



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 4, 2024 – 12:32 AM JST

PDB ID : 6KJ0
Title : Bifunctional xylosidase/glucosidase LXYL mutant E529Q C2221
Authors : Gong, W.M.; Yang, L.Y.
Deposited on : 2019-07-20
Resolution : 2.27 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 : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

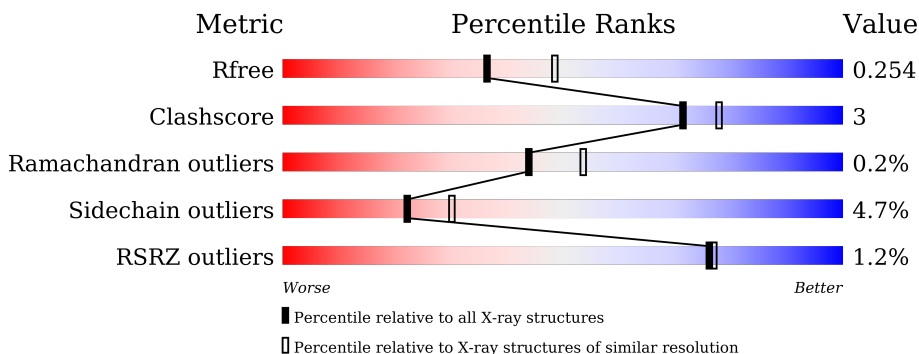
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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.



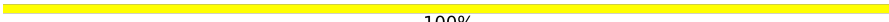
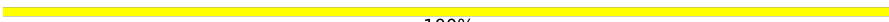
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	809	 82% 9% 7%
1	B	809	 84% 8% 7%
2	C	3	 100%
2	F	3	 67% 33%
3	D	7	 100%
3	G	7	 86% 14%

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Mol	Chain	Length	Quality of chain
4	E	4	 100%
4	H	4	 100%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12707 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 Beta-D-xylosidase/beta-D-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	756	5713	3618	957	1121	17	0	0	0
1	B	756	5720	3622	959	1122	17	0	2	0

There are 14 discrepancies between the modelled and reference sequences:

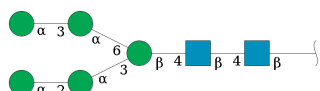
Chain	Residue	Modelled	Actual	Comment	Reference
A	529	GLN	GLU	engineered mutation	UNP G8GLP2
A	804	HIS	-	expression tag	UNP G8GLP2
A	805	HIS	-	expression tag	UNP G8GLP2
A	806	HIS	-	expression tag	UNP G8GLP2
A	807	HIS	-	expression tag	UNP G8GLP2
A	808	HIS	-	expression tag	UNP G8GLP2
A	809	HIS	-	expression tag	UNP G8GLP2
B	529	GLN	GLU	engineered mutation	UNP G8GLP2
B	804	HIS	-	expression tag	UNP G8GLP2
B	805	HIS	-	expression tag	UNP G8GLP2
B	806	HIS	-	expression tag	UNP G8GLP2
B	807	HIS	-	expression tag	UNP G8GLP2
B	808	HIS	-	expression tag	UNP G8GLP2
B	809	HIS	-	expression tag	UNP G8GLP2

- Molecule 2 is an oligosaccharide called alpha-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
2	C	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
3	D	7	Total	C	N	O	0	0	0
			83	46	2	35			
3	G	7	Total	C	N	O	0	0	0
			83	46	2	35			

- 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.



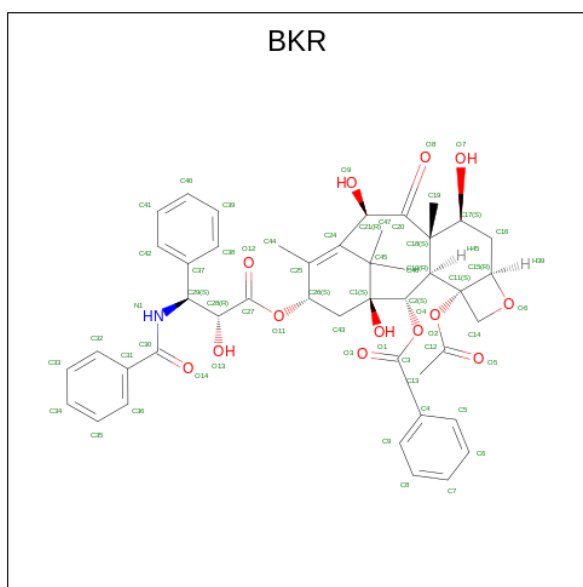
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
4	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



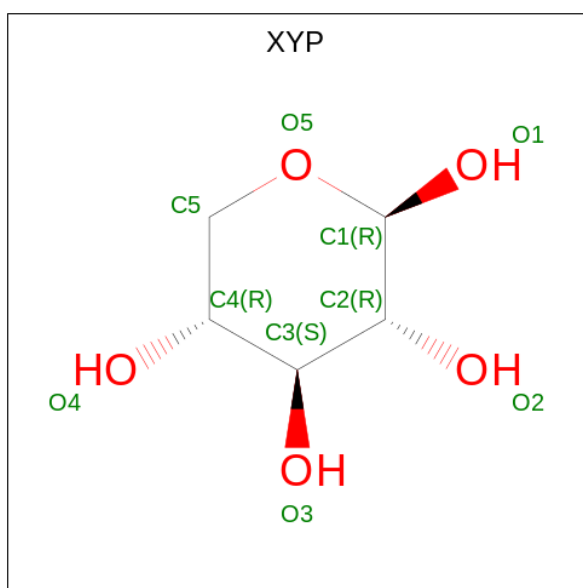
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total 14	8	1	5	0	0
5	A	1	Total 14	8	1	5	0	0
5	A	1	Total 14	8	1	5	0	0
5	A	1	Total 14	8	1	5	0	0
5	B	1	Total 14	8	1	5	0	0
5	B	1	Total 14	8	1	5	0	0
5	B	1	Total 14	8	1	5	0	0
5	B	1	Total 14	8	1	5	0	0

- Molecule 6 is Deacetyltaxol (three-letter code: BKR) (formula: $C_{45}H_{49}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
6	A	1	Total	C	N	O	0	0
			59	45	1	13		
6	B	1	Total	C	N	O	0	0
			59	45	1	13		

- Molecule 7 is beta-D-xylopyranose (three-letter code: XYP) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	A	1	Total	C	O	0	0
			10	5	5		
7	B	1	Total	C	O	0	0
			10	5	5		

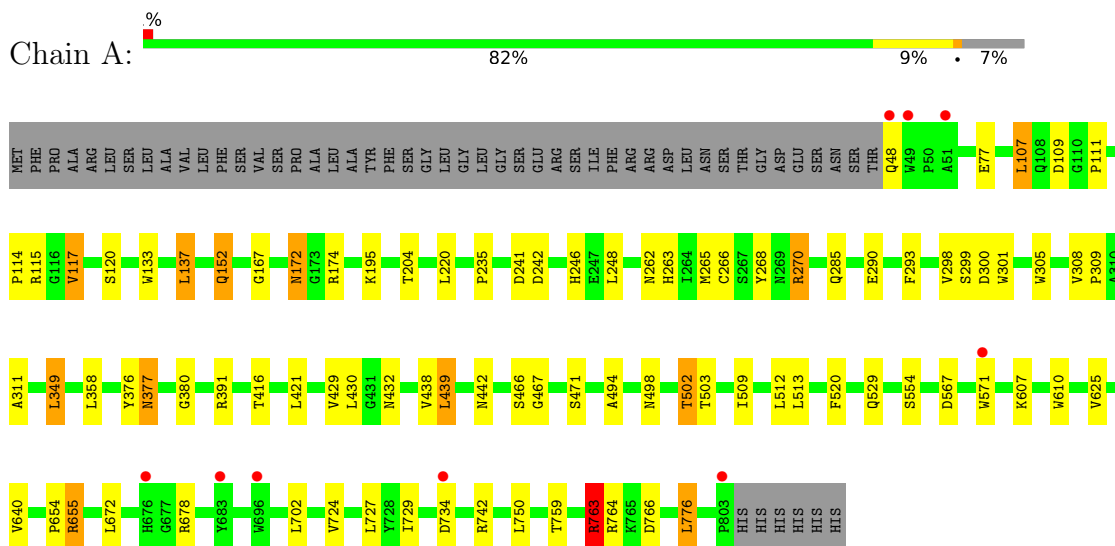
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	343	Total 343	O 343	0	0
8	B	337	Total 337	O 337	0	0

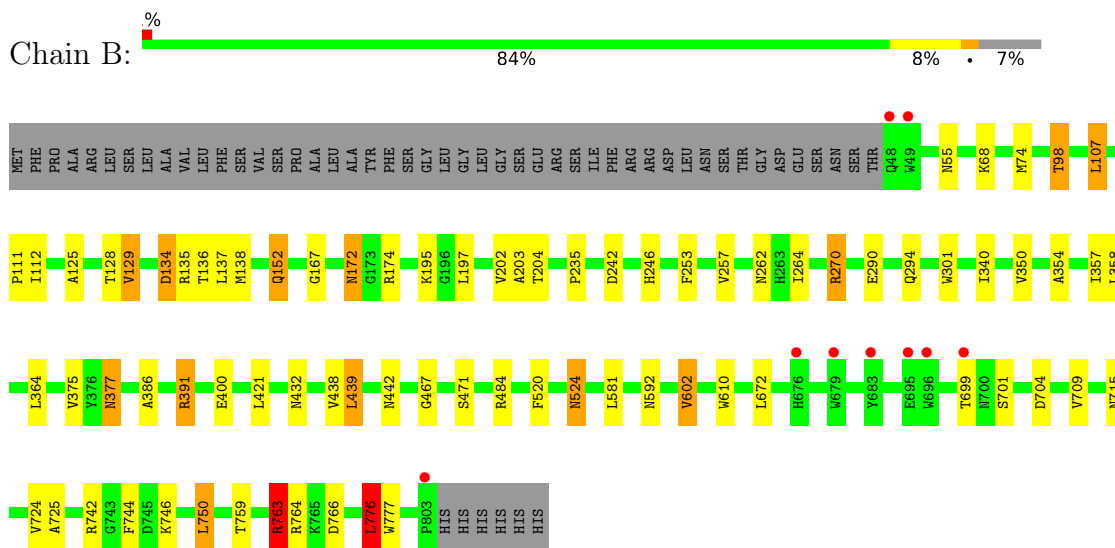
3 Residue-property plots [i](#)

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


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase



- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

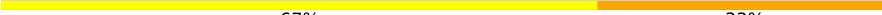


- Molecule 2: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  100%

MAG1
MAG2
MAN3

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

Chain F:  67% 33%


MAG1
MAG2
MAN3

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 D:  100%

MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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:  86% 14%


MAG1
MAG2
BMA3
MAN4
MAN5
MAN6
MAN7

- 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 E:  100%

MAG1
MAG2
BMA3
MAN4

- 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 H:  100%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	80.00Å 182.23Å 241.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	120.76 – 2.27 120.76 – 2.27	Depositor EDS
% Data completeness (in resolution range)	93.1 (120.76-2.27) 93.2 (120.76-2.27)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.27Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.192 , 0.252 0.203 , 0.254	Depositor DCC
R_{free} test set	4078 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtrriage
Anisotropy	0.030	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12707	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 58.33 % 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 2.0776e-05. 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.86	1/5854 (0.0%)	0.95	17/8009 (0.2%)
1	B	0.89	2/5860 (0.0%)	0.94	17/8018 (0.2%)
All	All	0.88	3/11714 (0.0%)	0.94	34/16027 (0.2%)

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
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	TRP	CE3-CZ3	5.67	1.48	1.38
1	B	400	GLU	CG-CD	5.62	1.60	1.51
1	B	777	TRP	CB-CG	5.36	1.59	1.50

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	763	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	270	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	391	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	B	270	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	391	ARG	NE-CZ-NH1	8.22	124.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	699	THR	Peptide

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	5713	0	5506	39	0
1	B	5720	0	5515	36	0
2	C	39	0	34	0	0
2	F	39	0	34	1	0
3	D	83	0	70	0	0
3	G	83	0	70	1	0
4	E	50	0	43	0	0
4	H	50	0	43	0	0
5	A	56	0	52	0	0
5	B	56	0	52	0	0
6	A	59	0	0	0	0
6	B	59	0	0	0	0
7	A	10	0	0	1	0
7	B	10	0	0	0	0
8	A	343	0	0	5	0
8	B	337	0	0	2	0
All	All	12707	0	11419	76	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 3.

The worst 5 of 76 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:A:502:THR:HG21	8:A:1260:HOH:O	1.80	0.81
1:B:246:HIS:HE1	1:B:290:GLU:OE2	1.68	0.77
1:A:421:LEU:HD11	1:A:520:PHE:HZ	1.53	0.72
1:B:421:LEU:HD11	1:B:520:PHE:HZ	1.54	0.72
1:B:55:ASN:H	1:B:294:GLN:HE22	1.38	0.72

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	754/809 (93%)	718 (95%)	35 (5%)	1 (0%)	48	59
1	B	756/809 (93%)	719 (95%)	35 (5%)	2 (0%)	37	45
All	All	1510/1618 (93%)	1437 (95%)	70 (5%)	3 (0%)	44	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	ALA
1	B	167	GLY
1	A	167	GLY

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	609/654 (93%)	576 (95%)	33 (5%)	18	24
1	B	610/654 (93%)	586 (96%)	24 (4%)	27	39
All	All	1219/1308 (93%)	1162 (95%)	57 (5%)	22	30

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	734	ASP
1	B	763	ARG
1	B	107	LEU

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Mol	Chain	Res	Type
1	B	759	THR
1	B	602	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	262	ASN
1	B	377	ASN
1	B	294	GLN
1	B	442	ASN
1	A	377	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](#)

28 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1	2,1	14,14,15	1.26	2 (14%)	17,19,21	1.95	5 (29%)
2	NAG	C	2	2	14,14,15	1.16	0	17,19,21	1.61	4 (23%)
2	MAN	C	3	2	11,11,12	0.98	0	15,15,17	3.18	5 (33%)
3	NAG	D	1	3,1	14,14,15	1.63	3 (21%)	17,19,21	2.98	7 (41%)
3	NAG	D	2	3	14,14,15	0.84	0	17,19,21	1.29	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	D	3	3	11,11,12	0.86	0	15,15,17	2.35	3 (20%)
3	MAN	D	4	3	11,11,12	1.22	1 (9%)	15,15,17	2.30	4 (26%)
3	MAN	D	5	3	11,11,12	0.90	0	15,15,17	2.31	3 (20%)
3	MAN	D	6	3	11,11,12	0.78	0	15,15,17	1.28	1 (6%)
3	MAN	D	7	3	11,11,12	0.76	0	15,15,17	1.19	2 (13%)
4	NAG	E	1	1,4	14,14,15	0.60	0	17,19,21	1.91	4 (23%)
4	NAG	E	2	4	14,14,15	0.61	0	17,19,21	2.05	5 (29%)
4	BMA	E	3	4	11,11,12	0.98	0	15,15,17	2.44	6 (40%)
4	MAN	E	4	4	11,11,12	1.09	0	15,15,17	1.76	4 (26%)
2	NAG	F	1	2,1	14,14,15	1.34	2 (14%)	17,19,21	1.10	1 (5%)
2	NAG	F	2	2	14,14,15	0.98	0	17,19,21	1.53	3 (17%)
2	MAN	F	3	2	11,11,12	1.09	0	15,15,17	1.66	3 (20%)
3	NAG	G	1	3,1	14,14,15	1.28	2 (14%)	17,19,21	1.64	2 (11%)
3	NAG	G	2	3	14,14,15	0.63	0	17,19,21	1.10	0
3	BMA	G	3	3	11,11,12	0.54	0	15,15,17	0.94	1 (6%)
3	MAN	G	4	3	11,11,12	0.83	0	15,15,17	2.60	2 (13%)
3	MAN	G	5	3	11,11,12	1.31	1 (9%)	15,15,17	1.34	2 (13%)
3	MAN	G	6	3	11,11,12	0.91	1 (9%)	15,15,17	2.57	4 (26%)
3	MAN	G	7	3	11,11,12	0.65	0	15,15,17	0.94	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.82	1 (7%)	17,19,21	1.24	3 (17%)
4	NAG	H	2	4	14,14,15	0.78	0	17,19,21	1.50	2 (11%)
4	BMA	H	3	4	11,11,12	1.03	1 (9%)	15,15,17	1.93	4 (26%)
4	MAN	H	4	4	11,11,12	0.84	0	15,15,17	2.12	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	MAN	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	D	2	3	-	1/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	MAN	D	6	3	-	0/2/19/22	0/1/1/1
3	MAN	D	7	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	2/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	1/6/23/26	0/1/1/1
2	MAN	F	3	2	-	2/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	MAN	G	4	3	-	0/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	0/1/1/1
3	MAN	G	6	3	-	2/2/19/22	0/1/1/1
3	MAN	G	7	3	-	0/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	BMA	H	3	4	-	0/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	5	MAN	C2-C3	2.89	1.56	1.52
3	D	1	NAG	O5-C1	-2.89	1.39	1.43
3	D	1	NAG	C2-N2	-2.83	1.41	1.46
3	D	1	NAG	O7-C7	-2.76	1.17	1.23
3	D	4	MAN	O5-C1	-2.69	1.39	1.43

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4	MAN	C1-O5-C5	8.58	123.81	112.19
2	C	3	MAN	C1-C2-C3	7.75	119.19	109.67
3	D	1	NAG	O5-C5-C6	-7.62	95.26	107.20
3	G	6	MAN	C1-O5-C5	7.45	122.29	112.19
2	C	3	MAN	C1-O5-C5	7.30	122.08	112.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

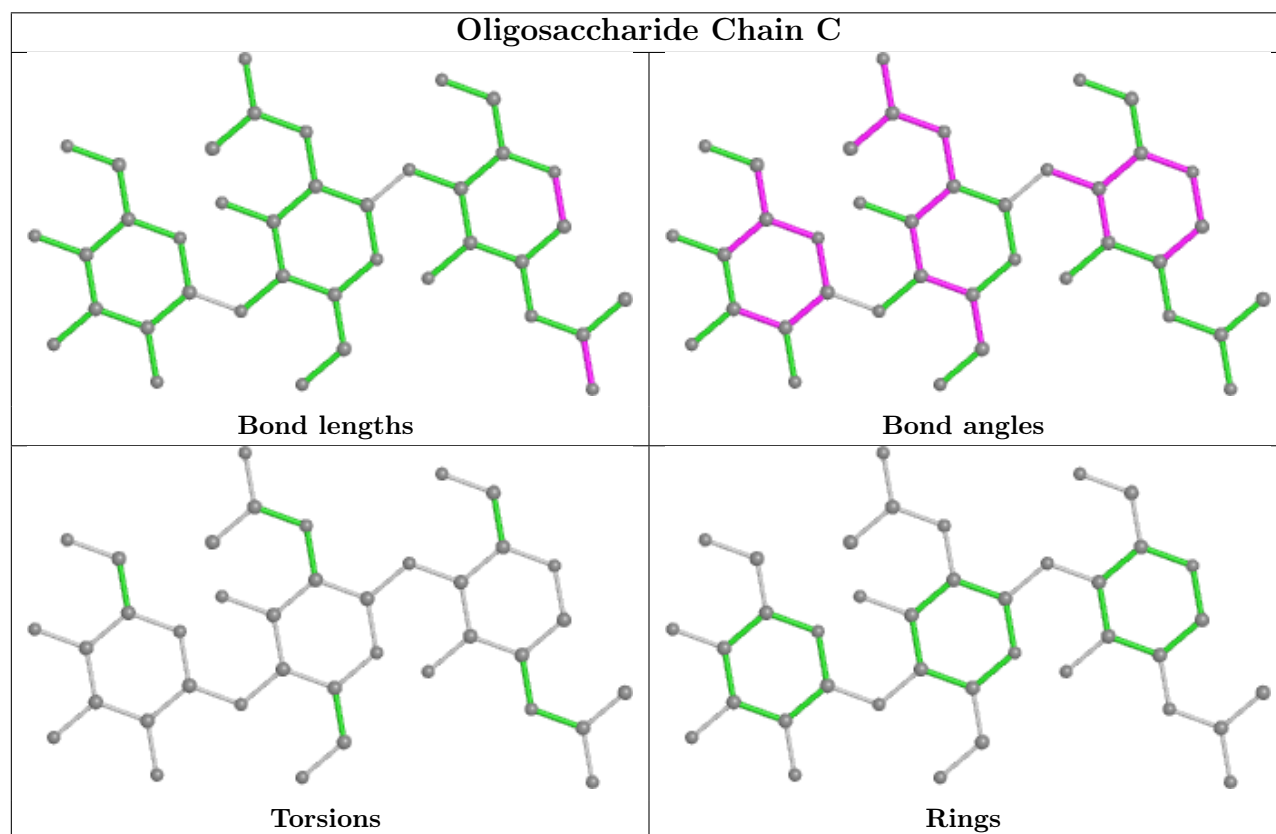
Mol	Chain	Res	Type	Atoms
4	E	4	MAN	O5-C5-C6-O6
2	F	3	MAN	O5-C5-C6-O6
4	E	4	MAN	C4-C5-C6-O6
3	D	4	MAN	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6

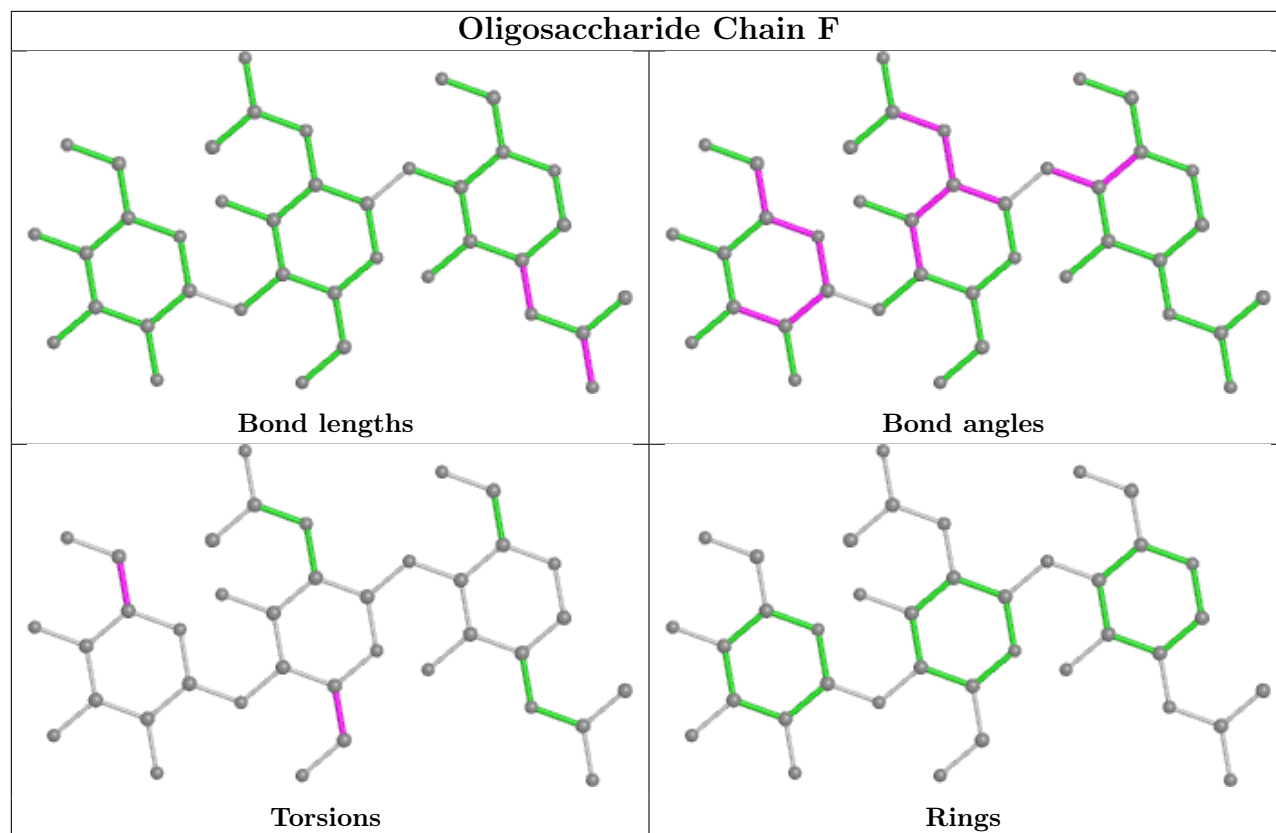
There are no ring outliers.

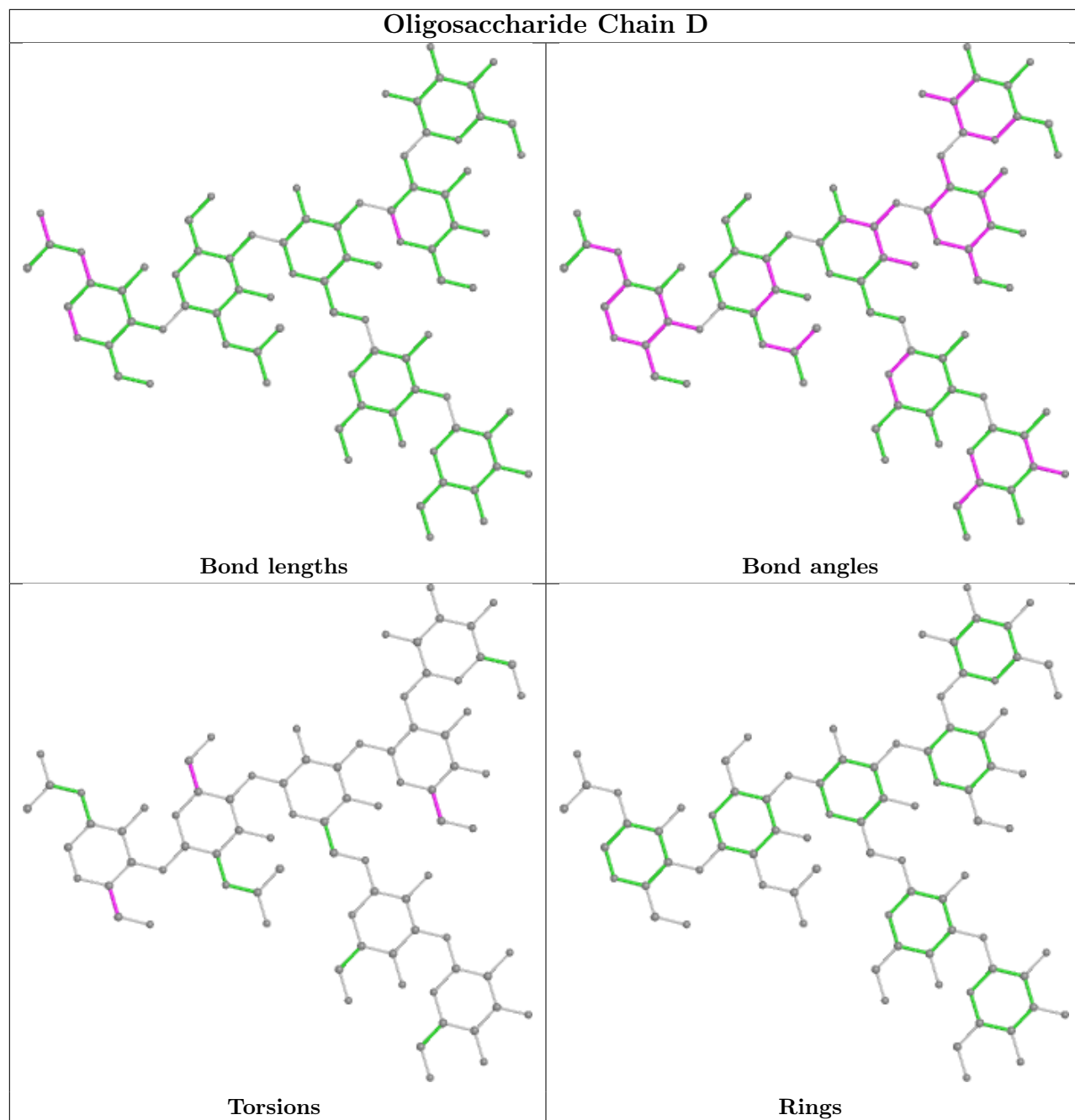
3 monomers are involved in 2 short contacts:

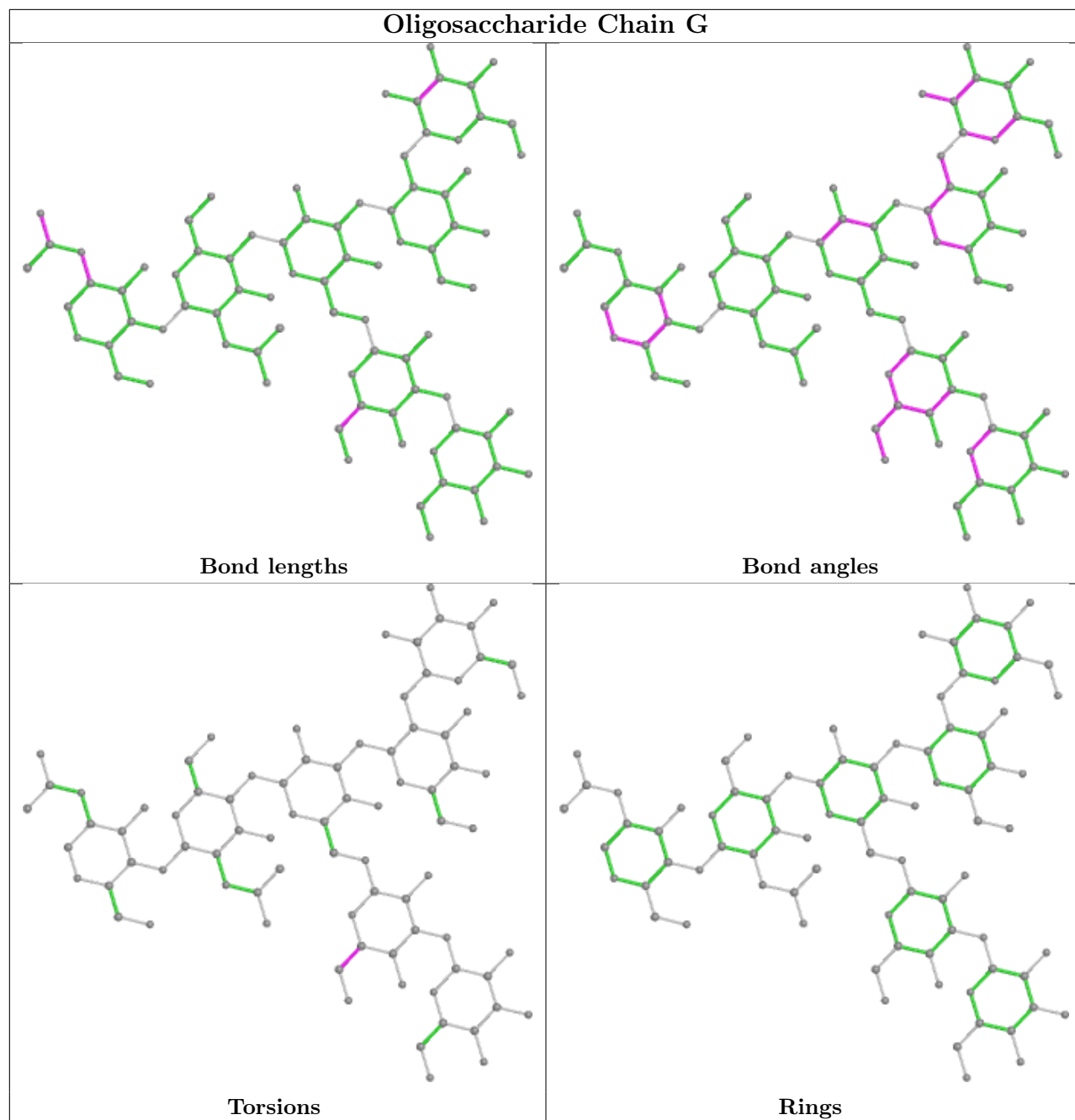
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	1	0
3	G	1	NAG	1	0
2	F	1	NAG	1	0

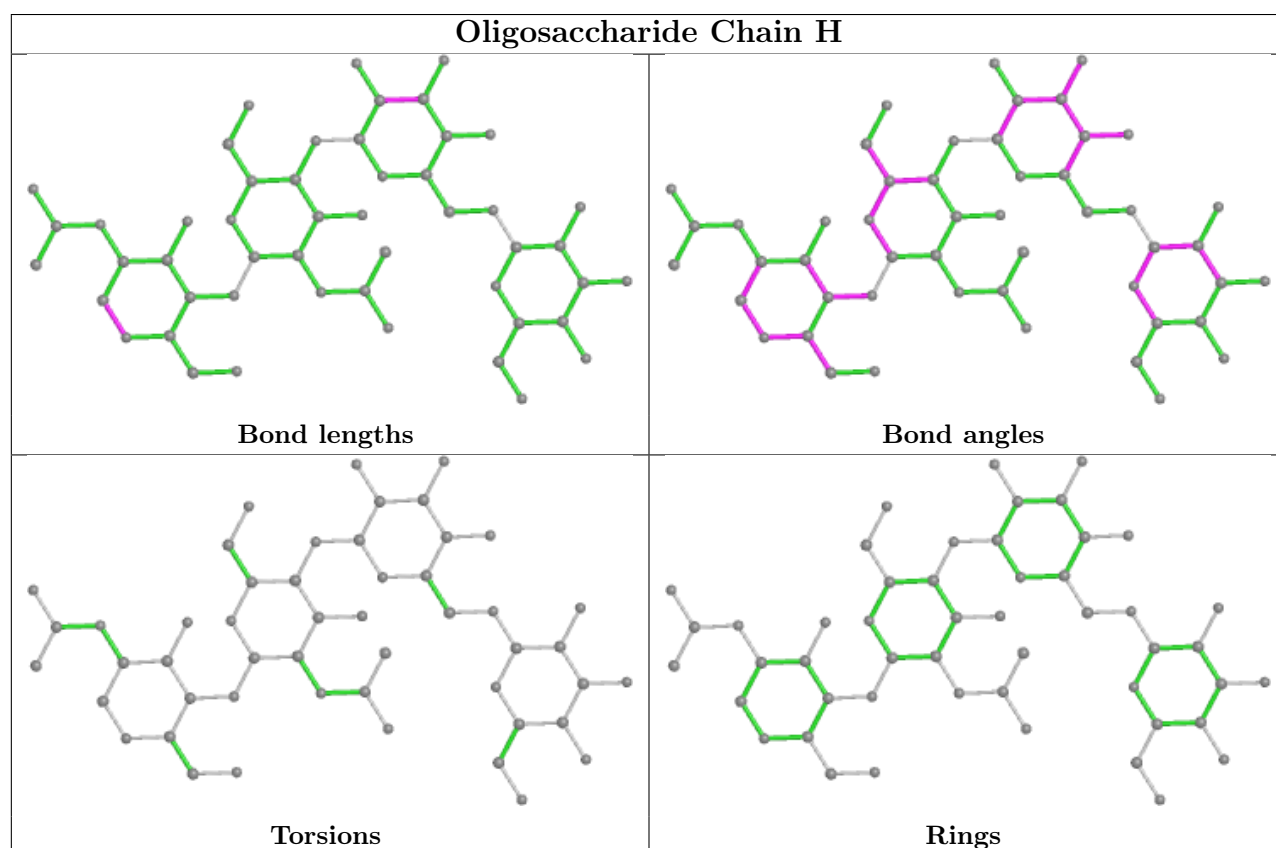
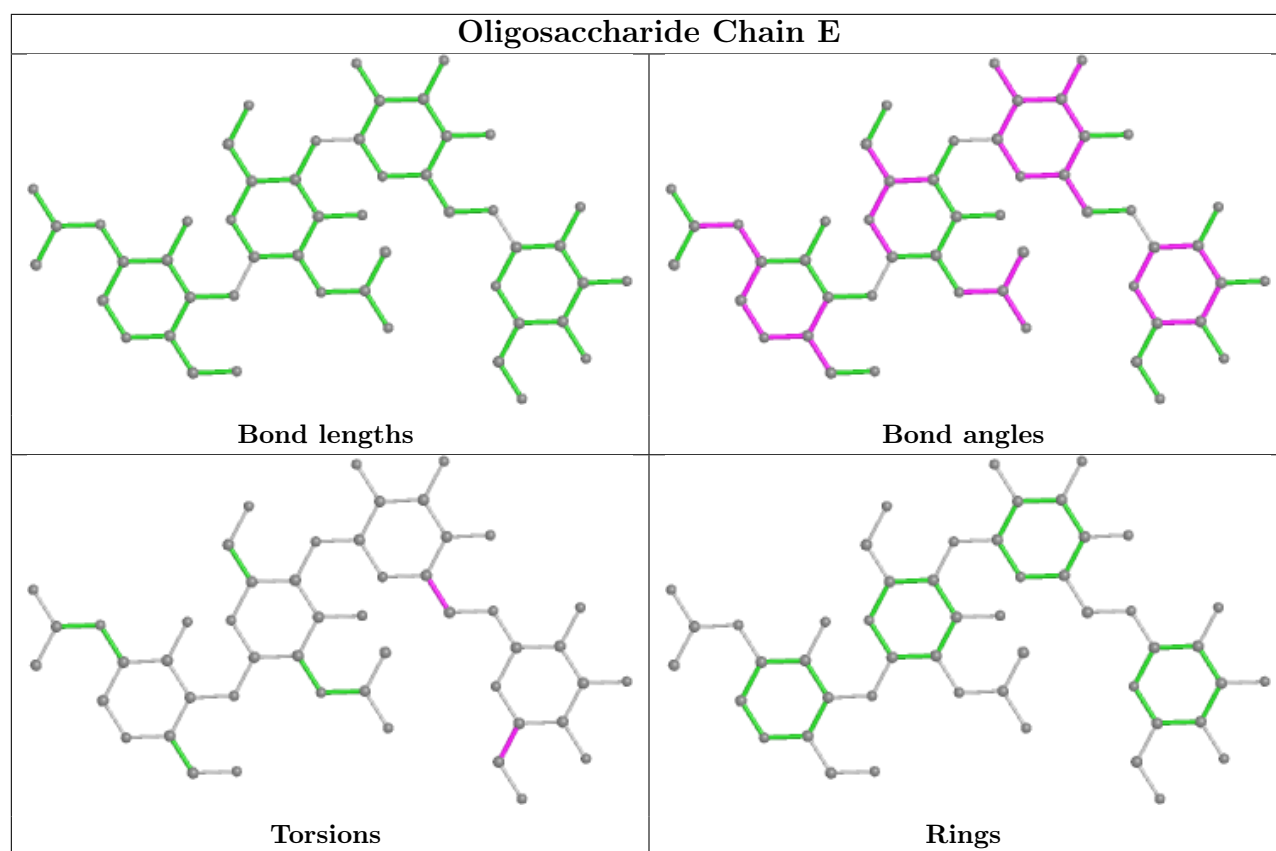
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

12 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$
5	NAG	B	911	1	14,14,15	0.40	0	17,19,21	1.79	2 (11%)
5	NAG	B	918	1	14,14,15	0.91	1 (7%)	17,19,21	1.31	2 (11%)
6	BKR	A	919	-	65,65,65	1.33	4 (6%)	101,101,101	1.37	13 (12%)
5	NAG	A	911	1	14,14,15	0.65	0	17,19,21	1.54	2 (11%)
5	NAG	B	917	1	14,14,15	0.49	0	17,19,21	1.47	1 (5%)
5	NAG	B	912	1	14,14,15	0.72	0	17,19,21	1.17	1 (5%)
5	NAG	A	918	1	14,14,15	0.49	0	17,19,21	1.50	2 (11%)
7	XYP	B	920	-	10,10,10	2.09	4 (40%)	14,14,14	3.74	8 (57%)
7	XYP	A	920	-	10,10,10	1.32	1 (10%)	14,14,14	3.21	7 (50%)
6	BKR	B	919	-	65,65,65	1.34	3 (4%)	101,101,101	1.23	9 (8%)
5	NAG	A	917	1	14,14,15	0.61	0	17,19,21	1.13	1 (5%)
5	NAG	A	912	1	14,14,15	0.62	0	17,19,21	1.31	2 (11%)

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	B	911	1	-	1/6/23/26	0/1/1/1
5	NAG	B	918	1	-	0/6/23/26	0/1/1/1
6	BKR	A	919	-	-	14/37/123/123	0/7/7/7
5	NAG	A	911	1	-	0/6/23/26	0/1/1/1
5	NAG	B	917	1	-	0/6/23/26	0/1/1/1
5	NAG	B	912	1	-	0/6/23/26	0/1/1/1
5	NAG	A	918	1	-	2/6/23/26	0/1/1/1
7	XYP	B	920	-	-	-	0/1/1/1
7	XYP	A	920	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BKR	B	919	-	-	3/37/123/123	0/7/7/7
5	NAG	A	917	1	-	0/6/23/26	0/1/1/1
5	NAG	A	912	1	-	1/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	919	BKR	O2-C3	5.64	1.46	1.34
6	B	919	BKR	O2-C3	5.46	1.45	1.34
6	B	919	BKR	O11-C27	5.10	1.46	1.34
6	A	919	BKR	O11-C27	4.67	1.45	1.34
6	A	919	BKR	O4-C12	3.92	1.44	1.35

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	920	XYP	C5-C4-C3	-8.66	99.02	109.67
7	B	920	XYP	O4-C4-C3	6.97	124.10	110.14
7	A	920	XYP	C5-C4-C3	-6.37	101.84	109.67
5	B	911	NAG	C1-O5-C5	5.52	119.67	112.19
7	A	920	XYP	O4-C4-C3	5.46	121.07	110.14

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	918	NAG	O5-C5-C6-O6
5	A	918	NAG	C4-C5-C6-O6
6	B	919	BKR	O12-C27-C28-O13
6	A	919	BKR	O11-C27-C28-O13
6	A	919	BKR	O12-C27-C28-O13

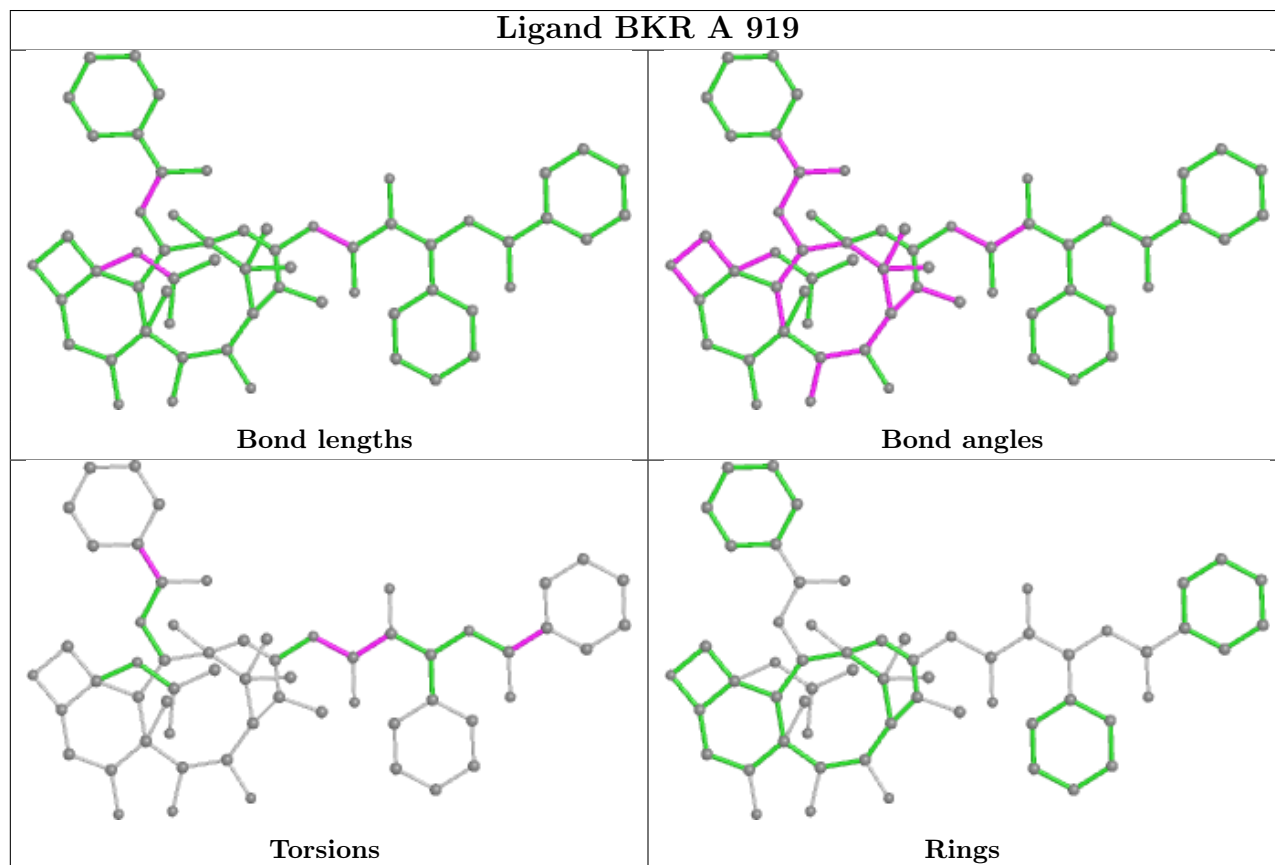
There are no ring outliers.

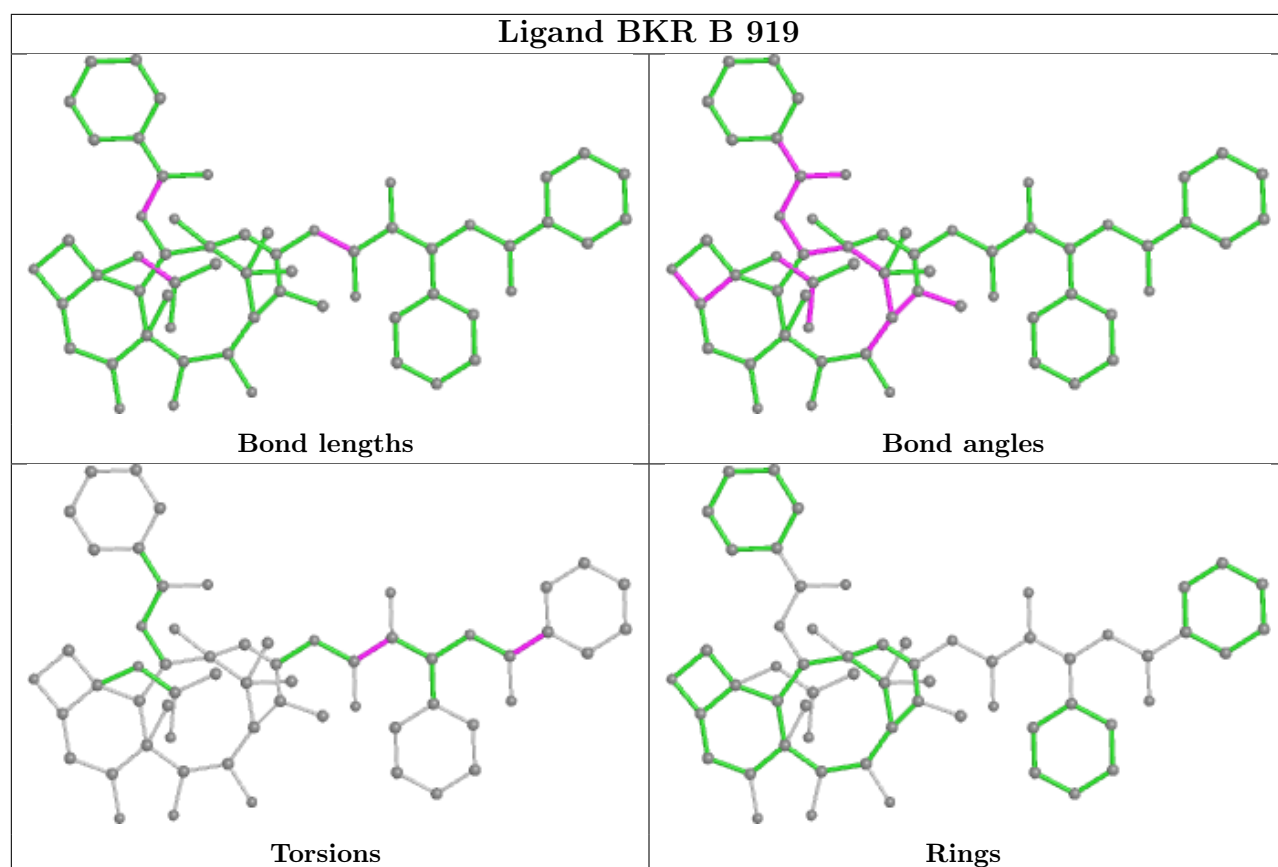
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	920	XYP	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	756/809 (93%)	-0.13	9 (1%) 76 77	19, 31, 49, 104	0
1	B	756/809 (93%)	-0.12	9 (1%) 76 77	12, 32, 48, 91	2 (0%)
All	All	1512/1618 (93%)	-0.13	18 (1%) 76 77	12, 31, 49, 104	2 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	696	TRP	4.7
1	A	683	TYR	3.9
1	A	48	GLN	3.9
1	B	696	TRP	3.8
1	B	803	PRO	3.7

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
4	BMA	E	3	11/12	0.53	0.17	62,80,85,87	0
2	MAN	C	3	11/12	0.60	0.16	69,78,83,89	0
4	MAN	E	4	11/12	0.60	0.17	72,89,91,94	0
4	BMA	H	3	11/12	0.61	0.15	75,85,98,99	0
2	MAN	F	3	11/12	0.63	0.14	60,76,80,83	0

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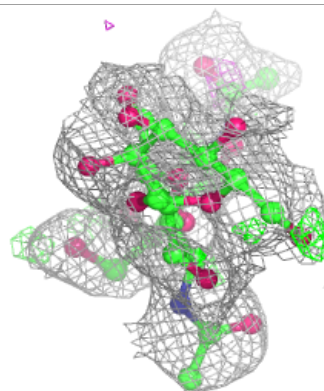
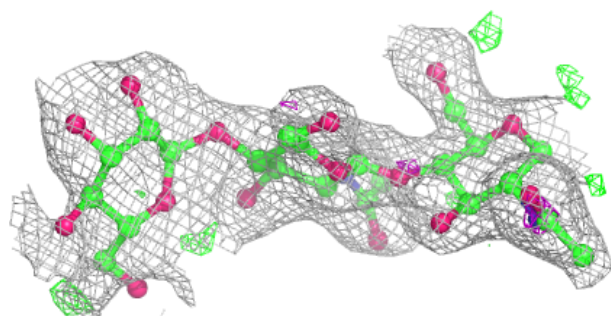
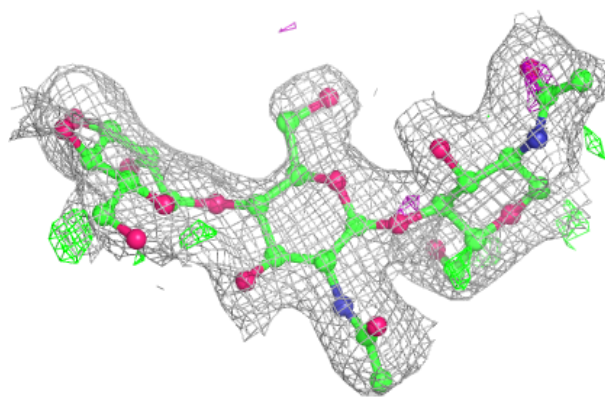
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MAN	H	4	11/12	0.65	0.14	83,95,103,107	0
3	MAN	D	4	11/12	0.72	0.17	20,20,20,20	0
3	MAN	G	5	11/12	0.77	0.14	59,69,74,75	0
3	MAN	D	6	11/12	0.78	0.11	40,43,55,60	0
3	MAN	D	5	11/12	0.78	0.12	46,53,56,57	0
3	MAN	G	4	11/12	0.81	0.11	51,60,64,66	0
3	MAN	G	6	11/12	0.84	0.10	42,45,48,50	0
4	NAG	E	2	14/15	0.85	0.14	41,48,58,72	0
3	NAG	D	1	14/15	0.86	0.11	20,20,20,20	0
2	NAG	F	2	14/15	0.87	0.12	45,50,66,79	0
3	NAG	G	1	14/15	0.88	0.12	20,20,20,20	0
3	NAG	D	2	14/15	0.88	0.10	31,37,39,40	0
2	NAG	C	2	14/15	0.88	0.11	46,50,58,66	0
3	MAN	G	7	11/12	0.90	0.09	52,55,58,64	0
3	MAN	D	7	11/12	0.91	0.09	46,49,52,53	0
3	NAG	G	2	14/15	0.92	0.08	34,41,44,46	0
2	NAG	F	1	14/15	0.93	0.10	20,20,20,20	0
4	NAG	H	2	14/15	0.93	0.10	39,46,62,67	0
3	BMA	D	3	11/12	0.93	0.07	35,40,42,44	0
3	BMA	G	3	11/12	0.93	0.07	41,45,49,50	0
2	NAG	C	1	14/15	0.94	0.10	20,20,20,20	0
4	NAG	H	1	14/15	0.96	0.05	25,27,31,38	0
4	NAG	E	1	14/15	0.96	0.05	23,26,28,36	0

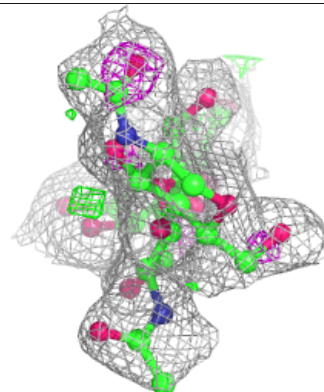
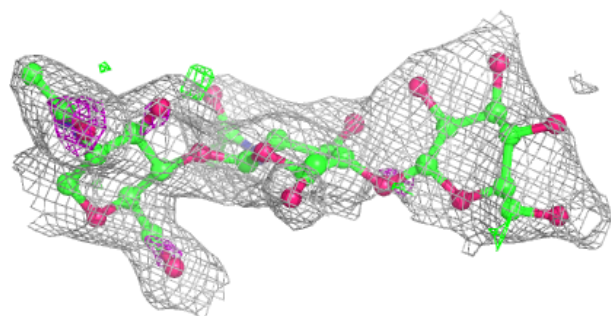
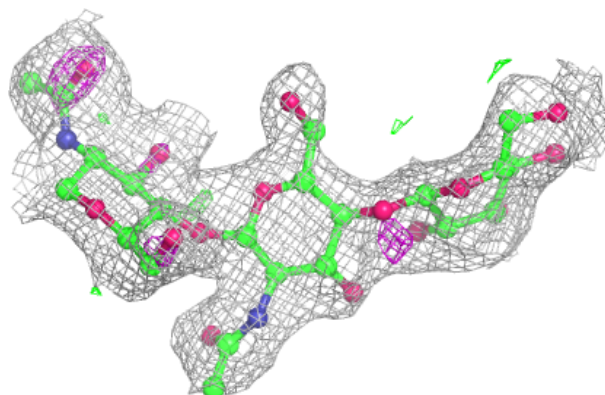
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

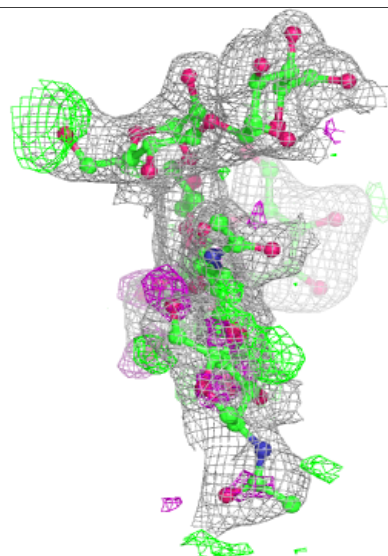
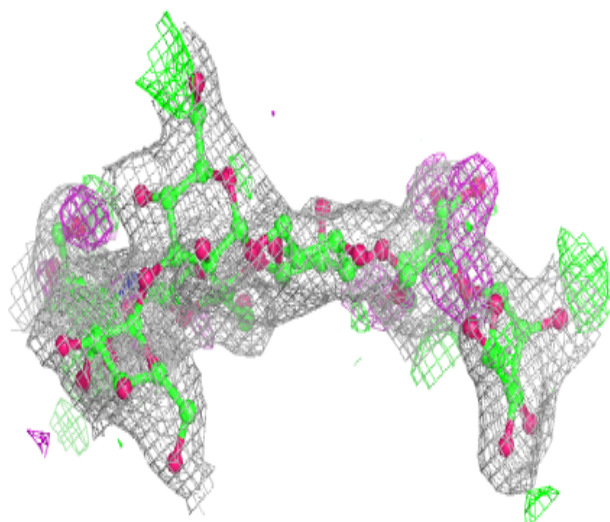
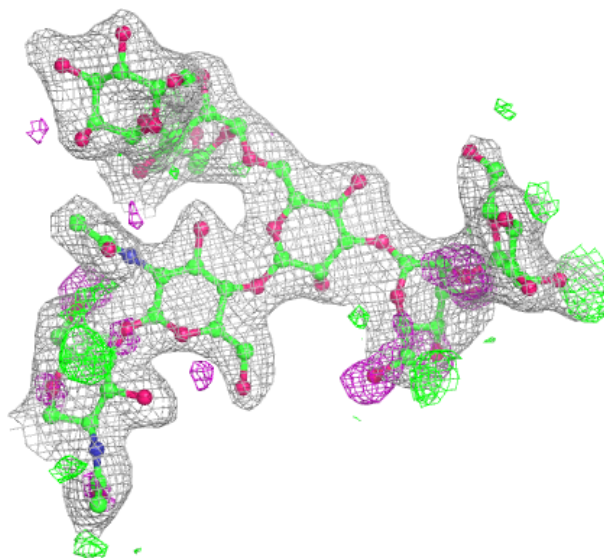
**Electron density around Chain F:**

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



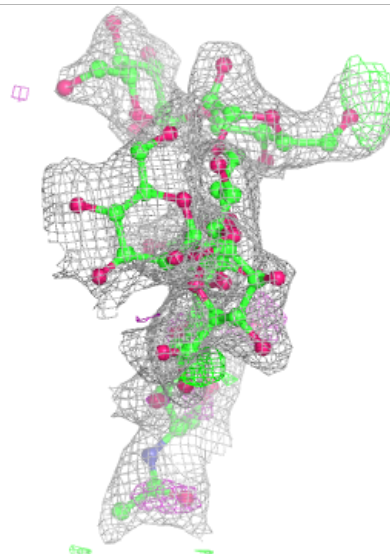
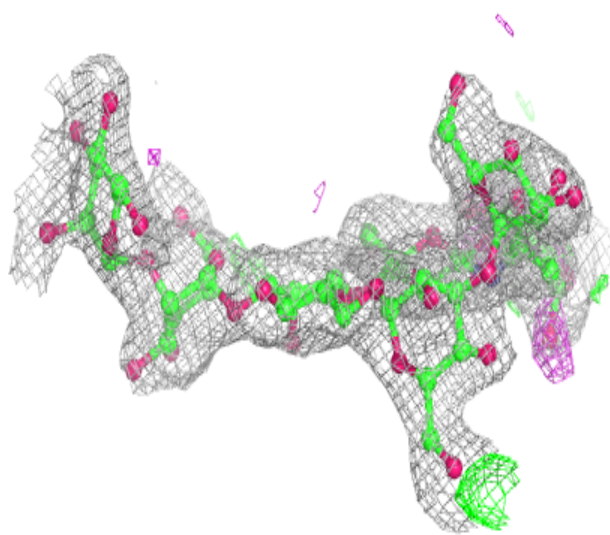
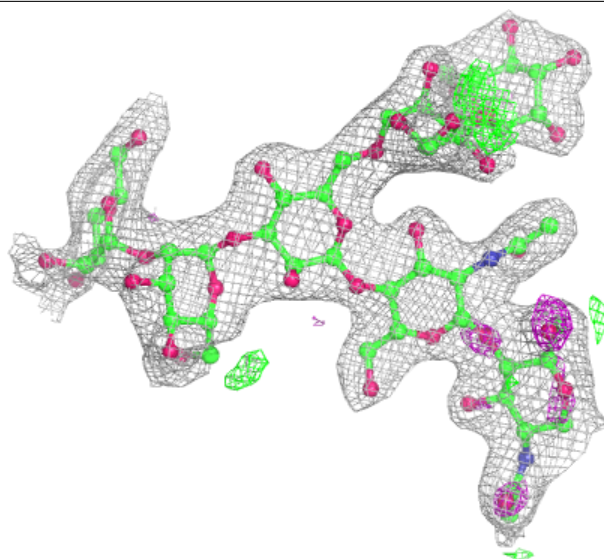
Electron density around Chain D:

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



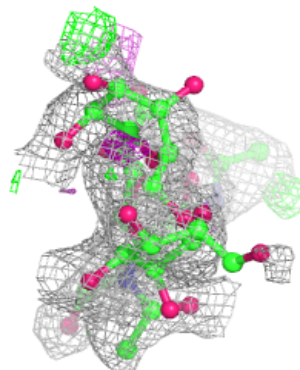
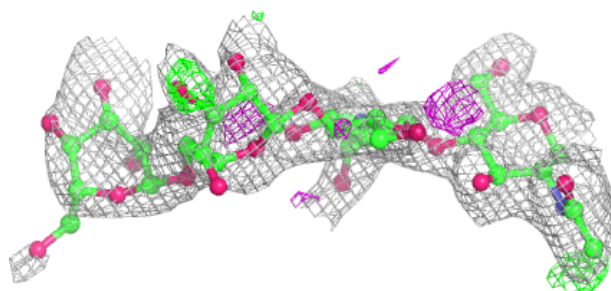
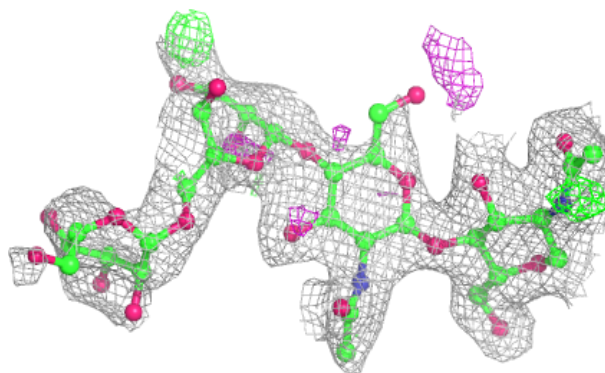
Electron density around Chain G:

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

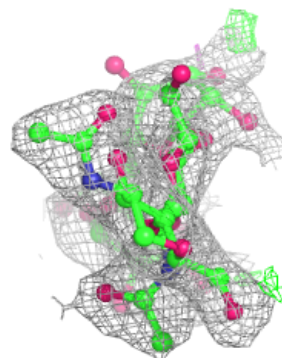
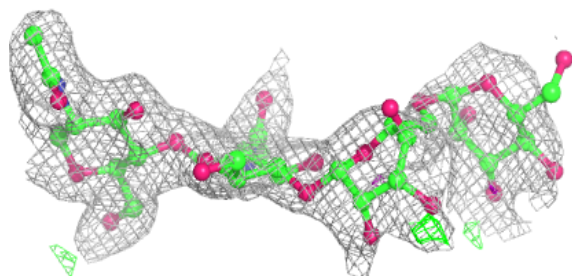
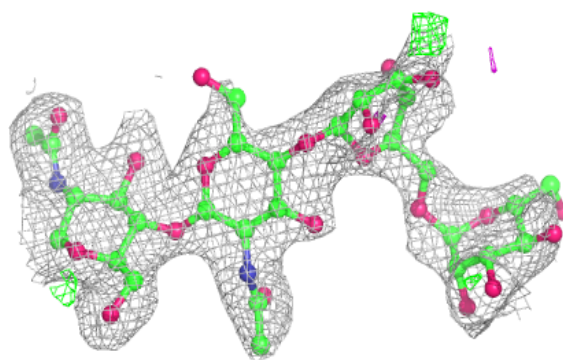


Electron density around Chain E:

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

**Electron density around Chain H:**

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



6.4 Ligands

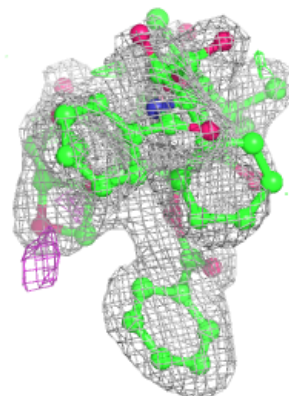
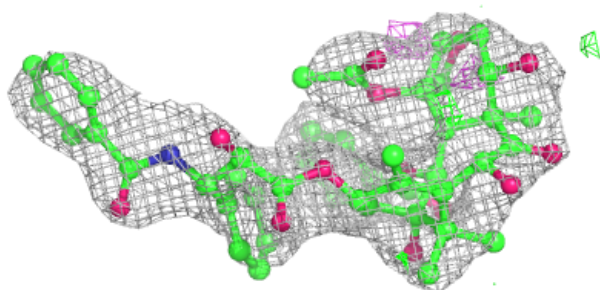
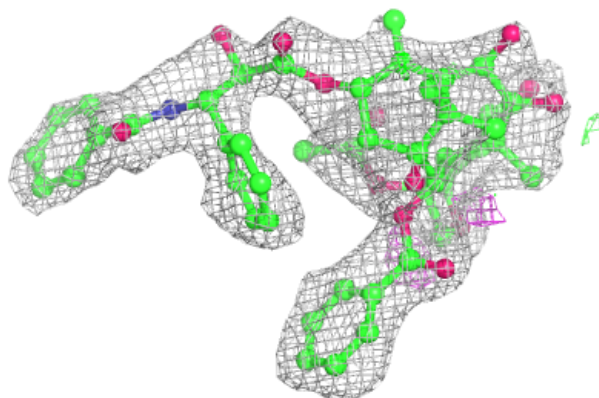
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	918	14/15	0.67	0.17	78,89,96,99	0
5	NAG	A	918	14/15	0.69	0.16	62,77,84,85	0
5	NAG	A	911	14/15	0.78	0.14	61,69,76,78	0
7	XYP	A	920	10/10	0.81	0.12	31,34,36,39	0
5	NAG	B	911	14/15	0.84	0.12	61,65,70,73	0
6	BKR	B	919	59/59	0.86	0.12	42,53,68,70	0
6	BKR	A	919	59/59	0.86	0.13	38,53,68,74	0
7	XYP	B	920	10/10	0.87	0.11	32,37,39,40	0
5	NAG	B	912	14/15	0.89	0.09	41,48,51,51	0
5	NAG	A	912	14/15	0.91	0.09	42,47,49,50	0
5	NAG	A	917	14/15	0.94	0.07	34,38,40,46	0
5	NAG	B	917	14/15	0.95	0.06	35,38,41,44	0

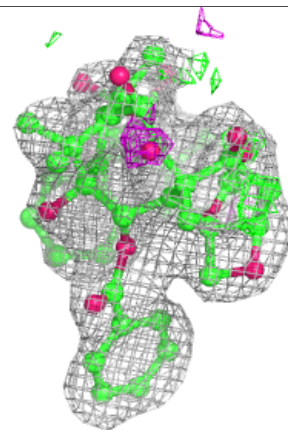
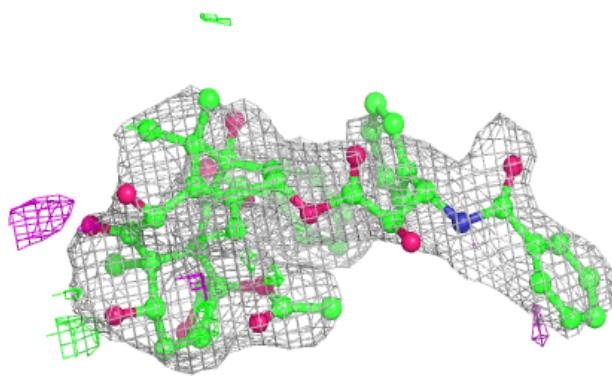
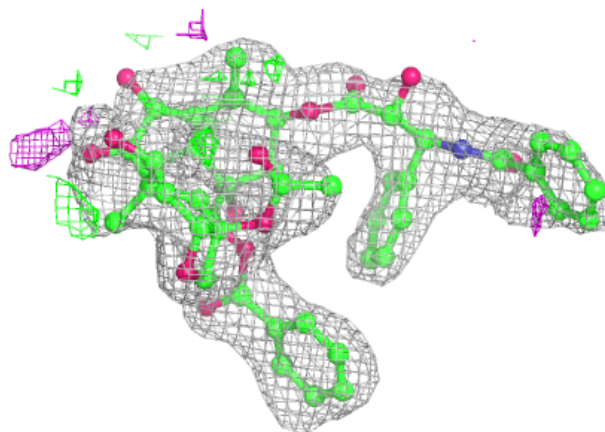
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BKR B 919:

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

**Electron density around BKR A 919:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.