



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 6, 2023 – 02:47 PM EDT

PDB ID : 4FQK
Title : Influenza B/Brisbane/60/2008 hemagglutinin Fab CR8059 complex
Authors : Dreyfus, C.; Laursen, N.S.; Wilson, I.A.
Deposited on : 2012-06-25
Resolution : 5.65 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

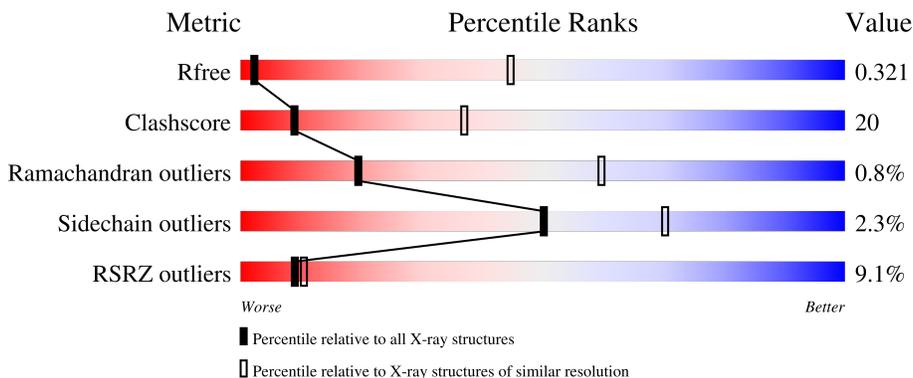
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.65 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.



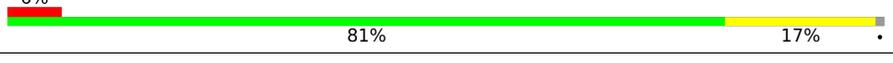
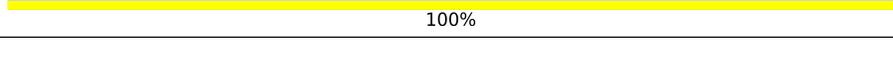
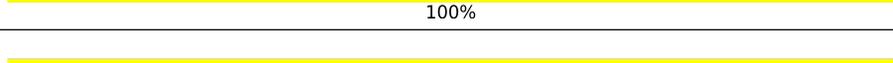
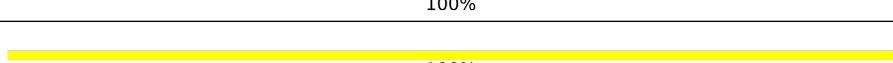
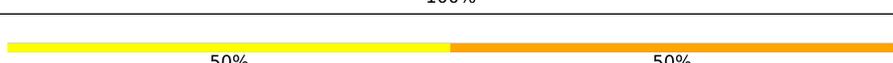
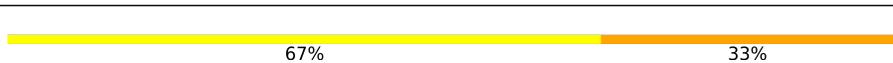
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1006 (7.40-3.84)
Clashscore	141614	1018 (7.40-3.90)
Ramachandran outliers	138981	1001 (7.40-3.84)
Sidechain outliers	138945	1203 (7.50-3.80)
RSRZ outliers	127900	1000 (7.54-3.78)

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 $\leq 5\%$. 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	347	
1	C	347	
2	B	179	
2	D	179	
3	E	234	

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Mol	Chain	Length	Quality of chain
3	H	234	
4	F	216	
4	L	216	
5	G	2	
5	I	2	
5	J	2	
5	N	2	
5	O	2	
5	P	2	
6	K	3	
6	M	3	

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
5	NAG	G	2	-	-	-	X
5	NAG	J	2	-	-	-	X
5	NAG	O	2	-	-	-	X
6	NAG	K	1	-	-	-	X
7	NAG	A	410	-	-	-	X
7	NAG	C	410	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14080 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2560	1607	458	480	15	0	0	0
1	C	337	2560	1607	458	480	15	0	0	0

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	139	1054	652	182	215	5	0	0	0
2	D	140	1062	658	183	216	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	524	SER	-	linker	UNP C0LT38
B	525	GLY	-	linker	UNP C0LT38
B	526	ARG	-	linker	UNP C0LT38
D	524	SER	-	linker	UNP C0LT38
D	525	GLY	-	linker	UNP C0LT38
D	526	ARG	-	linker	UNP C0LT38

- Molecule 3 is a protein called Antibody CR8059 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	220	1673	1061	278	327	7	0	0	0
3	H	221	1679	1064	279	328	8	0	0	0

- Molecule 4 is a protein called Antibody CR8059 Light Chain.

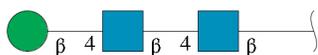
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	213	Total	C	N	O	S	0	0	0
			1606	1006	269	327	4			
4	L	214	Total	C	N	O	S	0	0	0
			1612	1009	270	328	5			

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



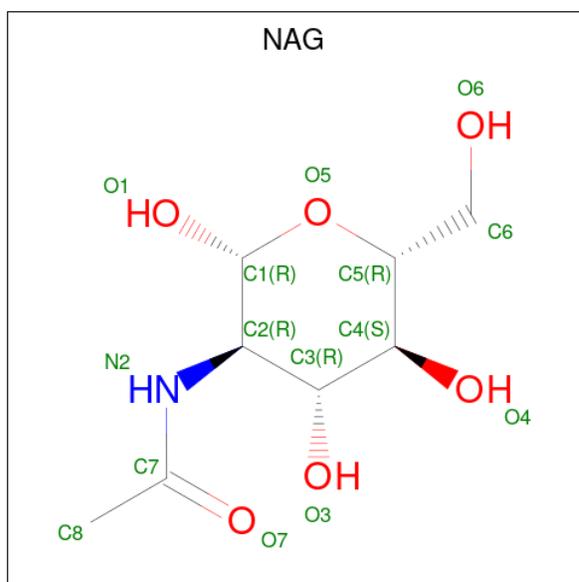
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 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
6	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

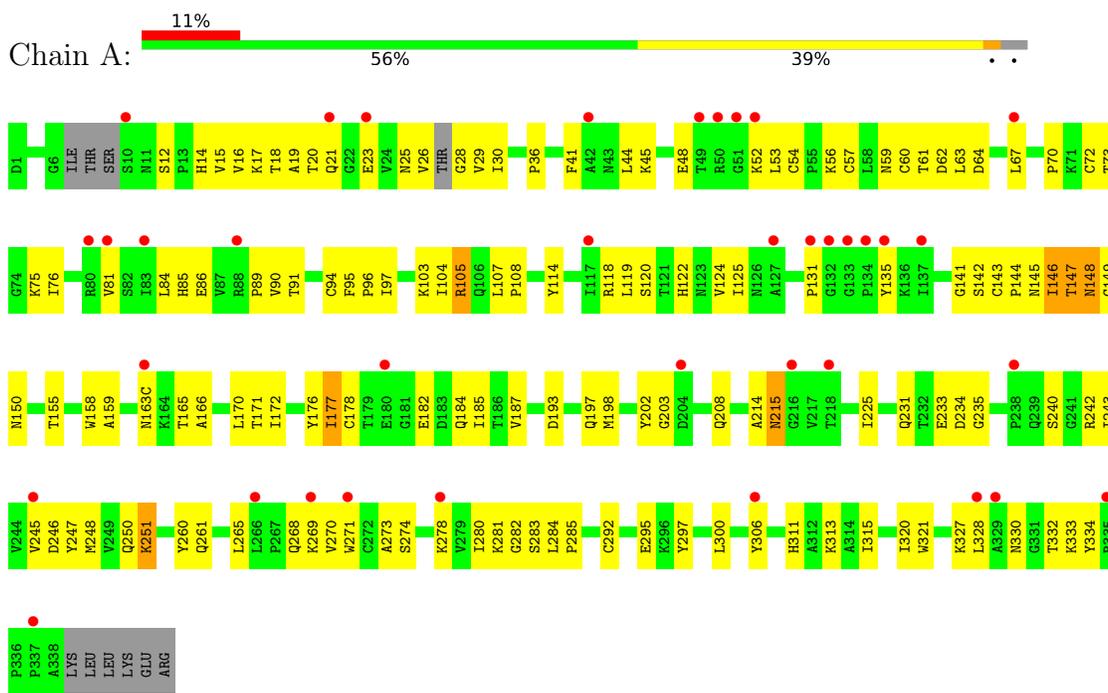


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

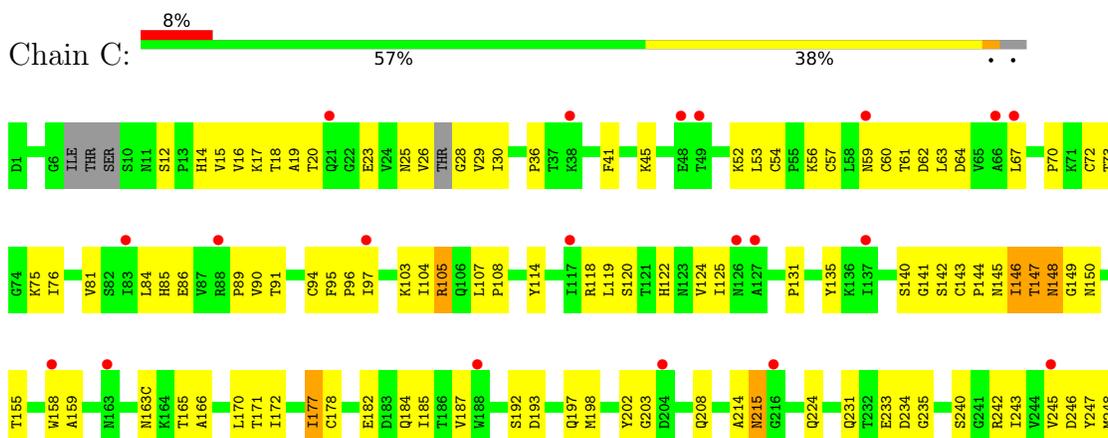
3 Residue-property plots [i](#)

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

- Molecule 1: Hemagglutinin HA1



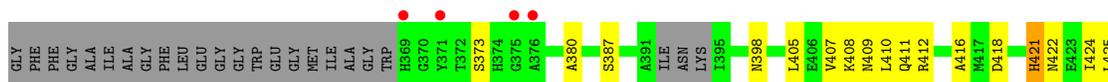
- Molecule 1: Hemagglutinin HA1





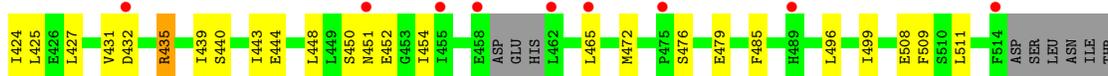
ARG

• Molecule 2: Hemagglutinin HA2



GLY ARG

• Molecule 2: Hemagglutinin HA2



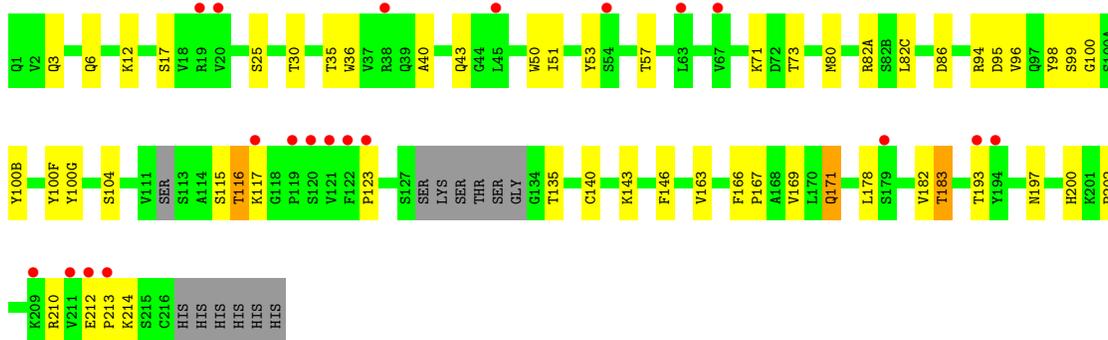
ALA ALA SER SER GLY ARG

• Molecule 3: Antibody CR8059 Heavy Chain



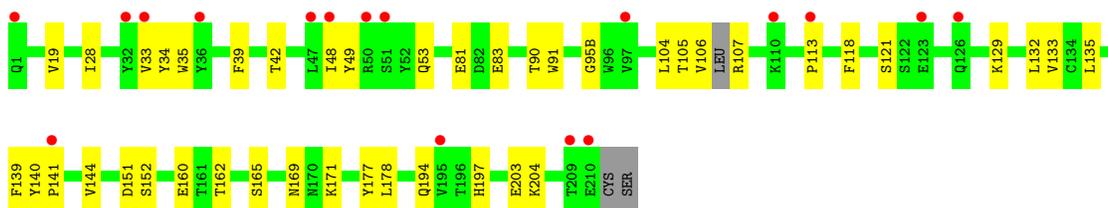
• Molecule 3: Antibody CR8059 Heavy Chain

Chain H: 



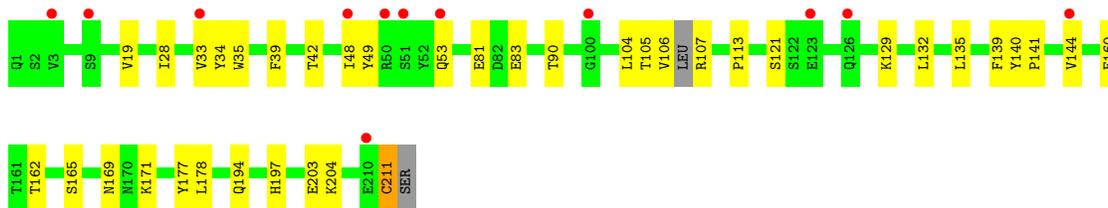
• Molecule 4: Antibody CR8059 Light Chain

Chain F: 



• Molecule 4: Antibody CR8059 Light Chain

Chain L: 

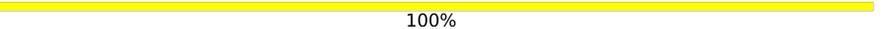


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 

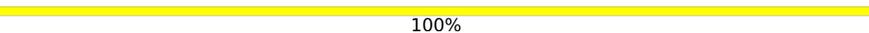


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

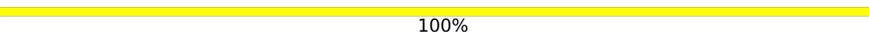


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

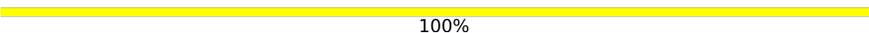
MAG1
MAG2

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

Chain N:  100%

MAG1
MAG2

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

Chain O:  100%

MAG1
MAG2

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

Chain P:  50% 50%

MAG1
MAG2

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

Chain K:  67% 33%

MAG1
MAG2
BMA3

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

Chain M:  67% 33%

MAG1
MAG2
BMA3

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	189.20Å 189.20Å 319.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.93 – 5.65 48.93 – 5.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.93-5.65) 99.9 (48.93-5.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 5.73Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.306 , 0.324 0.298 , 0.321	Depositor DCC
R_{free} test set	1275 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	243.5	Xtrriage
Anisotropy	0.141	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 139.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.429 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	14080	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

5.1 Standard geometry

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	0.64	0/2618	0.94	3/3553 (0.1%)
1	C	0.64	0/2618	0.94	2/3553 (0.1%)
2	B	0.45	0/1063	0.70	0/1429
2	D	0.45	0/1071	0.71	0/1440
3	E	0.44	0/1714	0.61	0/2335
3	H	0.44	0/1720	0.61	0/2343
4	F	0.43	0/1648	0.57	0/2250
4	L	0.43	0/1654	0.57	0/2258
All	All	0.52	0/14106	0.75	5/19161 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	A	84	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	C	67	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	A	67	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	A	44	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2559	201	0
1	C	2560	0	2559	195	0
2	B	1054	0	1043	65	0
2	D	1062	0	1054	59	0
3	E	1673	0	1633	50	0
3	H	1679	0	1638	49	0
4	F	1606	0	1541	34	0
4	L	1612	0	1546	29	0
5	G	28	0	25	1	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	5	0
6	K	39	0	34	3	0
6	M	39	0	34	1	0
7	A	14	0	13	0	0
7	C	14	0	13	0	0
All	All	14080	0	13817	567	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 20.

The worst 5 of 567 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:214:ALA:HB2	1:C:248:MET:CE	1.62	1.29
1:A:214:ALA:HB2	1:A:248:MET:CE	1.62	1.27
1:A:20:THR:CG2	2:B:452:GLU:HG3	1.78	1.13
1:A:320:ILE:CD1	2:B:405:LEU:HD22	1.78	1.12
1:C:320:ILE:CD1	2:D:405:LEU:HD22	1.80	1.11

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	331/347 (95%)	303 (92%)	22 (7%)	6 (2%)	8	40
1	C	331/347 (95%)	303 (92%)	22 (7%)	6 (2%)	8	40
2	B	133/179 (74%)	128 (96%)	5 (4%)	0	100	100
2	D	134/179 (75%)	129 (96%)	5 (4%)	0	100	100
3	E	214/234 (92%)	202 (94%)	11 (5%)	1 (0%)	29	69
3	H	215/234 (92%)	203 (94%)	11 (5%)	1 (0%)	29	69
4	F	209/216 (97%)	202 (97%)	7 (3%)	0	100	100
4	L	210/216 (97%)	203 (97%)	7 (3%)	0	100	100
All	All	1777/1952 (91%)	1673 (94%)	90 (5%)	14 (1%)	19	60

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ILE
1	A	251	LYS
1	C	177	ILE
1	C	251	LYS
1	A	148	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/294 (97%)	279 (98%)	5 (2%)	59	77
1	C	284/294 (97%)	279 (98%)	5 (2%)	59	77
2	B	116/143 (81%)	114 (98%)	2 (2%)	60	78
2	D	117/143 (82%)	115 (98%)	2 (2%)	60	78
3	E	185/198 (93%)	177 (96%)	8 (4%)	29	54
3	H	186/198 (94%)	178 (96%)	8 (4%)	29	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	180/183 (98%)	178 (99%)	2 (1%)	73	84
4	L	181/183 (99%)	178 (98%)	3 (2%)	60	78
All	All	1533/1636 (94%)	1498 (98%)	35 (2%)	50	70

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	171	GLN
3	H	178	LEU
4	L	81	GLU
2	D	421	HIS
1	C	215	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	85	HIS
1	C	126	ASN
2	D	409	ASN
1	C	129	ASN
1	A	129	ASN

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](#)

18 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	5,1	14,14,15	0.52	0	17,19,21	0.95	1 (5%)
5	NAG	G	2	5	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
5	NAG	I	1	5,1	14,14,15	0.40	0	17,19,21	1.80	3 (17%)
5	NAG	I	2	5	14,14,15	0.45	0	17,19,21	1.27	3 (17%)
5	NAG	J	1	5,1	14,14,15	0.53	0	17,19,21	0.96	1 (5%)
5	NAG	J	2	5	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
6	NAG	K	1	6,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
6	NAG	K	2	6	14,14,15	0.50	0	17,19,21	1.40	3 (17%)
6	BMA	K	3	6	11,11,12	0.66	0	15,15,17	1.46	3 (20%)
6	NAG	M	1	6,1	14,14,15	0.52	0	17,19,21	0.95	1 (5%)
6	NAG	M	2	6	14,14,15	0.49	0	17,19,21	0.86	1 (5%)
6	BMA	M	3	6	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
5	NAG	N	1	5,1	14,14,15	0.40	0	17,19,21	1.80	3 (17%)
5	NAG	N	2	5	14,14,15	0.44	0	17,19,21	1.27	3 (17%)
5	NAG	O	1	5,1	14,14,15	0.51	0	17,19,21	0.96	1 (5%)
5	NAG	O	2	5	14,14,15	0.49	0	17,19,21	0.85	1 (5%)
5	NAG	P	1	5,1	14,14,15	0.51	0	17,19,21	2.24	3 (17%)
5	NAG	P	2	5	14,14,15	0.49	0	17,19,21	1.40	3 (17%)

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	5,1	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	J	2	5	-	3/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1

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

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1	NAG	O5-C1-C2	-7.39	99.63	111.29
6	K	1	NAG	O5-C1-C2	-7.38	99.64	111.29
5	I	1	NAG	C1-O5-C5	5.94	120.24	112.19
5	N	1	NAG	C1-O5-C5	5.92	120.21	112.19
6	K	2	NAG	O5-C5-C6	-3.58	101.59	107.20

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C8-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	I	1	NAG	O7-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	N	1	NAG	O5-C5-C6-O6

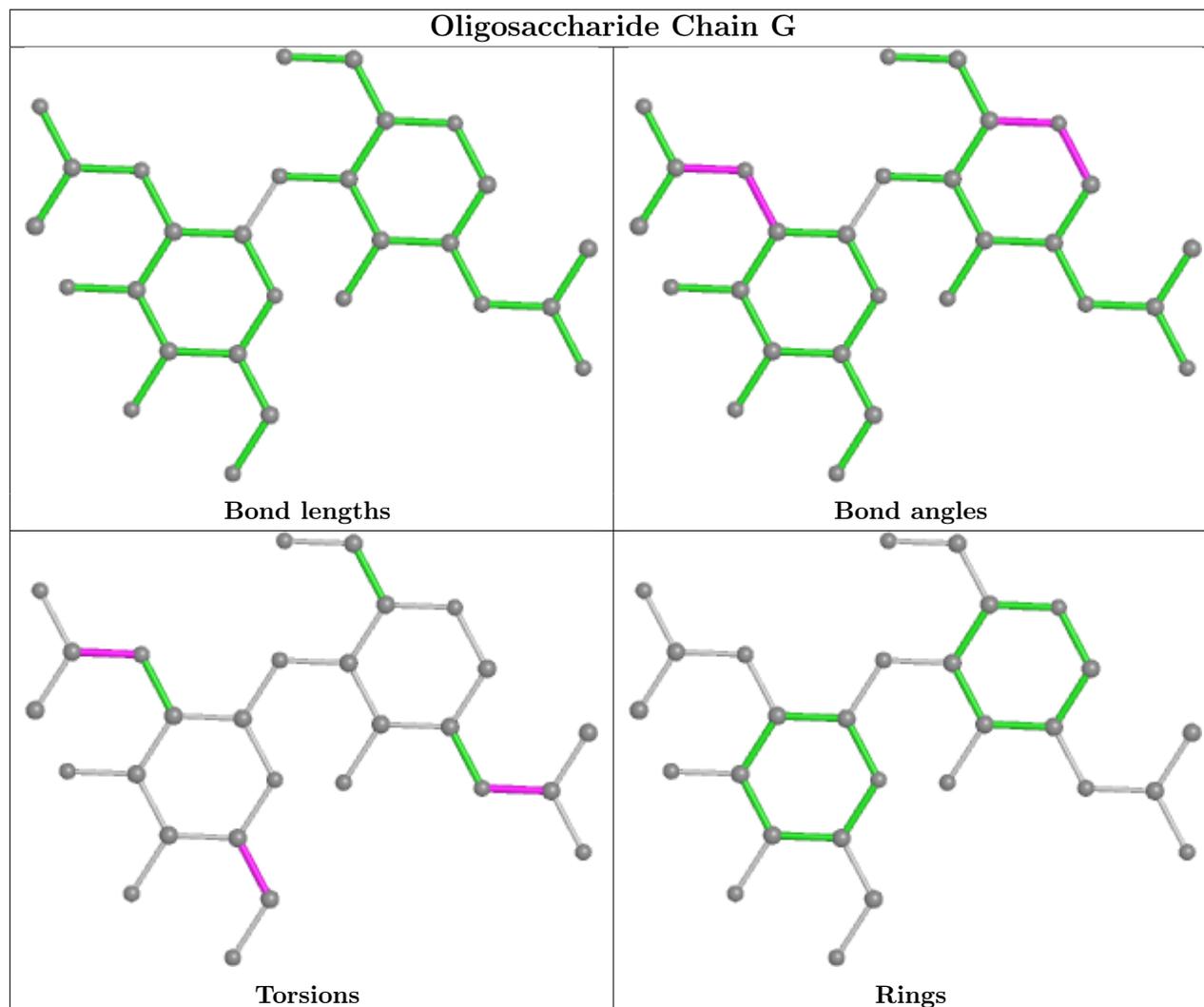
There are no ring outliers.

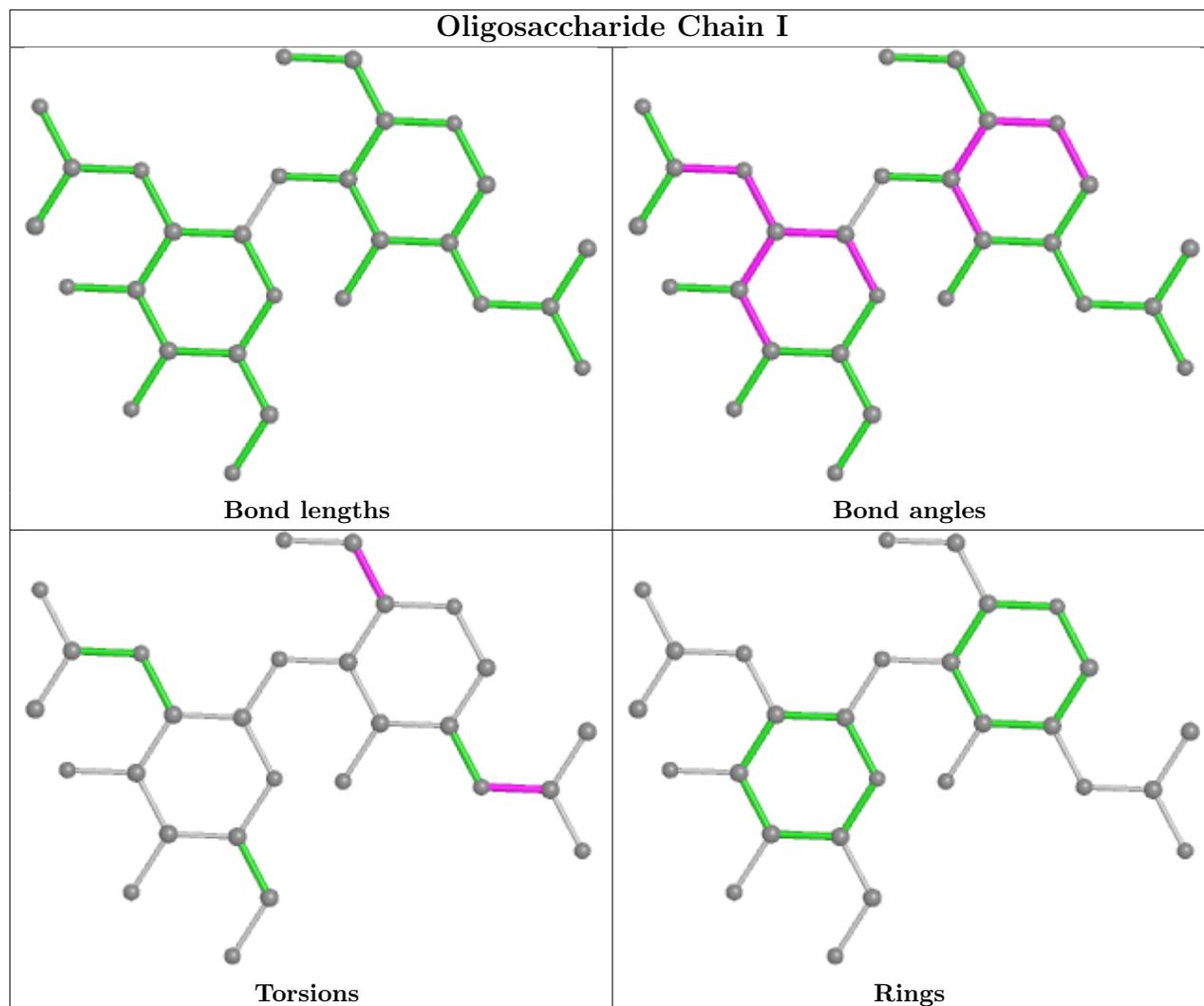
4 monomers are involved in 10 short contacts:

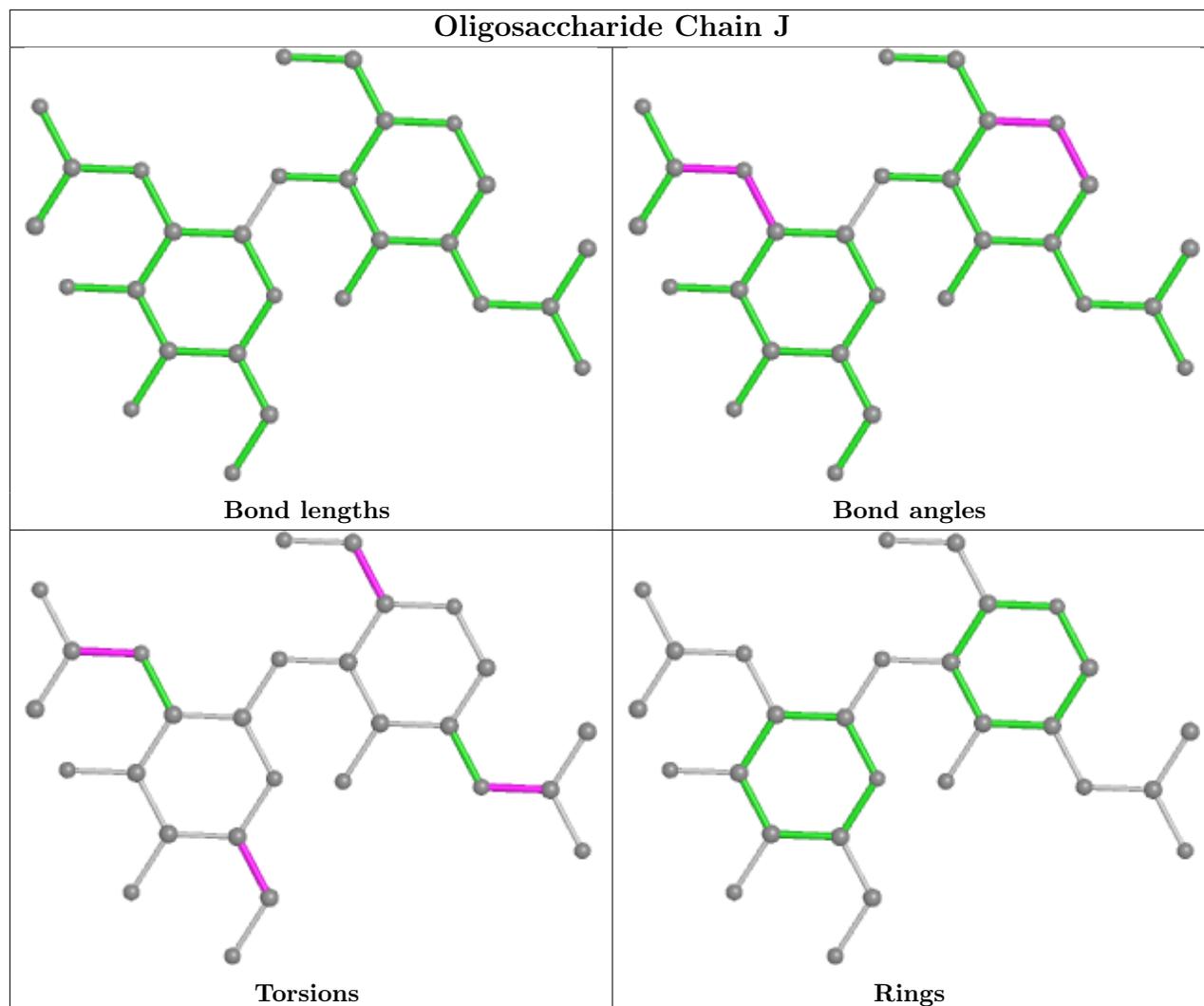
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1	NAG	1	0
6	K	1	NAG	3	0
5	P	1	NAG	5	0
5	G	1	NAG	1	0

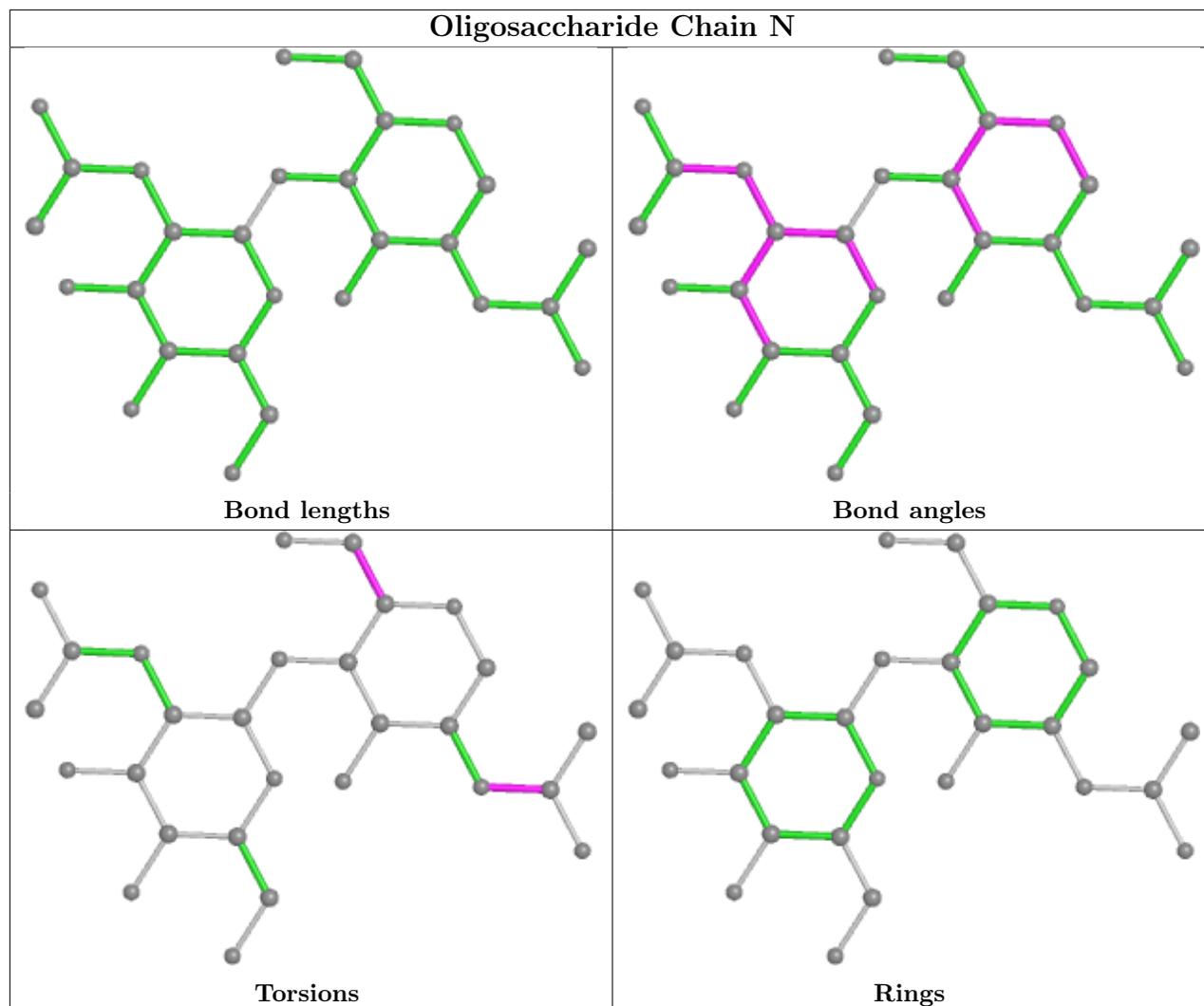
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

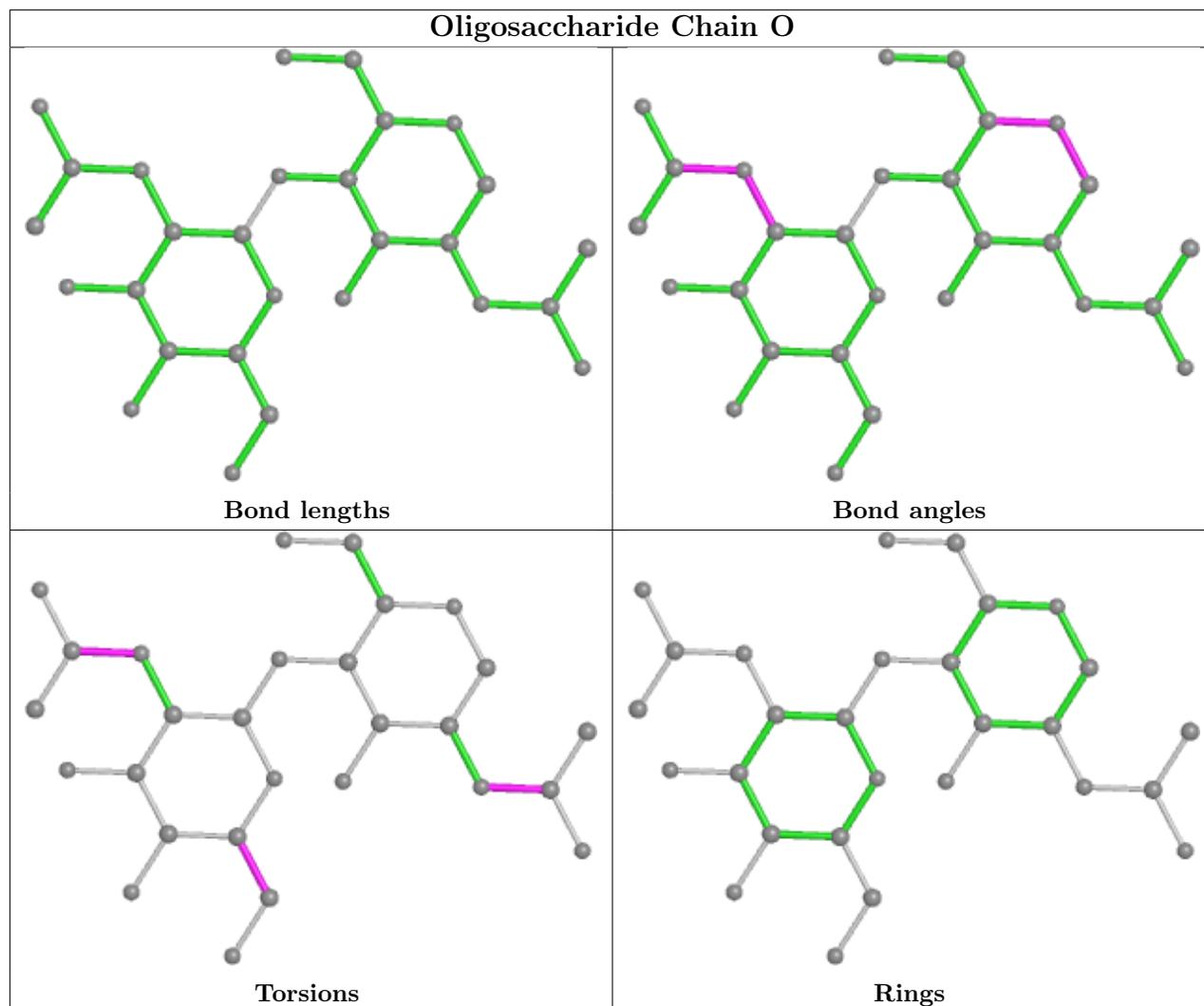
bond angles, torsion angles, and ring geometry for oligosaccharide.

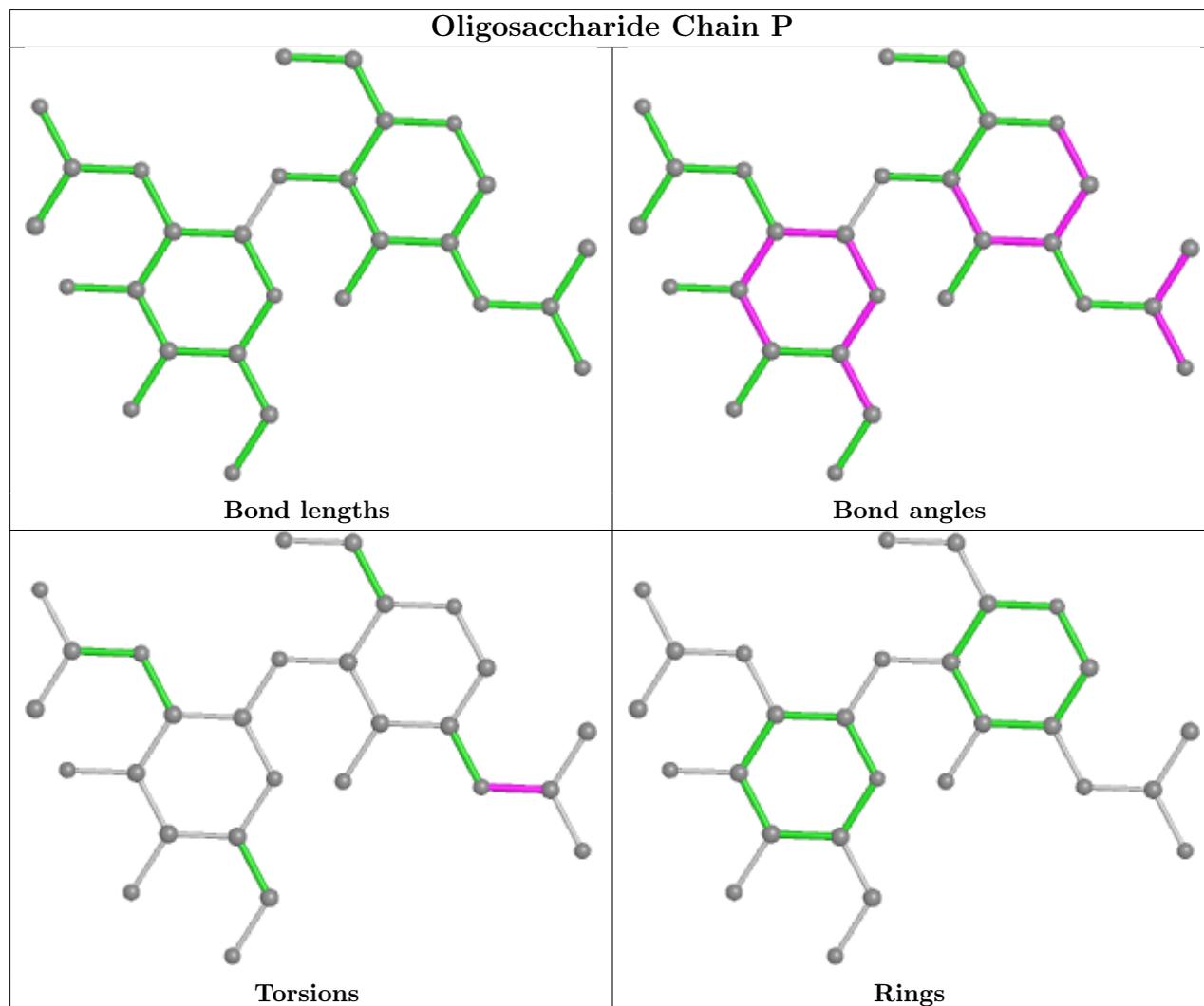


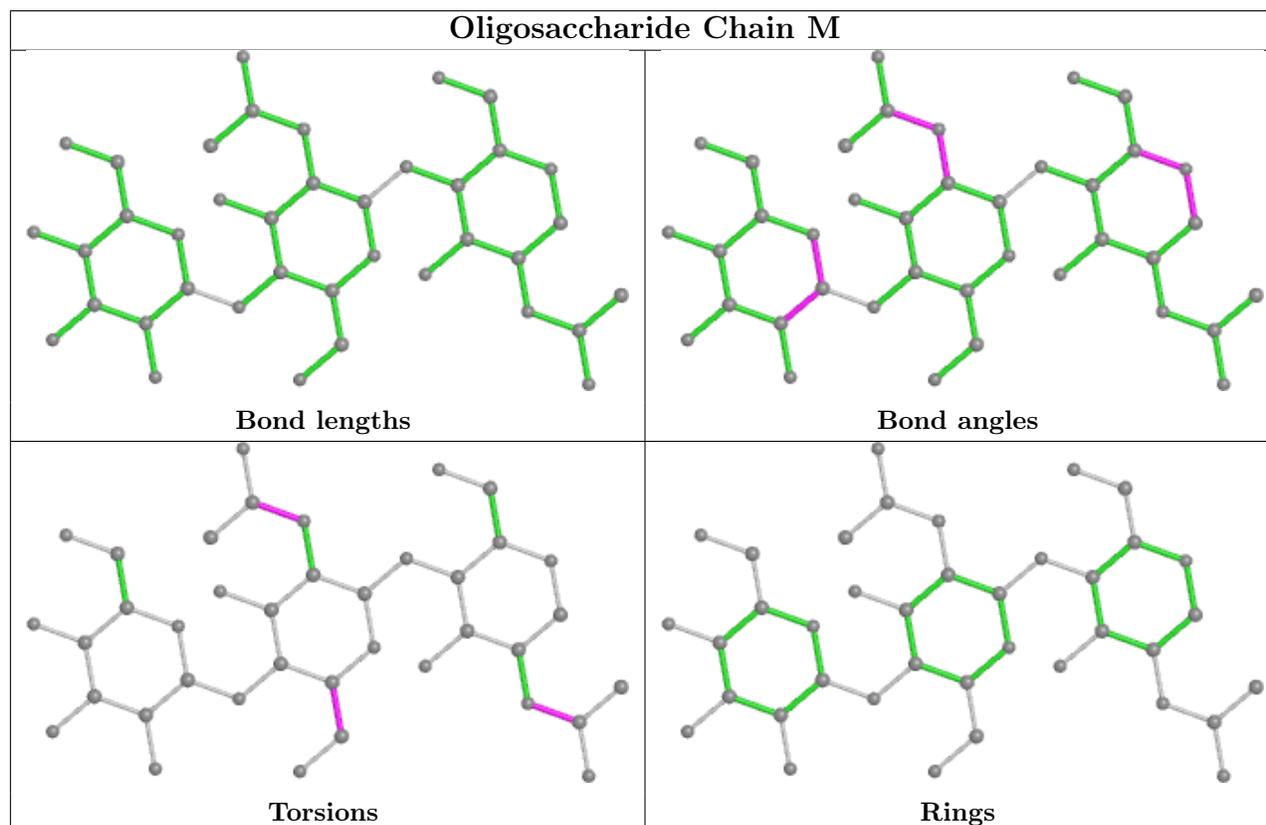
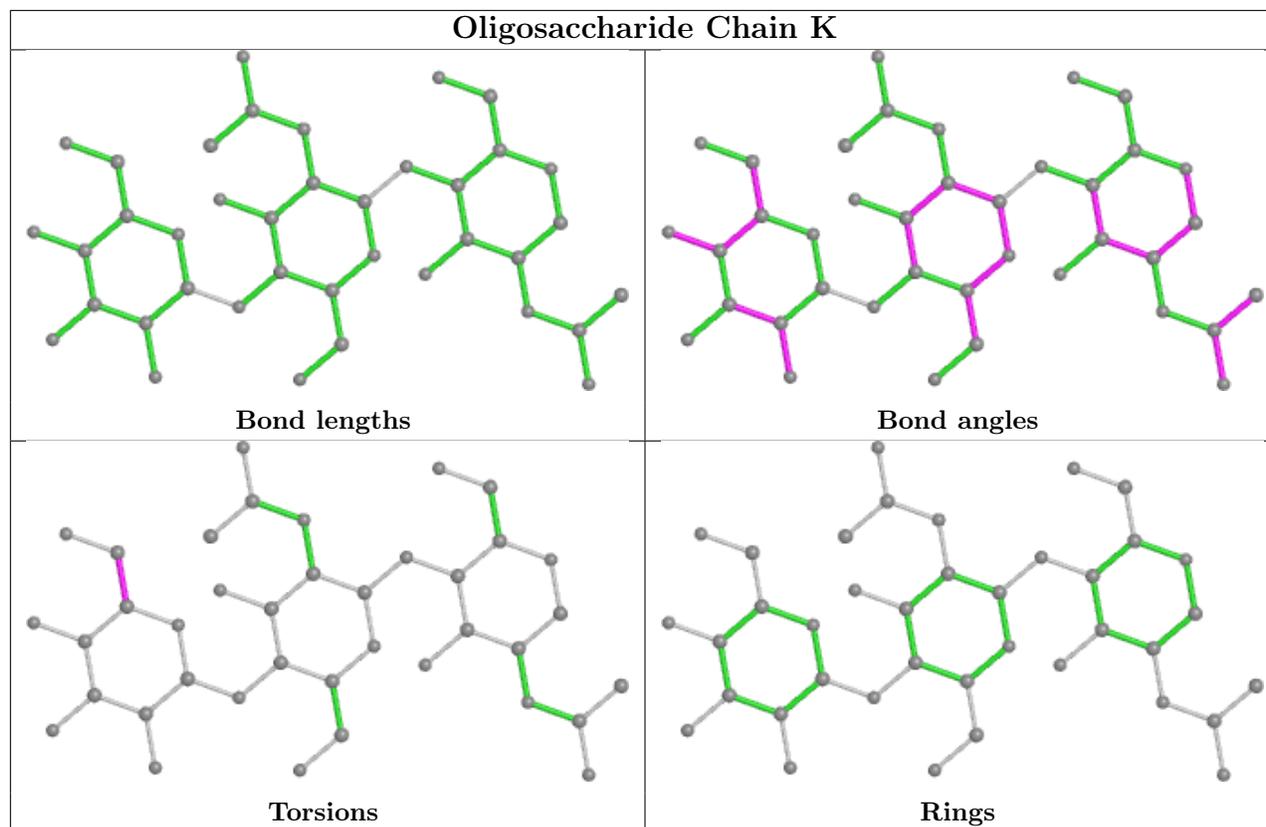












5.6 Ligand geometry

2 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
7	NAG	C	410	1	14,14,15	0.50	0	17,19,21	0.98	1 (5%)
7	NAG	A	410	1	14,14,15	0.49	0	17,19,21	0.98	1 (5%)

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
7	NAG	C	410	1	-	2/6/23/26	0/1/1/1
7	NAG	A	410	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	410	NAG	C1-O5-C5	2.46	115.53	112.19
7	C	410	NAG	C1-O5-C5	2.46	115.52	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	410	NAG	C8-C7-N2-C2
7	C	410	NAG	C8-C7-N2-C2
7	C	410	NAG	O7-C7-N2-C2
7	A	410	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	337/347 (97%)	0.56	37 (10%) 5 8	100, 100, 100, 100	0
1	C	337/347 (97%)	0.52	28 (8%) 11 12	100, 100, 100, 100	0
2	B	139/179 (77%)	0.65	11 (7%) 12 13	100, 100, 100, 100	0
2	D	140/179 (78%)	0.79	14 (10%) 7 9	100, 100, 100, 100	0
3	E	220/234 (94%)	0.66	26 (11%) 4 7	100, 100, 100, 100	0
3	H	221/234 (94%)	0.57	20 (9%) 9 11	100, 100, 100, 100	0
4	F	213/216 (98%)	0.38	17 (7%) 12 13	100, 100, 100, 100	0
4	L	214/216 (99%)	0.30	12 (5%) 24 23	100, 100, 100, 100	0
All	All	1821/1952 (93%)	0.54	165 (9%) 9 10	100, 100, 100, 100	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	194	TYR	6.7
1	C	329	ALA	6.1
4	L	123	GLU	5.4
1	A	329	ALA	4.9
4	F	210	GLU	4.8

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,

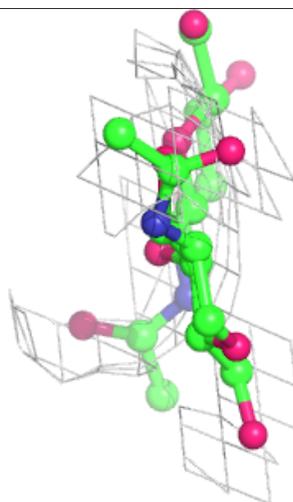
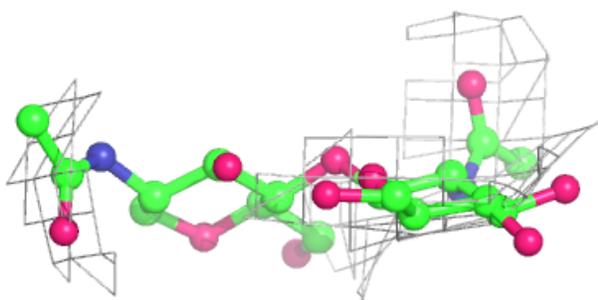
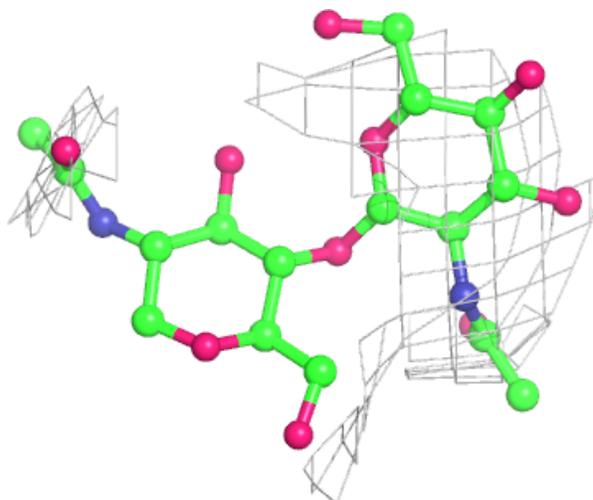
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

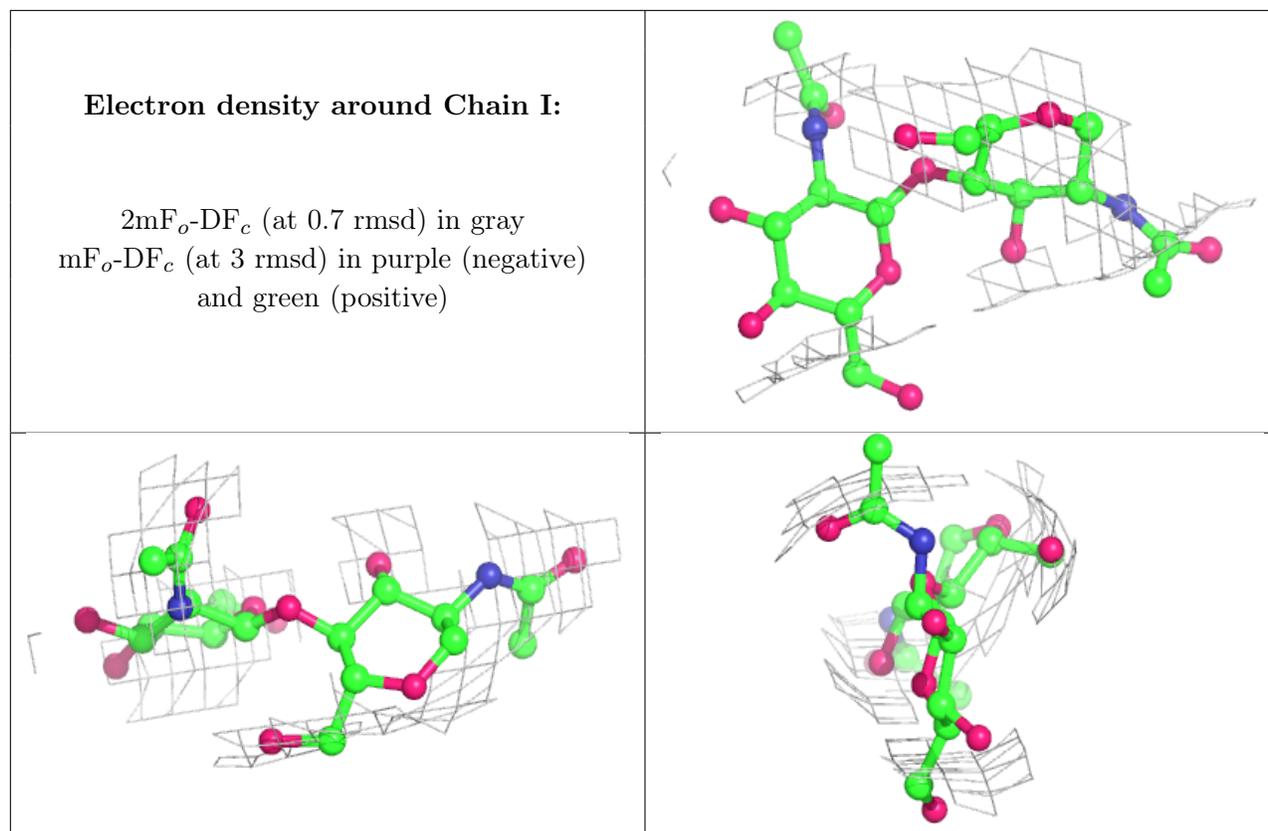
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	G	2	14/15	0.60	0.57	100,100,100,100	0
5	NAG	J	2	14/15	0.67	0.45	100,100,100,100	0
6	BMA	M	3	11/12	0.67	0.38	100,100,100,100	0
5	NAG	P	2	14/15	0.76	0.31	100,100,100,100	0
6	BMA	K	3	11/12	0.76	0.34	100,100,100,100	0
5	NAG	O	2	14/15	0.76	0.41	100,100,100,100	0
6	NAG	K	1	14/15	0.77	0.47	100,100,100,100	0
6	NAG	K	2	14/15	0.80	0.25	100,100,100,100	0
6	NAG	M	2	14/15	0.81	0.38	100,100,100,100	0
5	NAG	I	2	14/15	0.81	0.37	100,100,100,100	0
5	NAG	J	1	14/15	0.82	0.45	100,100,100,100	0
5	NAG	O	1	14/15	0.85	0.50	100,100,100,100	0
5	NAG	P	1	14/15	0.85	0.35	100,100,100,100	0
5	NAG	N	2	14/15	0.89	0.32	100,100,100,100	0
6	NAG	M	1	14/15	0.89	0.29	100,100,100,100	0
5	NAG	G	1	14/15	0.91	0.27	100,100,100,100	0
5	NAG	I	1	14/15	0.91	0.36	100,100,100,100	0
5	NAG	N	1	14/15	0.96	0.19	100,100,100,100	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:

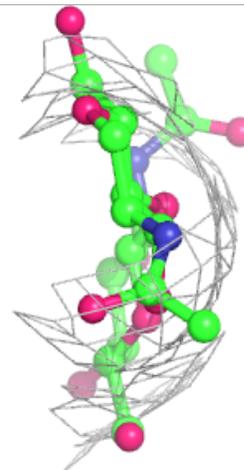
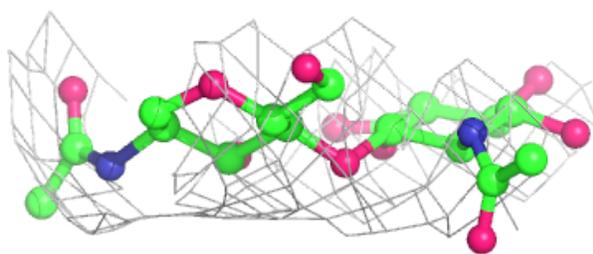
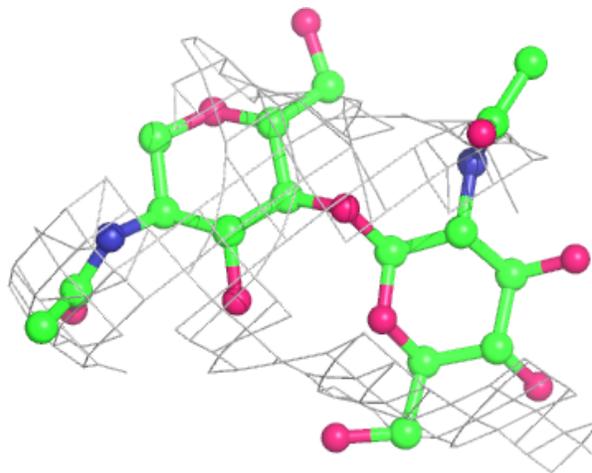
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





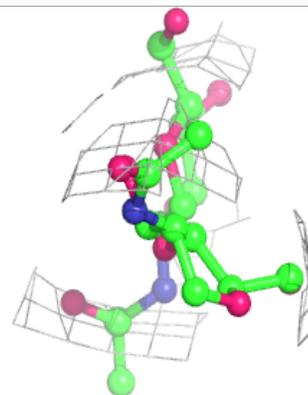
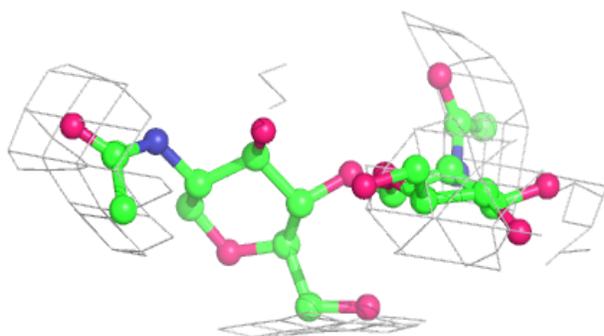
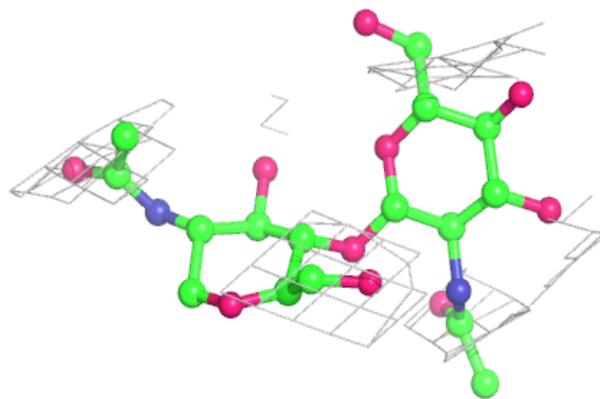
Electron density around Chain J:

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

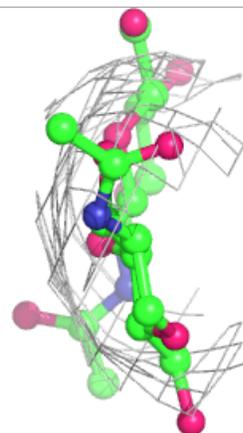
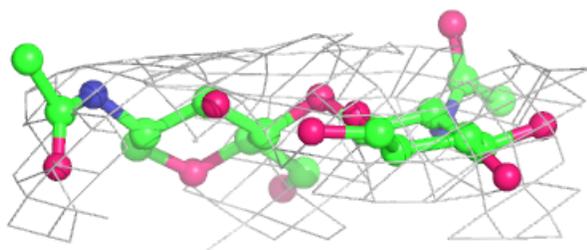
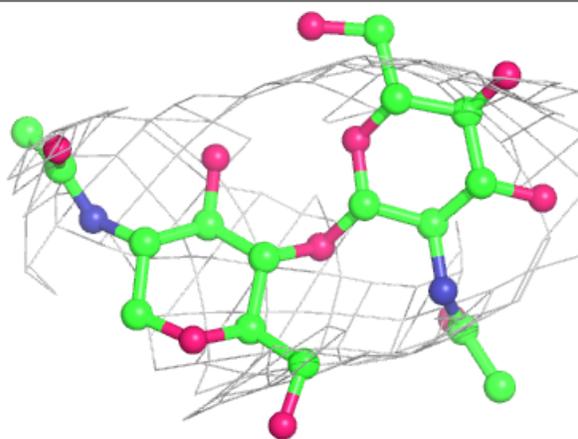


Electron density around Chain N:

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

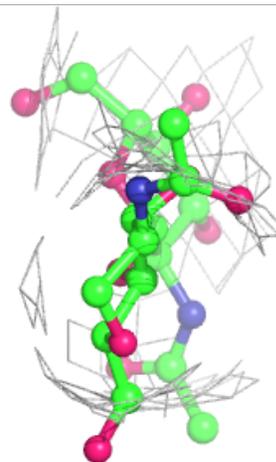
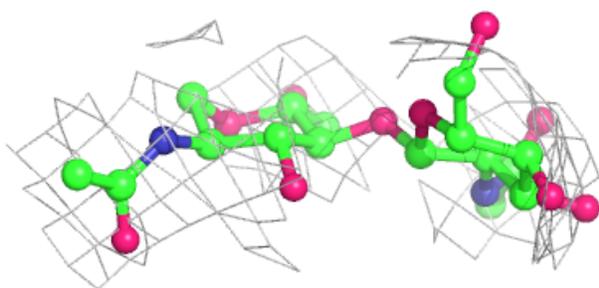
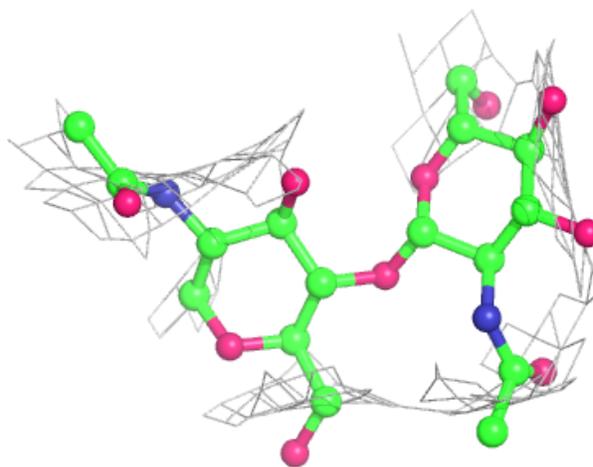
**Electron density around Chain O:**

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



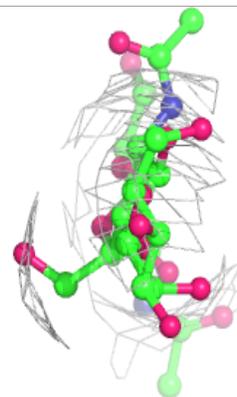
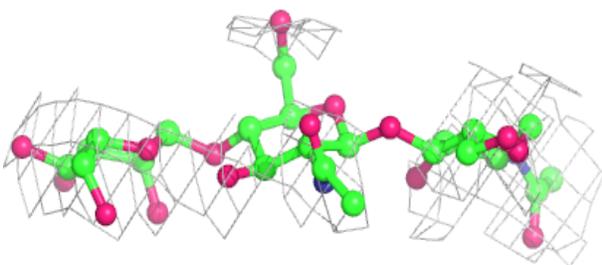
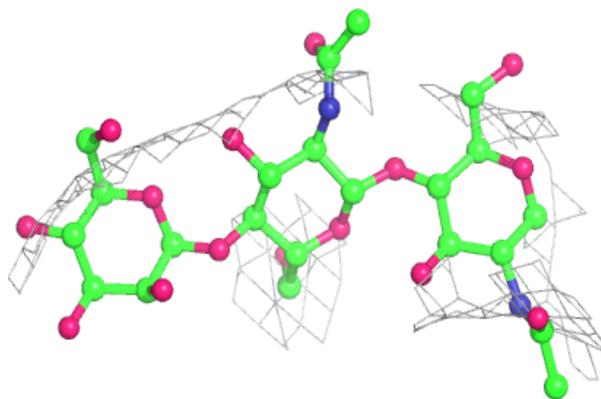
Electron density around Chain P:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

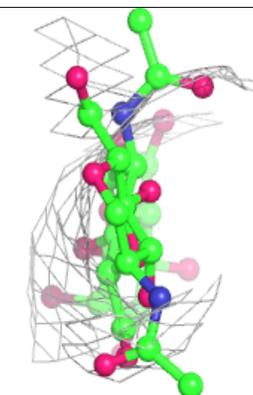
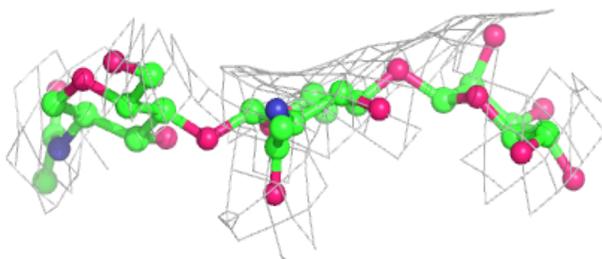
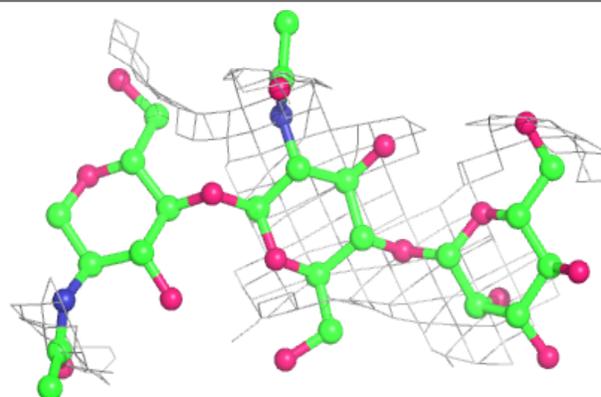


Electron density around Chain K:

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

**Electron density around Chain M:**

$2mF_o-DF_c$ (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
7	NAG	C	410	14/15	0.62	0.50	100,100,100,100	0
7	NAG	A	410	14/15	0.73	0.47	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.