



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 5, 2022 – 04:26 PM EST

PDB ID : 7RFB
Title : Crystal structure of broadly neutralizing antibody mAb1198 in complex with Hepatitis C virus envelope glycoprotein E2 ectodomain
Authors : Flyak, A.I.; Bjorkman, P.J.
Deposited on : 2021-07-14
Resolution : 2.70 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	:	2.25
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)	:	2.25

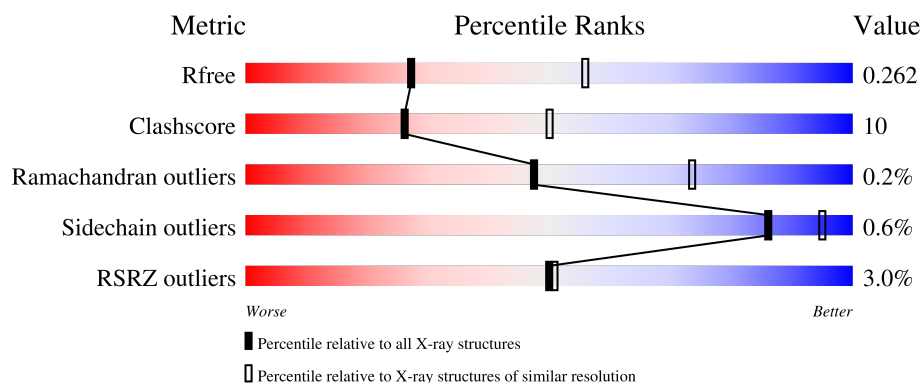
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	237	<div> <div>0%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
1	H	237	<div> <div>3%</div> <div>74%</div> <div>18%</div> <div>8%</div> </div>
2	B	220	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	L	220	<div> <div>3%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
3	C	262	<div> <div>3%</div> <div>75%</div> <div>10%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	262	
4	E	4	
4	F	4	
4	J	4	
5	G	5	
5	I	5	
5	K	5	

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
4	BMA	J	3	-	-	-	X
5	MAN	G	4	-	-	-	X
5	MAN	K	5	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10487 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 mAb1198 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1634	1029	282	317	6			
1	H	219	Total	C	N	O	S	0	0	0
			1621	1021	279	315	6			

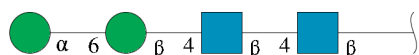
- Molecule 2 is a protein called mAb1198 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1665	1047	279	333	6			
2	L	219	Total	C	N	O	S	0	0	0
			1673	1051	280	336	6			

- Molecule 3 is a protein called envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	226	Total	C	N	O	S	0	0	0
			1771	1123	313	316	19			
3	D	217	Total	C	N	O	S	0	0	0
			1706	1088	298	301	19			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



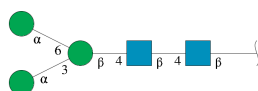
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

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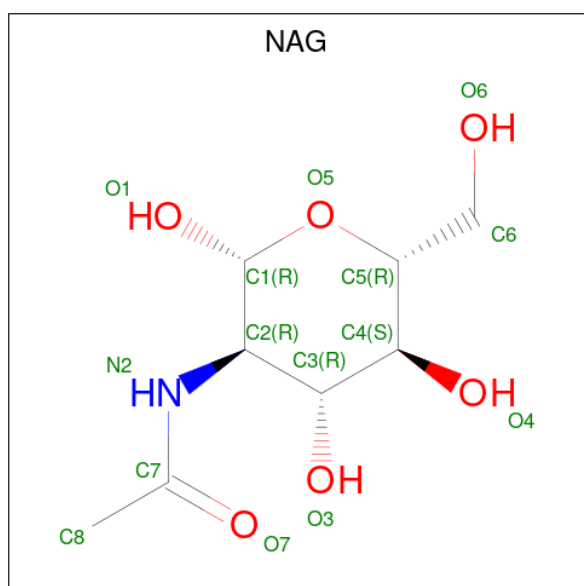
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 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.

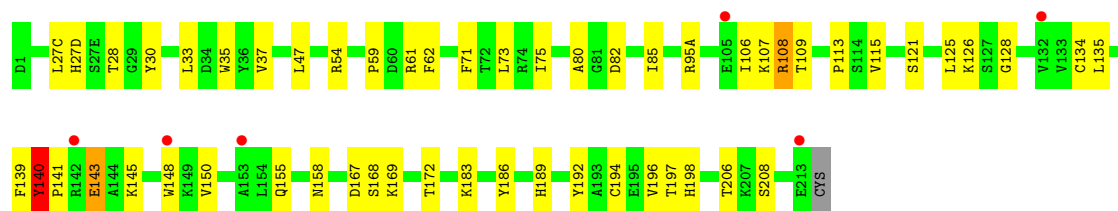


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	K	5	Total	C	N	O	0	0	0
			61	34	2	25			

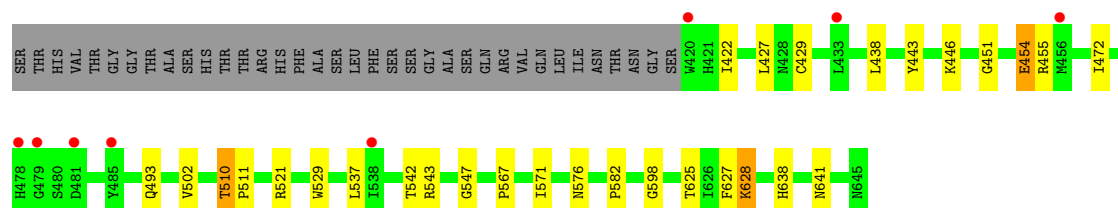
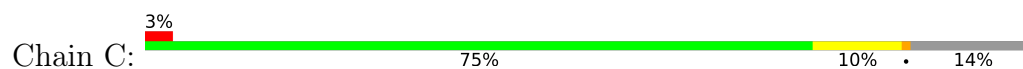
- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



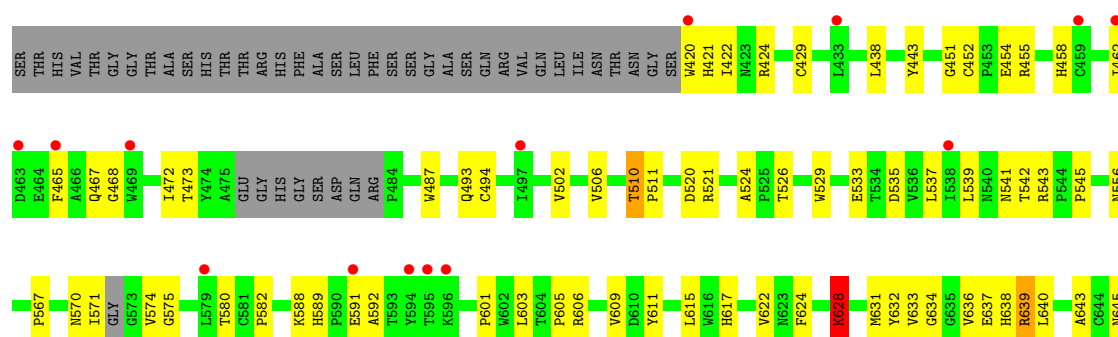
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		



• Molecule 3: envelope glycoprotein E2



• Molecule 3: envelope glycoprotein E2



• Molecule 4: 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



• Molecule 4: 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



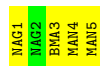
• Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 25% 25%



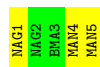
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  20% 80%



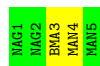
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  40% 60%



- Molecule 5: 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 K:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.09Å 102.43Å 131.52Å 90.00° 92.73° 90.00°	Depositor
Resolution (Å)	46.16 – 2.70 46.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (46.16-2.70) 95.9 (46.16-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.215 , 0.262 0.215 , 0.262	Depositor DCC
R_{free} test set	2318 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10487	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9516e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, MAN, BMA

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	0.41	0/1675	1.50	3/2288 (0.1%)
1	H	0.41	0/1662	0.65	0/2272
2	B	0.43	1/1701 (0.1%)	0.68	2/2311 (0.1%)
2	L	0.46	1/1709 (0.1%)	0.75	4/2322 (0.2%)
3	C	0.44	2/1837 (0.1%)	0.65	1/2517 (0.0%)
3	D	0.48	1/1769 (0.1%)	0.76	4/2423 (0.2%)
All	All	0.44	5/10353 (0.0%)	0.88	14/14133 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
3	D	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	542	THR	C-N	8.13	1.52	1.34
2	B	79	GLU	CD-OE2	5.82	1.32	1.25
3	C	454	GLU	CB-CG	-5.62	1.41	1.52
2	L	143	GLU	CD-OE2	5.61	1.31	1.25
3	C	454	GLU	CD-OE2	-5.11	1.20	1.25

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	CB-CG-OD1	48.20	161.68	118.30
1	A	101	ASP	CB-CG-OD2	-35.92	85.97	118.30
1	A	101	ASP	OD1-CG-OD2	-24.86	76.06	123.30
3	D	628	LYS	CD-CE-NZ	-13.56	80.51	111.70
3	D	542	THR	C-N-CA	-9.42	98.15	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	637	GLU	Sidechain
2	L	140	TYR	Sidechain

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	1634	0	1611	28	0
1	H	1621	0	1595	33	1
2	B	1665	0	1635	28	0
2	L	1673	0	1642	42	0
3	C	1771	0	1628	27	0
3	D	1706	0	1577	67	1
4	E	50	0	43	1	0
4	F	50	0	43	1	0
4	J	50	0	43	1	0
5	G	61	0	52	0	0
5	I	61	0	52	0	0
5	K	61	0	52	0	0
6	C	56	0	52	1	0
6	D	28	0	26	0	0
All	All	10487	0	10051	213	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 213 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:543:ARG:NH2	3:C:567:PRO:O	2.07	0.88
1:H:18:VAL:HG23	1:H:82(C):LEU:HD11	1.60	0.82
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.13	0.80
2:L:28:THR:HG22	2:L:30:TYR:HD1	1.48	0.78
1:H:12:LYS:HG3	1:H:18:VAL:HG22	1.65	0.78

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:628:LYS:NZ	1:H:191:THR:OG1[2_545]	1.98	0.22

5.3 Torsion angles

5.3.1 Protein backbone

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	217/237 (92%)	212 (98%)	5 (2%)	0	100	100
1	H	215/237 (91%)	208 (97%)	7 (3%)	0	100	100
2	B	216/220 (98%)	210 (97%)	6 (3%)	0	100	100
2	L	217/220 (99%)	207 (95%)	10 (5%)	0	100	100
3	C	224/262 (86%)	212 (95%)	10 (4%)	2 (1%)	17	40
3	D	211/262 (80%)	199 (94%)	11 (5%)	1 (0%)	29	54
All	All	1300/1438 (90%)	1248 (96%)	49 (4%)	3 (0%)	47	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	510	THR
3	C	582	PRO
3	D	510	THR

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	183/199 (92%)	183 (100%)	0	100	100
1	H	182/199 (92%)	181 (100%)	1 (0%)	88	96
2	B	190/192 (99%)	189 (100%)	1 (0%)	88	96
2	L	191/192 (100%)	189 (99%)	2 (1%)	76	91
3	C	190/219 (87%)	189 (100%)	1 (0%)	88	96
3	D	184/219 (84%)	182 (99%)	2 (1%)	73	90
All	All	1120/1220 (92%)	1113 (99%)	7 (1%)	86	95

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	639	ARG
1	H	94	LYS
2	L	140	TYR
2	L	108	ARG
3	D	628	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	532	ASN
3	D	421	HIS
3	D	638	HIS
2	B	152	ASN
2	B	45	GLN

5.3.3 RNA [i](#)

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 ⓘ

27 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	$\# Z > 2$
4	NAG	E	1	3,4	14,14,15	0.35	0	17,19,21	1.04	1 (5%)
4	NAG	E	2	4	14,14,15	0.39	0	17,19,21	0.90	0
4	BMA	E	3	4	11,11,12	0.37	0	15,15,17	1.07	1 (6%)
4	MAN	E	4	4	11,11,12	0.46	0	15,15,17	0.88	1 (6%)
4	NAG	F	1	3,4	14,14,15	0.37	0	17,19,21	0.91	0
4	NAG	F	2	4	14,14,15	0.34	0	17,19,21	0.52	0
4	BMA	F	3	4	11,11,12	0.35	0	15,15,17	0.70	0
4	MAN	F	4	4	11,11,12	0.37	0	15,15,17	0.74	0
5	NAG	G	1	3,5	14,14,15	0.32	0	17,19,21	0.75	1 (5%)
5	NAG	G	2	5	14,14,15	0.41	0	17,19,21	0.67	0
5	BMA	G	3	5	11,11,12	0.79	0	15,15,17	1.60	2 (13%)
5	MAN	G	4	5	11,11,12	0.42	0	15,15,17	1.21	3 (20%)
5	MAN	G	5	5	11,11,12	0.43	0	15,15,17	0.91	1 (6%)
5	NAG	I	1	3,5	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
5	NAG	I	2	5	14,14,15	0.35	0	17,19,21	0.81	0
5	BMA	I	3	5	11,11,12	0.36	0	15,15,17	0.83	0
5	MAN	I	4	5	11,11,12	0.42	0	15,15,17	0.99	1 (6%)
5	MAN	I	5	5	11,11,12	0.36	0	15,15,17	0.91	2 (13%)
4	NAG	J	1	3,4	14,14,15	0.50	0	17,19,21	1.33	2 (11%)
4	NAG	J	2	4	14,14,15	0.42	0	17,19,21	0.66	0
4	BMA	J	3	4	11,11,12	0.40	0	15,15,17	1.07	2 (13%)
4	MAN	J	4	4	11,11,12	0.36	0	15,15,17	0.84	0
5	NAG	K	1	3,5	14,14,15	0.34	0	17,19,21	0.52	0
5	NAG	K	2	5	14,14,15	0.24	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	K	3	5	11,11,12	0.36	0	15,15,17	1.00	1 (6%)
5	MAN	K	4	5	11,11,12	0.37	0	15,15,17	0.84	1 (6%)
5	MAN	K	5	5	11,11,12	0.31	0	15,15,17	0.68	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	E	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	3/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	1/2/19/22	0/1/1/1
4	NAG	F	1	3,4	-	2/6/23/26	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
5	NAG	G	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
5	NAG	I	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
5	MAN	I	5	5	-	0/2/19/22	0/1/1/1
4	NAG	J	1	3,4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
4	MAN	J	4	4	-	1/2/19/22	0/1/1/1
5	NAG	K	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	5/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	O3-C3-C2	4.88	119.34	109.99
4	J	1	NAG	O5-C1-C2	-3.80	105.29	111.29
5	I	4	MAN	O5-C1-C2	-2.88	106.33	110.77
4	J	3	BMA	O5-C5-C6	2.83	111.64	107.20
4	J	1	NAG	C1-O5-C5	2.77	115.95	112.19

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

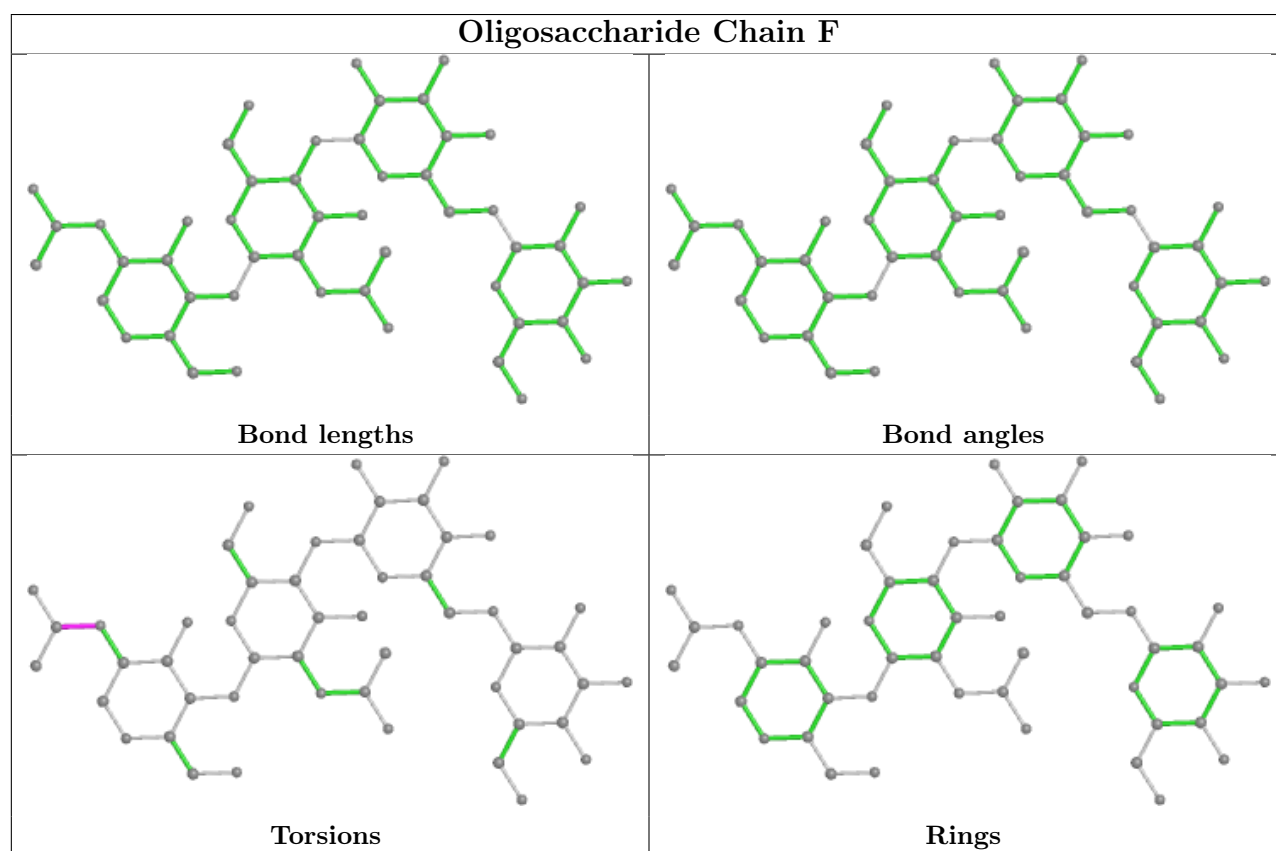
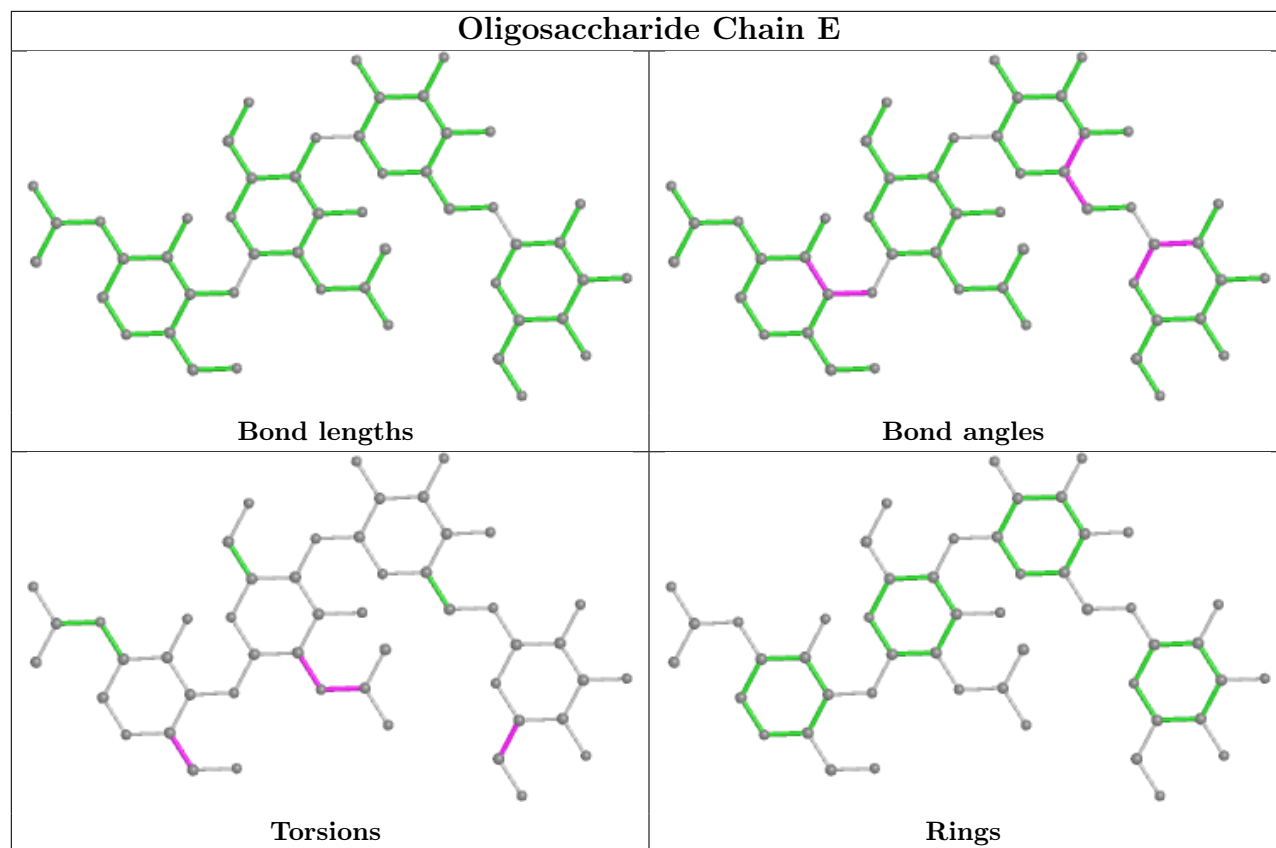
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2

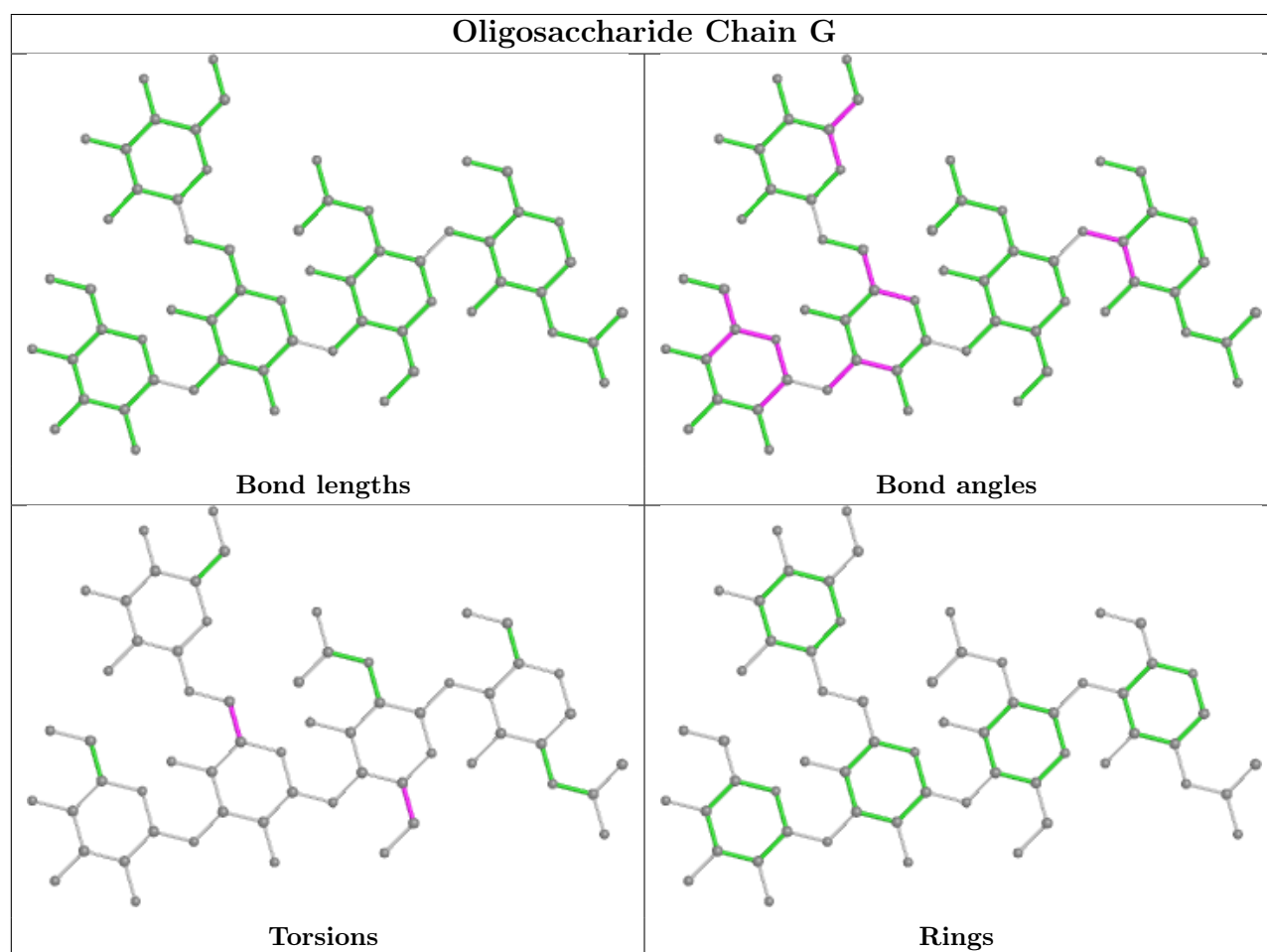
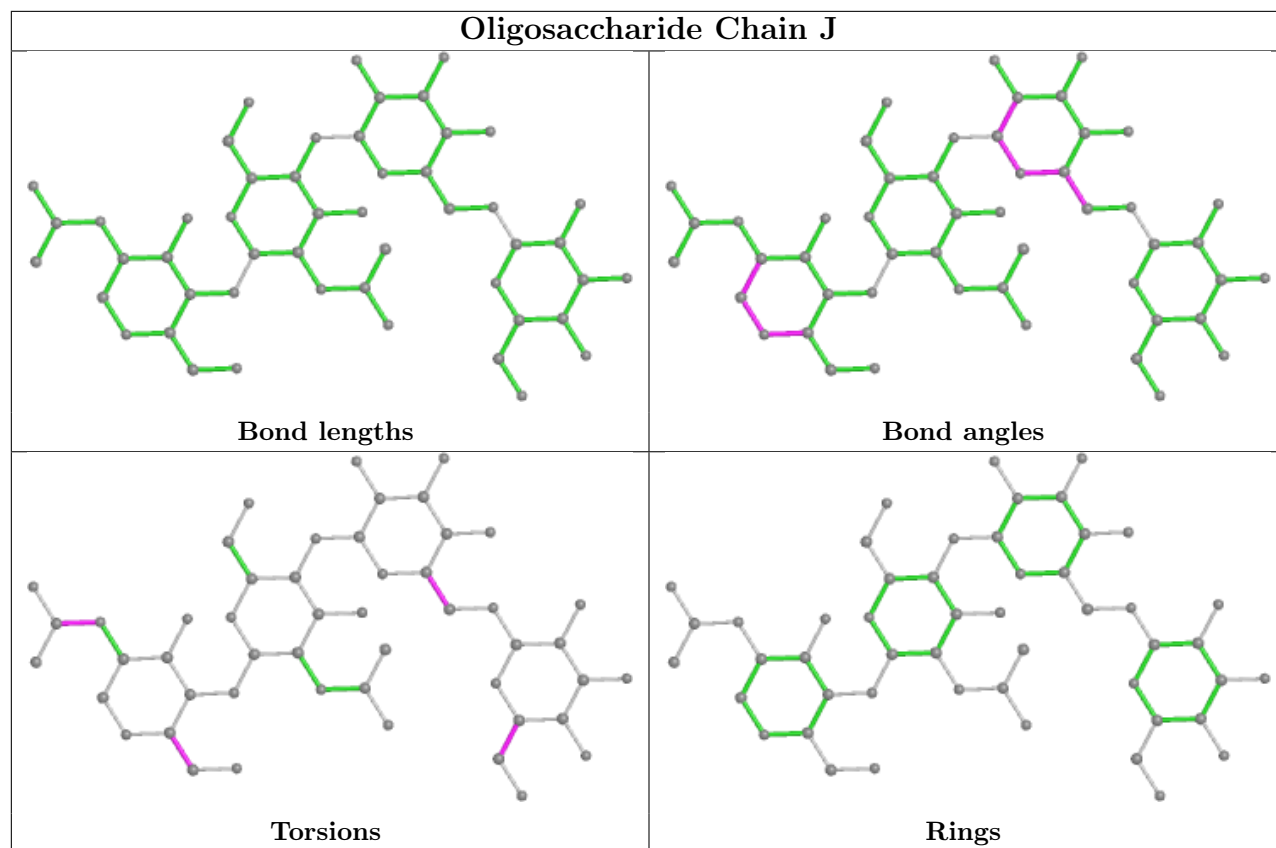
There are no ring outliers.

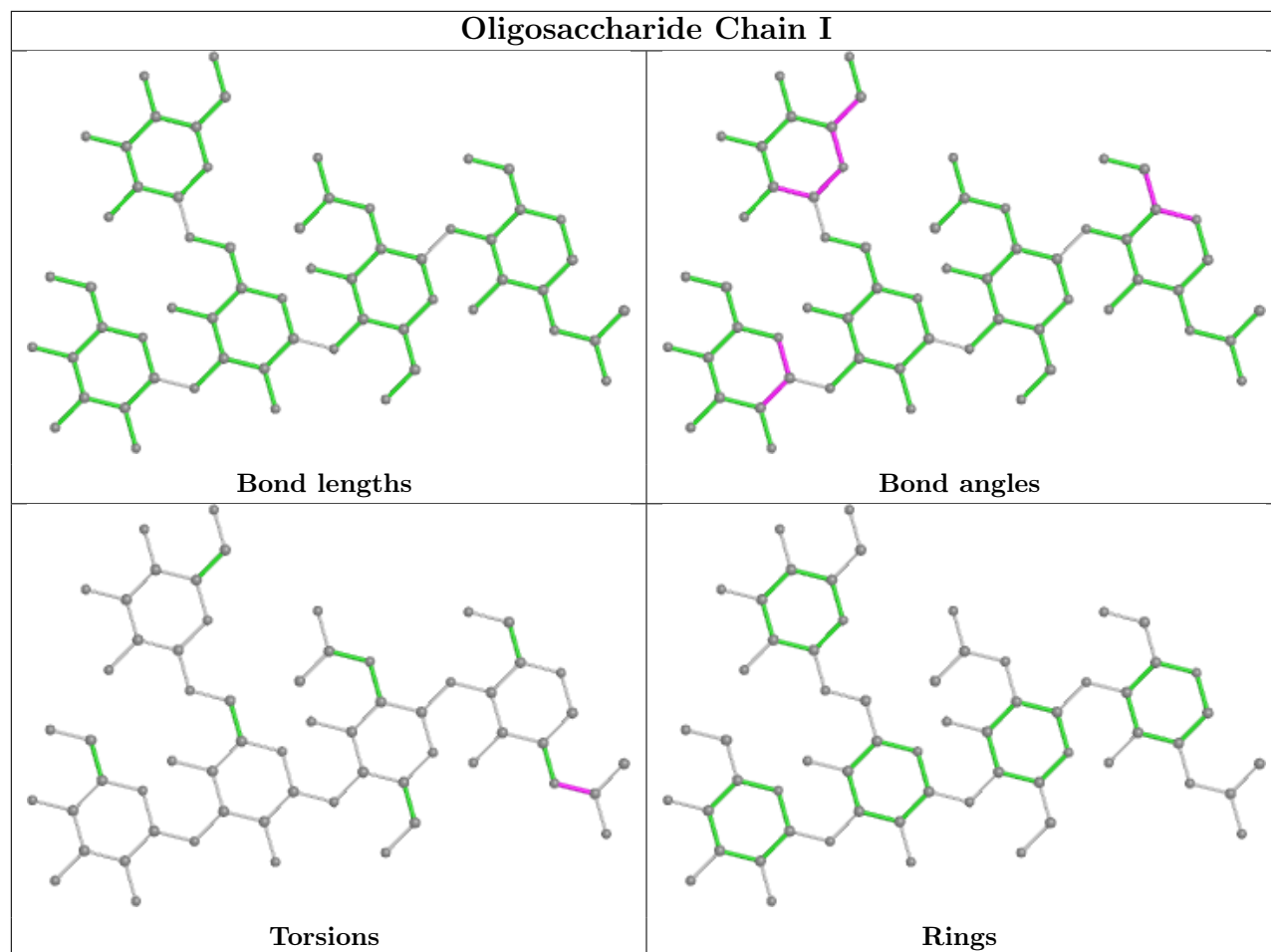
3 monomers are involved in 3 short contacts:

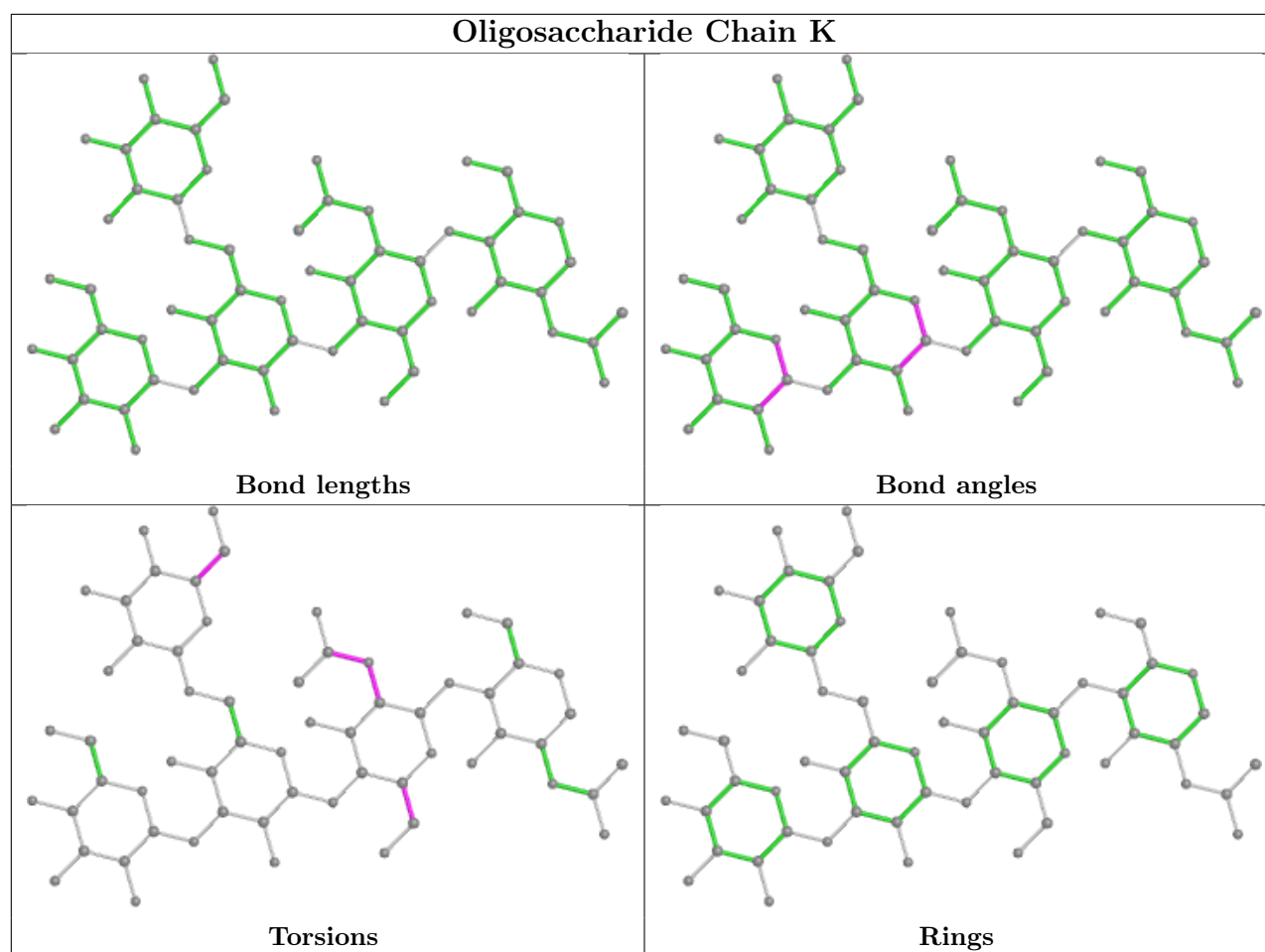
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	1	0
4	F	1	NAG	1	0
4	E	2	NAG	1	0

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](#)

6 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	D	4301	3	14,14,15	0.31	0	17,19,21	0.76	0
6	NAG	C	702	3	14,14,15	0.35	0	17,19,21	1.04	1 (5%)
6	NAG	C	704	3	14,14,15	0.47	0	17,19,21	1.13	2 (11%)
6	NAG	D	4302	3	14,14,15	0.34	0	17,19,21	0.70	0
6	NAG	C	703	3	14,14,15	0.36	0	17,19,21	0.65	0
6	NAG	C	701	3	14,14,15	0.38	0	17,19,21	0.86	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
6	NAG	D	4301	3	-	3/6/23/26	0/1/1/1
6	NAG	C	702	3	-	1/6/23/26	0/1/1/1
6	NAG	C	704	3	-	4/6/23/26	0/1/1/1
6	NAG	D	4302	3	-	2/6/23/26	0/1/1/1
6	NAG	C	703	3	-	2/6/23/26	0/1/1/1
6	NAG	C	701	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	704	NAG	O5-C5-C6	3.11	112.08	107.20
6	C	704	NAG	C4-C3-C2	-2.32	107.62	111.02
6	C	702	NAG	O5-C1-C2	-2.27	107.70	111.29
6	C	701	NAG	O5-C5-C6	2.03	110.38	107.20

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	704	NAG	C8-C7-N2-C2
6	C	704	NAG	O7-C7-N2-C2
6	D	4302	NAG	C8-C7-N2-C2
6	D	4302	NAG	O7-C7-N2-C2
6	D	4301	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	704	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	221/237 (93%)	0.13	3 (1%) 75 77	50, 68, 97, 131	0
1	H	219/237 (92%)	0.34	8 (3%) 41 41	53, 86, 123, 176	0
2	B	218/220 (99%)	0.10	1 (0%) 91 92	50, 87, 115, 132	0
2	L	219/220 (99%)	0.35	6 (2%) 54 55	55, 101, 150, 184	0
3	C	226/262 (86%)	0.34	8 (3%) 44 44	51, 80, 125, 179	0
3	D	217/262 (82%)	0.57	14 (6%) 18 17	62, 103, 161, 201	0
All	All	1320/1438 (91%)	0.31	40 (3%) 50 51	50, 86, 143, 201	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	433	LEU	6.2
3	D	538	ILE	5.9
3	D	469	TRP	5.7
1	A	214	LYS	5.1
2	L	142	ARG	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](#)

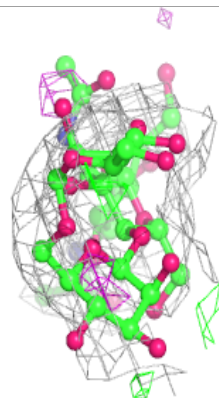
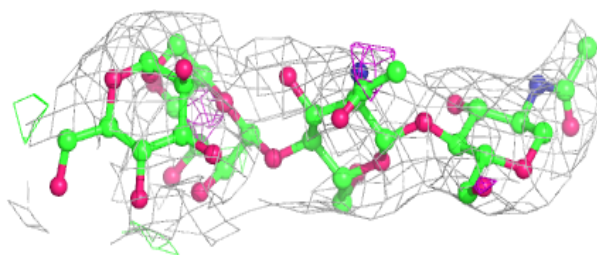
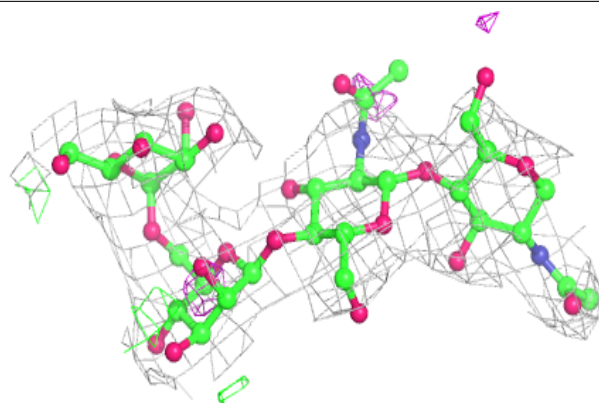
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	J	4	11/12	0.38	0.34	118,133,138,139	0
4	MAN	F	4	11/12	0.52	0.21	123,128,133,135	0
4	MAN	E	4	11/12	0.63	0.23	117,123,125,126	0
5	MAN	G	4	11/12	0.63	0.41	123,127,131,132	0
4	BMA	J	3	11/12	0.67	0.42	136,140,142,142	0
5	MAN	I	4	11/12	0.67	0.28	126,131,135,135	0
5	MAN	I	5	11/12	0.67	0.21	132,137,138,139	0
5	MAN	K	4	11/12	0.67	0.34	131,136,138,139	0
5	MAN	G	5	11/12	0.69	0.35	127,131,133,136	0
5	MAN	K	5	11/12	0.69	0.42	131,140,142,143	0
5	BMA	G	3	11/12	0.70	0.38	126,129,131,132	0
5	BMA	K	3	11/12	0.73	0.39	134,138,141,141	0
4	BMA	F	3	11/12	0.76	0.29	119,124,129,132	0
5	BMA	I	3	11/12	0.77	0.20	133,136,137,137	0
5	NAG	I	2	14/15	0.79	0.29	124,132,133,136	0
4	NAG	J	1	14/15	0.81	0.24	98,105,112,116	0
4	BMA	E	3	11/12	0.82	0.16	119,123,124,125	0
4	NAG	E	2	14/15	0.83	0.26	106,115,121,121	0
5	NAG	G	2	14/15	0.85	0.18	107,112,123,125	0
4	NAG	J	2	14/15	0.90	0.31	113,123,131,135	0
5	NAG	I	1	14/15	0.90	0.22	119,126,130,131	0
4	NAG	E	1	14/15	0.90	0.22	83,97,106,113	0
5	NAG	K	2	14/15	0.92	0.18	111,118,125,132	0
4	NAG	F	2	14/15	0.93	0.24	83,101,110,116	0
4	NAG	F	1	14/15	0.93	0.14	76,82,89,92	0
5	NAG	G	1	14/15	0.94	0.10	79,87,96,104	0
5	NAG	K	1	14/15	0.95	0.11	95,100,106,113	0

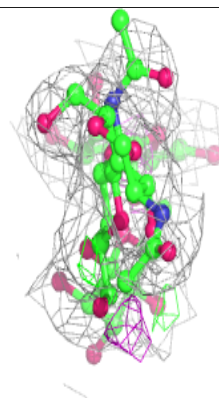
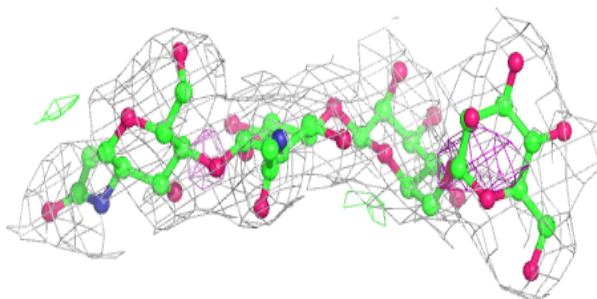
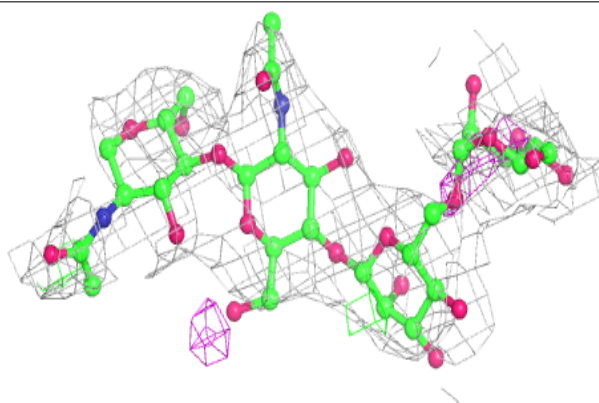
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

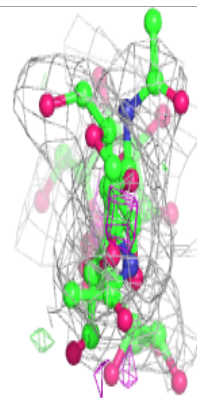
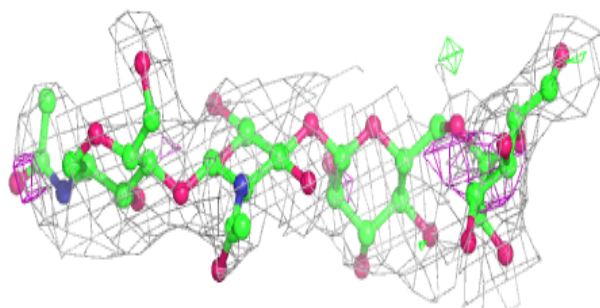
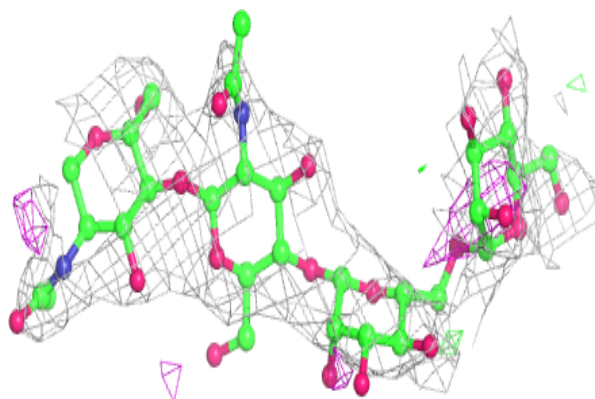
**Electron density around Chain F:**

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

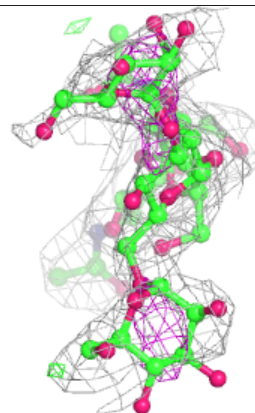
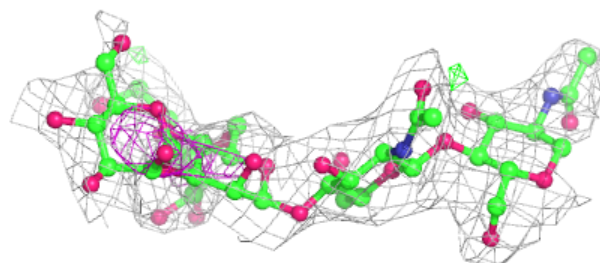
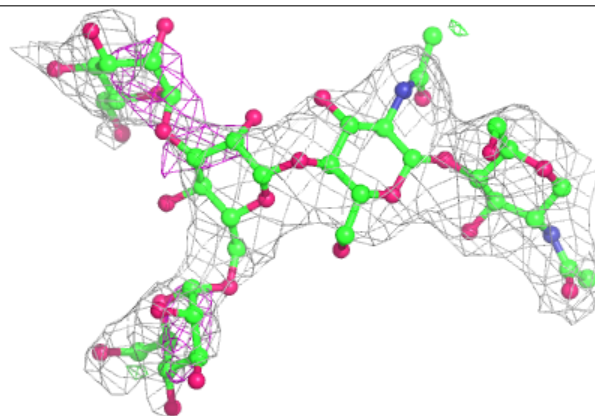


Electron density around Chain J:

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

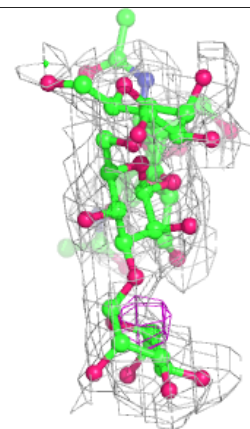
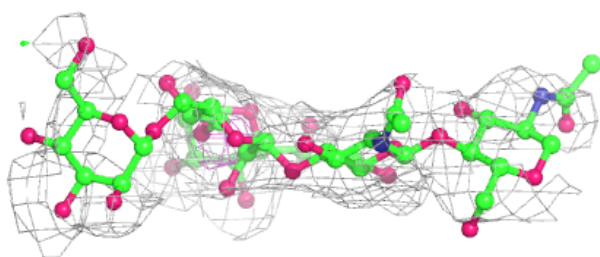
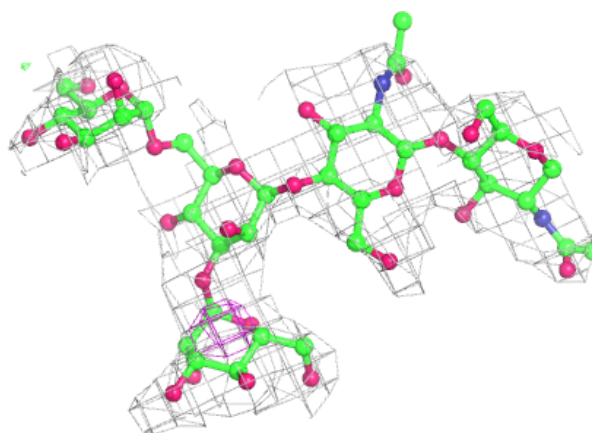
**Electron density around Chain G:**

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

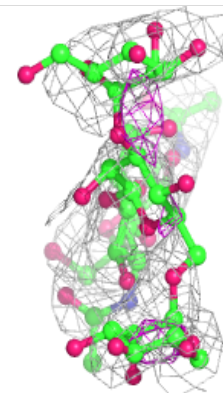
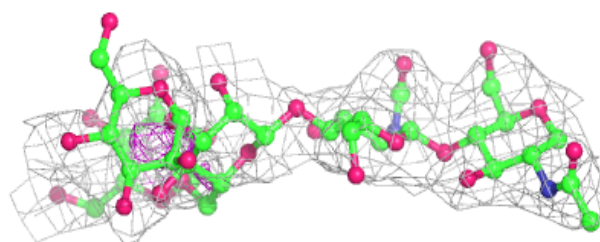
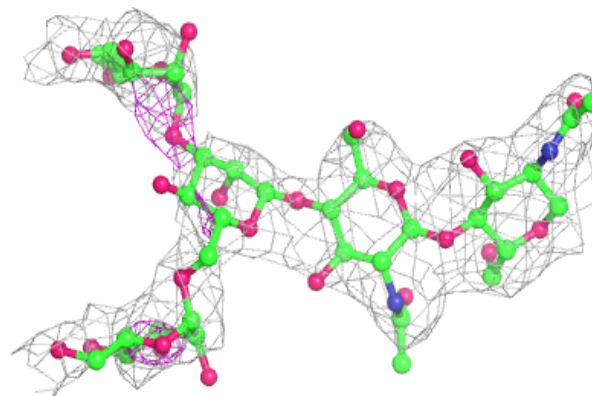


Electron density around Chain I:

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

**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)



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(\AA^2)	Q<0.9
6	NAG	C	704	14/15	0.78	0.25	96,99,108,111	0
6	NAG	C	702	14/15	0.79	0.33	106,115,120,121	0
6	NAG	D	4301	14/15	0.80	0.38	142,146,147,148	0
6	NAG	C	701	14/15	0.85	0.42	98,105,108,111	0
6	NAG	C	703	14/15	0.90	0.16	86,92,98,101	0
6	NAG	D	4302	14/15	0.93	0.12	101,106,111,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.