



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 10:59 AM UTC

PDB ID : 7RFB / pdb_00007rfb
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

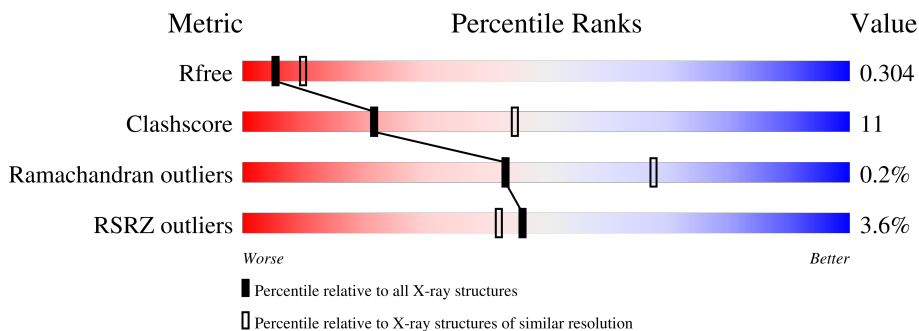
1 Overall quality at a glance

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.



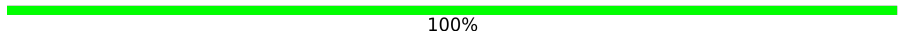
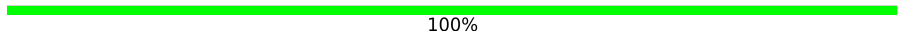
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	
1	H	237	
2	B	220	
2	L	220	
3	C	262	
3	D	262	

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Mol	Chain	Length	Quality of chain
4	E	4	 50% 50%
4	F	4	 75% 25%
4	J	4	 50% 25% 25%
5	G	5	 60% 40%
5	I	5	 100%
5	K	5	 100%

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
			Total	C	N	O	S			
1	A	221	Total 1634	C 1029	N 282	O 317	S 6	0	0	0
1	H	219	Total 1621	C 1021	N 279	O 315	S 6	0	0	0

- Molecule 2 is a protein called mAb1198 Light Chain.

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

- Molecule 3 is a protein called envelope glycoprotein E2.

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

- 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.



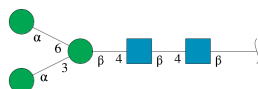
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	4	Total 50	C 28	N 2	O 20	0	0	0

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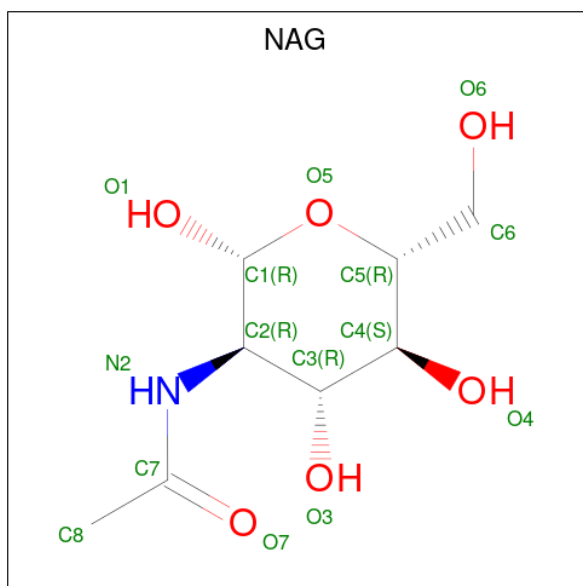
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).




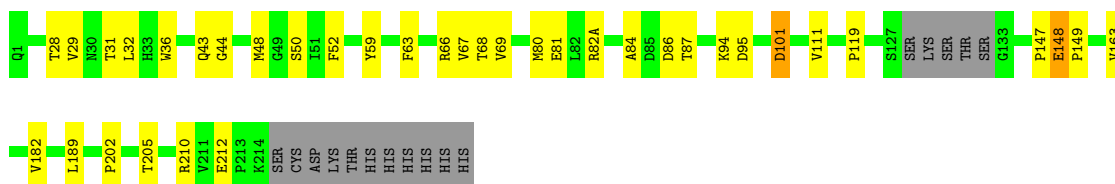
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

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.

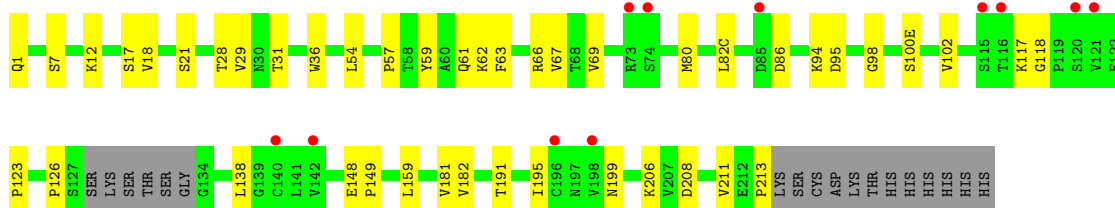
- Molecule 1: mAb1198 Heavy Chain

Chain A: 




- Molecule 1: mAb1198 Heavy Chain

Chain H: 




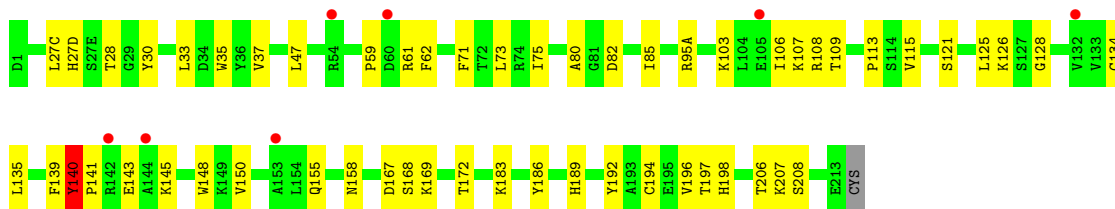
- Molecule 2: mAb1198 Light Chain

Chain B: 

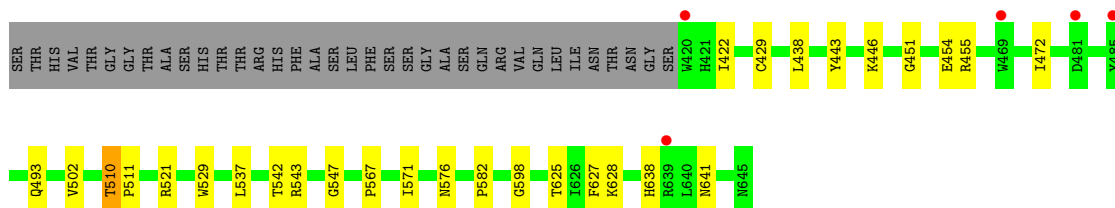
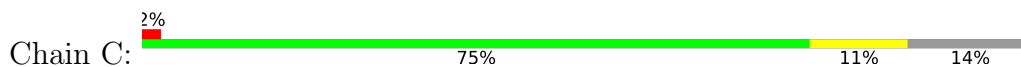


- Molecule 2: mAb1198 Light Chain

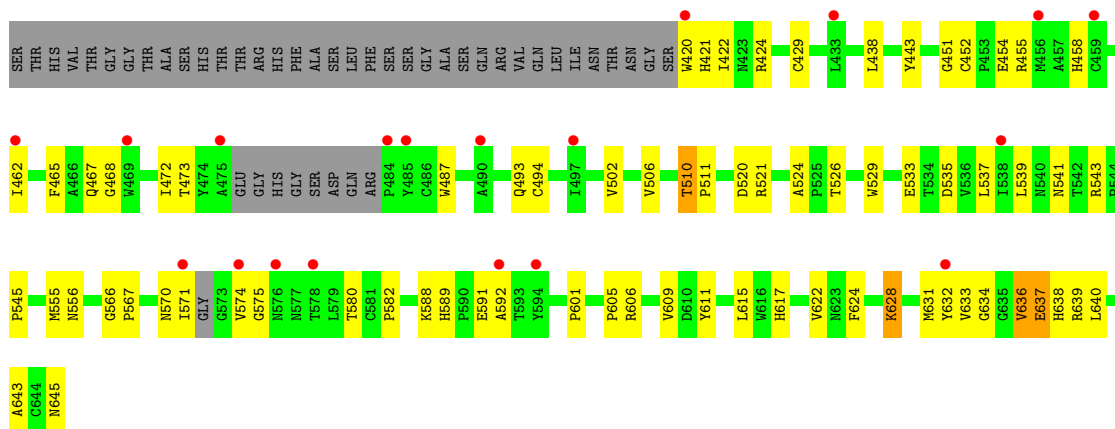
Chain L: 



- 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:  60% 40%



- 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:  100%



- 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:  100%



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)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.215 , 0.262 (Not available) , 0.304	Depositor DCC
R_{free} test set	2325 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10487	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage'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: BMA, NAG, MAN

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	0.33	0/1675	0.88	5/2288 (0.2%)
1	H	0.36	0/1662	0.64	0/2272
2	B	0.34	0/1701	0.66	2/2311 (0.1%)
2	L	0.37	0/1709	0.71	2/2322 (0.1%)
3	C	0.35	0/1837	0.68	0/2517
3	D	0.36	0/1769	0.75	7/2423 (0.3%)
All	All	0.35	0/10353	0.72	16/14133 (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

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	OD1-CG-OD2	-19.52	76.06	122.90
1	A	101	ASP	CB-CG-OD1	18.82	161.68	118.40
1	A	101	ASP	CB-CG-OD2	-14.10	85.97	118.40
3	D	628	LYS	CD-CE-NZ	-9.81	80.51	111.90
2	B	78	VAL	CA-C-N	7.15	133.81	122.59

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	32	1
2	B	1665	0	1635	27	0
2	L	1673	0	1642	44	0
3	C	1771	0	1628	29	0
3	D	1706	0	1577	71	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	221	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 11.

The worst 5 of 221 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 [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	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%)	14	35
3	D	211/262 (80%)	199 (94%)	11 (5%)	1 (0%)	24	48
All	All	1300/1438 (90%)	1248 (96%)	49 (4%)	3 (0%)	43	68

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](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

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	1.01	1 (5%)
4	NAG	E	2	4	14,14,15	0.41	0	17,19,21	0.89	0
4	BMA	E	3	4	11,11,12	0.36	0	15,15,17	0.99	0
4	MAN	E	4	4	11,11,12	0.46	0	15,15,17	0.70	0
4	NAG	F	1	3,4	14,14,15	0.40	0	17,19,21	0.94	0
4	NAG	F	2	4	14,14,15	0.35	0	17,19,21	0.53	0
4	BMA	F	3	4	11,11,12	0.34	0	15,15,17	0.62	0
4	MAN	F	4	4	11,11,12	0.37	0	15,15,17	0.63	0
5	NAG	G	1	3,5	14,14,15	0.31	0	17,19,21	0.75	1 (5%)
5	NAG	G	2	5	14,14,15	0.41	0	17,19,21	0.69	0
5	BMA	G	3	5	11,11,12	0.77	0	15,15,17	1.44	1 (6%)
5	MAN	G	4	5	11,11,12	0.41	0	15,15,17	0.99	0
5	MAN	G	5	5	11,11,12	0.42	0	15,15,17	0.72	0
5	NAG	I	1	3,5	14,14,15	0.36	0	17,19,21	0.71	0
5	NAG	I	2	5	14,14,15	0.37	0	17,19,21	0.82	0
5	BMA	I	3	5	11,11,12	0.35	0	15,15,17	0.72	0
5	MAN	I	4	5	11,11,12	0.41	0	15,15,17	0.76	0
5	MAN	I	5	5	11,11,12	0.36	0	15,15,17	0.70	0
4	NAG	J	1	3,4	14,14,15	0.52	0	17,19,21	1.36	2 (11%)
4	NAG	J	2	4	14,14,15	0.43	0	17,19,21	0.64	0
4	BMA	J	3	4	11,11,12	0.40	0	15,15,17	0.81	1 (6%)
4	MAN	J	4	4	11,11,12	0.36	0	15,15,17	0.65	0
5	NAG	K	1	3,5	14,14,15	0.35	0	17,19,21	0.52	0
5	NAG	K	2	5	14,14,15	0.25	0	17,19,21	0.82	0
5	BMA	K	3	5	11,11,12	0.36	0	15,15,17	0.80	0
5	MAN	K	4	5	11,11,12	0.37	0	15,15,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	K	5	5	11,11,12	0.30	0	15,15,17	0.54	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	-	2/6/23/26	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 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3	BMA	O3-C3-C2	4.55	119.34	110.05
4	J	1	NAG	O5-C1-C2	-3.88	105.29	111.29
4	J	1	NAG	C1-O5-C5	2.81	115.95	112.19
5	G	1	NAG	O4-C4-C3	-2.28	104.99	110.38
4	E	1	NAG	O4-C4-C3	-2.12	105.39	110.38

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

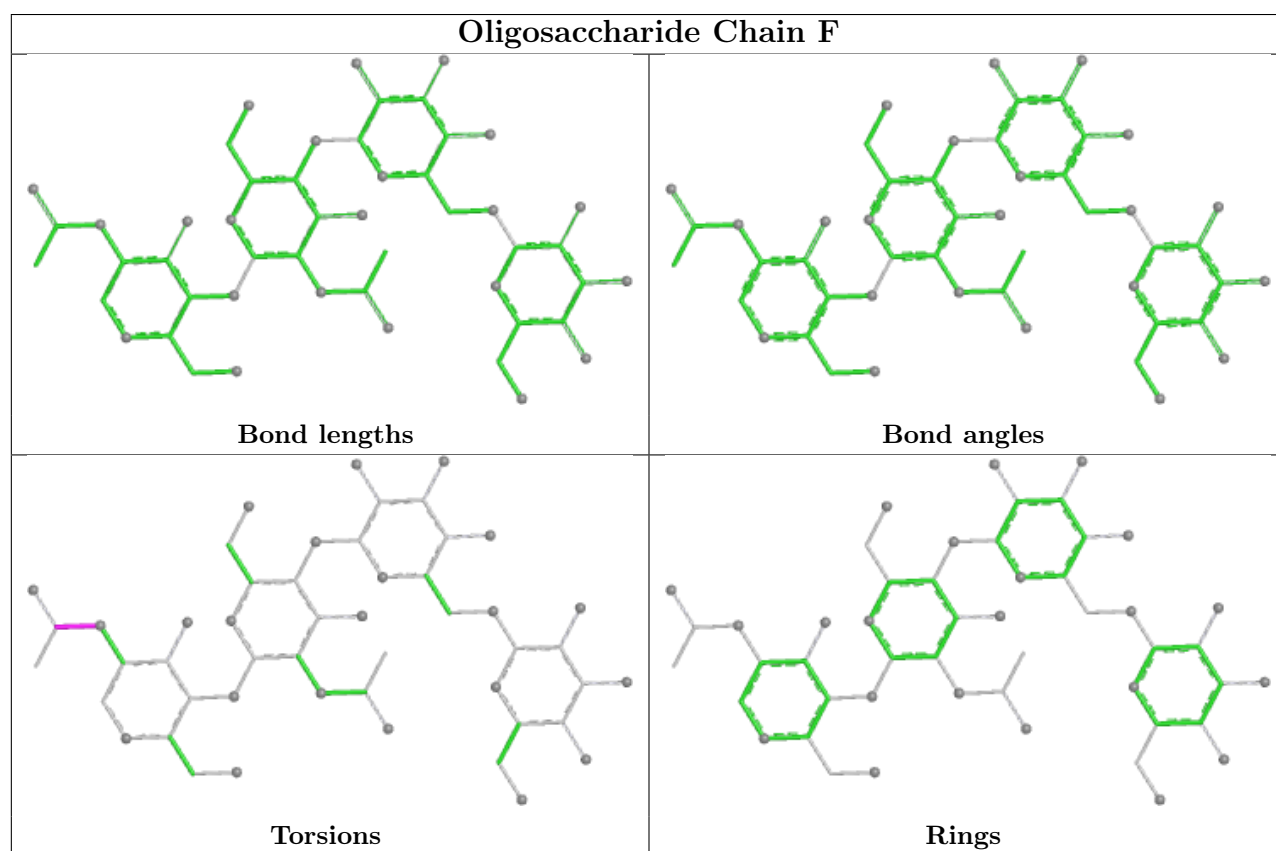
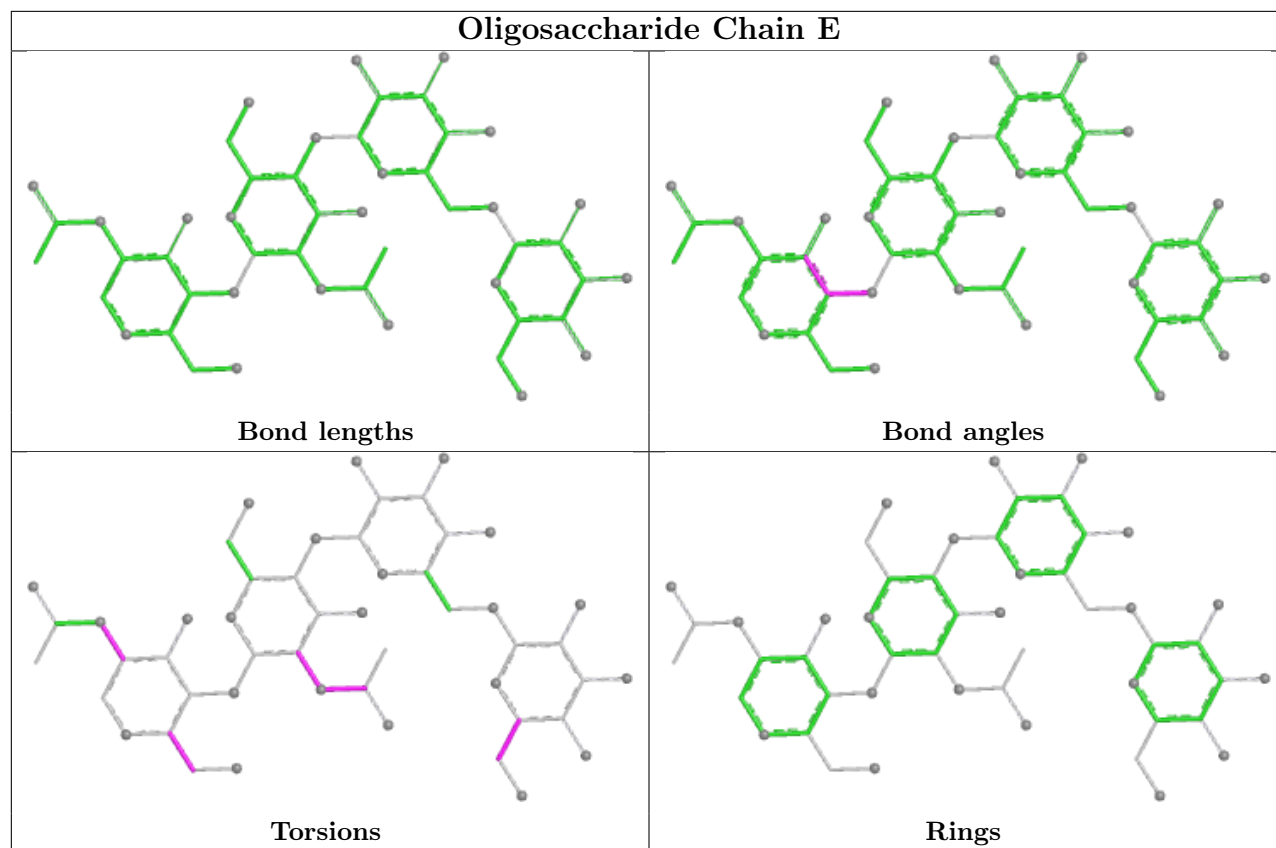
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C1-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2

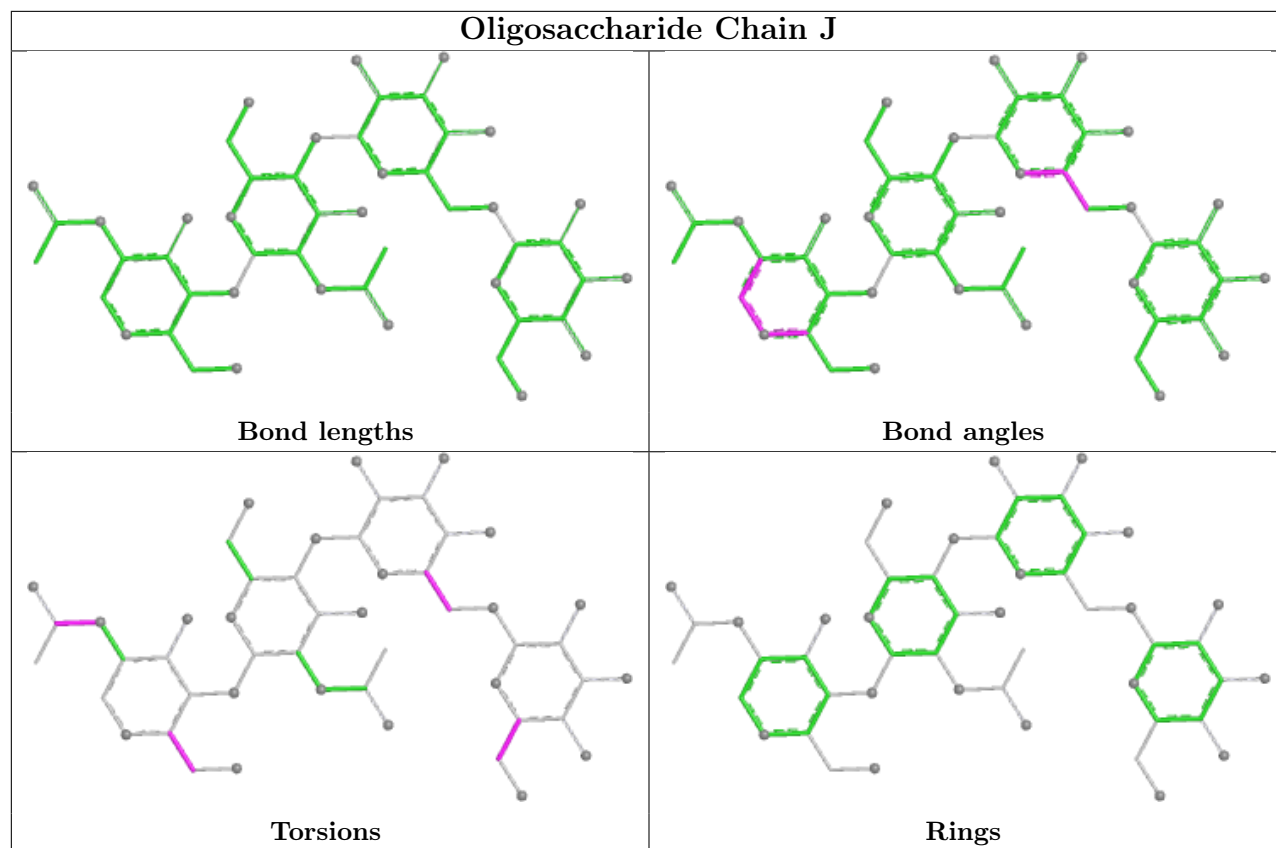
There are no ring outliers.

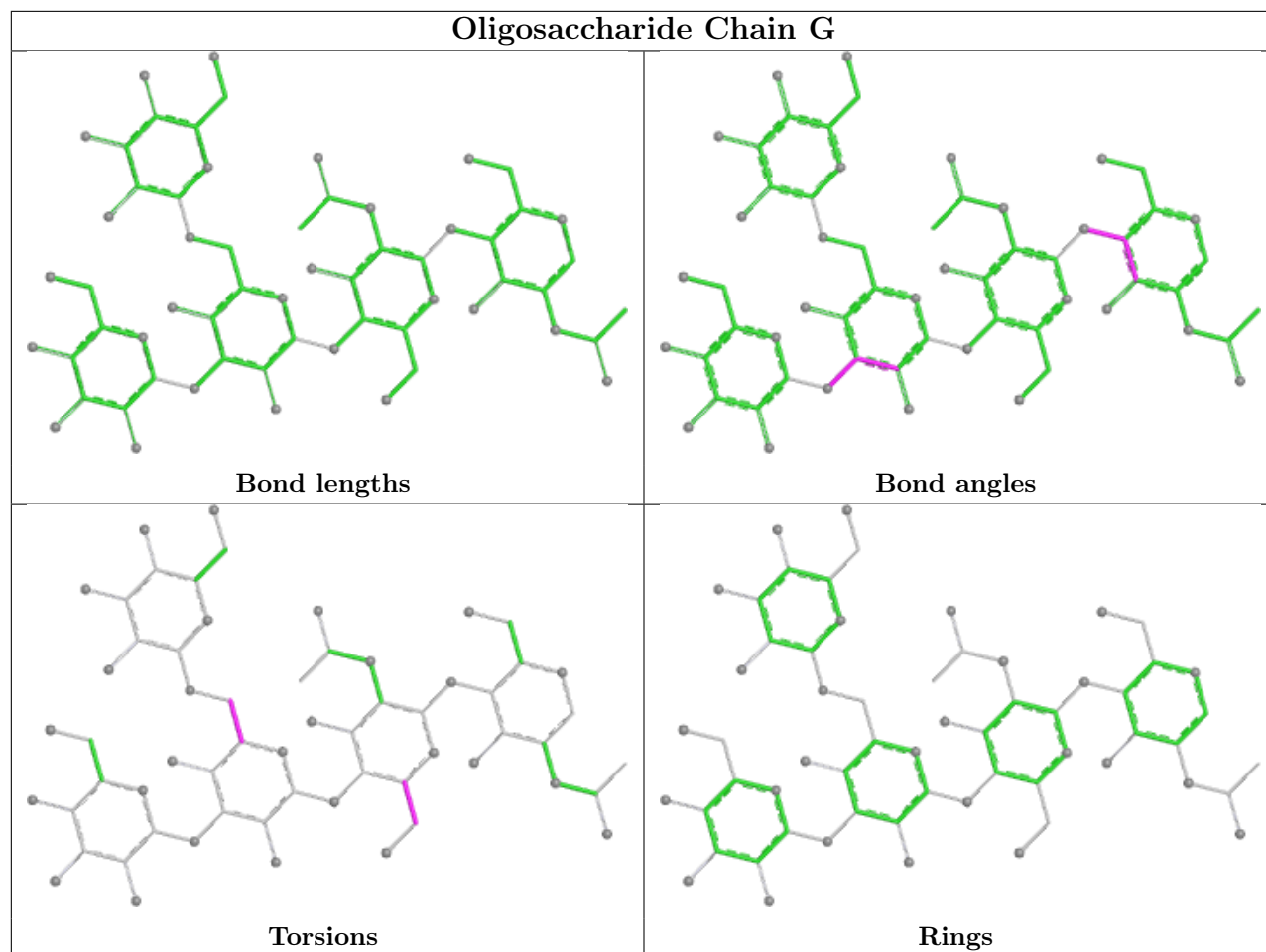
3 monomers are involved in 3 short contacts:

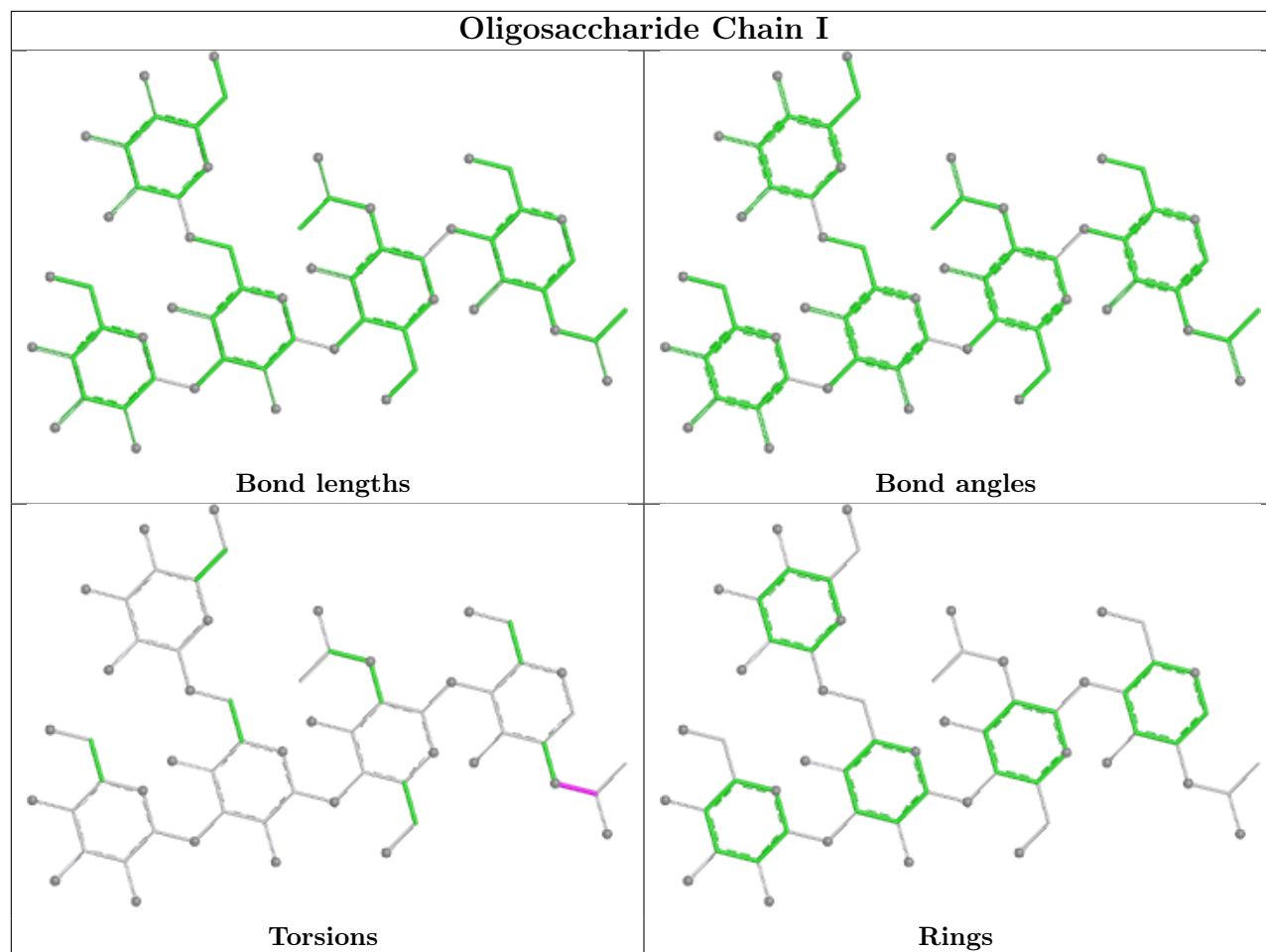
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	1	0
4	E	2	NAG	1	0
4	F	1	NAG	1	0

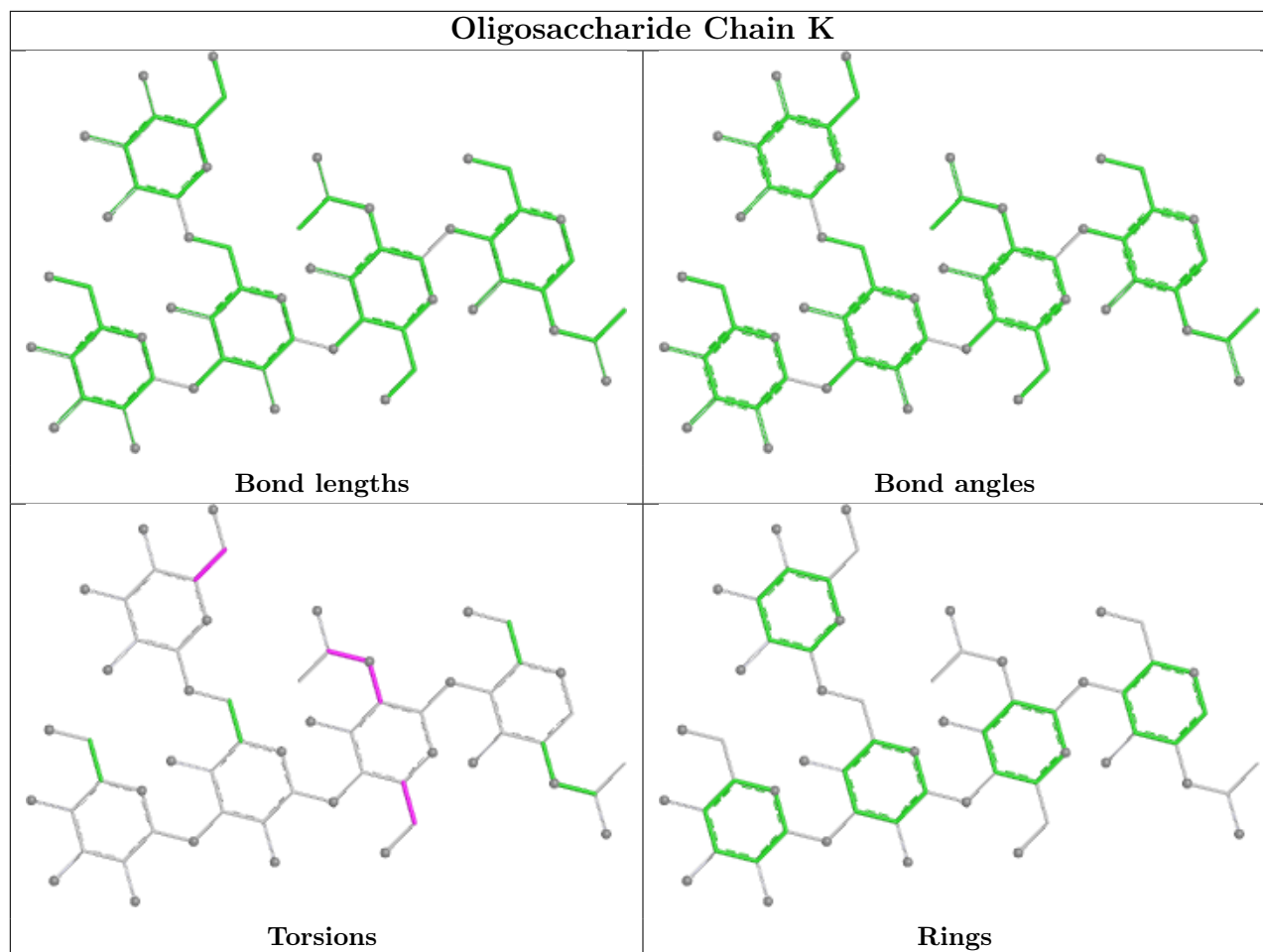
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

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	0.32	0	17,19,21	0.71	0
6	NAG	D	4302	3	14,14,15	0.35	0	17,19,21	0.67	0
6	NAG	C	701	3	14,14,15	0.39	0	17,19,21	0.79	0
6	NAG	C	702	3	14,14,15	0.37	0	17,19,21	1.07	1 (5%)
6	NAG	C	704	3	14,14,15	0.48	0	17,19,21	1.00	2 (11%)
6	NAG	C	703	3	14,14,15	0.37	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	4301	3	-	3/6/23/26	0/1/1/1
6	NAG	D	4302	3	-	2/6/23/26	0/1/1/1
6	NAG	C	701	3	-	0/6/23/26	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	C	703	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	704	NAG	C4-C3-C2	-2.32	107.62	111.02
6	C	702	NAG	O5-C1-C2	-2.32	107.70	111.29
6	C	704	NAG	O5-C5-C6	2.27	112.08	107.66

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 [i](#)

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%)	-0.06	0 100 100	50, 68, 97, 131	0
1	H	219/237 (92%)	0.36	11 (5%) 34 30	53, 86, 123, 176	0
2	B	218/220 (99%)	0.21	6 (2%) 55 51	50, 87, 115, 132	0
2	L	219/220 (99%)	0.44	7 (3%) 50 46	55, 101, 150, 184	0
3	C	226/262 (86%)	0.31	5 (2%) 62 59	51, 80, 125, 179	0
3	D	217/262 (82%)	0.73	19 (8%) 15 13	62, 103, 161, 201	0
All	All	1320/1438 (91%)	0.33	48 (3%) 46 42	50, 86, 143, 201	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	420	TRP	4.5
3	D	538	ILE	4.2
3	D	420	TRP	3.9
1	H	140	CYS	3.7
3	D	475	ALA	3.5

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](#)

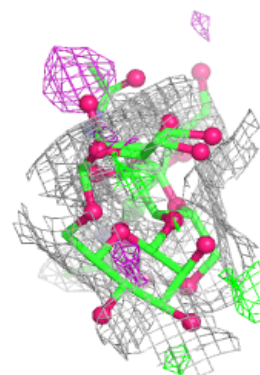
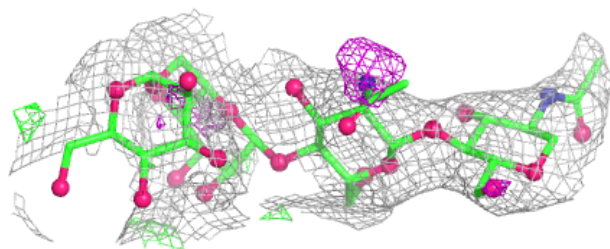
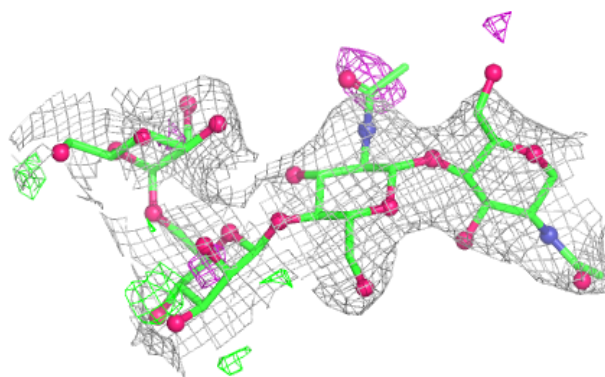
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	NAG	E	1	14/15	-	-	83,97,106,113	0
4	NAG	E	2	14/15	-	-	106,115,121,121	0
4	BMA	E	3	11/12	-	-	119,123,124,125	0
4	MAN	E	4	11/12	-	-	117,123,125,126	0
4	NAG	F	1	14/15	-	-	76,82,89,92	0
4	NAG	F	2	14/15	-	-	83,101,110,116	0
4	BMA	F	3	11/12	-	-	119,124,129,132	0
4	MAN	F	4	11/12	-	-	123,128,133,135	0
5	BMA	G	3	11/12	0.23	0.15	126,129,131,132	0
5	MAN	K	4	11/12	0.31	0.17	131,136,138,139	0
5	MAN	G	4	11/12	0.32	0.15	123,127,131,132	0
5	BMA	K	3	11/12	0.35	0.13	134,138,141,141	0
5	MAN	I	4	11/12	0.37	0.13	126,131,135,135	0
5	MAN	I	5	11/12	0.42	0.14	132,137,138,139	0
5	BMA	I	3	11/12	0.43	0.15	133,136,137,137	0
4	BMA	J	3	11/12	0.45	0.12	136,140,142,142	0
5	MAN	G	5	11/12	-	-	127,131,133,136	0
5	NAG	I	2	14/15	0.54	0.14	124,132,133,136	0
4	MAN	J	4	11/12	0.55	0.10	118,133,138,139	0
4	NAG	J	2	14/15	0.68	0.13	113,123,131,135	0
5	NAG	G	2	14/15	0.70	0.14	107,112,123,125	0
5	NAG	K	1	14/15	0.72	0.12	95,100,106,113	0
5	NAG	K	2	14/15	0.72	0.10	111,118,125,132	0
5	NAG	G	1	14/15	0.76	0.12	79,87,96,104	0
4	NAG	J	1	14/15	0.79	0.11	98,105,112,116	0
5	NAG	I	1	14/15	0.84	0.10	119,126,130,131	0
5	MAN	K	5	11/12	-	-	131,140,142,143	0

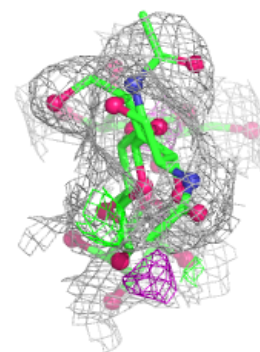
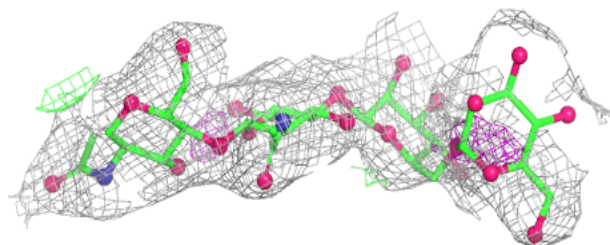
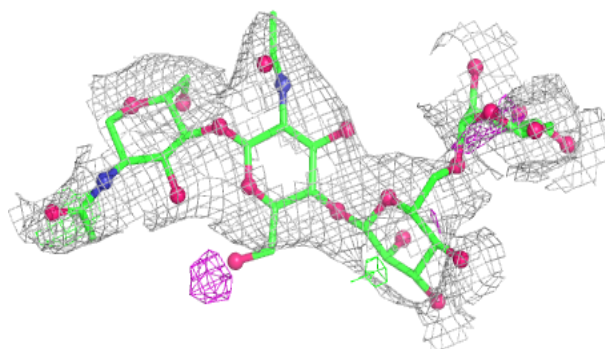
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

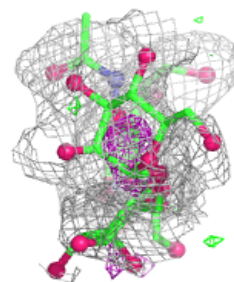
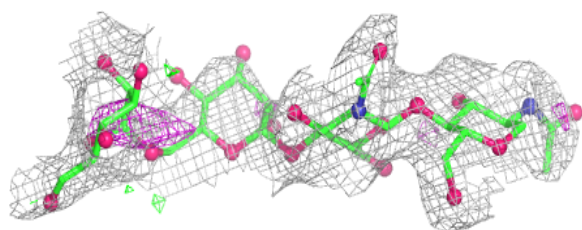
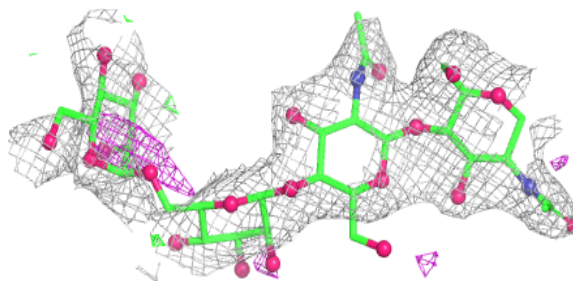
**Electron density around Chain F:**

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

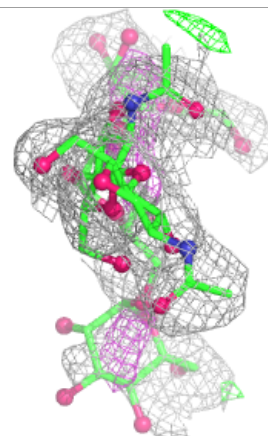
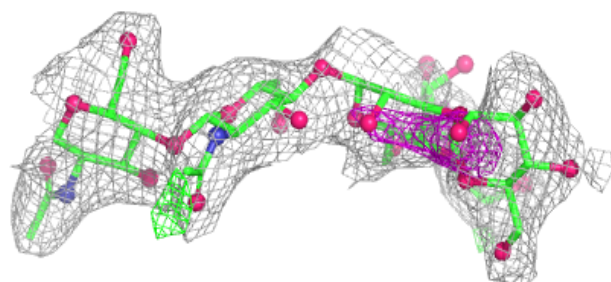
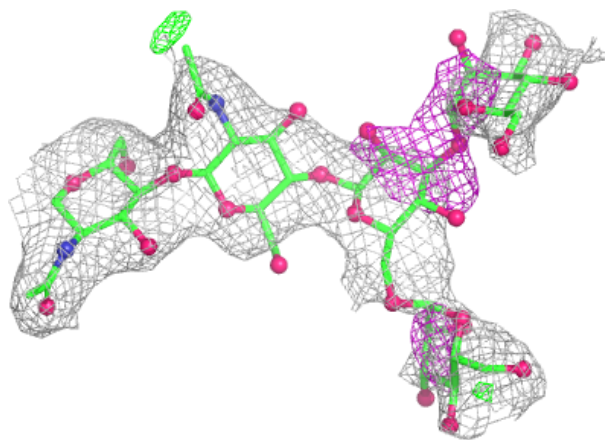


Electron density around Chain J:

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

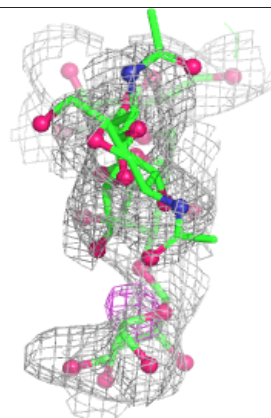
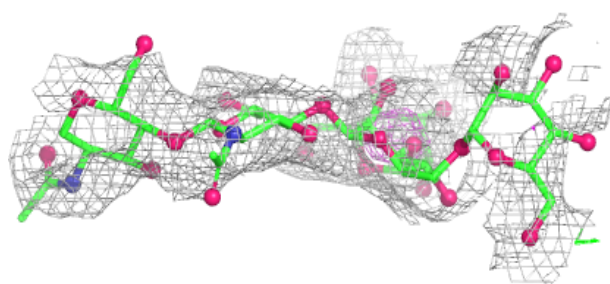
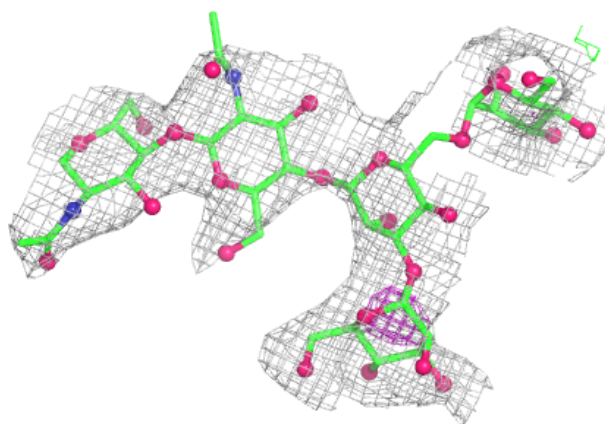
**Electron density around Chain G:**

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

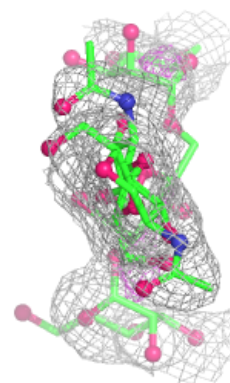
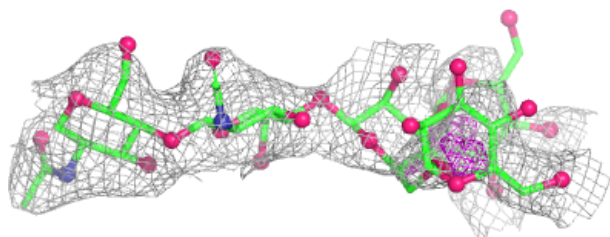
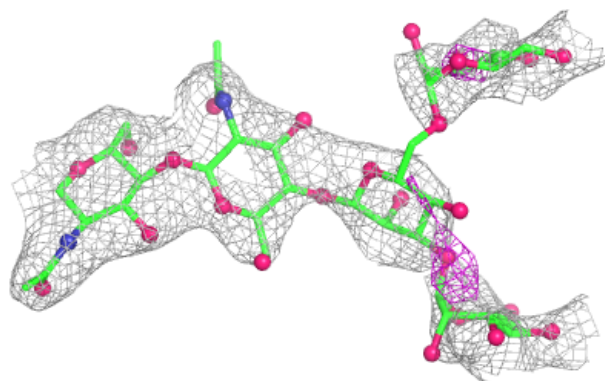


Electron density around Chain I:

$2mF_o-DF_c$ (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	702	14/15	0.49	0.13	106,115,120,121	0
6	NAG	C	704	14/15	0.53	0.15	96,99,108,111	0
6	NAG	D	4301	14/15	0.60	0.11	142,146,147,148	0
6	NAG	C	701	14/15	0.64	0.15	98,105,108,111	0
6	NAG	C	703	14/15	0.73	0.10	86,92,98,101	0
6	NAG	D	4302	14/15	0.78	0.08	101,106,111,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.