



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:34 PM BST

PDB ID : 6MZK
Title : Crystal structure of hemagglutinin from influenza virus A/Pennsylvania/14/2010 (H3N2)
Authors : Dai, Y.N.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2018-11-05
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

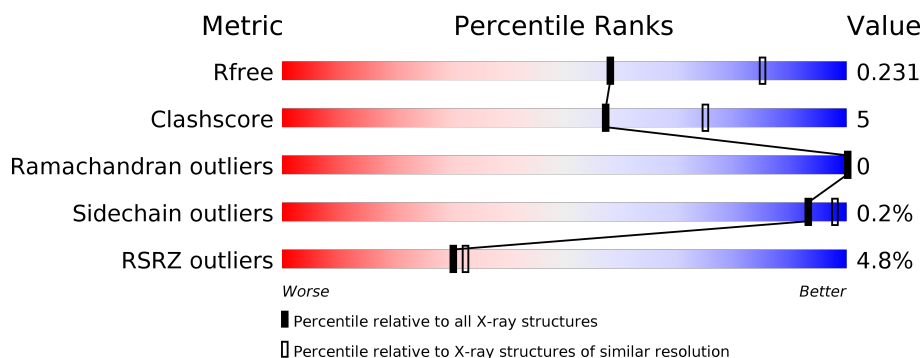
1 Overall quality at a glance

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.





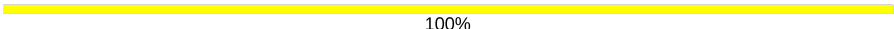
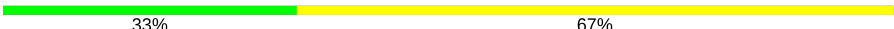
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	497	<div> <div>3%</div> <div>88%</div> <div>10%</div> <div>.</div> </div>
1	B	497	<div> <div>6%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
1	C	497	<div> <div>6%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
2	D	2	<div> <div>100%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>
2	H	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	2	 50% 50%
3	E	3	 33% 67%
3	G	3	 100%
3	I	3	 33% 67%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12075 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.

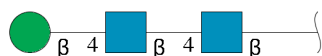
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3844	2403	677	746	18			
1	B	484	Total	C	N	O	S	0	0	0
			3845	2402	678	747	18			
1	C	482	Total	C	N	O	S	0	0	0
			3827	2392	675	742	18			

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



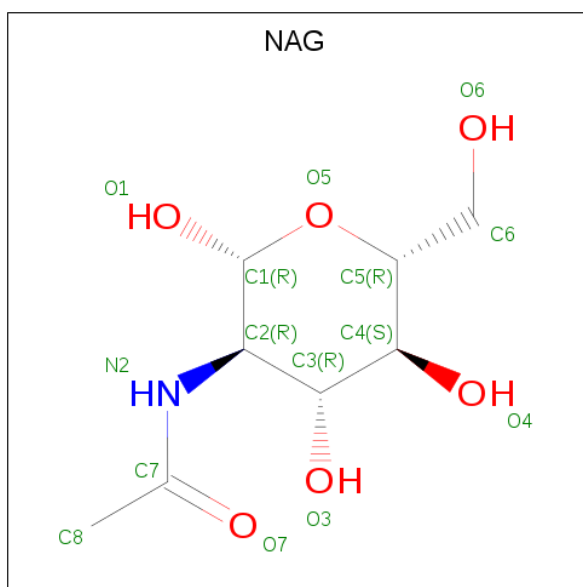
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

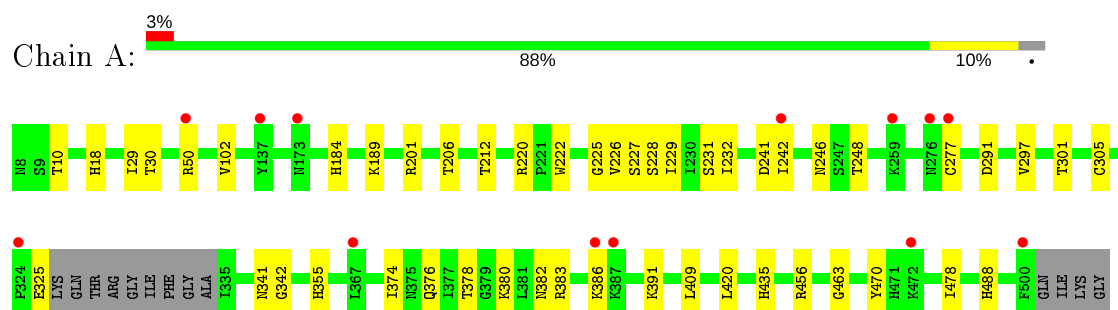
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total 77	O 77	0	0
5	B	65	Total 65	O 65	0	0
5	C	76	Total 76	O 76	0	0

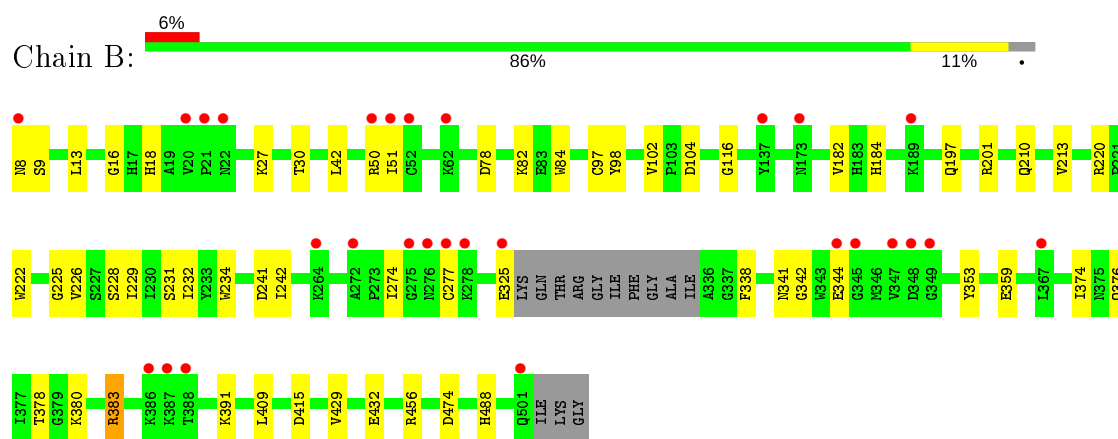
3 Residue-property plots [i](#)

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.

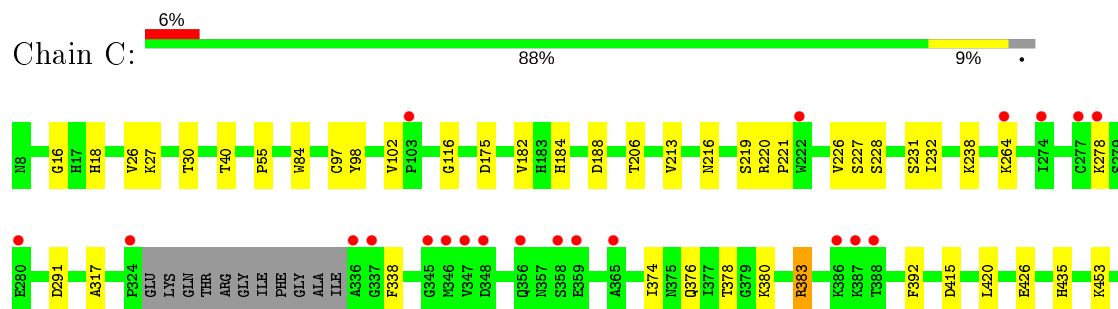
- Molecule 1: Hemagglutinin

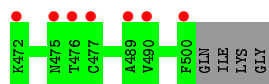


- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin





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

Chain D: 100%



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

Chain F: 50% 50%



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

Chain H: 100%



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

Chain J: 50% 50%



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

Chain E: 33% 67%



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

Chain G: 100%



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

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	170.72Å 394.90Å 102.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.50 49.56 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.56-2.50) 99.8 (49.56-2.50)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.207 , 0.231 0.206 , 0.231	Depositor DCC
R_{free} test set	5971 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12075	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 2.53% 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: BMA, NAG

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	0.28	0/3926	0.49	0/5326
1	B	0.28	0/3927	0.50	1/5327 (0.0%)
1	C	0.29	0/3909	0.56	3/5303 (0.1%)
All	All	0.29	0/11762	0.52	4/15956 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	ARG	NE-CZ-NH2	-14.37	113.12	120.30
1	C	383	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	C	383	ARG	CD-NE-CZ	-7.21	113.51	123.60
1	B	383	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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	3844	0	3708	44	0
1	B	3845	0	3705	39	0
1	C	3827	0	3691	49	0
2	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	28	0	25	3	0
2	H	28	0	25	4	0
2	J	28	0	25	0	0
3	E	39	0	34	1	0
3	G	39	0	34	2	0
3	I	39	0	34	0	0
4	A	28	0	26	1	0
4	B	42	0	39	0	0
4	C	42	0	39	2	0
5	A	77	0	0	0	0
5	B	65	0	0	0	0
5	C	76	0	0	0	0
All	All	12075	0	11410	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (114) 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:380:LYS:HA	1:C:383:ARG:HH11	1.03	1.14
1:C:380:LYS:HA	1:C:383:ARG:NH1	1.79	0.96
1:B:325:GLU:HA	1:B:341:ASN:HD21	1.33	0.93
1:A:383:ARG:O	1:B:27:LYS:NZ	2.07	0.87
1:A:248:THR:HG23	2:F:1:NAG:H82	1.62	0.80
1:A:30:THR:C	1:C:383:ARG:HH22	1.86	0.79
2:H:1:NAG:O3	2:H:1:NAG:O7	1.99	0.78
1:B:383:ARG:NH2	1:C:30:THR:O	2.16	0.77
1:B:383:ARG:O	1:C:27:LYS:NZ	2.20	0.74
1:B:325:GLU:HG3	1:B:344:GLU:H	1.54	0.72
1:A:206:THR:O	1:B:220:ARG:NH1	2.22	0.72
1:B:210:GLN:HE22	1:C:216:ASN:HB3	1.56	0.70
1:A:376:GLN:HG2	1:B:30:THR:HG23	1.72	0.70
1:C:380:LYS:CA	1:C:383:ARG:HH11	1.95	0.70
1:A:29:ILE:O	1:C:383:ARG:NH2	2.26	0.68
1:A:325:GLU:HG3	1:A:341:ASN:HD21	1.57	0.68
1:A:30:THR:C	1:C:383:ARG:NH2	2.47	0.67
1:C:55:PRO:HB3	1:C:278:LYS:NZ	2.09	0.67
1:B:226:VAL:HG12	1:B:228:SER:H	1.60	0.66
1:A:184:HIS:NE2	1:A:231:SER:OG	2.30	0.65
1:C:55:PRO:HB3	1:C:278:LYS:HZ2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ARG:NH2	1:C:216:ASN:OD1	2.29	0.64
1:B:197:GLN:N	1:B:197:GLN:OE1	2.29	0.63
1:C:175:ASP:OD1	1:C:238:LYS:HD2	1.98	0.63
2:H:1:NAG:HO3	2:H:1:NAG:C7	2.06	0.63
1:C:380:LYS:NZ	1:C:435:HIS:HD2	1.98	0.62
1:A:30:THR:HG23	1:C:376:GLN:HG2	1.81	0.61
1:C:380:LYS:HZ1	1:C:435:HIS:CD2	2.19	0.61
1:C:380:LYS:NZ	1:C:435:HIS:CD2	2.71	0.59
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.38	0.58
1:A:325:GLU:HA	1:A:341:ASN:ND2	2.18	0.58
1:A:325:GLU:HA	1:A:341:ASN:HD21	1.68	0.58
1:A:355:HIS:CD2	1:A:478:ILE:HG21	2.38	0.58
1:B:376:GLN:HG2	1:C:30:THR:HG23	1.84	0.57
1:A:220:ARG:NH2	1:C:206:THR:O	2.37	0.56
1:C:226:VAL:HG12	1:C:228:SER:H	1.68	0.56
1:A:382:ASN:HB3	1:A:386:LYS:HE3	1.89	0.54
1:B:325:GLU:HA	1:B:341:ASN:ND2	2.12	0.54
1:C:184:HIS:NE2	1:C:231:SER:OG	2.41	0.54
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.90	0.53
1:C:380:LYS:HZ1	1:C:435:HIS:HD2	1.53	0.53
1:A:325:GLU:HA	1:A:341:ASN:OD1	2.09	0.52
1:A:226:VAL:HG12	1:A:228:SER:H	1.74	0.52
1:C:188:ASP:CG	2:H:2:NAG:H5	2.30	0.52
1:A:380:LYS:NZ	1:A:435:HIS:HD2	2.07	0.52
1:A:30:THR:CA	1:C:383:ARG:HH22	2.22	0.52
1:B:359:GLU:OE2	1:B:474:ASP:HB2	2.11	0.51
1:B:456:ARG:HG3	1:B:488:HIS:CD2	2.46	0.50
1:B:383:ARG:NH2	1:C:30:THR:C	2.64	0.49
1:B:374:ILE:O	1:B:378:THR:HG23	2.12	0.49
1:A:325:GLU:HG3	1:A:341:ASN:ND2	2.27	0.49
1:A:297:VAL:HG13	4:A:609:NAG:H82	1.95	0.49
1:A:50:ARG:NH1	1:A:277:CYS:SG	2.86	0.49
1:C:27:LYS:NZ	1:C:426:GLU:OE2	2.26	0.48
1:C:16:GLY:HA2	1:C:338:PHE:HB3	1.94	0.48
1:A:301:THR:HB	1:A:305:CYS:SG	2.54	0.48
1:B:184:HIS:NE2	1:B:231:SER:OG	2.45	0.47
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.49	0.47
1:B:13:LEU:HD11	1:B:353:TYR:HB3	1.96	0.47
1:A:291:ASP:OD1	1:A:291:ASP:N	2.47	0.47
1:B:210:GLN:HE22	1:C:216:ASN:CB	2.25	0.47
1:C:380:LYS:HG3	1:C:380:LYS:HZ3	1.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASN:HB3	1:B:9:SER:H	1.56	0.46
1:A:30:THR:O	1:C:383:ARG:NH2	2.47	0.46
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.97	0.46
1:B:380:LYS:HG2	1:B:432:GLU:OE1	2.16	0.46
1:C:374:ILE:O	1:C:378:THR:HG23	2.14	0.46
1:C:221:PRO:HA	3:G:2:NAG:O7	2.16	0.46
1:C:188:ASP:OD1	2:H:2:NAG:H5	2.16	0.45
1:A:325:GLU:HA	1:A:341:ASN:CG	2.37	0.45
1:C:380:LYS:CE	1:C:435:HIS:HD2	2.29	0.45
1:B:42:LEU:HD12	1:B:429:VAL:HG22	1.99	0.45
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.51	0.45
1:A:391:LYS:NZ	1:B:415:ASP:OD2	2.41	0.44
1:B:241:ASP:OD1	1:B:242:ILE:N	2.42	0.44
1:C:182:VAL:HG21	1:C:213:VAL:HB	1.98	0.44
1:B:104:ASP:HB3	1:B:234:TRP:CH2	2.52	0.44
4:C:601:NAG:H83	4:C:601:NAG:H3	1.98	0.44
1:A:409:LEU:HG	1:B:409:LEU:HD21	1.99	0.43
1:A:10:THR:HG22	1:A:470:TYR:HA	2.00	0.43
1:C:220:ARG:HB2	1:C:227:SER:O	2.19	0.43
3:E:1:NAG:H81	2:F:2:NAG:H82	1.99	0.43
1:B:16:GLY:HA2	1:B:338:PHE:HB3	2.01	0.43
1:B:84:TRP:CE2	1:B:116:GLY:HA2	2.54	0.42
1:A:374:ILE:O	1:A:378:THR:HG23	2.19	0.42
1:B:220:ARG:HD3	1:B:229:ILE:HB	2.01	0.42
1:A:241:ASP:OD1	1:A:242:ILE:N	2.45	0.42
1:A:220:ARG:HD3	1:A:229:ILE:HB	2.00	0.42
1:C:26:VAL:HG21	1:C:317:ALA:HB2	2.01	0.42
1:A:463:GLY:HA2	1:C:453:LYS:HD3	2.01	0.42
1:B:222:TRP:NE1	1:B:225:GLY:HA2	2.34	0.42
1:B:97:CYS:SG	1:B:98:TYR:N	2.92	0.42
1:A:220:ARG:HB2	1:A:227:SER:O	2.20	0.42
1:A:456:ARG:HG3	1:A:488:HIS:CG	2.55	0.42
1:A:226:VAL:CG1	1:A:228:SER:H	2.32	0.42
1:B:78:ASP:O	1:B:82:LYS:HD2	2.18	0.42
1:C:98:TYR:OH	1:C:228:SER:HB2	2.20	0.41
1:B:182:VAL:HG21	1:B:213:VAL:HB	2.02	0.41
1:C:97:CYS:SG	1:C:98:TYR:N	2.90	0.41
1:A:189:LYS:HA	1:A:189:LYS:HD3	1.91	0.41
1:C:291:ASP:N	1:C:291:ASP:OD1	2.50	0.41
1:A:201:ARG:HH21	1:A:212:THR:HG21	1.86	0.41
1:B:102:VAL:HG22	1:B:232:ILE:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLU:HG2	1:B:342:GLY:O	2.20	0.41
1:A:246:ASN:OD1	2:F:1:NAG:H83	2.20	0.41
1:B:50:ARG:NH2	1:B:277:CYS:SG	2.94	0.41
1:C:40:THR:HB	4:C:601:NAG:H62	2.02	0.41
1:B:391:LYS:NZ	1:C:415:ASP:OD2	2.42	0.41
1:A:420:LEU:HD13	1:C:420:LEU:HD13	2.03	0.41
1:B:51:ILE:HB	1:B:274:ILE:HD13	2.03	0.41
1:C:219:SER:OG	3:G:1:NAG:N2	2.45	0.41
1:A:341:ASN:OD1	1:A:342:GLY:N	2.54	0.40
1:C:264:LYS:HB3	1:C:392:PHE:CG	2.56	0.40
1:C:264:LYS:HD3	1:C:392:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/497 (97%)	462 (96%)	18 (4%)	0	100	100
1	B	480/497 (97%)	458 (95%)	22 (5%)	0	100	100
1	C	478/497 (96%)	459 (96%)	19 (4%)	0	100	100
All	All	1438/1491 (96%)	1379 (96%)	59 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/436 (98%)	426 (100%)	1 (0%)	93	98
1	B	427/436 (98%)	426 (100%)	1 (0%)	93	98
1	C	425/436 (98%)	424 (100%)	1 (0%)	93	98
All	All	1279/1308 (98%)	1276 (100%)	3 (0%)	93	98

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

Mol	Chain	Res	Type
1	A	18	HIS
1	B	18	HIS
1	C	18	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	GLN
1	C	435	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

17 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	0.48	0
2	NAG	D	2	2	14,14,15	0.23	0	17,19,21	0.53	0
3	NAG	E	1	1,3	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.44	0
3	BMA	E	3	3	11,11,12	0.85	1 (9%)	15,15,17	1.07	0
2	NAG	F	1	1,2	14,14,15	0.18	0	17,19,21	0.72	0
2	NAG	F	2	2	14,14,15	0.21	0	17,19,21	0.67	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.22	0	17,19,21	0.54	0
3	BMA	G	3	3	11,11,12	0.66	0	15,15,17	1.00	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.25	0	17,19,21	1.06	1 (5%)
2	NAG	H	2	2	14,14,15	0.46	0	17,19,21	1.12	2 (11%)
3	NAG	I	1	1,3	14,14,15	0.54	0	17,19,21	0.77	1 (5%)
3	NAG	I	2	3	14,14,15	0.51	0	17,19,21	0.52	0
3	BMA	I	3	3	11,11,12	0.72	0	15,15,17	0.98	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.66	0	17,19,21	0.42	0
2	NAG	J	2	2	14,14,15	0.59	1 (7%)	17,19,21	0.44	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	BMA	C1-C2	2.11	1.57	1.52
2	J	2	NAG	O5-C1	-2.09	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	NAG	C1-O5-C5	2.65	115.79	112.19
3	I	3	BMA	O5-C5-C6	2.47	111.08	107.20
3	G	3	BMA	C1-O5-C5	2.38	115.41	112.19
2	F	2	NAG	C1-O5-C5	2.23	115.22	112.19
2	H	2	NAG	C4-C3-C2	-2.12	107.91	111.02
2	H	1	NAG	C2-N2-C7	2.03	125.79	122.90
3	I	1	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6

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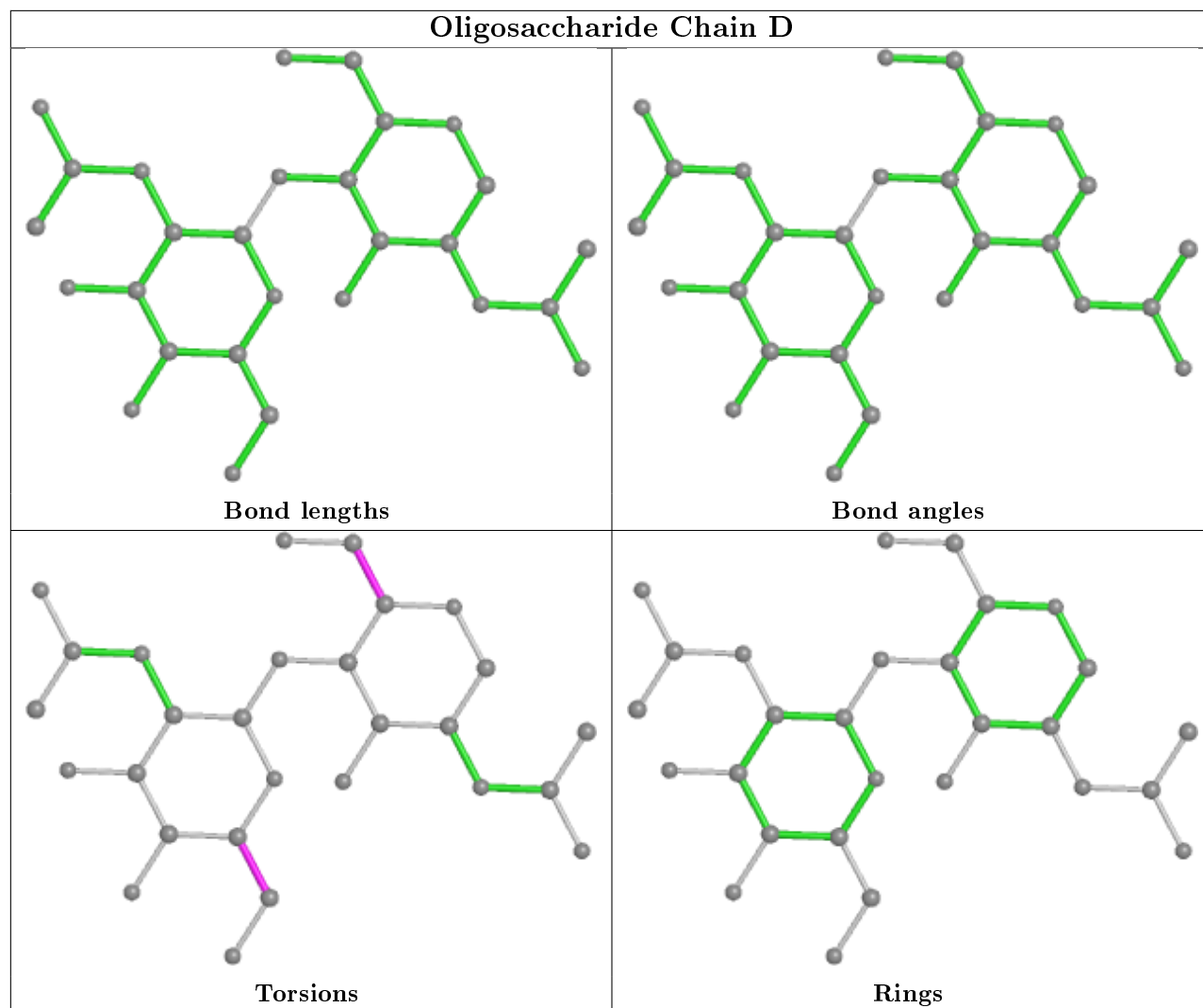
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6

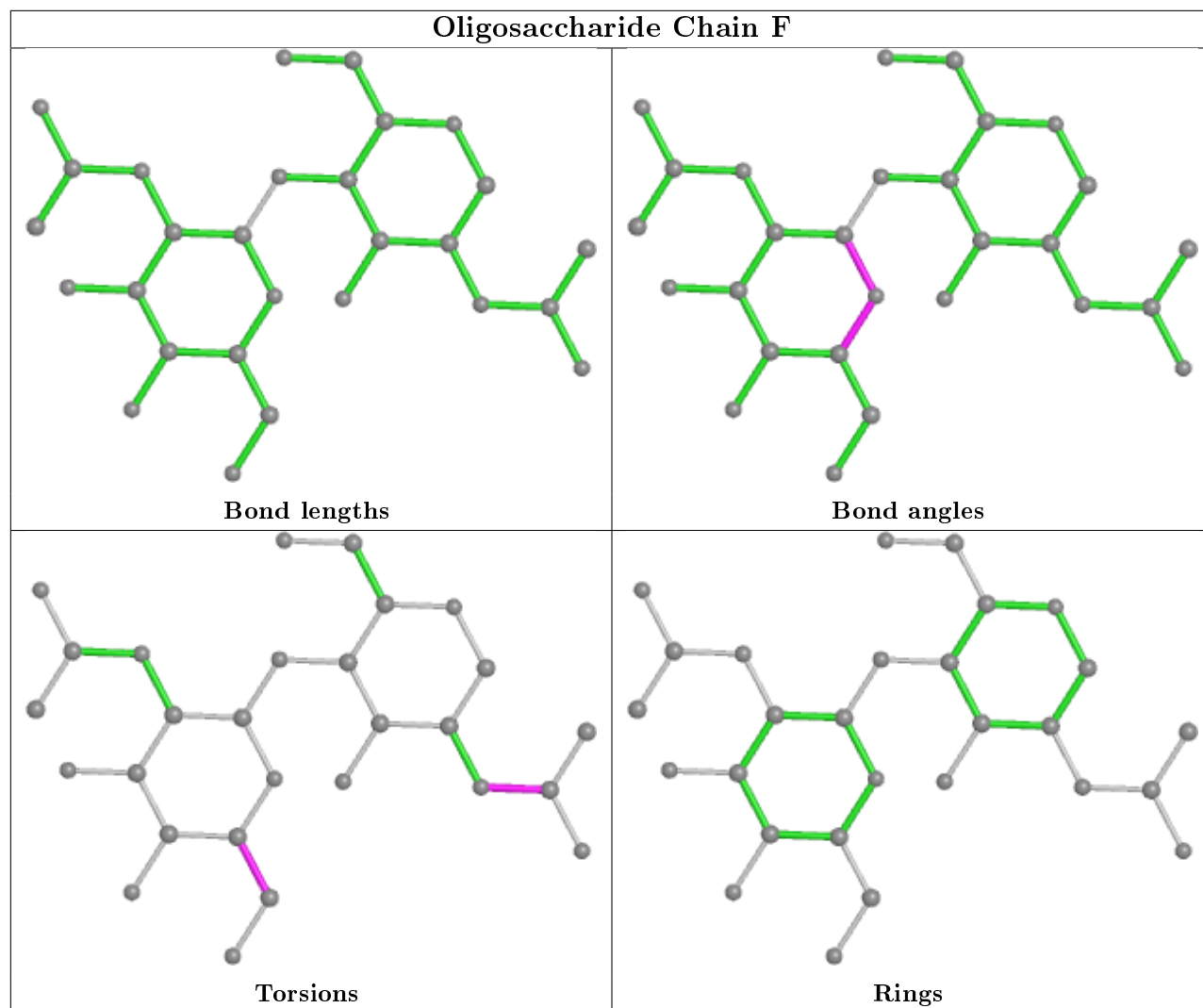
There are no ring outliers.

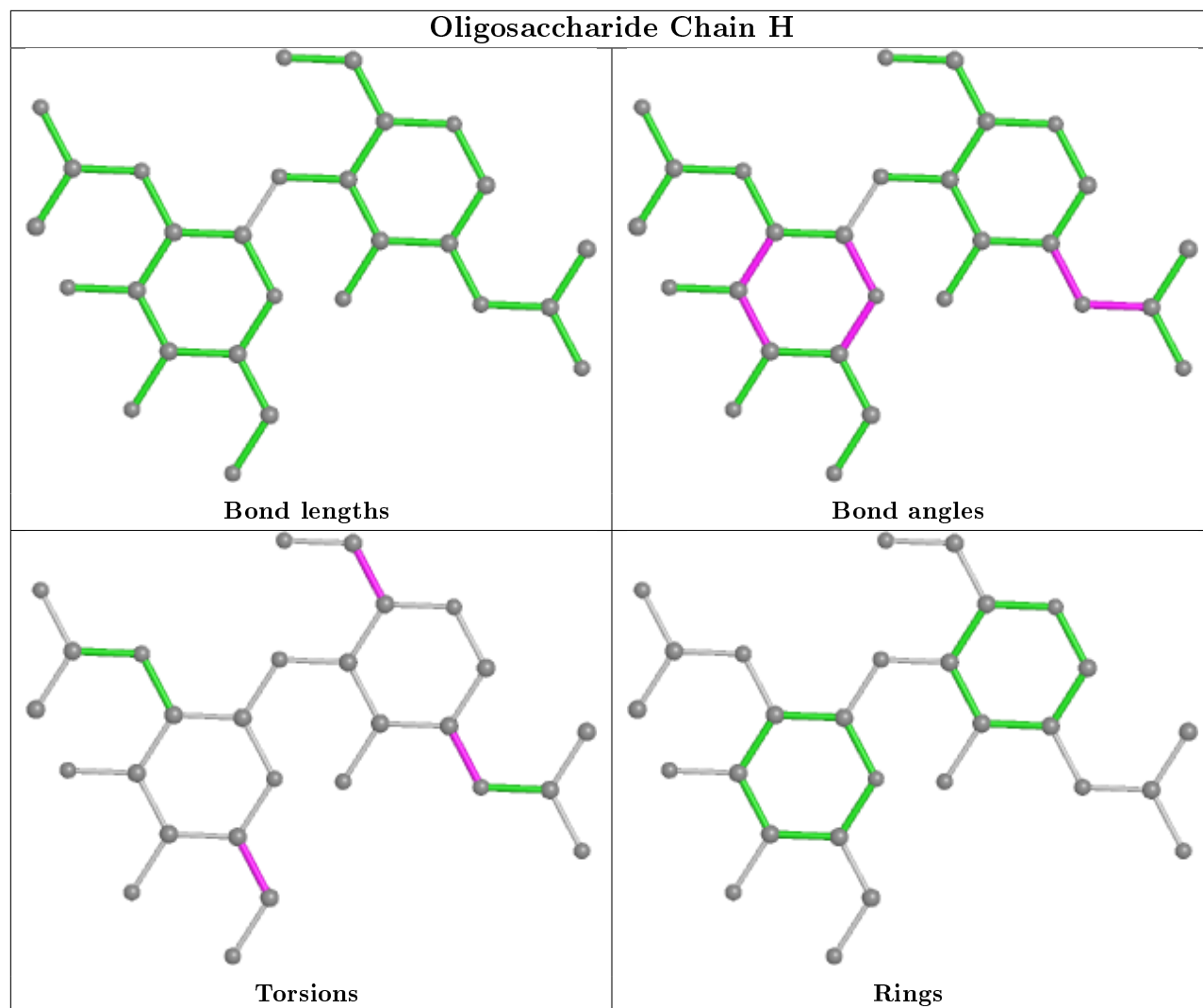
7 monomers are involved in 9 short contacts:

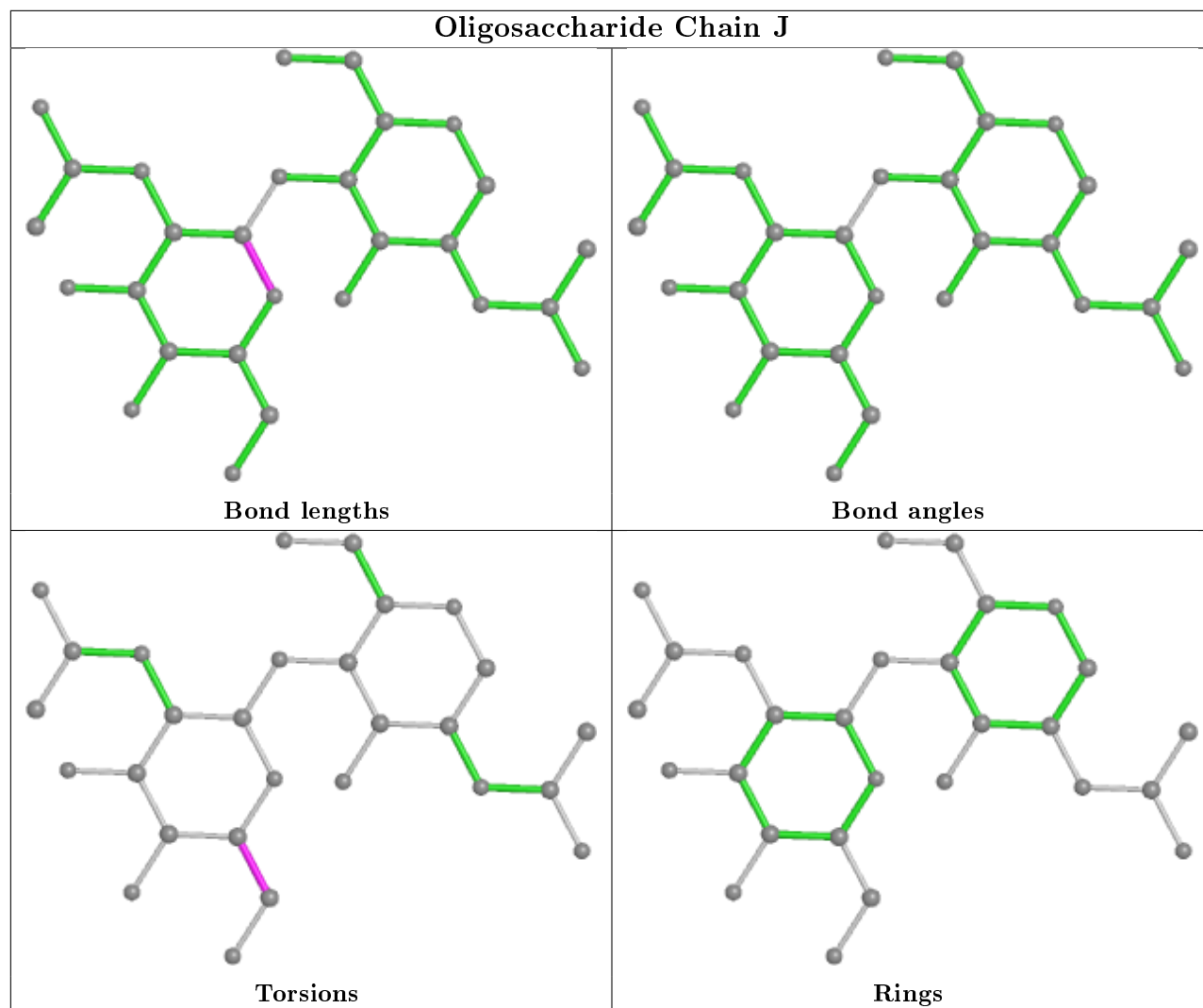
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	2	0
2	H	1	NAG	2	0
2	F	1	NAG	2	0
3	G	1	NAG	1	0
2	F	2	NAG	1	0
3	G	2	NAG	1	0
3	E	1	NAG	1	0

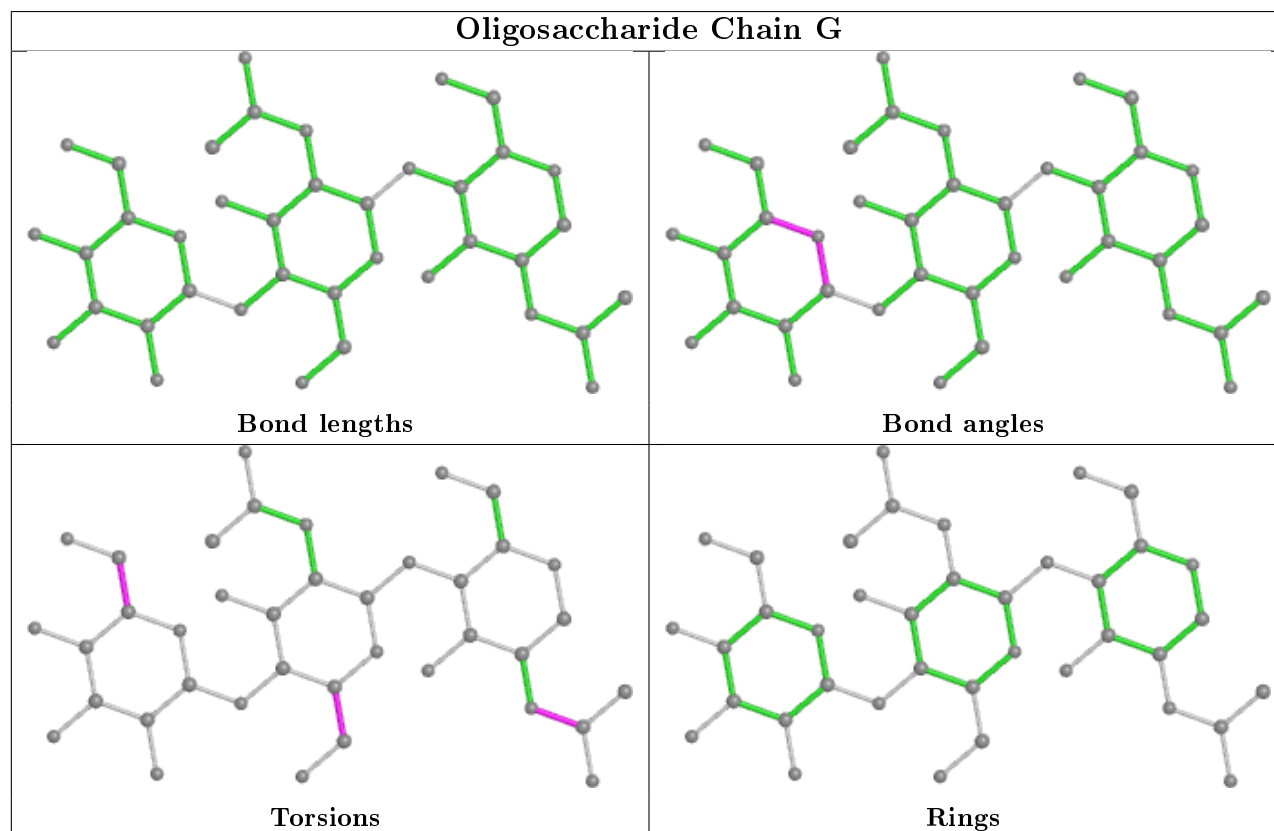
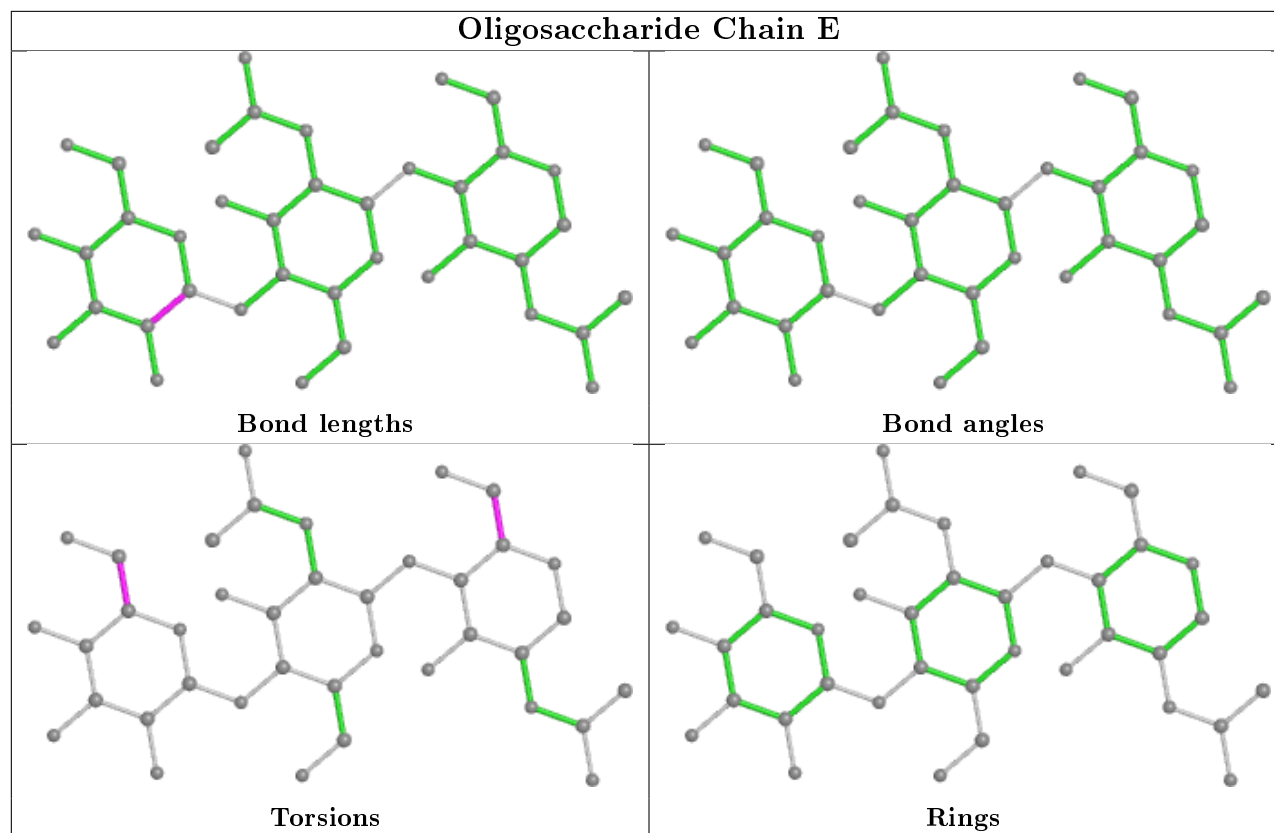
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

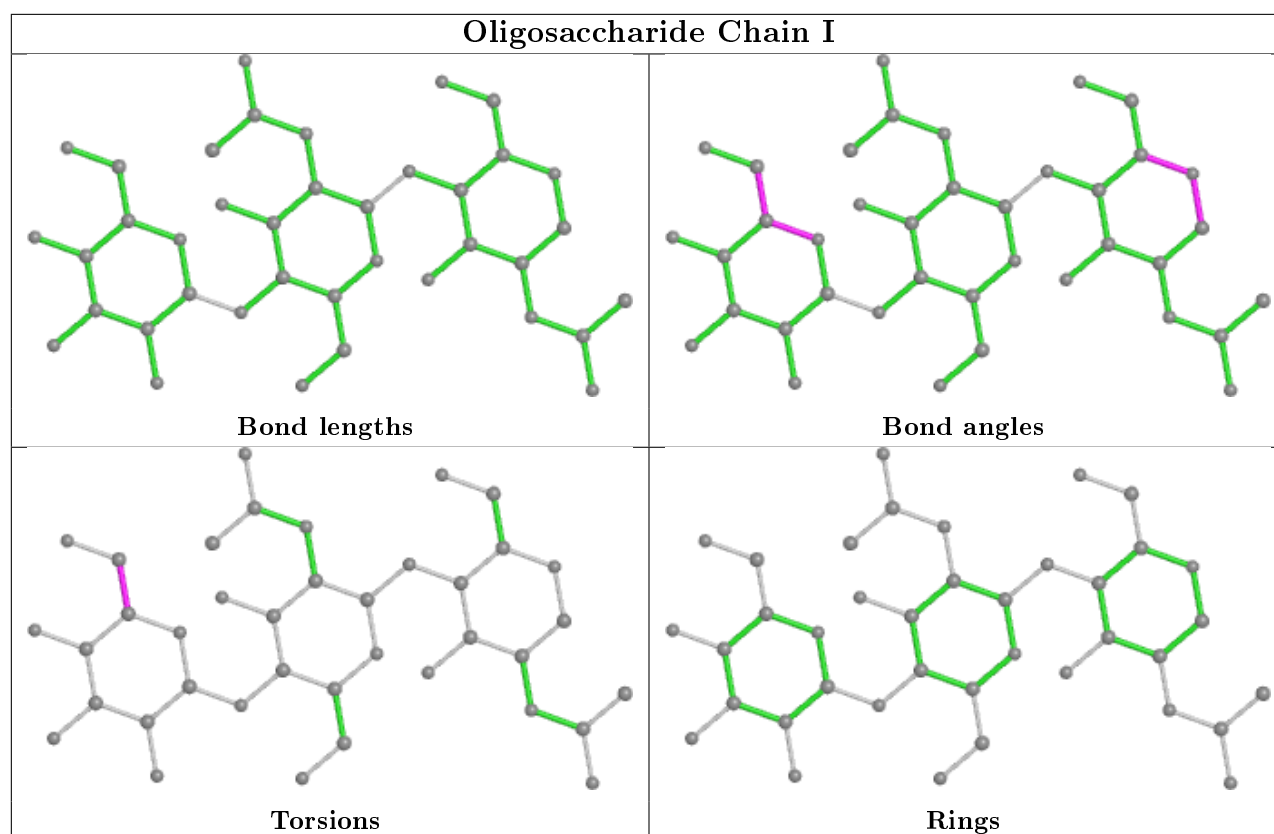












5.6 Ligand geometry [i](#)

8 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	$\# Z > 2$
4	NAG	C	601	1	14,14,15	0.76	1 (7%)	17,19,21	1.31	2 (11%)
4	NAG	A	609	1	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	C	608	1	14,14,15	0.42	0	17,19,21	0.50	0
4	NAG	C	607	1	14,14,15	0.66	0	17,19,21	0.47	0
4	NAG	A	608	1	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	B	608	1	14,14,15	0.90	2 (14%)	17,19,21	0.85	1 (5%)
4	NAG	B	607	1	14,14,15	0.51	0	17,19,21	0.50	0
4	NAG	B	601	1	14,14,15	0.34	0	17,19,21	0.50	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
4	NAG	C	601	1	-	4/6/23/26	0/1/1/1
4	NAG	A	609	1	-	0/6/23/26	0/1/1/1
4	NAG	C	608	1	-	2/6/23/26	0/1/1/1
4	NAG	C	607	1	-	1/6/23/26	0/1/1/1
4	NAG	A	608	1	-	2/6/23/26	0/1/1/1
4	NAG	B	608	1	-	3/6/23/26	0/1/1/1
4	NAG	B	607	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	608	NAG	C1-C2	2.58	1.56	1.52
4	C	601	NAG	O5-C1	-2.53	1.39	1.43
4	B	608	NAG	O5-C1	-2.05	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	NAG	C2-N2-C7	4.14	128.80	122.90
4	C	601	NAG	C1-C2-N2	2.41	114.61	110.49
4	B	608	NAG	C2-N2-C7	2.22	126.06	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	608	NAG	C3-C2-N2-C7
4	C	608	NAG	O5-C5-C6-O6
4	B	608	NAG	O5-C5-C6-O6
4	C	608	NAG	C4-C5-C6-O6
4	C	601	NAG	C8-C7-N2-C2
4	C	601	NAG	O7-C7-N2-C2
4	B	608	NAG	C4-C5-C6-O6
4	A	608	NAG	O5-C5-C6-O6
4	A	608	NAG	C4-C5-C6-O6
4	C	607	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	601	NAG	C1-C2-N2-C7
4	C	601	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	NAG	2	0
4	A	609	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/497 (97%)	0.30	13 (2%) 54 58	36, 55, 86, 114	0
1	B	484/497 (97%)	0.40	28 (5%) 23 24	37, 60, 86, 110	0
1	C	482/497 (96%)	0.43	28 (5%) 23 24	37, 60, 96, 120	0
All	All	1450/1491 (97%)	0.38	69 (4%) 30 32	36, 58, 90, 120	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	ASN	5.1
1	B	8	ASN	5.1
1	B	20	VAL	4.5
1	B	278	LYS	4.3
1	C	348	ASP	4.2
1	C	346	MET	4.1
1	C	336	ALA	3.9
1	C	222	TRP	3.9
1	C	278	LYS	3.7
1	B	137	TYR	3.7
1	C	387	LYS	3.7
1	A	277	CYS	3.7
1	C	345	GLY	3.5
1	A	137	TYR	3.3
1	B	347	VAL	3.3
1	C	365	ALA	3.2
1	B	349	GLY	3.2
1	B	21	PRO	3.2
1	C	489	ALA	3.2
1	C	472	LYS	3.2
1	A	500	PHE	3.1
1	C	500	PHE	3.1
1	C	347	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	337	GLY	3.1
1	B	276	ASN	3.0
1	B	275	GLY	3.0
1	A	276	ASN	3.0
1	C	280	GLU	2.9
1	C	359	GLU	2.8
1	C	358	SER	2.8
1	B	345	GLY	2.8
1	C	490	VAL	2.8
1	C	475	ASN	2.7
1	C	264	LYS	2.7
1	A	387	LYS	2.7
1	C	476	THR	2.6
1	B	52	CYS	2.6
1	B	348	ASP	2.6
1	C	386	LYS	2.5
1	C	274	ILE	2.5
1	B	264	LYS	2.4
1	C	103	PRO	2.4
1	A	386	LYS	2.4
1	A	472	LYS	2.4
1	A	324	PRO	2.3
1	B	387	LYS	2.3
1	A	50	ARG	2.3
1	C	277	CYS	2.3
1	C	388	THR	2.3
1	B	50	ARG	2.3
1	A	173	ASN	2.3
1	B	189	LYS	2.2
1	A	242	ILE	2.2
1	A	259	LYS	2.2
1	C	356	GLN	2.2
1	B	386	LYS	2.2
1	A	367	LEU	2.2
1	B	367	LEU	2.2
1	B	277	CYS	2.2
1	B	173	ASN	2.2
1	B	325	GLU	2.2
1	C	324	PRO	2.2
1	B	62	LYS	2.1
1	B	501	GLN	2.1
1	B	272	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	388	THR	2.1
1	B	51	ILE	2.0
1	C	477	CYS	2.0
1	B	344	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

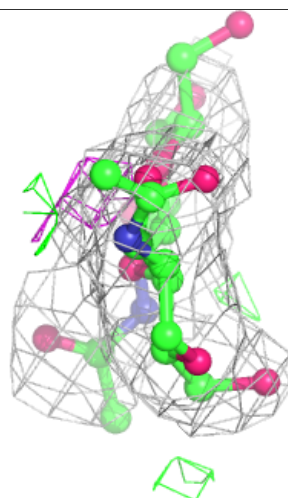
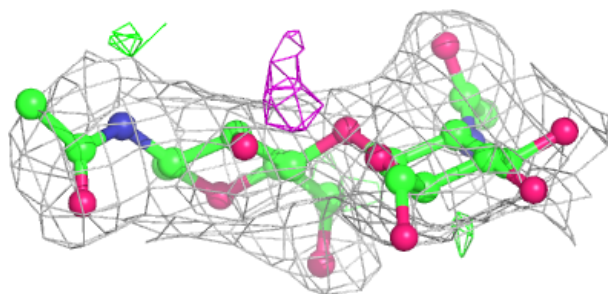
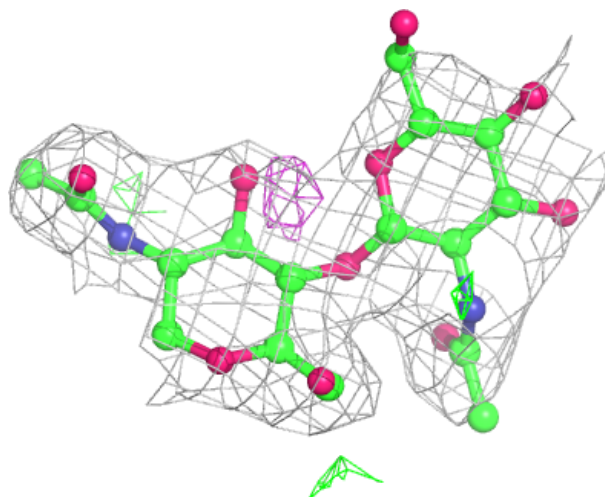
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	H	2	14/15	0.71	0.34	84,107,118,120	0
3	BMA	G	3	11/12	0.81	0.27	76,105,118,122	0
3	BMA	E	3	11/12	0.83	0.23	61,105,114,114	0
3	BMA	I	3	11/12	0.85	0.24	80,98,102,107	0
2	NAG	D	2	14/15	0.86	0.30	82,115,126,129	0
2	NAG	H	1	14/15	0.88	0.20	66,92,105,112	0
2	NAG	D	1	14/15	0.93	0.20	64,81,84,91	0
2	NAG	F	1	14/15	0.93	0.17	50,60,78,78	0
2	NAG	J	2	14/15	0.93	0.19	62,71,81,89	0
2	NAG	F	2	14/15	0.94	0.14	67,89,101,105	0
3	NAG	G	2	14/15	0.95	0.24	70,94,112,112	0
2	NAG	J	1	14/15	0.95	0.15	45,56,64,65	0
3	NAG	E	2	14/15	0.95	0.18	45,72,101,111	0
3	NAG	E	1	14/15	0.96	0.13	49,58,78,84	0
3	NAG	G	1	14/15	0.96	0.18	65,78,96,107	0
3	NAG	I	1	14/15	0.97	0.14	48,58,73,86	0
3	NAG	I	2	14/15	0.97	0.26	54,71,80,96	0

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

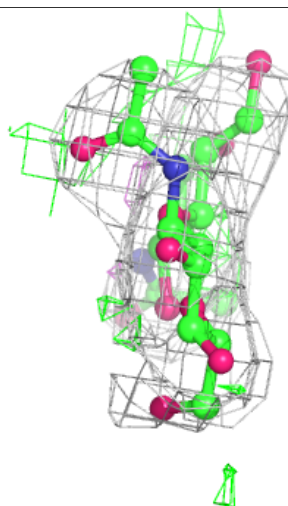
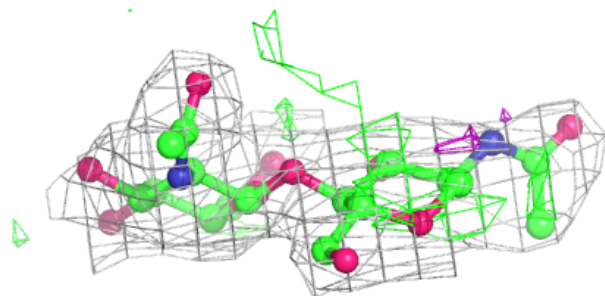
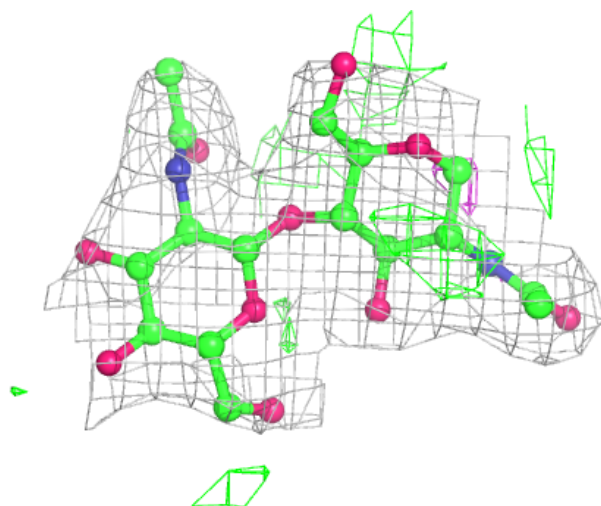
Electron density around Chain D:

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



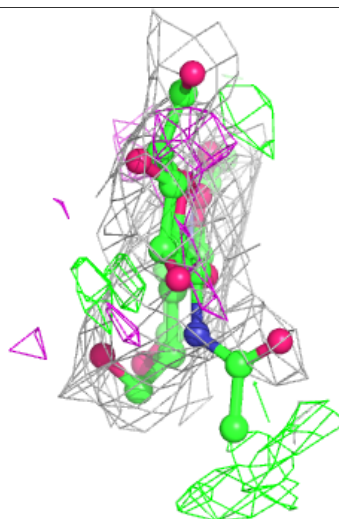
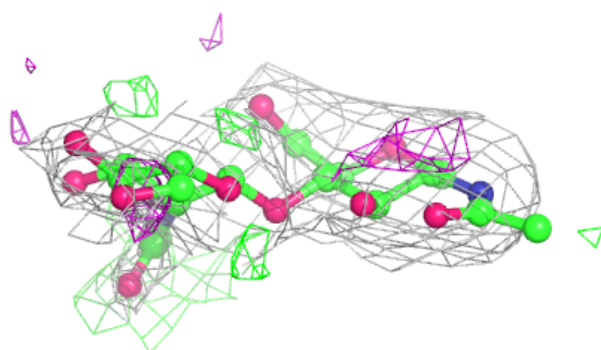
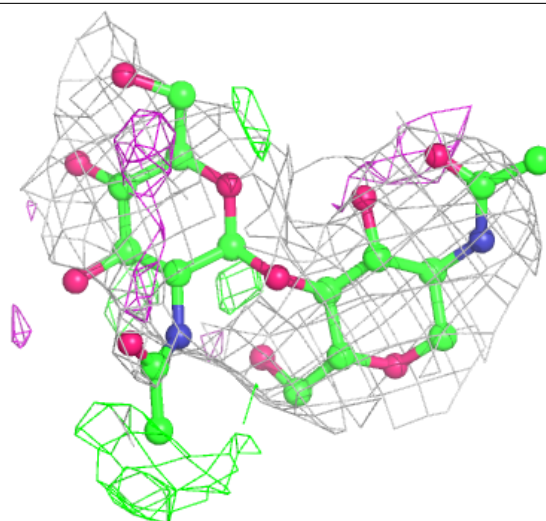
Electron density around Chain F:

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



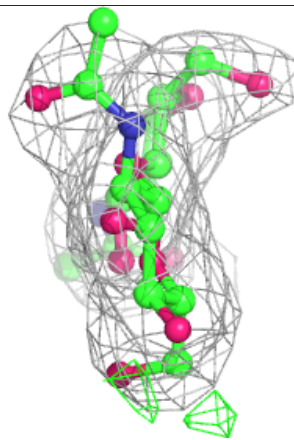
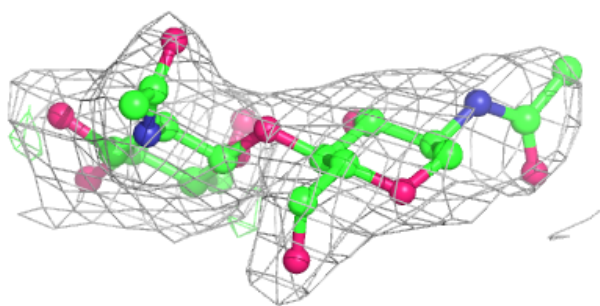
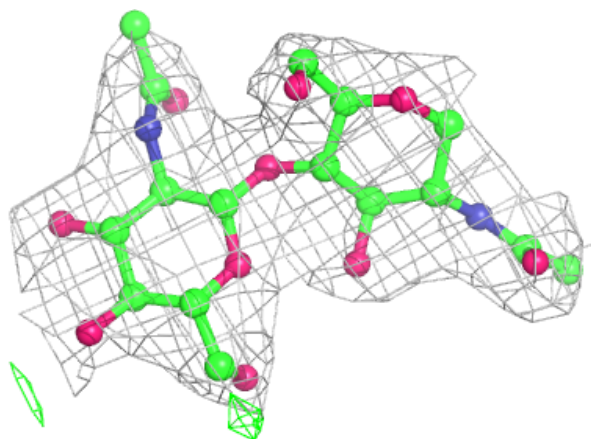
Electron density around Chain H:

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

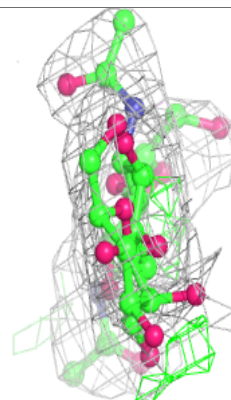
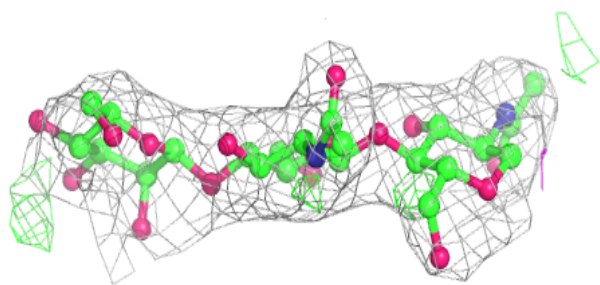
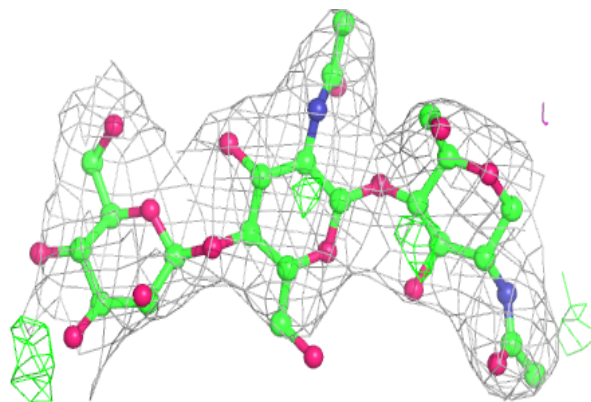


Electron density around Chain J:

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

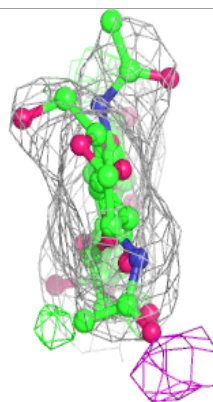
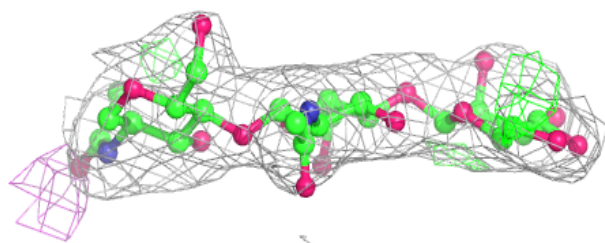
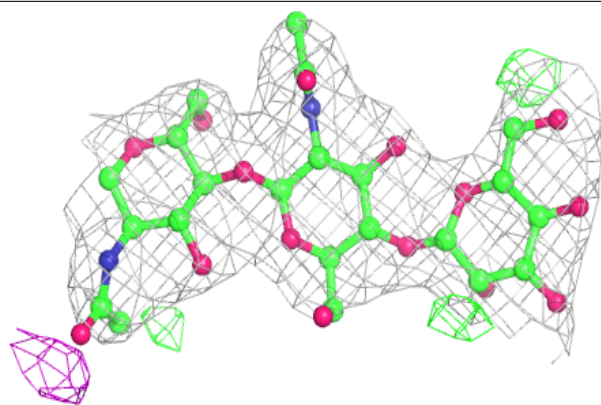
**Electron density around Chain E:**

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

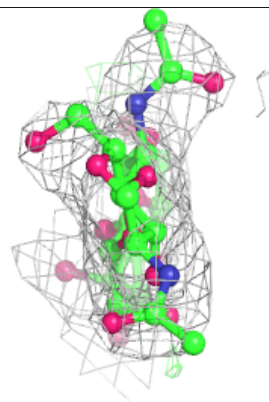
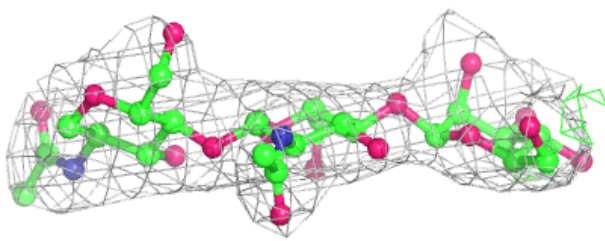
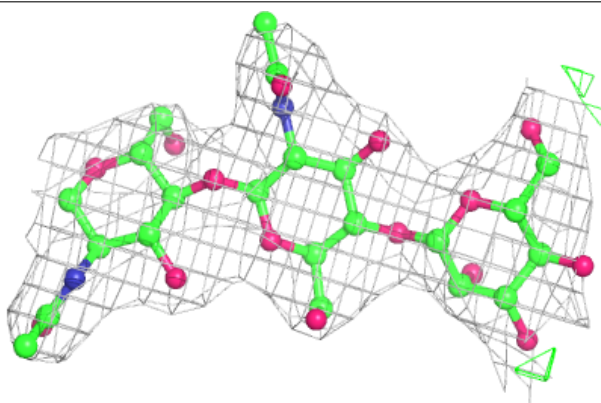


Electron density around Chain G:

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

**Electron density around Chain I:**

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



6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	NAG	B	608	14/15	0.64	0.29	64,95,104,107	0
4	NAG	B	601	14/15	0.85	0.29	76,88,94,94	0
4	NAG	C	608	14/15	0.86	0.24	73,91,99,99	0
4	NAG	B	607	14/15	0.88	0.24	77,98,107,110	0
4	NAG	A	608	14/15	0.88	0.21	78,95,103,110	0
4	NAG	C	601	14/15	0.89	0.19	75,96,102,104	0
4	NAG	C	607	14/15	0.90	0.24	87,102,111,117	0
4	NAG	A	609	14/15	0.91	0.29	74,90,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.