



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 01:05 PM BST

PDB ID : 6N41
Title : Crystal structure of InvbM.18715.a.KN11: Influenza hemagglutinin from strain A/Netherlands/002P1/1951
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-11-16
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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

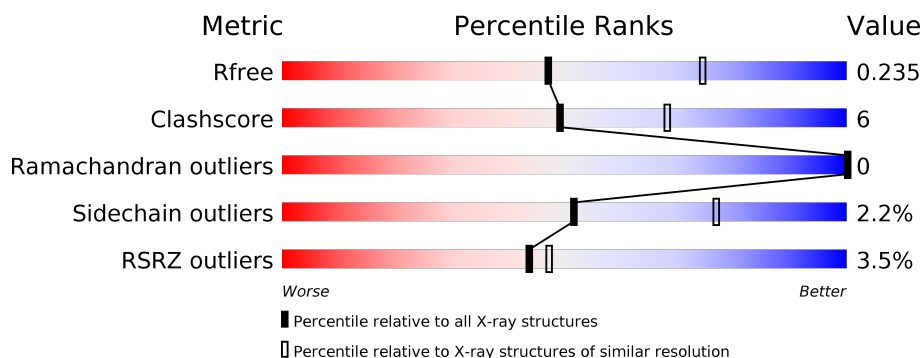
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.




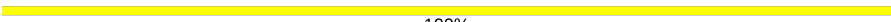
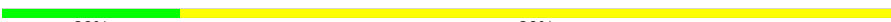
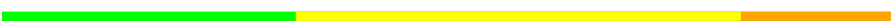
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div></div> </div> <div></div> </div>
1	B	499	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div></div> </div> <div></div> </div>
1	C	499	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div></div> </div> <div></div> </div>
2	D	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
3	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
3	G	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	H	2	 100%
3	I	2	 100%
4	F	5	 20% 80%
5	J	6	 33% 50% 17%

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
6	NAG	C	501	-	-	-	X
6	NAG	C	505	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11831 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.

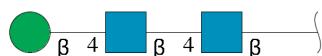
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3690	2307	643	720	20			
1	B	486	Total	C	N	O	S	0	0	0
			3765	2359	653	733	20			
1	C	479	Total	C	N	O	S	0	0	0
			3646	2288	634	704	20			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP E6XTV3
A	2	SER	-	expression tag	UNP E6XTV3
A	495	PHE	-	expression tag	UNP E6XTV3
A	496	LEU	-	expression tag	UNP E6XTV3
A	497	VAL	-	expression tag	UNP E6XTV3
A	498	PRO	-	expression tag	UNP E6XTV3
A	499	ARG	-	expression tag	UNP E6XTV3
B	1	GLY	-	expression tag	UNP E6XTV3
B	2	SER	-	expression tag	UNP E6XTV3
B	495	PHE	-	expression tag	UNP E6XTV3
B	496	LEU	-	expression tag	UNP E6XTV3
B	497	VAL	-	expression tag	UNP E6XTV3
B	498	PRO	-	expression tag	UNP E6XTV3
B	499	ARG	-	expression tag	UNP E6XTV3
C	1	GLY	-	expression tag	UNP E6XTV3
C	2	SER	-	expression tag	UNP E6XTV3
C	495	PHE	-	expression tag	UNP E6XTV3
C	496	LEU	-	expression tag	UNP E6XTV3
C	497	VAL	-	expression tag	UNP E6XTV3
C	498	PRO	-	expression tag	UNP E6XTV3
C	499	ARG	-	expression tag	UNP E6XTV3

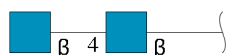
- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



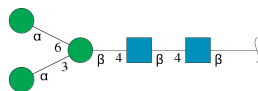
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



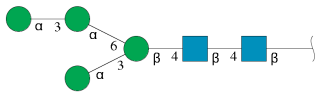
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 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.



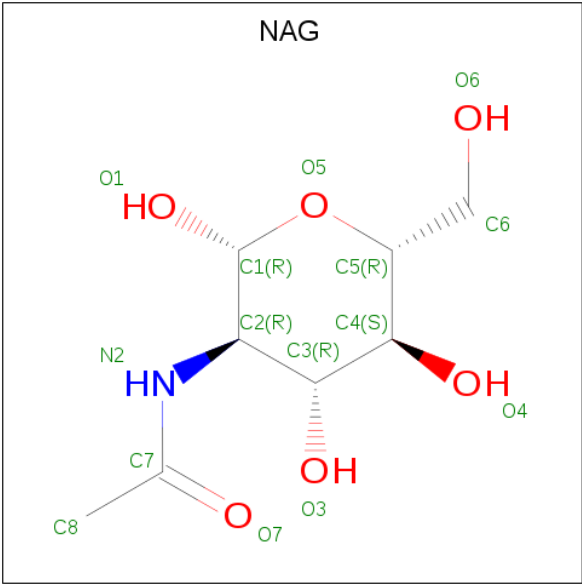
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 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
5	J	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



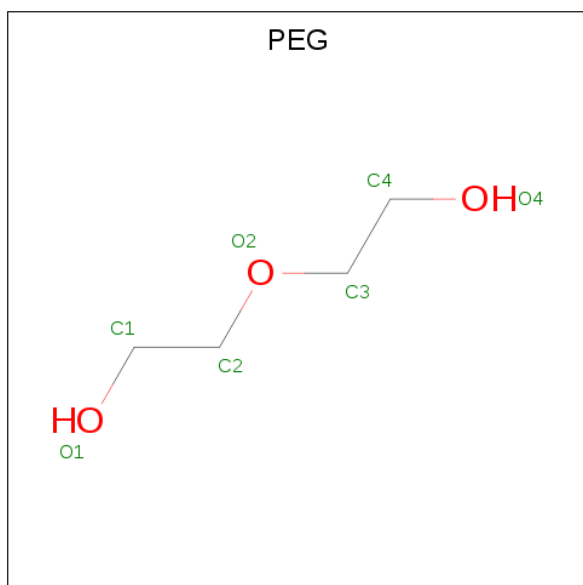
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

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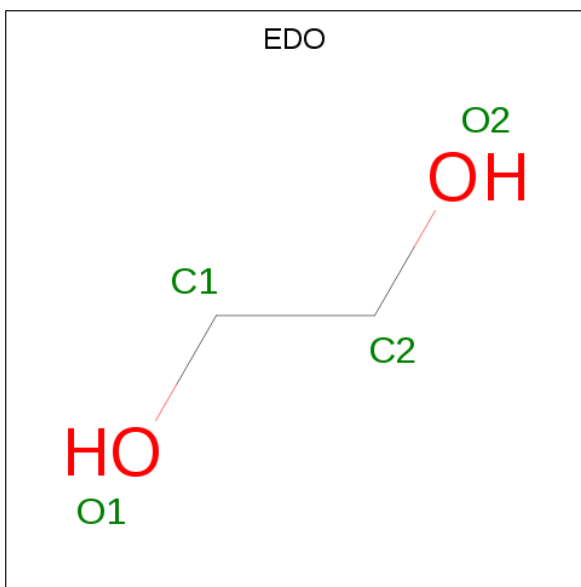
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

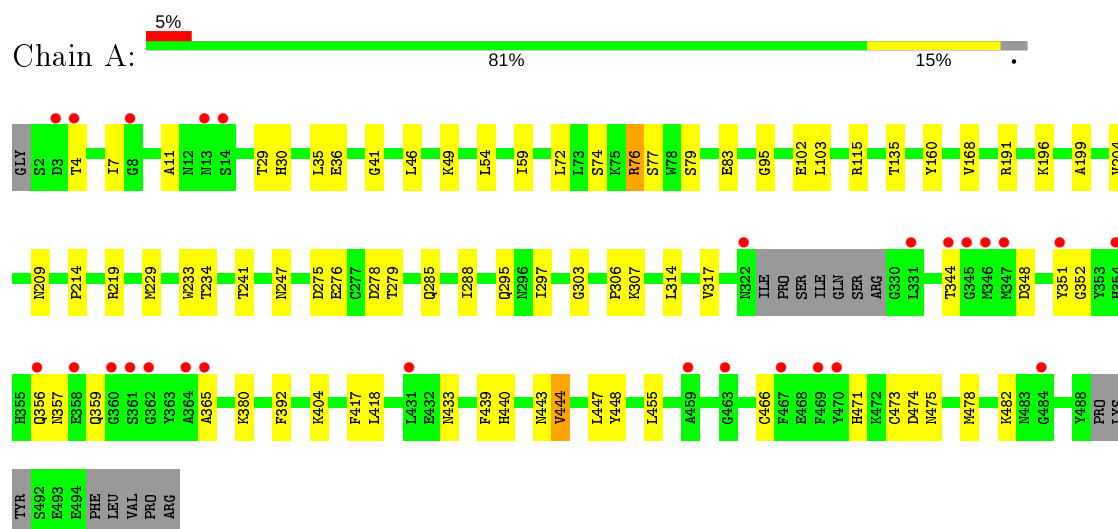
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	82	Total 82	O 82	0	0
9	B	81	Total 81	O 81	0	0
9	C	73	Total 73	O 73	0	0

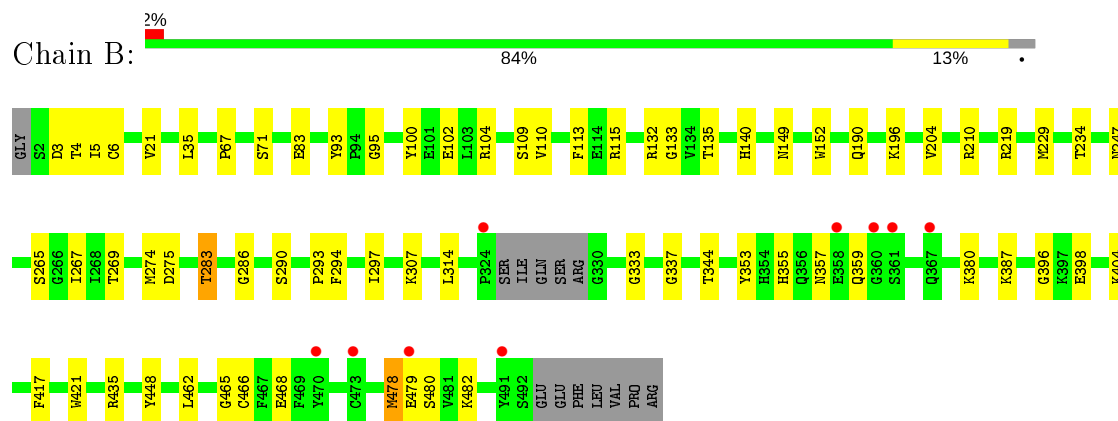
3 Residue-property plots [i](#)

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.

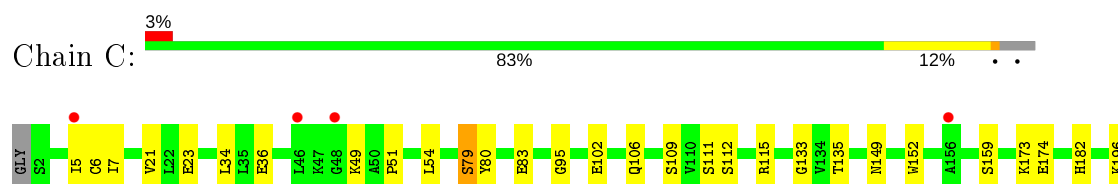
• Molecule 1: Hemagglutinin

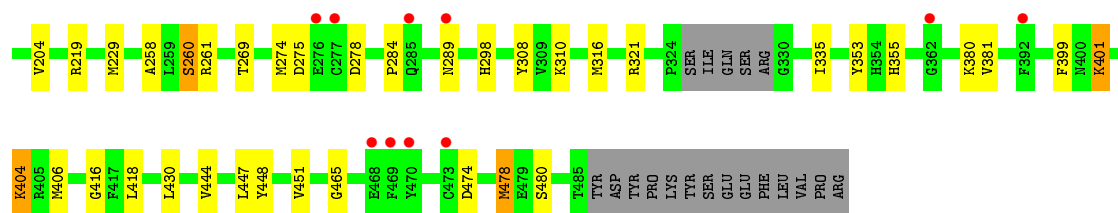


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





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

Chain D: 33% 67%



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

Chain E: 50% 50%



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

Chain G: 50% 50%



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

Chain H: 100%



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

Chain I: 100%



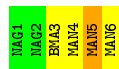
- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  20% 80%



- Molecule 5: α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain J:  33% 50% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.28Å 123.41Å 119.97Å 90.00° 95.54° 90.00°	Depositor
Resolution (Å)	46.27 – 2.50 46.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.27-2.50) 99.9 (46.27-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_3297	Depositor
R, R_{free}	0.187 , 0.235 0.188 , 0.235	Depositor DCC
R_{free} test set	2037 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11831	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, MAN, BMA, NAG, EDO

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	0.40	0/3772	0.59	1/5129 (0.0%)
1	B	0.43	0/3853	0.61	0/5238
1	C	0.40	0/3730	0.57	0/5076
All	All	0.41	0/11355	0.59	1/15443 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3690	0	3392	52	0
1	B	3765	0	3490	45	0
1	C	3646	0	3355	44	0
2	D	39	0	34	0	0
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	28	0	25	0	0
4	F	61	0	52	0	0
5	J	72	0	61	1	0
6	A	28	0	26	0	0
6	B	70	0	65	2	0
6	C	42	0	39	1	0
7	A	7	0	10	2	0
7	B	7	0	10	0	0
8	A	12	0	18	3	0
8	B	24	0	36	7	0
8	C	20	0	30	2	0
9	A	82	0	0	1	0
9	B	81	0	0	3	0
9	C	73	0	0	0	0
All	All	11831	0	10718	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 132 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:C:34:LEU:HD21	1:C:316:MET:HE2	1.72	0.71
1:B:234:THR:HA	8:B:511:EDO:H21	1.75	0.69
1:B:204:VAL:HG11	1:C:219:ARG:HG2	1.77	0.65
1:C:23:GLU:OE1	1:C:321:ARG:NH2	2.24	0.65
8:B:511:EDO:H12	1:C:401:LYS:HD2	1.80	0.63

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	477/499 (96%)	466 (98%)	11 (2%)	0	100	100
1	B	482/499 (97%)	467 (97%)	15 (3%)	0	100	100
1	C	475/499 (95%)	464 (98%)	11 (2%)	0	100	100
All	All	1434/1497 (96%)	1397 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/436 (88%)	374 (97%)	10 (3%)	46	72
1	B	398/436 (91%)	392 (98%)	6 (2%)	65	85
1	C	377/436 (86%)	367 (97%)	10 (3%)	44	71
All	All	1159/1308 (89%)	1133 (98%)	26 (2%)	52	77

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

Mol	Chain	Res	Type
1	B	135	THR
1	B	478	MET
1	C	478	MET
1	B	283	THR
1	B	344	THR

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

22 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	D	1	1,2	14,14,15	0.48	0	17,19,21	0.73	1 (5%)
2	NAG	D	2	2	14,14,15	0.73	0	17,19,21	0.50	0
2	BMA	D	3	2	11,11,12	1.26	1 (9%)	15,15,17	1.13	2 (13%)
3	NAG	E	1	1,3	14,14,15	0.39	0	17,19,21	0.40	0
3	NAG	E	2	3	14,14,15	0.20	0	17,19,21	0.73	1 (5%)
4	NAG	F	1	1,4	14,14,15	0.27	0	17,19,21	0.75	1 (5%)
4	NAG	F	2	4	14,14,15	0.43	0	17,19,21	0.47	0
4	BMA	F	3	4	11,11,12	0.79	0	15,15,17	1.01	1 (6%)
4	MAN	F	4	4	11,11,12	1.17	1 (9%)	15,15,17	1.20	2 (13%)
4	MAN	F	5	4	11,11,12	1.30	2 (18%)	15,15,17	1.13	2 (13%)
3	NAG	G	1	1,3	14,14,15	0.44	0	17,19,21	0.62	0
3	NAG	G	2	3	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
3	NAG	H	1	1,3	14,14,15	0.31	0	17,19,21	1.09	2 (11%)
3	NAG	H	2	3	14,14,15	0.20	0	17,19,21	0.61	1 (5%)
3	NAG	I	1	1,3	14,14,15	0.40	0	17,19,21	1.37	2 (11%)
3	NAG	I	2	3	14,14,15	0.72	1 (7%)	17,19,21	1.28	2 (11%)
5	NAG	J	1	1,5	14,14,15	0.42	0	17,19,21	0.38	0
5	NAG	J	2	5	14,14,15	0.37	0	17,19,21	0.60	0
5	BMA	J	3	5	11,11,12	1.07	1 (9%)	15,15,17	0.96	0
5	MAN	J	4	5	11,11,12	1.51	2 (18%)	15,15,17	2.15	6 (40%)
5	MAN	J	5	5	11,11,12	1.05	0	15,15,17	1.42	2 (13%)
5	MAN	J	6	5	11,11,12	0.99	1 (9%)	15,15,17	1.17	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	MAN	F	5	4	-	2/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
5	MAN	J	4	5	-	1/2/19/22	0/1/1/1
5	MAN	J	5	5	-	1/2/19/22	0/1/1/1
5	MAN	J	6	5	-	2/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4	MAN	C4-C5	3.26	1.59	1.53
5	J	4	MAN	O5-C5	3.13	1.49	1.43
2	D	3	BMA	C4-C3	2.76	1.59	1.52
3	I	2	NAG	O5-C1	-2.34	1.40	1.43
4	F	4	MAN	C1-C2	2.33	1.57	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	4	MAN	C1-O5-C5	5.69	119.90	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C1-O5-C5	4.32	118.05	112.19
5	J	5	MAN	C1-O5-C5	4.15	117.81	112.19
3	I	1	NAG	O4-C4-C5	4.06	119.38	109.30
3	I	1	NAG	C1-O5-C5	3.08	116.36	112.19

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

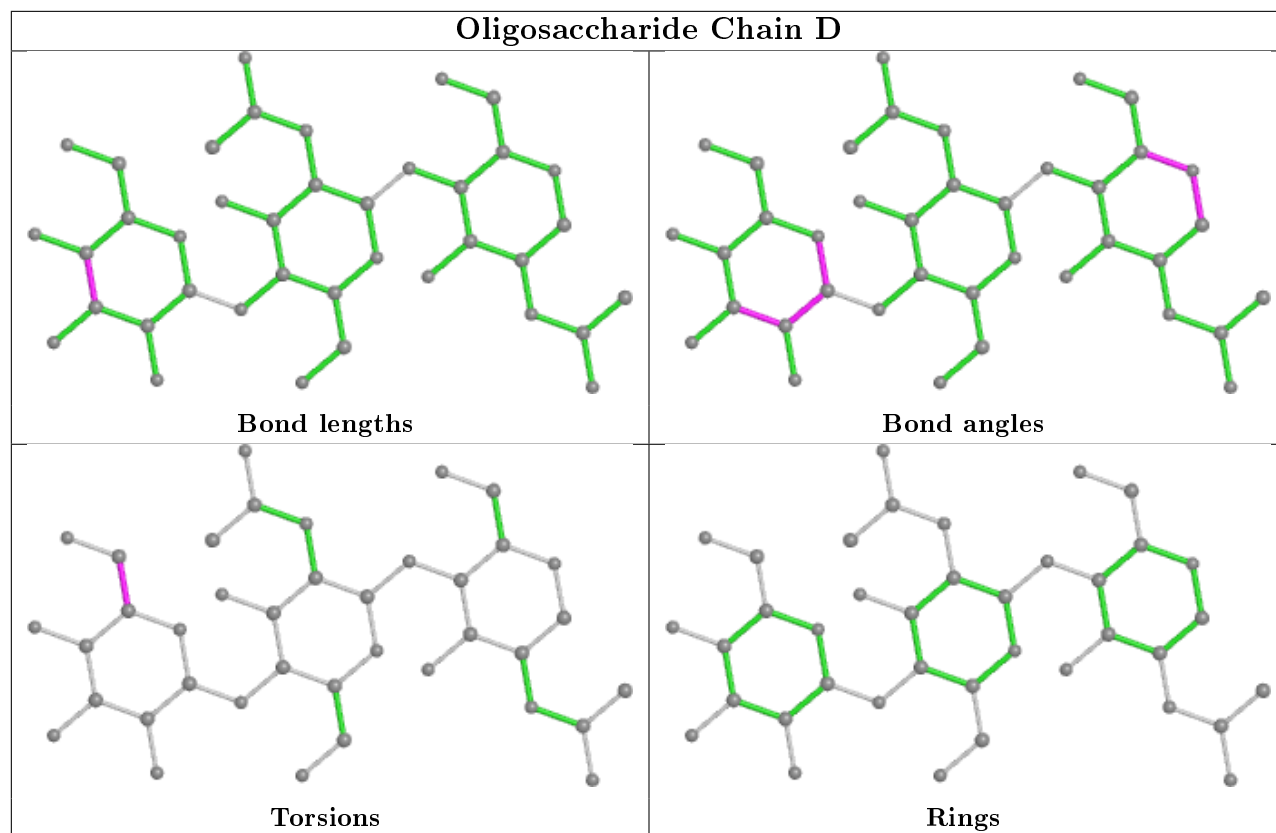
Mol	Chain	Res	Type	Atoms
5	J	2	NAG	O5-C5-C6-O6
4	F	5	MAN	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6

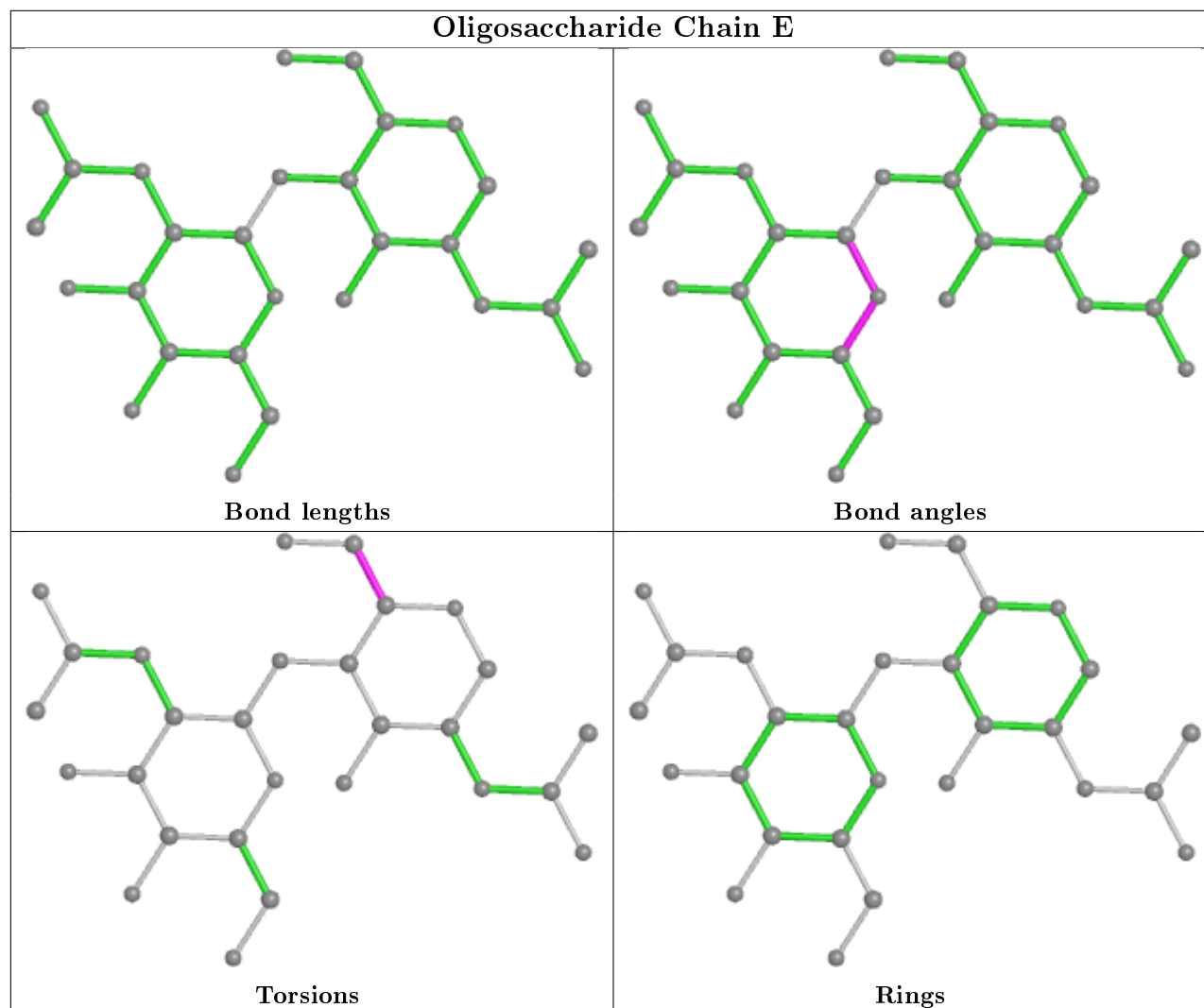
There are no ring outliers.

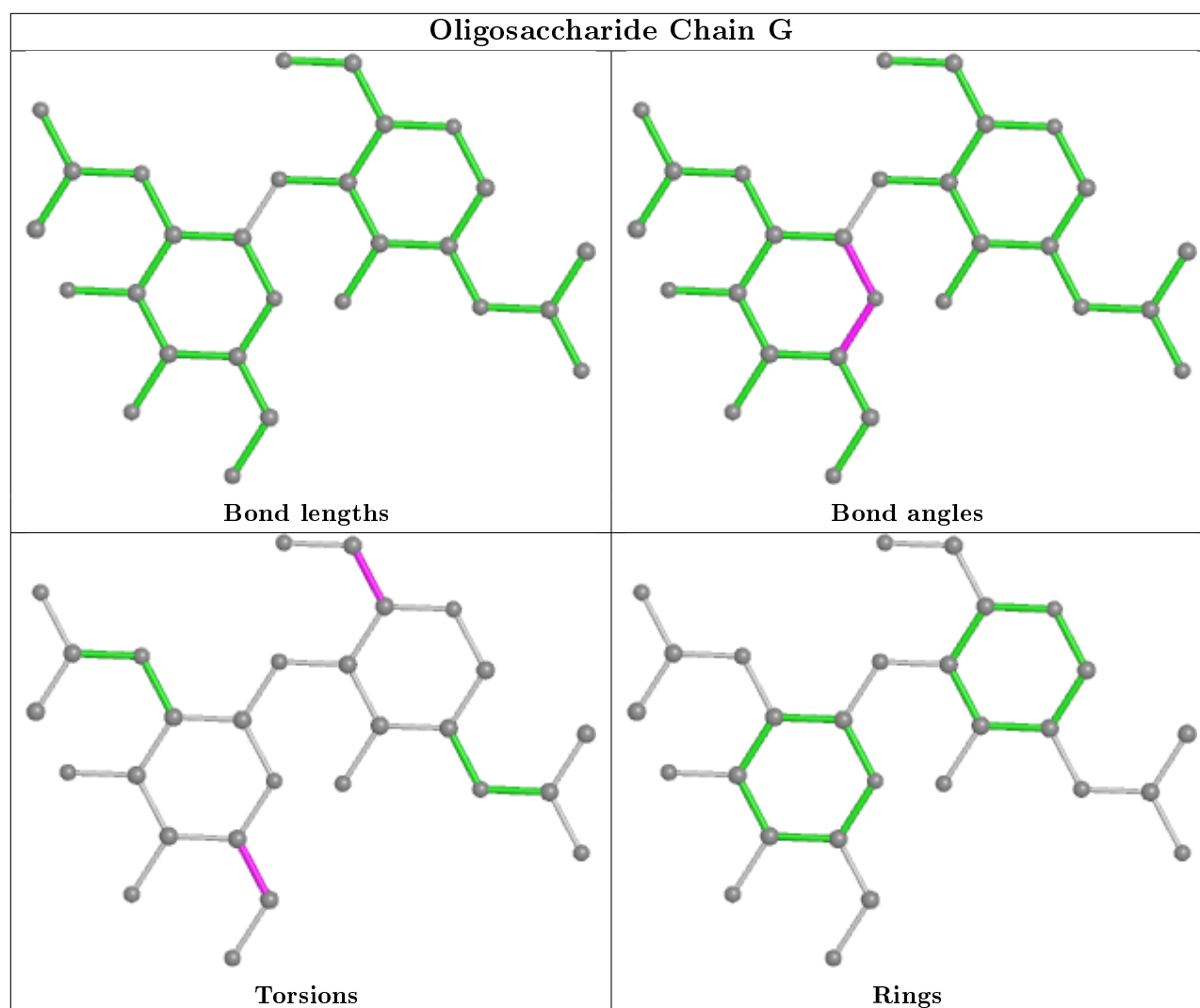
3 monomers are involved in 2 short contacts:

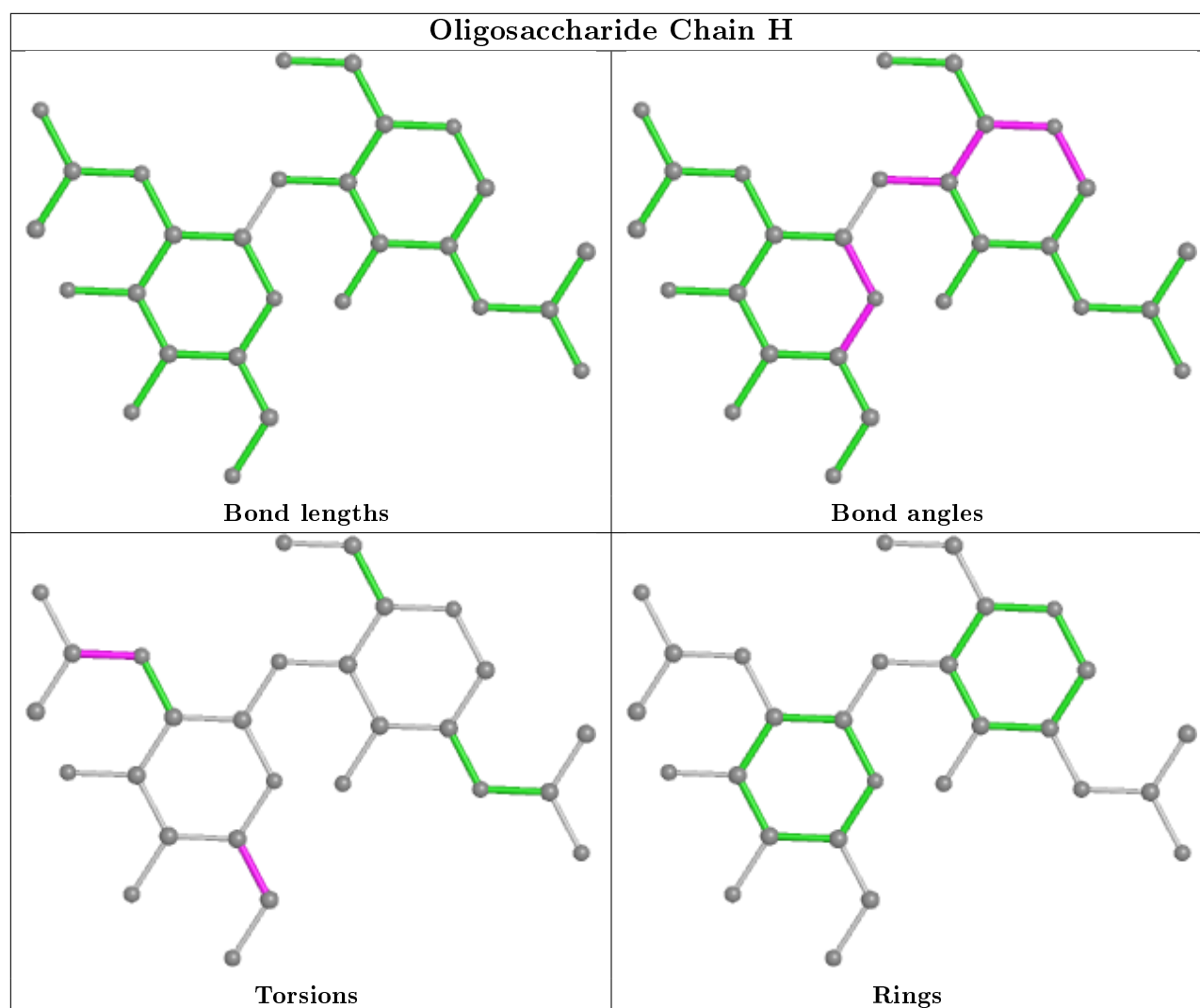
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1	NAG	1	0
3	H	2	NAG	1	0
5	J	5	MAN	1	0

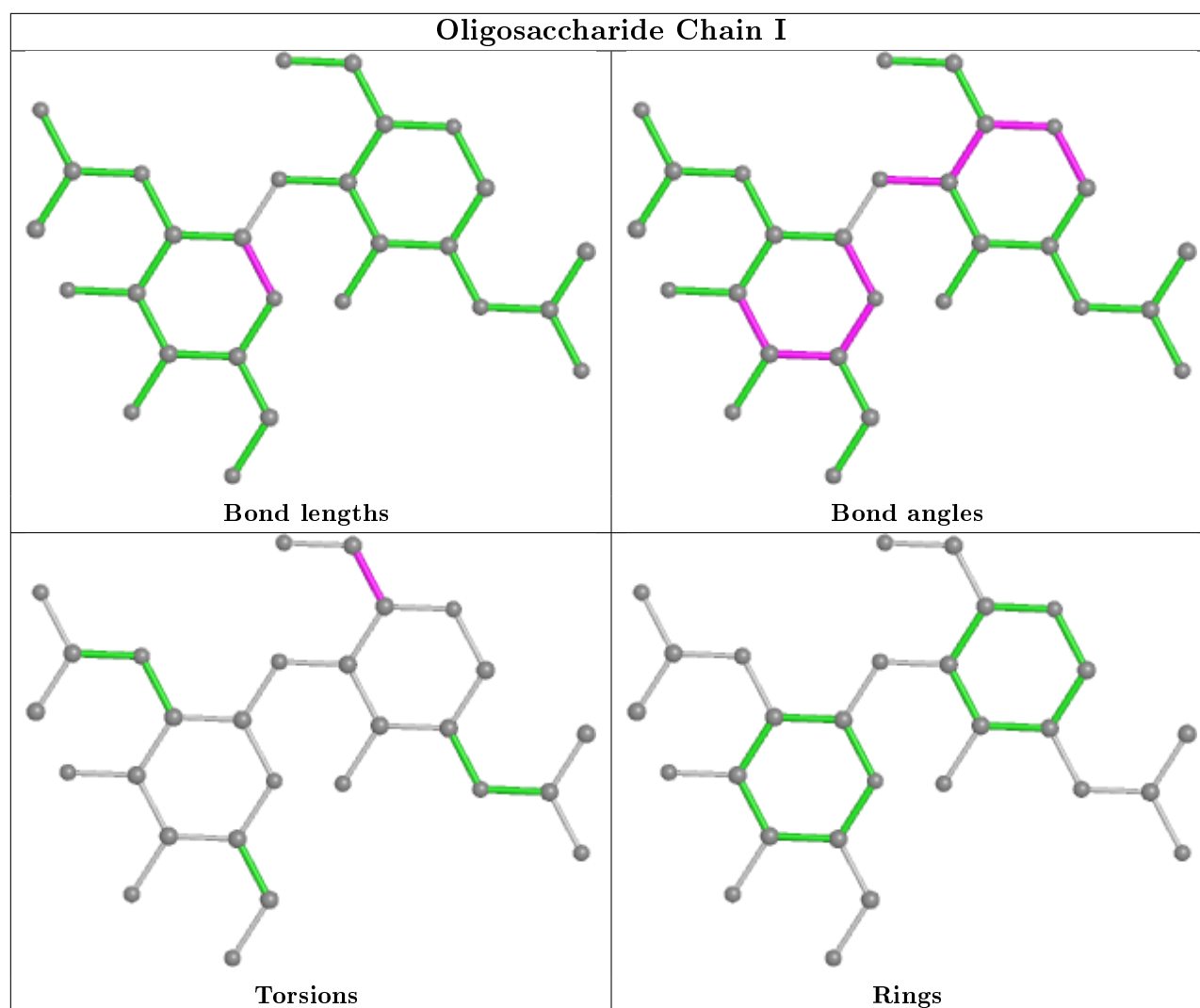
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

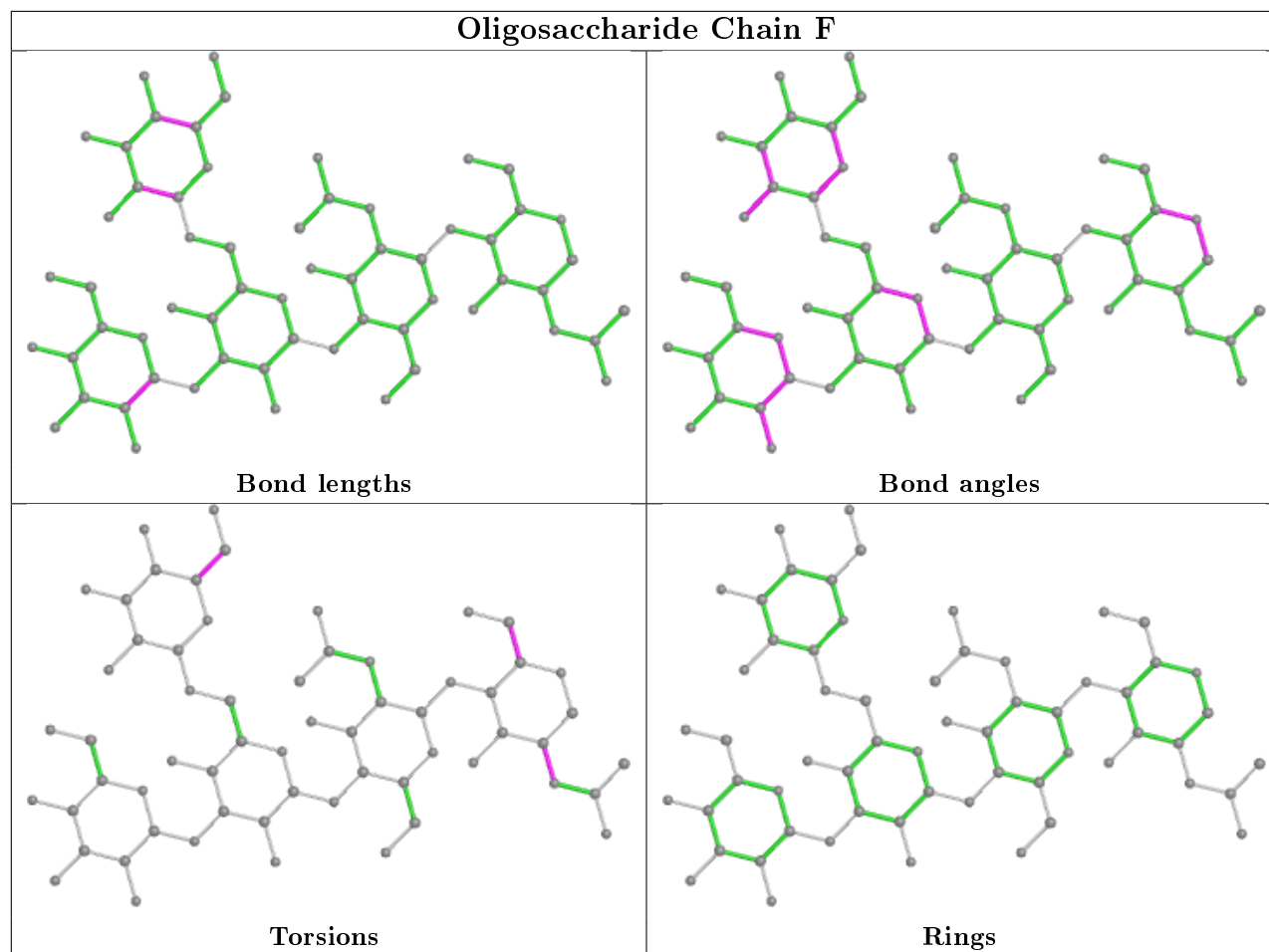


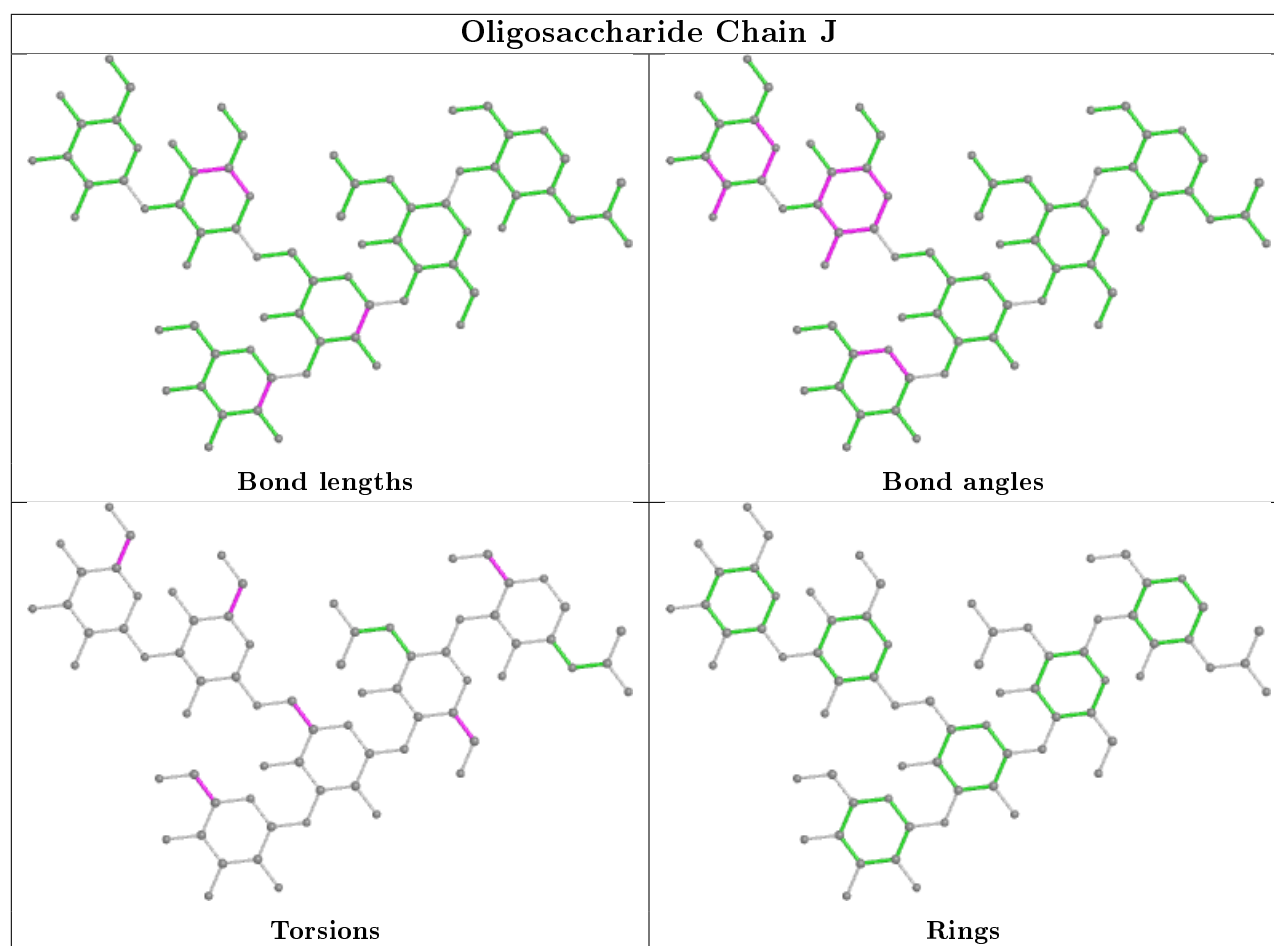












5.6 Ligand geometry [i](#)

26 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	$\# Z > 2$
6	NAG	B	505	1	14,14,15	0.38	0	17,19,21	0.57	0
6	NAG	C	505	1	14,14,15	0.34	0	17,19,21	0.69	0
8	EDO	C	512	-	3,3,3	0.49	0	2,2,2	0.32	0
8	EDO	B	511	-	3,3,3	0.52	0	2,2,2	0.12	0
8	EDO	A	509	-	3,3,3	0.44	0	2,2,2	0.43	0
8	EDO	B	509	-	3,3,3	0.48	0	2,2,2	0.40	0
8	EDO	C	513	-	3,3,3	0.60	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	506	1	14,14,15	0.31	0	17,19,21	0.31	0
8	EDO	B	515	-	3,3,3	0.54	0	2,2,2	0.08	0
6	NAG	B	504	1	14,14,15	0.38	0	17,19,21	0.56	0
6	NAG	C	501	1	14,14,15	0.52	0	17,19,21	0.63	0
8	EDO	C	514	-	3,3,3	0.40	0	2,2,2	0.49	0
8	EDO	A	508	-	3,3,3	0.52	0	2,2,2	0.33	0
6	NAG	C	504	1	14,14,15	0.51	0	17,19,21	0.54	0
7	PEG	B	516	-	6,6,6	0.25	0	5,5,5	0.17	0
6	NAG	B	501	1	14,14,15	0.40	0	17,19,21	1.13	2 (11%)
6	NAG	B	508	1	14,14,15	0.57	0	17,19,21	0.49	0
6	NAG	A	515	1	14,14,15	0.28	0	17,19,21	0.38	0
8	EDO	B	514	-	3,3,3	0.54	0	2,2,2	0.19	0
8	EDO	B	510	-	3,3,3	0.37	0	2,2,2	0.46	0
7	PEG	A	507	-	6,6,6	0.38	0	5,5,5	0.35	0
8	EDO	B	512	-	3,3,3	0.45	0	2,2,2	0.53	0
8	EDO	A	516	-	3,3,3	0.57	0	2,2,2	0.21	0
8	EDO	C	516	-	3,3,3	0.52	0	2,2,2	0.22	0
6	NAG	B	513	1	14,14,15	0.62	0	17,19,21	0.64	0
8	EDO	C	515	-	3,3,3	0.52	0	2,2,2	0.03	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
6	NAG	B	505	1	-	2/6/23/26	0/1/1/1
6	NAG	C	505	1	-	4/6/23/26	0/1/1/1
8	EDO	C	512	-	-	0/1/1/1	-
8	EDO	B	511	-	-	0/1/1/1	-
8	EDO	A	509	-	-	0/1/1/1	-
8	EDO	B	509	-	-	0/1/1/1	-
8	EDO	C	513	-	-	1/1/1/1	-
6	NAG	A	506	1	-	3/6/23/26	0/1/1/1
8	EDO	B	515	-	-	0/1/1/1	-
6	NAG	B	504	1	-	2/6/23/26	0/1/1/1
6	NAG	C	501	1	-	3/6/23/26	0/1/1/1
8	EDO	C	514	-	-	0/1/1/1	-
8	EDO	A	508	-	-	1/1/1/1	-
6	NAG	C	504	1	-	2/6/23/26	0/1/1/1
7	PEG	B	516	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	501	1	-	1/6/23/26	0/1/1/1
6	NAG	B	508	1	-	0/6/23/26	0/1/1/1
6	NAG	A	515	1	-	2/6/23/26	0/1/1/1
8	EDO	B	514	-	-	1/1/1/1	-
8	EDO	B	510	-	-	0/1/1/1	-
7	PEG	A	507	-	-	2/4/4/4	-
8	EDO	B	512	-	-	0/1/1/1	-
8	EDO	A	516	-	-	1/1/1/1	-
8	EDO	C	516	-	-	1/1/1/1	-
6	NAG	B	513	1	-	4/6/23/26	0/1/1/1
8	EDO	C	515	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	NAG	C2-N2-C7	3.45	127.81	122.90
6	B	501	NAG	C1-C2-N2	2.34	114.48	110.49

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	501	NAG	C1-C2-N2-C7
6	C	504	NAG	O5-C5-C6-O6
6	C	505	NAG	O5-C5-C6-O6
6	C	504	NAG	C4-C5-C6-O6
6	A	506	NAG	C8-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	505	NAG	1	0
8	B	511	EDO	2	0
8	B	509	EDO	1	0
8	C	513	EDO	1	0
8	B	515	EDO	3	0
6	B	504	NAG	1	0
8	C	514	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	504	NAG	1	0
8	B	510	EDO	1	0
7	A	507	PEG	2	0
8	A	516	EDO	3	0
6	B	513	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	483/499 (96%)	0.15	27 (5%) 24 25	33, 59, 115, 141	0
1	B	486/499 (97%)	0.02	9 (1%) 66 69	30, 54, 86, 103	0
1	C	479/499 (95%)	0.12	14 (2%) 51 55	30, 56, 104, 128	0
All	All	1448/1497 (96%)	0.10	50 (3%) 44 47	30, 56, 105, 141	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	GLY	8.6
1	A	360	GLY	6.9
1	A	469	PHE	5.9
1	C	469	PHE	5.4
1	C	277	CYS	4.6

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.

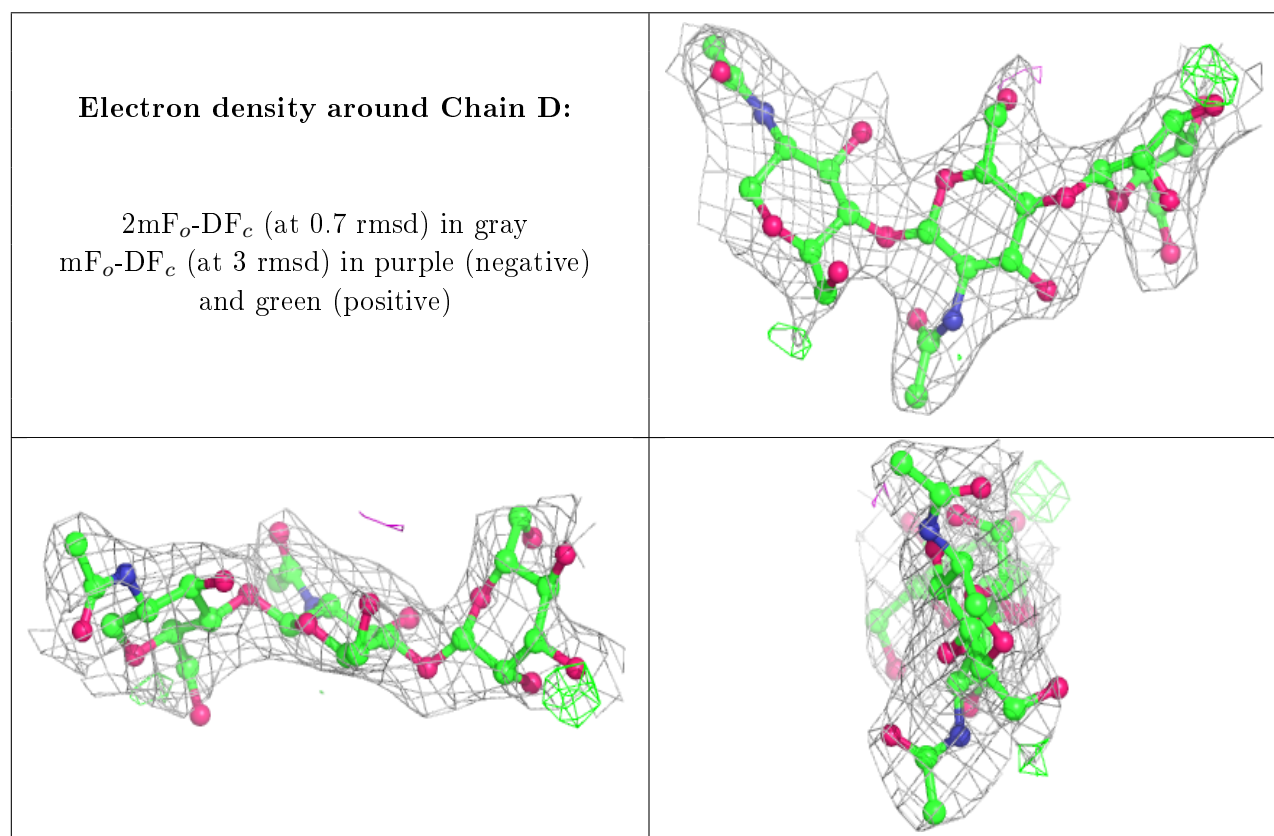
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MAN	J	5	11/12	0.57	0.33	111,121,125,125	0
4	MAN	F	5	11/12	0.68	0.27	97,105,111,111	0
2	BMA	D	3	11/12	0.68	0.32	100,108,114,116	0

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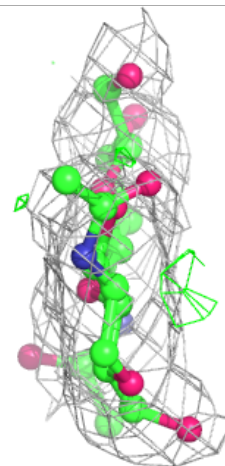
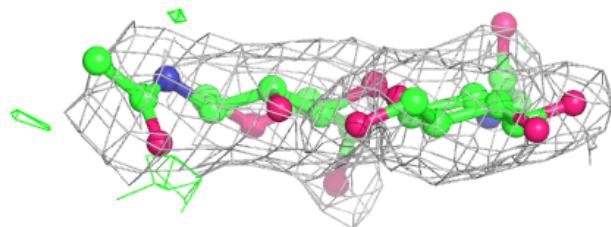
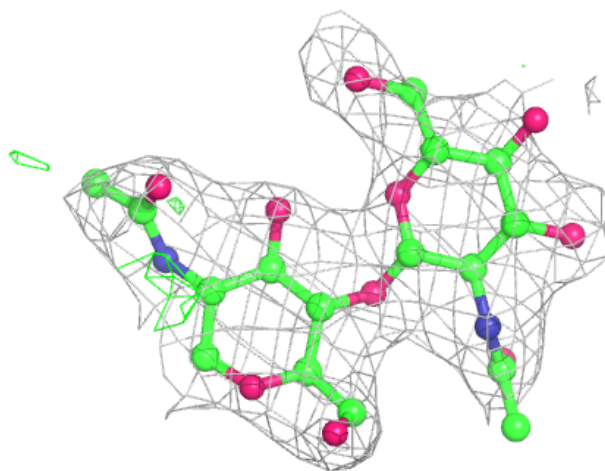
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	I	2	14/15	0.77	0.32	98,108,109,111	0
5	MAN	J	6	11/12	0.81	0.28	119,124,127,129	0
3	NAG	H	2	14/15	0.81	0.25	100,107,112,114	0
5	MAN	J	4	11/12	0.86	0.16	108,112,115,115	0
4	MAN	F	4	11/12	0.86	0.38	105,108,110,110	0
4	NAG	F	2	14/15	0.86	0.23	88,92,102,103	0
3	NAG	E	2	14/15	0.87	0.25	88,95,101,105	0
5	BMA	J	3	11/12	0.89	0.22	91,99,104,111	0
4	NAG	F	1	14/15	0.90	0.23	60,84,91,92	0
2	NAG	D	2	14/15	0.90	0.23	74,81,86,93	0
4	BMA	F	3	11/12	0.90	0.29	96,98,107,110	0
3	NAG	E	1	14/15	0.91	0.23	61,79,84,86	0
5	NAG	J	1	14/15	0.91	0.17	57,77,82,87	0
3	NAG	G	2	14/15	0.92	0.25	87,96,106,109	0
5	NAG	J	2	14/15	0.92	0.19	83,93,103,104	0
3	NAG	G	1	14/15	0.95	0.14	34,51,64,78	0
3	NAG	H	1	14/15	0.95	0.14	52,76,86,88	0
2	NAG	D	1	14/15	0.96	0.16	44,55,71,78	0
3	NAG	I	1	14/15	0.96	0.18	51,62,87,88	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.



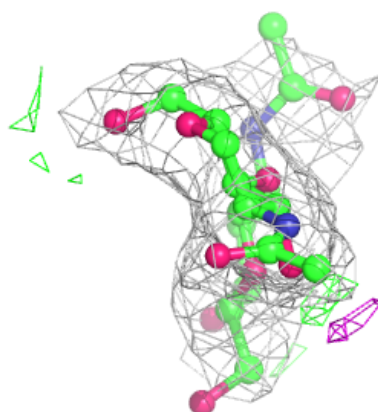
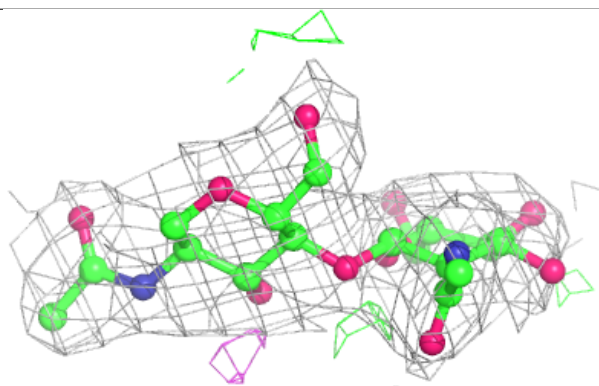
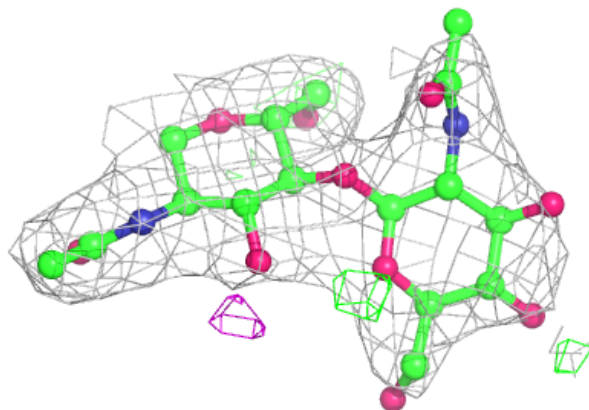
Electron density around Chain E:

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



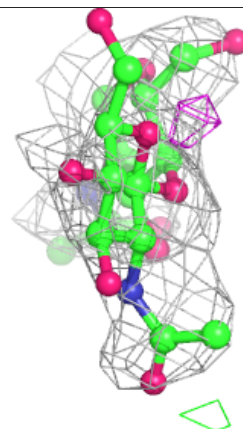
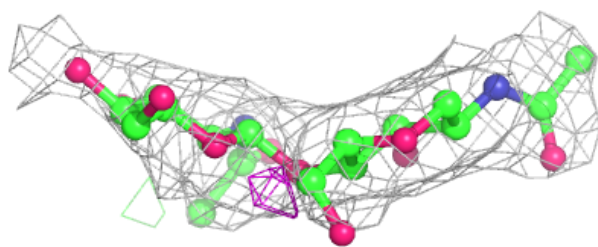
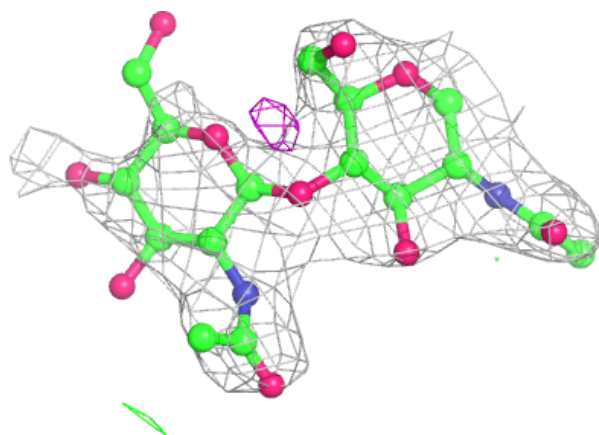
Electron density around Chain G:

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



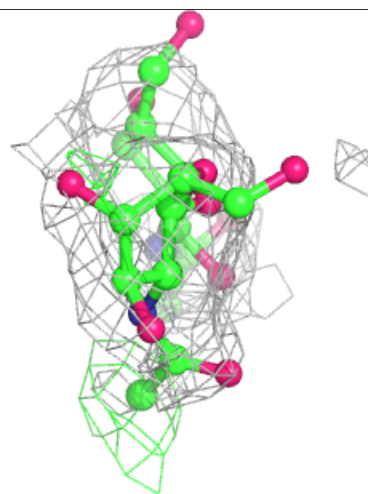
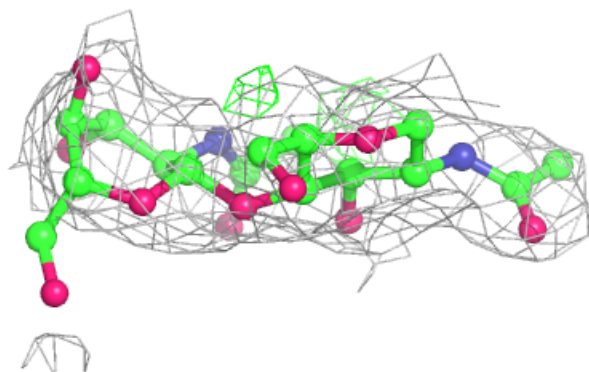
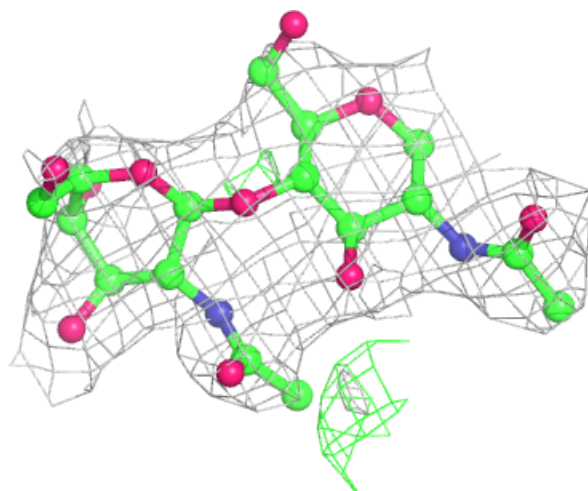
Electron density around Chain H:

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



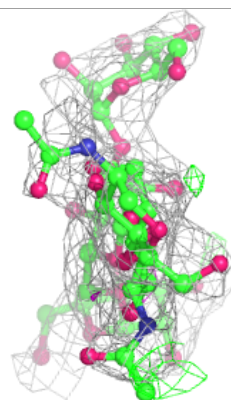
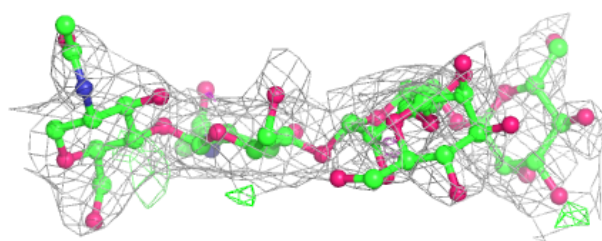
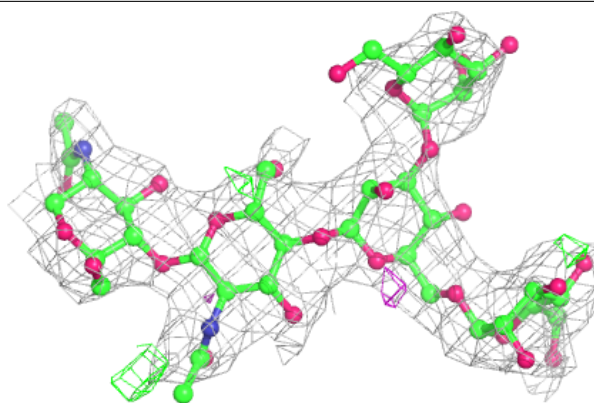
Electron density around Chain I:

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

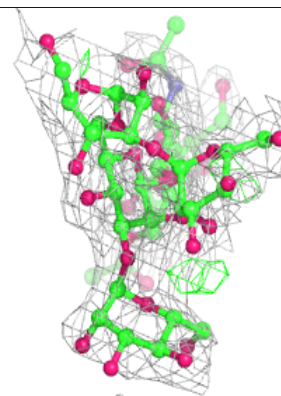
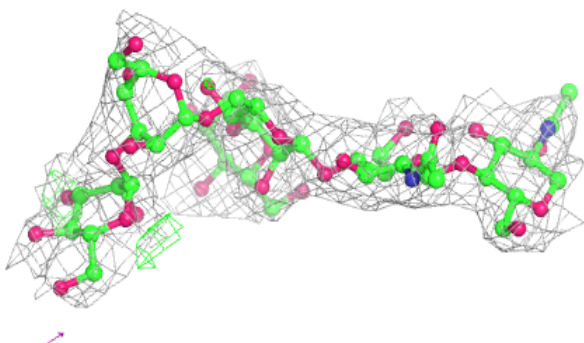
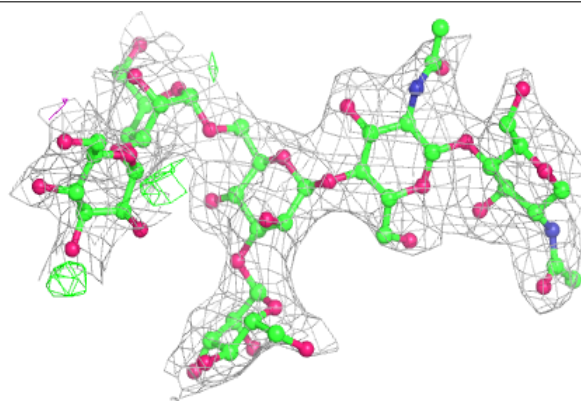


Electron density around Chain F:

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

**Electron density around Chain J:**

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



6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	A	515	14/15	0.67	0.32	93,109,114,117	0
6	NAG	C	501	14/15	0.68	0.45	90,110,122,126	0
6	NAG	C	505	14/15	0.69	0.50	106,118,132,135	0
6	NAG	B	505	14/15	0.70	0.40	81,100,111,119	0
6	NAG	B	508	14/15	0.79	0.35	82,98,111,116	0
6	NAG	B	501	14/15	0.80	0.44	89,102,109,111	0
6	NAG	B	513	14/15	0.80	0.41	76,93,97,98	0
8	EDO	A	508	4/4	0.81	0.13	67,73,77,81	0
7	PEG	A	507	7/7	0.82	0.28	43,50,61,64	0
8	EDO	A	516	4/4	0.83	0.27	63,66,68,69	0
6	NAG	A	506	14/15	0.84	0.48	90,111,116,116	0
8	EDO	B	509	4/4	0.86	0.18	59,59,62,66	0
8	EDO	C	512	4/4	0.87	0.22	59,59,62,63	0
6	NAG	C	504	14/15	0.87	0.20	74,79,96,102	0
7	PEG	B	516	7/7	0.88	0.26	79,96,102,110	0
8	EDO	C	515	4/4	0.88	0.28	70,70,72,75	0
6	NAG	B	504	14/15	0.89	0.30	81,93,96,100	0
8	EDO	B	514	4/4	0.89	0.17	55,55,57,58	0
8	EDO	C	513	4/4	0.91	0.18	50,52,54,58	0
8	EDO	C	516	4/4	0.91	0.25	67,72,76,78	0
8	EDO	B	511	4/4	0.92	0.26	53,54,57,61	0
8	EDO	B	515	4/4	0.92	0.26	69,69,74,75	0
8	EDO	A	509	4/4	0.94	0.16	73,73,75,78	0
8	EDO	B	510	4/4	0.95	0.36	47,49,50,55	0
8	EDO	B	512	4/4	0.95	0.17	50,51,54,58	0
8	EDO	C	514	4/4	0.97	0.37	55,56,57,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.