMA	I	3	11/12	0.85	0.16	107,119,144,153	0
7	MAN	I	4	11/12	0.85	0.27	159,163,172,181	0
6	MAN	H	4	11/12	0.86	0.25	129,146,154,158	0
6	NAG	H	2	14/15	0.87	0.21	76,98,120,144	0
7	MAN	N	4	11/12	0.87	0.28	149,154,169,176	0
5	NAG	L	1	14/15	0.88	0.15	80,106,126,149	0
5	NAG	P	1	14/15	0.90	0.16	91,107,140,155	0
7	BMA	N	3	11/12	0.92	0.11	55,96,131,138	0
5	NAG	J	1	14/15	0.92	0.17	67,82,97,103	0
5	NAG	M	1	14/15	0.94	0.20	68,90,100,117	0
8	NAG	O	1	14/15	0.94	0.09	45,78,89,102	0
7	NAG	I	2	14/15	0.95	0.13	47,80,87,98	0
5	NAG	G	1	14/15	0.96	0.11	45,54,69,72	0
7	NAG	N	2	14/15	0.96	0.12	39,65,89,97	0
7	NAG	I	1	14/15	0.96	0.13	42,49,60,64	0
6	NAG	H	1	14/15	0.97	0.11	46,63,72,79	0
7	NAG	N	1	14/15	0.97	0.12	41,55,65,71	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.

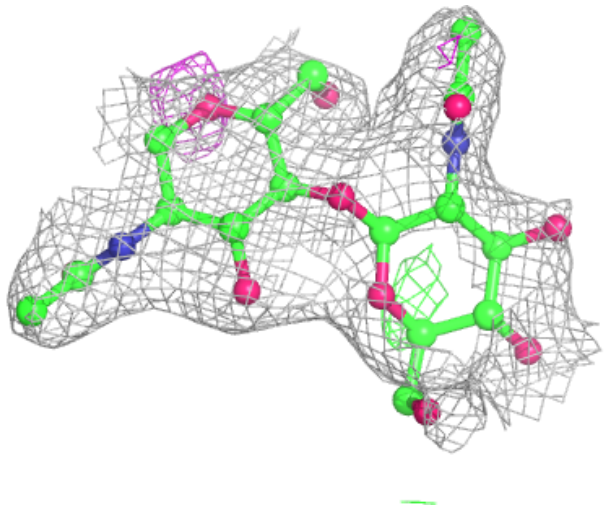
Electron density around Chain G:

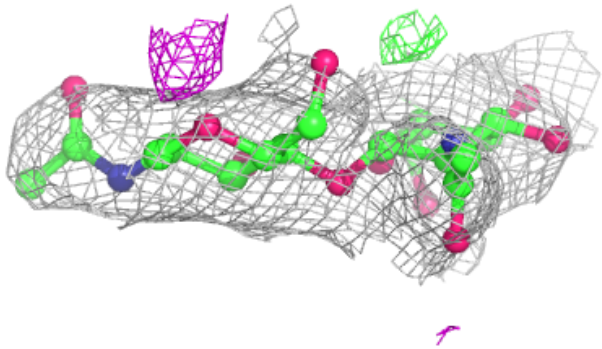
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

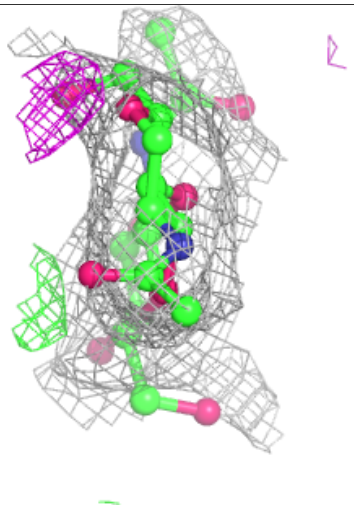


Electron density around Chain J:

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

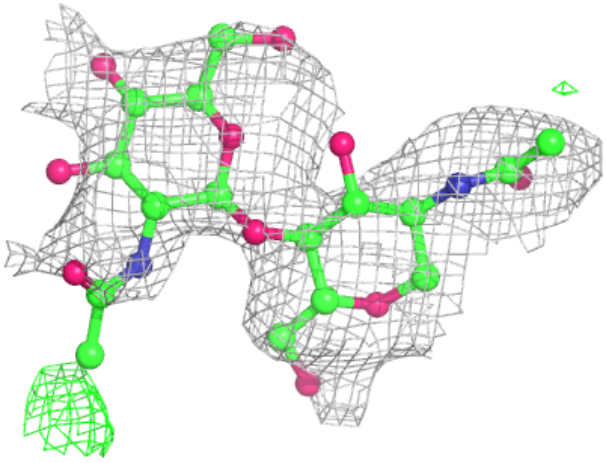


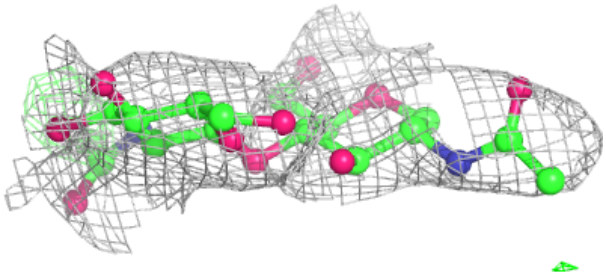


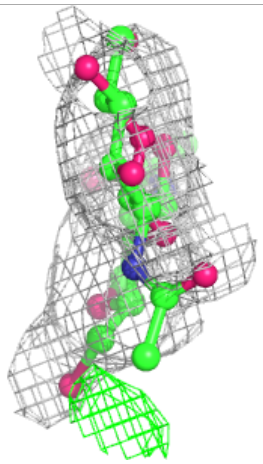


Electron density around Chain K:

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

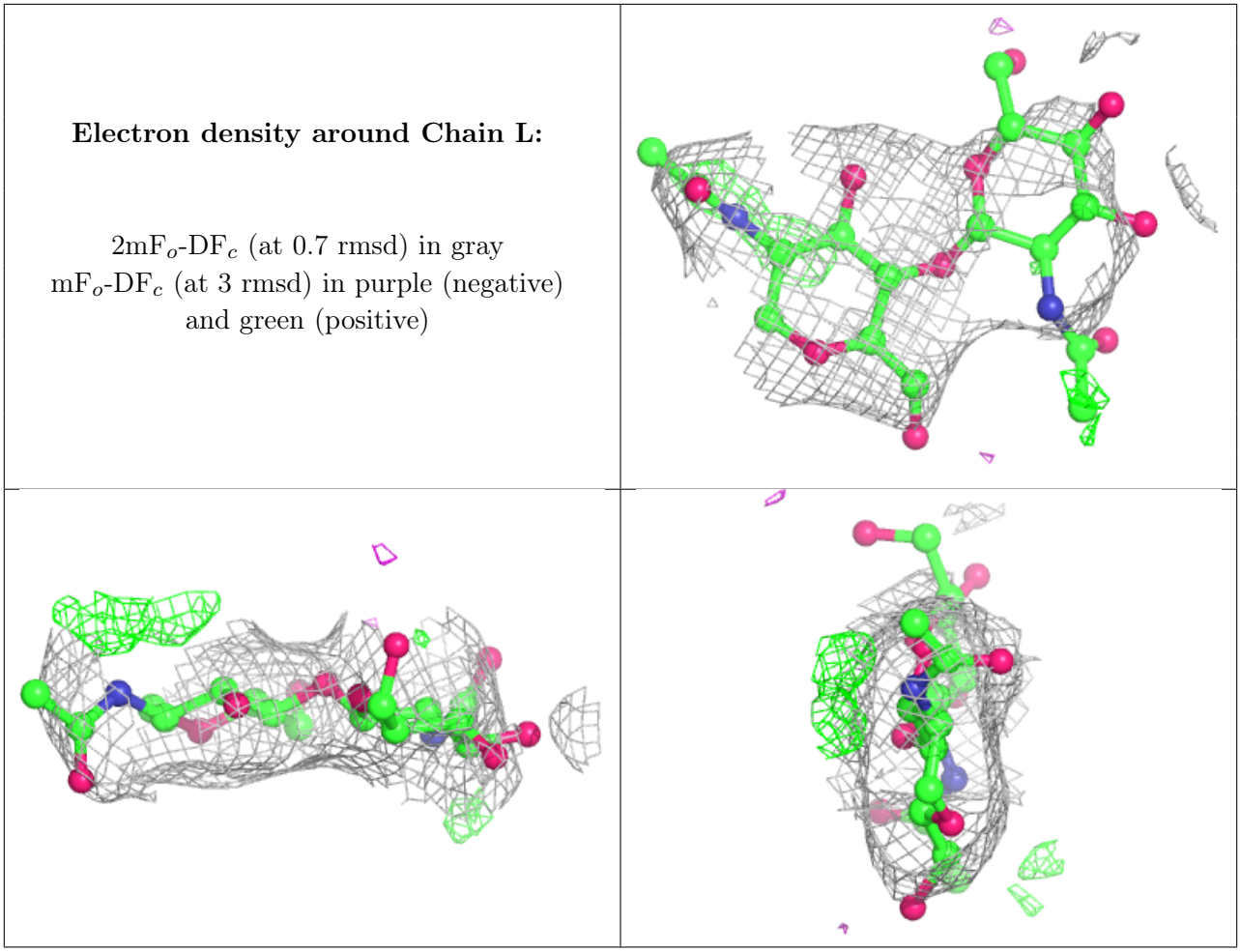






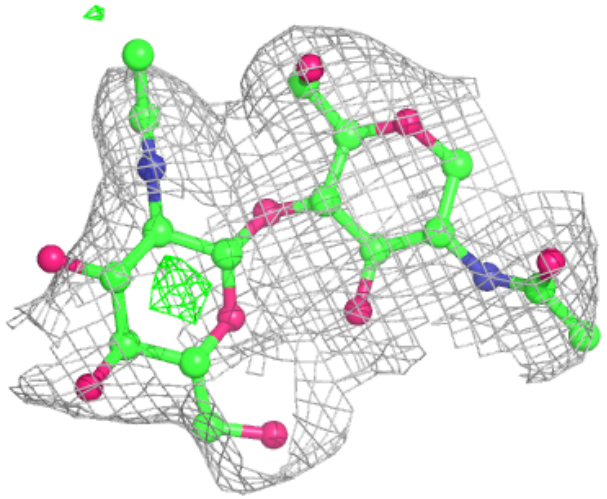
Electron density around Chain L:

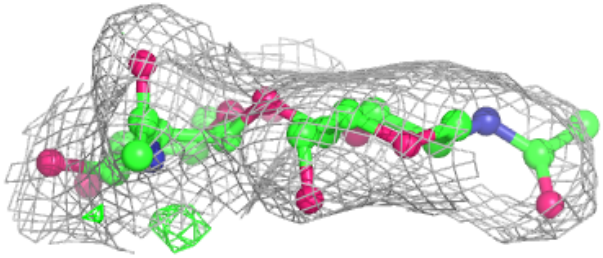
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

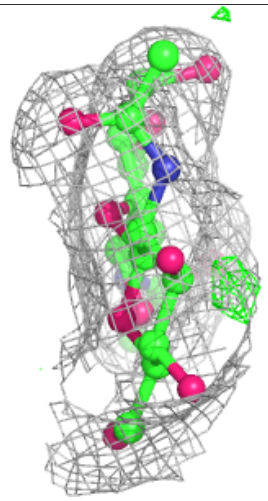


Electron density around Chain M:

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

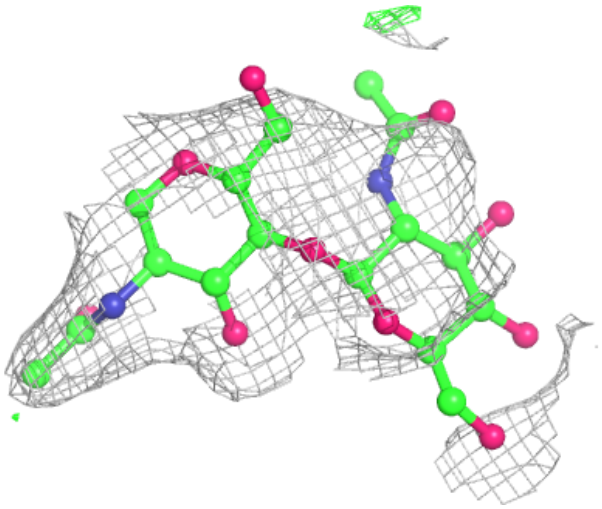


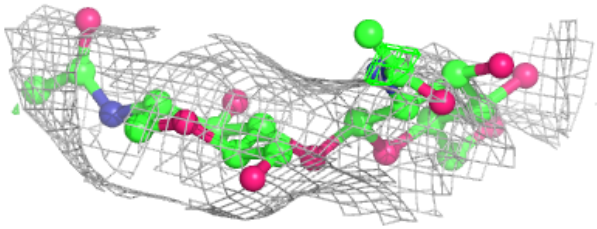


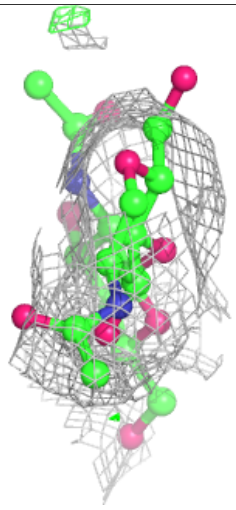


Electron density around Chain P:

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

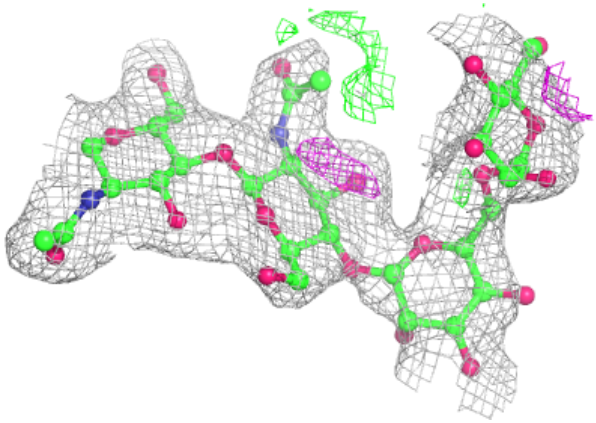


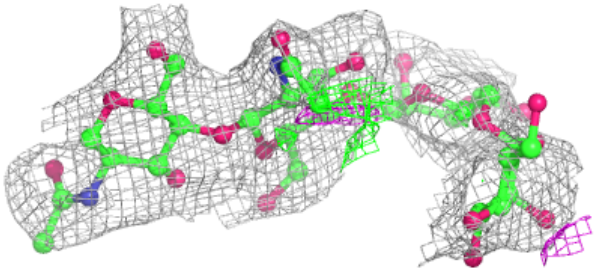


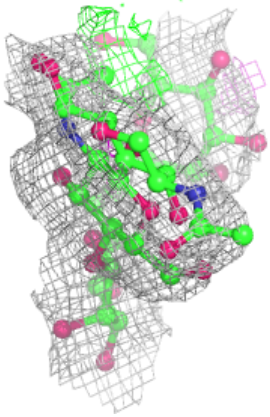


Electron density around Chain H:

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

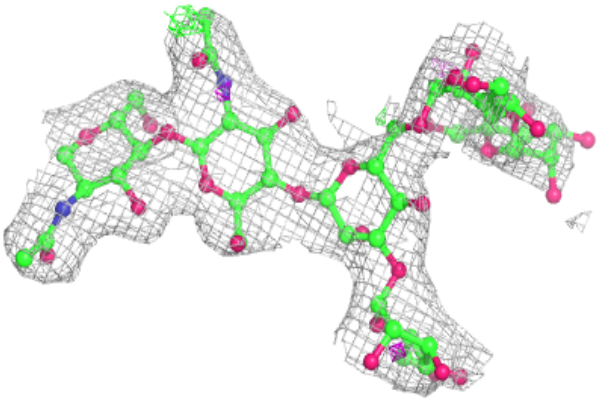


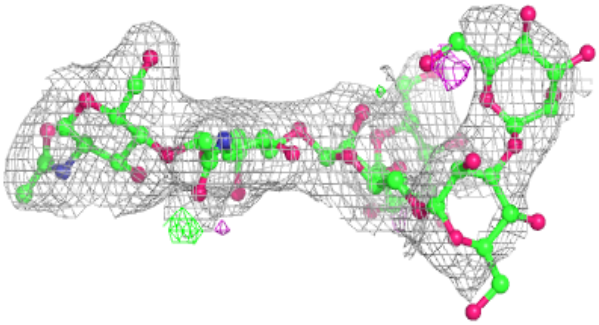


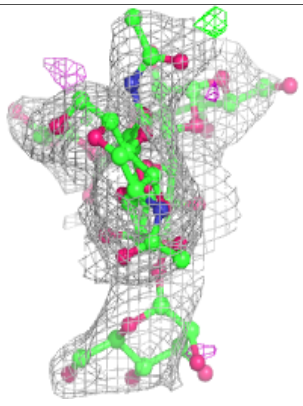


Electron density around Chain I:

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

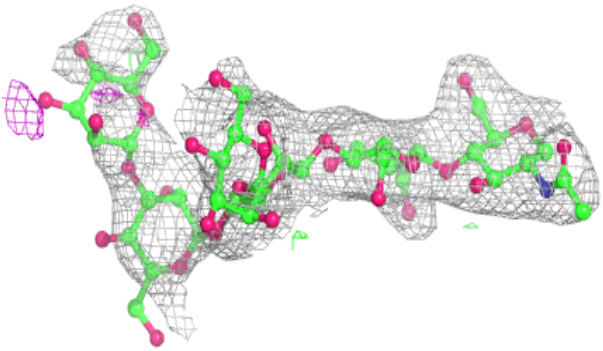


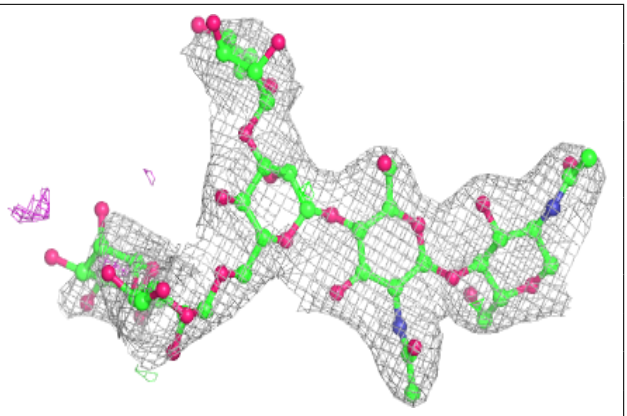


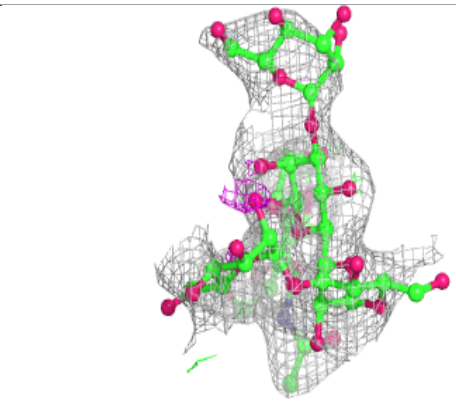


Electron density around Chain N:

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

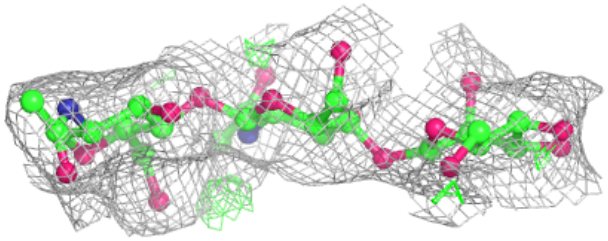


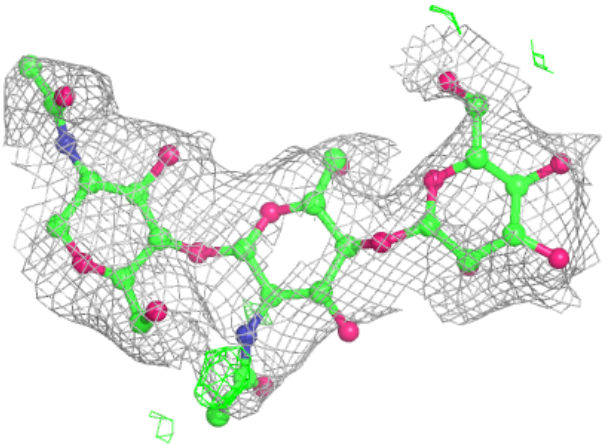


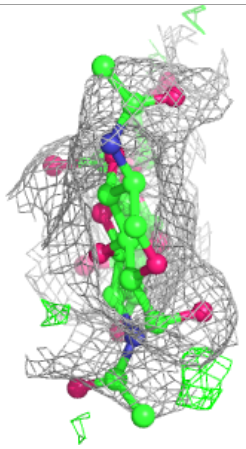


Electron density around Chain O:

$2mF_o$-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
10	CA	C	703	1/1	0.63	0.08	73,73,73,73	0
12	NAG	B	507	14/15	0.64	0.40	118,145,153,162	0
9	SO4	B	501	5/5	0.72	0.38	235,237,244,245	0
12	NAG	D	2004	14/15	0.74	0.48	116,141,156,158	0
12	NAG	D	2005	14/15	0.76	0.25	101,123,128,129	0
10	CA	D	2002	1/1	0.77	0.19	140,140,140,140	0
12	NAG	C	709	14/15	0.77	0.35	116,136,158,159	0
9	SO4	A	702	5/5	0.78	0.19	198,205,206,226	0
12	NAG	D	2006	14/15	0.78	0.21	100,134,147,151	0
12	NAG	B	505	14/15	0.84	0.40	109,130,164,168	0
13	MAN	C	708	11/12	0.85	0.17	98,105,113,115	0
12	NAG	B	506	14/15	0.87	0.18	105,111,118,120	0
12	NAG	C	707	14/15	0.93	0.11	55,65,78,85	0
10	CA	A	704	1/1	0.94	0.13	67,67,67,67	0
10	CA	C	705	1/1	0.94	0.07	66,66,66,66	0
10	CA	B	504	1/1	0.94	0.04	120,120,120,120	0
9	SO4	C	702	5/5	0.95	0.09	107,107,109,109	5
10	CA	C	706	1/1	0.95	0.08	62,62,62,62	0
10	CA	C	704	1/1	0.96	0.12	68,68,68,68	0
10	CA	D	2003	1/1	0.97	0.17	49,49,49,49	0
11	MG	B	502	1/1	0.97	0.09	61,61,61,61	0
11	MG	D	2001	1/1	0.97	0.10	81,81,81,81	0
9	SO4	C	701	5/5	0.97	0.11	66,69,86,93	0
10	CA	A	705	1/1	0.97	0.14	58,58,58,58	0
10	CA	A	706	1/1	0.97	0.13	53,53,53,53	0
9	SO4	A	703	5/5	0.98	0.16	82,89,99,101	0
10	CA	A	707	1/1	0.98	0.10	45,45,45,45	0
9	SO4	A	701	5/5	0.99	0.11	47,47,52,53	5
10	CA	B	503	1/1	0.99	0.18	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.