



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2022 – 02:30 PM EST

PDB ID : 7LER
Title : Netrin-1 filament assembly
Authors : McDougall, M.; Gupta, M.; Stetefeld, J.
Deposited on : 2021-01-14
Resolution : 5.99 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	:	2.26
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)	:	2.26

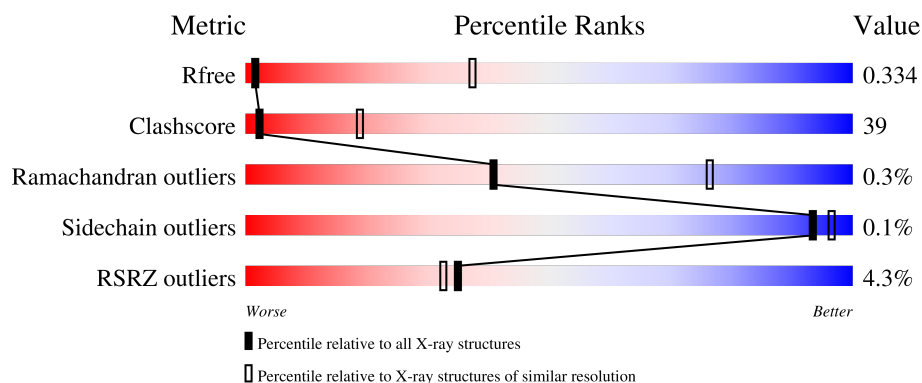
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.99 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	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)
RSRZ outliers	127900	1015 (8.20-3.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	443	<div> <div>6%</div> <div> <div></div> <div>37%</div> <div>55%</div> <div>7%</div> </div> </div>
1	B	443	<div> <div>4%</div> <div> <div></div> <div>34%</div> <div>56%</div> <div>9%</div> </div> </div>
1	C	443	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>58%</div> <div>8%</div> </div> </div>
1	D	443	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>56%</div> <div>9%</div> </div> </div>
1	E	443	<div> <div>5%</div> <div> <div></div> <div>37%</div> <div>55%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	443	
1	G	443	
1	H	443	
2	I	5	
2	K	5	
2	M	5	
2	O	5	
2	Q	5	
2	S	5	
2	U	5	
2	W	5	
3	J	2	
3	L	2	
3	N	2	
3	P	2	
3	R	2	
3	T	2	
3	V	2	
3	X	2	

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	NAG	A	502	-	-	-	X
4	NAG	E	502	-	-	-	X
4	NAG	G	502	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 26405 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 Netrin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3214	1977	599	600	38			
1	B	403	Total	C	N	O	S	0	0	0
			3161	1943	590	590	38			
1	C	409	Total	C	N	O	S	0	0	0
			3203	1971	595	599	38			
1	E	409	Total	C	N	O	S	0	0	0
			3209	1974	598	599	38			
1	D	402	Total	C	N	O	S	0	0	0
			3150	1937	586	589	38			
1	F	409	Total	C	N	O	S	0	0	0
			3209	1974	598	599	38			
1	G	403	Total	C	N	O	S	0	0	0
			3161	1943	590	590	38			
1	H	404	Total	C	N	O	S	0	0	0
			3162	1943	591	590	38			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP Q90922
A	23	PRO	-	expression tag	UNP Q90922
A	24	LEU	-	expression tag	UNP Q90922
A	25	ALA	-	expression tag	UNP Q90922
A	459	GLY	-	expression tag	UNP Q90922
A	460	SER	-	expression tag	UNP Q90922
A	461	LEU	-	expression tag	UNP Q90922
A	462	VAL	-	expression tag	UNP Q90922
A	463	PRO	-	expression tag	UNP Q90922
A	464	ARG	-	expression tag	UNP Q90922
B	22	ALA	-	expression tag	UNP Q90922
B	23	PRO	-	expression tag	UNP Q90922
B	24	LEU	-	expression tag	UNP Q90922

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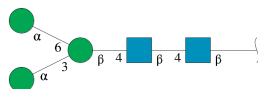
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ALA	-	expression tag	UNP Q90922
B	459	GLY	-	expression tag	UNP Q90922
B	460	SER	-	expression tag	UNP Q90922
B	461	LEU	-	expression tag	UNP Q90922
B	462	VAL	-	expression tag	UNP Q90922
B	463	PRO	-	expression tag	UNP Q90922
B	464	ARG	-	expression tag	UNP Q90922
C	22	ALA	-	expression tag	UNP Q90922
C	23	PRO	-	expression tag	UNP Q90922
C	24	LEU	-	expression tag	UNP Q90922
C	25	ALA	-	expression tag	UNP Q90922
C	459	GLY	-	expression tag	UNP Q90922
C	460	SER	-	expression tag	UNP Q90922
C	461	LEU	-	expression tag	UNP Q90922
C	462	VAL	-	expression tag	UNP Q90922
C	463	PRO	-	expression tag	UNP Q90922
C	464	ARG	-	expression tag	UNP Q90922
E	22	ALA	-	expression tag	UNP Q90922
E	23	PRO	-	expression tag	UNP Q90922
E	24	LEU	-	expression tag	UNP Q90922
E	25	ALA	-	expression tag	UNP Q90922
E	459	GLY	-	expression tag	UNP Q90922
E	460	SER	-	expression tag	UNP Q90922
E	461	LEU	-	expression tag	UNP Q90922
E	462	VAL	-	expression tag	UNP Q90922
E	463	PRO	-	expression tag	UNP Q90922
E	464	ARG	-	expression tag	UNP Q90922
D	22	ALA	-	expression tag	UNP Q90922
D	23	PRO	-	expression tag	UNP Q90922
D	24	LEU	-	expression tag	UNP Q90922
D	25	ALA	-	expression tag	UNP Q90922
D	459	GLY	-	expression tag	UNP Q90922
D	460	SER	-	expression tag	UNP Q90922
D	461	LEU	-	expression tag	UNP Q90922
D	462	VAL	-	expression tag	UNP Q90922
D	463	PRO	-	expression tag	UNP Q90922
D	464	ARG	-	expression tag	UNP Q90922
F	22	ALA	-	expression tag	UNP Q90922
F	23	PRO	-	expression tag	UNP Q90922
F	24	LEU	-	expression tag	UNP Q90922
F	25	ALA	-	expression tag	UNP Q90922
F	459	GLY	-	expression tag	UNP Q90922

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Chain	Residue	Modelled	Actual	Comment	Reference
F	460	SER	-	expression tag	UNP Q90922
F	461	LEU	-	expression tag	UNP Q90922
F	462	VAL	-	expression tag	UNP Q90922
F	463	PRO	-	expression tag	UNP Q90922
F	464	ARG	-	expression tag	UNP Q90922
G	22	ALA	-	expression tag	UNP Q90922
G	23	PRO	-	expression tag	UNP Q90922
G	24	LEU	-	expression tag	UNP Q90922
G	25	ALA	-	expression tag	UNP Q90922
G	459	GLY	-	expression tag	UNP Q90922
G	460	SER	-	expression tag	UNP Q90922
G	461	LEU	-	expression tag	UNP Q90922
G	462	VAL	-	expression tag	UNP Q90922
G	463	PRO	-	expression tag	UNP Q90922
G	464	ARG	-	expression tag	UNP Q90922
H	22	ALA	-	expression tag	UNP Q90922
H	23	PRO	-	expression tag	UNP Q90922
H	24	LEU	-	expression tag	UNP Q90922
H	25	ALA	-	expression tag	UNP Q90922
H	459	GLY	-	expression tag	UNP Q90922
H	460	SER	-	expression tag	UNP Q90922
H	461	LEU	-	expression tag	UNP Q90922
H	462	VAL	-	expression tag	UNP Q90922
H	463	PRO	-	expression tag	UNP Q90922
H	464	ARG	-	expression tag	UNP Q90922

- Molecule 2 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.



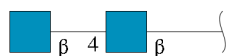
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	K	5	Total	C	N	O	0	0	0
			61	34	2	25			
2	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	5	Total 61	C 34	N 2	O 25	0	0	0
2	Q	5	Total 61	C 34	N 2	O 25	0	0	0
2	S	5	Total 61	C 34	N 2	O 25	0	0	0
2	U	5	Total 61	C 34	N 2	O 25	0	0	0
2	W	5	Total 61	C 34	N 2	O 25	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	J	2	Total 28	C 16	N 2	O 10	0	0	0
3	L	2	Total 28	C 16	N 2	O 10	0	0	0
3	N	2	Total 28	C 16	N 2	O 10	0	0	0
3	P	2	Total 28	C 16	N 2	O 10	0	0	0
3	R	2	Total 28	C 16	N 2	O 10	0	0	0
3	T	2	Total 28	C 16	N 2	O 10	0	0	0
3	V	2	Total 28	C 16	N 2	O 10	0	0	0
3	X	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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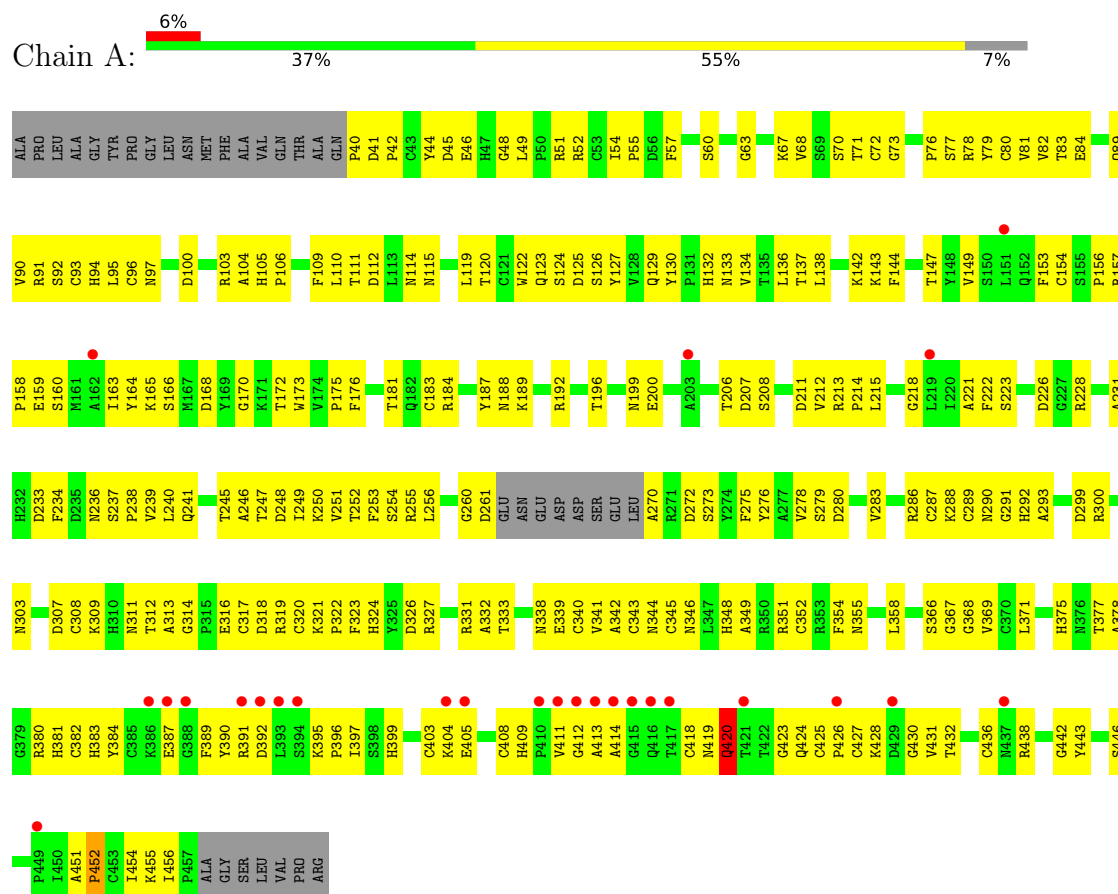
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

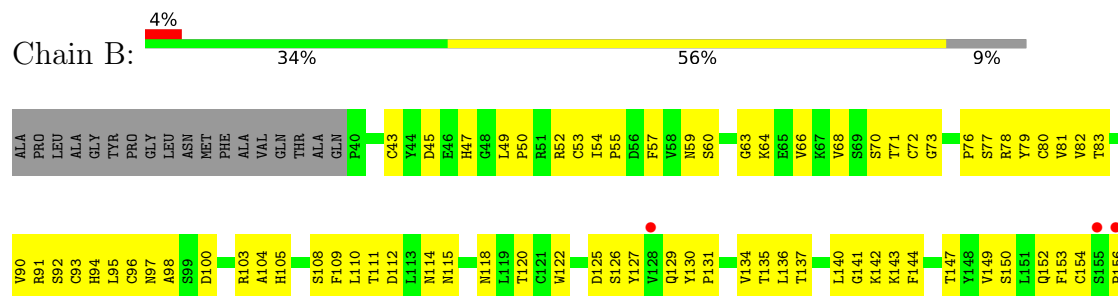
3 Residue-property plots

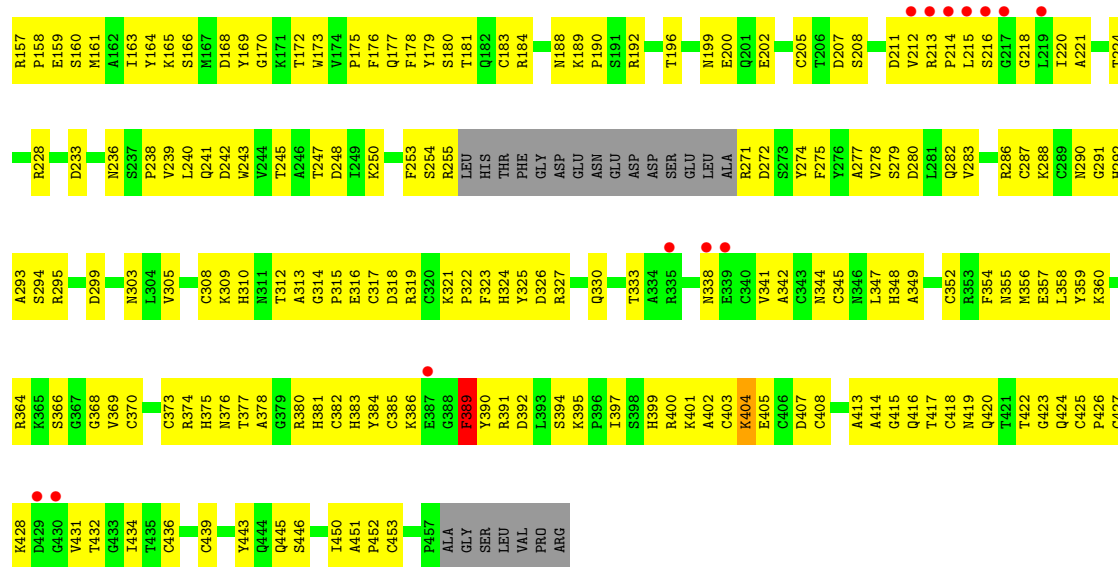
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Netrin-1

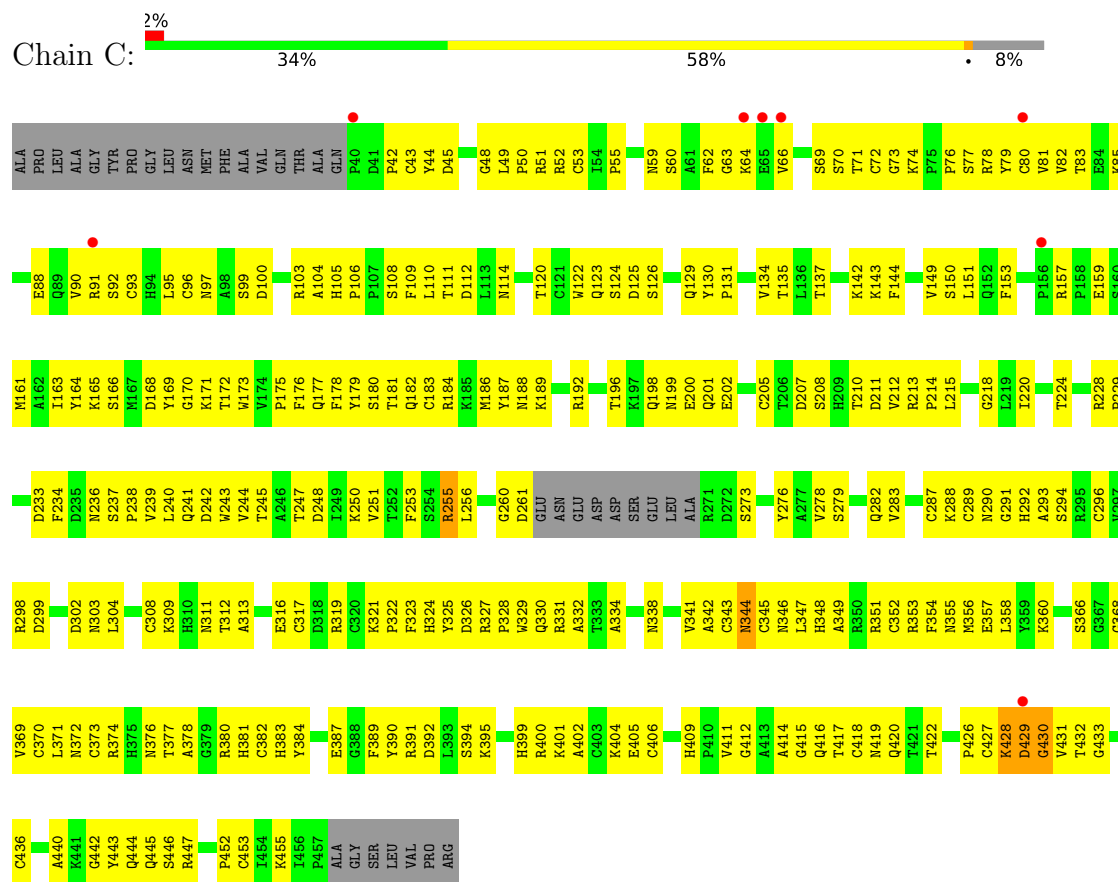


• Molecule 1: Netrin-1

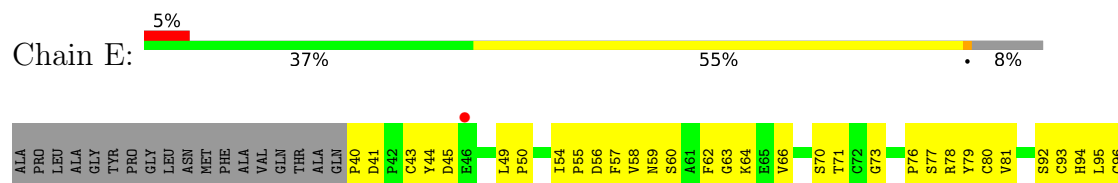


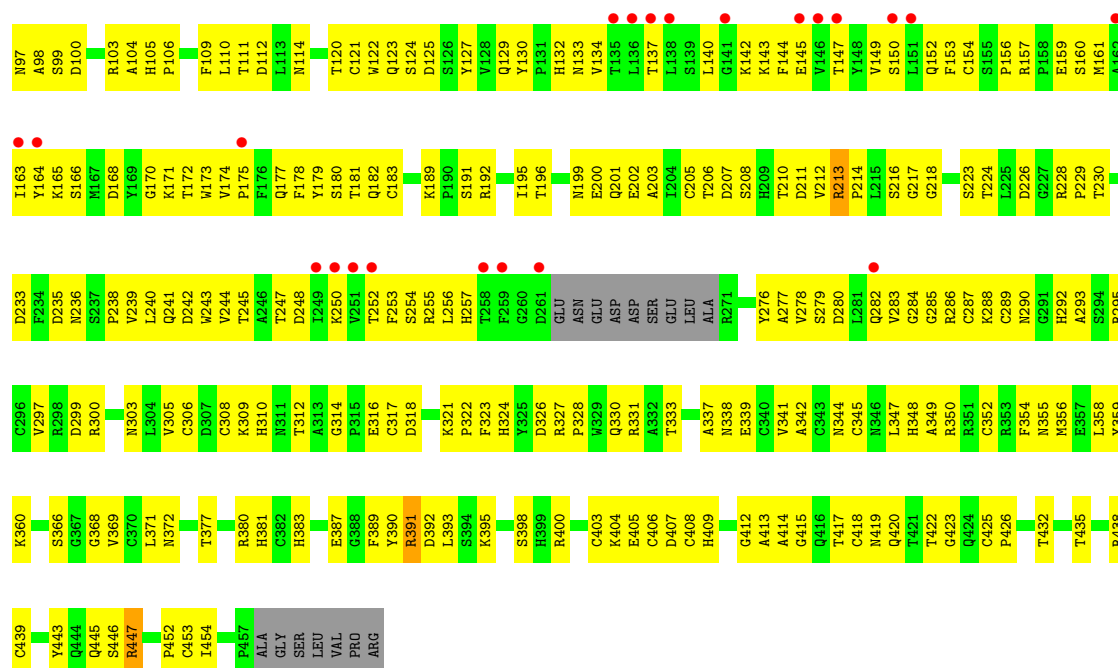


• Molecule 1: Netrin-1

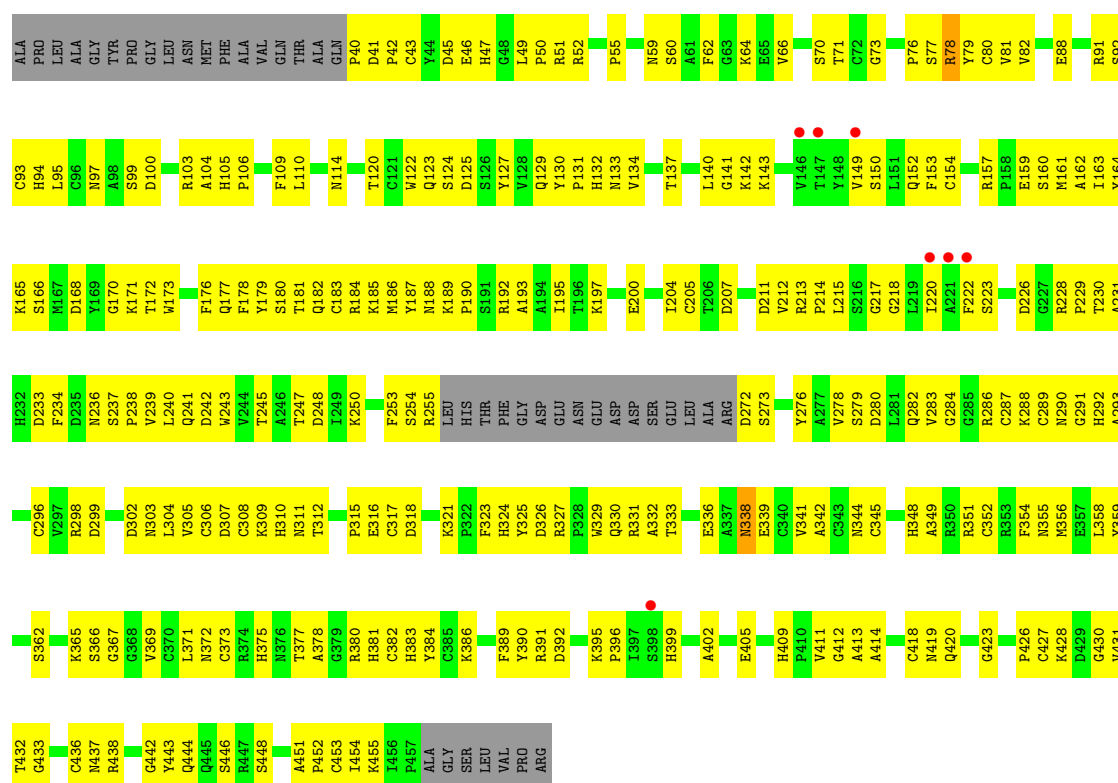


• Molecule 1: Netrin-1



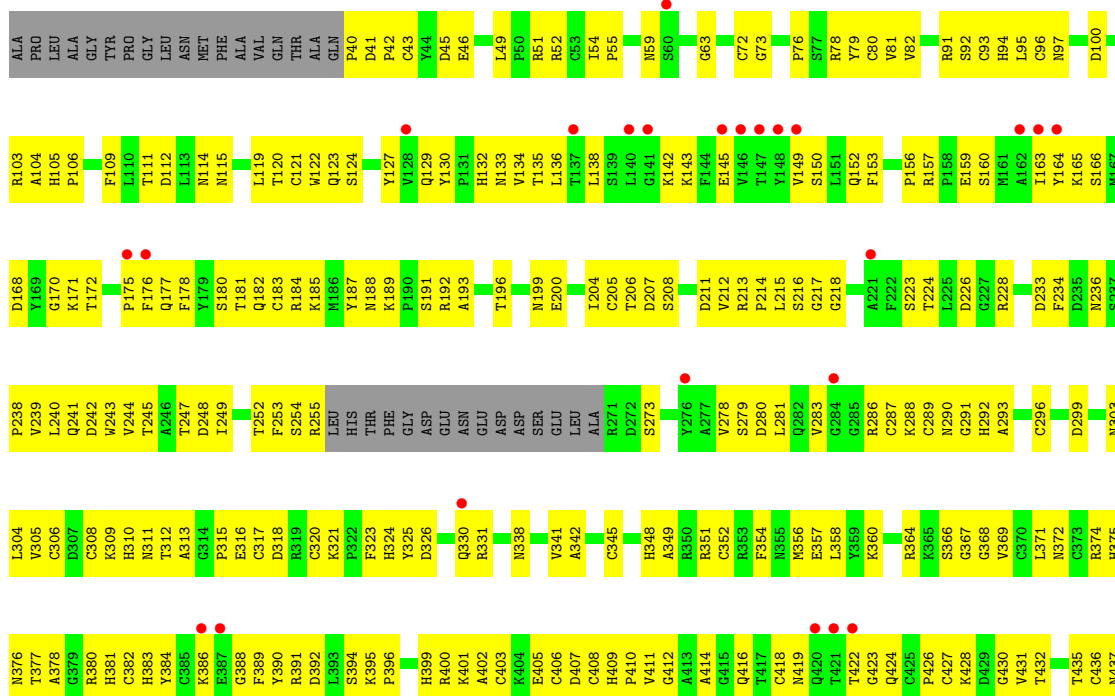


• Molecule 1: Netrin-1



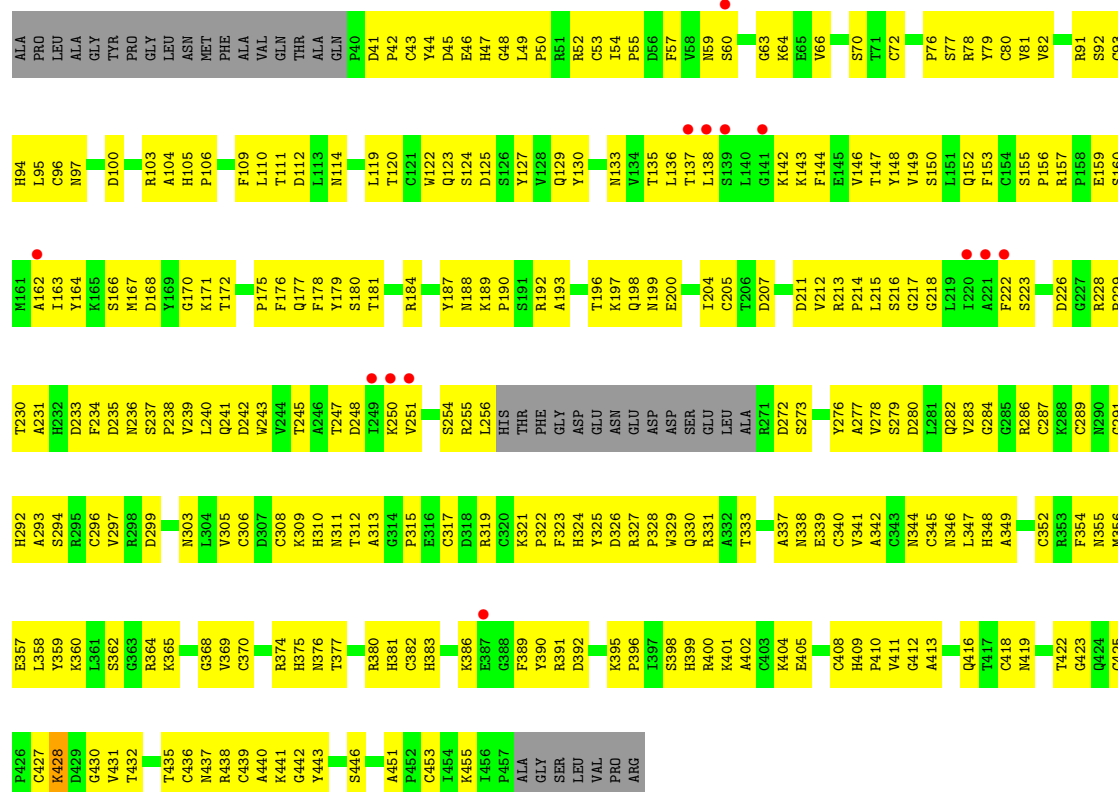
• Molecule 1: Netrin-1







• Molecule 1: Netrin-1



• Molecule 2: 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



• Molecule 2: 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



• Molecule 2: 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

nose

Chain M: 


NAG1
NAG2
BMA3
MAN4
MAN5

• Molecule 2: 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 O: 

NAG1
NAG2
BMA3
MAN4
MAN5

• Molecule 2: 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 Q: 

NAG1
NAG2
BMA3
MAN4
MAN5

• Molecule 2: 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 S: 


NAG1
NAG2
BMA3
MAN4
MAN5

• Molecule 2: 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 U: 

NAG1
NAG2
BMA3
MAN4
MAN5

• Molecule 2: 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 W: 

NAG1
NAG2
BMA3
MAN4
MAN5

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

Chain J:  50% 50%



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

Chain L:  50% 50%



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

Chain N:  50% 50%



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

Chain P:  50% 50%



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

Chain R:  50% 50%



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

Chain T:  50% 50%



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

Chain V:  50% 50%



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

Chain X:
The bar is divided into two segments: a yellow segment on the left and an orange segment on the right. The label '50%' is centered under each segment.



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	196.69Å 196.69Å 476.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.17 – 5.99 49.17 – 5.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.17-5.99) 91.7 (49.17-5.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 6.15Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874_3874	Depositor
R, R_{free}	0.304 , 0.368 0.282 , 0.334	Depositor DCC
R_{free} test set	1336 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	165.2	Xtriage
Anisotropy	0.931	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 400.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.419 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for k,h,-l	Depositor
Outliers	0 of 26041 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	26405	wwPDB-VP
Average B, all atoms (Å ²)	304.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	3/3295 (0.1%)	0.63	2/4459 (0.0%)
1	B	1.94	8/3240 (0.2%)	0.75	8/4384 (0.2%)
1	C	0.35	0/3284	0.62	0/4445
1	D	0.36	0/3229	0.60	0/4370
1	E	0.34	0/3290	0.60	1/4452 (0.0%)
1	F	0.34	0/3290	0.58	0/4452
1	G	0.35	0/3240	0.57	0/4384
1	H	0.34	0/3240	0.58	0/4384
All	All	0.76	11/26108 (0.0%)	0.62	11/35330 (0.0%)

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	A	0	1
1	B	0	1
1	C	0	1
1	H	0	1
All	All	0	4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389	PHE	CE2-CZ	53.47	2.38	1.37
1	B	389	PHE	CD2-CE2	49.39	2.38	1.39
1	B	389	PHE	CE1-CZ	48.51	2.29	1.37
1	B	389	PHE	CD1-CE1	44.40	2.28	1.39
1	B	389	PHE	CG-CD2	32.44	1.87	1.38

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	LYS	N-CA-CB	-13.11	87.00	110.60
1	B	404	LYS	CB-CA-C	12.66	135.71	110.40
1	B	389	PHE	CB-CG-CD1	-11.72	112.60	120.80
1	B	404	LYS	O-C-N	-11.40	104.47	122.70
1	A	420	GLN	CG-CD-OE1	-9.74	102.12	121.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	GLN	Mainchain
1	B	389	PHE	Sidechain
1	C	344	ASN	Peptide
1	H	428	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3214	0	3042	224	0
1	B	3161	0	2995	304	2
1	C	3203	0	3025	258	2
1	D	3150	0	2982	237	0
1	E	3209	0	3037	233	1
1	F	3209	0	3036	259	0
1	G	3161	0	2995	221	1
1	H	3162	0	2999	245	0
2	I	61	0	52	2	0
2	K	61	0	52	4	0
2	M	61	0	52	3	0
2	O	61	0	52	3	0
2	Q	61	0	52	3	0
2	S	61	0	52	2	0
2	U	61	0	52	1	0
2	W	61	0	52	1	0
3	J	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	28	0	25	1	0
3	N	28	0	25	1	0
3	P	28	0	25	1	0
3	R	28	0	25	1	0
3	T	28	0	25	0	0
3	V	28	0	25	1	0
3	X	28	0	25	2	0
4	A	28	0	26	1	0
4	B	28	0	26	1	0
4	C	28	0	26	2	0
4	D	28	0	26	1	0
4	E	28	0	26	1	0
4	F	28	0	26	2	0
4	G	28	0	26	1	0
4	H	28	0	26	2	0
All	All	26405	0	24935	1979	3

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 39.

The worst 5 of 1979 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:B:389:PHE:CD2	1:B:389:PHE:CG	1.87	1.60
1:B:389:PHE:CG	1:B:389:PHE:CD1	1.83	1.59
1:B:389:PHE:CE1	1:B:404:LYS:HA	1.42	1.54
1:B:404:LYS:CA	1:B:404:LYS:C	1.84	1.46
1:B:389:PHE:CD2	1:B:404:LYS:O	1.83	1.30

All (3) 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)
1:B:357:GLU:OE2	1:C:447:ARG:NH1[1_655]	2.02	0.18
1:E:447:ARG:N	1:G:357:GLU:OE2[1_455]	2.04	0.16
1:B:416:GLN:NE2	1:C:387:GLU:OE2[1_655]	2.06	0.14

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	406/443 (92%)	366 (90%)	38 (9%)	2 (0%)	29	69
1	B	399/443 (90%)	357 (90%)	42 (10%)	0	100	100
1	C	405/443 (91%)	361 (89%)	40 (10%)	4 (1%)	15	54
1	D	398/443 (90%)	356 (89%)	40 (10%)	2 (0%)	29	69
1	E	405/443 (91%)	363 (90%)	42 (10%)	0	100	100
1	F	405/443 (91%)	357 (88%)	46 (11%)	2 (0%)	29	69
1	G	399/443 (90%)	357 (90%)	42 (10%)	0	100	100
1	H	400/443 (90%)	358 (90%)	41 (10%)	1 (0%)	41	76
All	All	3217/3544 (91%)	2875 (89%)	331 (10%)	11 (0%)	41	76

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	429	ASP
1	C	430	GLY
1	A	420	GLN
1	C	428	LYS
1	C	255	ARG

5.3.2 Protein sidechains

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	360/385 (94%)	360 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	355/385 (92%)	355 (100%)	0	100	100
1	C	359/385 (93%)	359 (100%)	0	100	100
1	D	354/385 (92%)	353 (100%)	1 (0%)	92	94
1	E	360/385 (94%)	358 (99%)	2 (1%)	86	92
1	F	360/385 (94%)	360 (100%)	0	100	100
1	G	355/385 (92%)	355 (100%)	0	100	100
1	H	355/385 (92%)	355 (100%)	0	100	100
All	All	2858/3080 (93%)	2855 (100%)	3 (0%)	93	96

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

Mol	Chain	Res	Type
1	E	391	ARG
1	E	447	ARG
1	D	78	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	236	ASN
1	G	177	GLN
1	H	177	GLN
1	G	338	ASN
1	D	376	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

56 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	I	1	1,2	14,14,15	0.39	0	17,19,21	1.03	2 (11%)
2	NAG	I	2	2	14,14,15	0.45	0	17,19,21	0.50	0
2	BMA	I	3	2	11,11,12	1.38	1 (9%)	15,15,17	1.36	3 (20%)
2	MAN	I	4	2	11,11,12	0.84	0	15,15,17	1.61	4 (26%)
2	MAN	I	5	2	11,11,12	0.70	0	15,15,17	1.07	2 (13%)
3	NAG	J	1	1,3	14,14,15	0.80	1 (7%)	17,19,21	1.65	1 (5%)
3	NAG	J	2	3	14,14,15	0.62	0	17,19,21	0.46	0
2	NAG	K	1	1,2	14,14,15	0.31	0	17,19,21	1.05	2 (11%)
2	NAG	K	2	2	14,14,15	1.13	1 (7%)	17,19,21	1.14	2 (11%)
2	BMA	K	3	2	11,11,12	1.02	0	15,15,17	1.07	1 (6%)
2	MAN	K	4	2	11,11,12	0.91	0	15,15,17	1.64	4 (26%)
2	MAN	K	5	2	11,11,12	0.79	0	15,15,17	1.09	1 (6%)
3	NAG	L	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	1.66	2 (11%)
3	NAG	L	2	3	14,14,15	0.56	0	17,19,21	0.42	0
2	NAG	M	1	1,2	14,14,15	0.49	0	17,19,21	1.10	2 (11%)
2	NAG	M	2	2	14,14,15	0.99	1 (7%)	17,19,21	0.99	2 (11%)
2	BMA	M	3	2	11,11,12	1.10	1 (9%)	15,15,17	1.02	1 (6%)
2	MAN	M	4	2	11,11,12	0.81	0	15,15,17	1.56	3 (20%)
2	MAN	M	5	2	11,11,12	0.75	0	15,15,17	0.97	2 (13%)
3	NAG	N	1	1,3	14,14,15	0.95	1 (7%)	17,19,21	1.55	1 (5%)
3	NAG	N	2	3	14,14,15	0.64	0	17,19,21	0.47	0
2	NAG	O	1	1,2	14,14,15	0.44	0	17,19,21	1.16	2 (11%)
2	NAG	O	2	2	14,14,15	0.82	1 (7%)	17,19,21	1.01	2 (11%)
2	BMA	O	3	2	11,11,12	1.08	1 (9%)	15,15,17	1.15	1 (6%)
2	MAN	O	4	2	11,11,12	1.10	1 (9%)	15,15,17	1.58	2 (13%)
2	MAN	O	5	2	11,11,12	0.64	0	15,15,17	1.10	1 (6%)
3	NAG	P	1	1,3	14,14,15	0.85	1 (7%)	17,19,21	1.63	1 (5%)
3	NAG	P	2	3	14,14,15	0.62	0	17,19,21	0.48	0
2	NAG	Q	1	1,2	14,14,15	0.34	0	17,19,21	1.06	2 (11%)
2	NAG	Q	2	2	14,14,15	1.09	1 (7%)	17,19,21	1.00	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	Q	3	2	11,11,12	1.07	1 (9%)	15,15,17	1.06	1 (6%)
2	MAN	Q	4	2	11,11,12	0.84	1 (9%)	15,15,17	1.56	3 (20%)
2	MAN	Q	5	2	11,11,12	0.59	0	15,15,17	1.05	2 (13%)
3	NAG	R	1	1,3	14,14,15	0.86	1 (7%)	17,19,21	1.62	1 (5%)
3	NAG	R	2	3	14,14,15	0.53	0	17,19,21	0.45	0
2	NAG	S	1	1,2	14,14,15	0.47	0	17,19,21	0.96	2 (11%)
2	NAG	S	2	2	14,14,15	1.02	1 (7%)	17,19,21	1.07	2 (11%)
2	BMA	S	3	2	11,11,12	0.93	0	15,15,17	1.08	1 (6%)
2	MAN	S	4	2	11,11,12	0.82	0	15,15,17	1.56	3 (20%)
2	MAN	S	5	2	11,11,12	0.72	0	15,15,17	0.98	1 (6%)
3	NAG	T	1	1,3	14,14,15	0.98	1 (7%)	17,19,21	1.61	1 (5%)
3	NAG	T	2	3	14,14,15	0.60	0	17,19,21	0.41	0
2	NAG	U	1	1,2	14,14,15	0.53	0	17,19,21	0.94	1 (5%)
2	NAG	U	2	2	14,14,15	0.90	1 (7%)	17,19,21	1.01	2 (11%)
2	BMA	U	3	2	11,11,12	1.08	1 (9%)	15,15,17	1.06	1 (6%)
2	MAN	U	4	2	11,11,12	0.82	1 (9%)	15,15,17	1.57	4 (26%)
2	MAN	U	5	2	11,11,12	0.62	0	15,15,17	1.06	1 (6%)
3	NAG	V	1	1,3	14,14,15	0.90	1 (7%)	17,19,21	1.60	1 (5%)
3	NAG	V	2	3	14,14,15	0.63	0	17,19,21	0.48	0
2	NAG	W	1	1,2	14,14,15	0.47	0	17,19,21	0.98	1 (5%)
2	NAG	W	2	2	14,14,15	0.87	1 (7%)	17,19,21	0.99	2 (11%)
2	BMA	W	3	2	11,11,12	1.91	2 (18%)	15,15,17	1.36	2 (13%)
2	MAN	W	4	2	11,11,12	0.84	1 (9%)	15,15,17	1.53	3 (20%)
2	MAN	W	5	2	11,11,12	0.87	0	15,15,17	1.02	1 (6%)
3	NAG	X	1	1,3	14,14,15	0.91	1 (7%)	17,19,21	1.62	1 (5%)
3	NAG	X	2	3	14,14,15	0.58	0	17,19,21	0.46	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	I	5	2	-	0/2/19/22	1/1/1/1
3	NAG	J	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	J	2	3	-	4/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	1/2/19/22	1/1/1/1
2	MAN	K	4	2	-	0/2/19/22	0/1/1/1
2	MAN	K	5	2	-	0/2/19/22	1/1/1/1
3	NAG	L	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	L	2	3	-	4/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	3/6/23/26	0/1/1/1
2	BMA	M	3	2	-	1/2/19/22	1/1/1/1
2	MAN	M	4	2	-	0/2/19/22	0/1/1/1
2	MAN	M	5	2	-	0/2/19/22	1/1/1/1
3	NAG	N	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	4/6/23/26	0/1/1/1
2	BMA	O	3	2	-	1/2/19/22	1/1/1/1
2	MAN	O	4	2	-	0/2/19/22	0/1/1/1
2	MAN	O	5	2	-	0/2/19/22	1/1/1/1
3	NAG	P	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	P	2	3	-	4/6/23/26	0/1/1/1
2	NAG	Q	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Q	2	2	-	3/6/23/26	0/1/1/1
2	BMA	Q	3	2	-	1/2/19/22	1/1/1/1
2	MAN	Q	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Q	5	2	-	0/2/19/22	1/1/1/1
3	NAG	R	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	3/6/23/26	0/1/1/1
2	BMA	S	3	2	-	1/2/19/22	1/1/1/1
2	MAN	S	4	2	-	0/2/19/22	0/1/1/1
2	MAN	S	5	2	-	0/2/19/22	1/1/1/1
3	NAG	T	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	T	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	U	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	U	2	2	-	3/6/23/26	0/1/1/1
2	BMA	U	3	2	-	1/2/19/22	1/1/1/1
2	MAN	U	4	2	-	0/2/19/22	0/1/1/1
2	MAN	U	5	2	-	0/2/19/22	1/1/1/1
3	NAG	V	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
2	NAG	W	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	W	2	2	-	3/6/23/26	0/1/1/1
2	BMA	W	3	2	-	1/2/19/22	0/1/1/1
2	MAN	W	4	2	-	0/2/19/22	0/1/1/1
2	MAN	W	5	2	-	0/2/19/22	1/1/1/1
3	NAG	X	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	X	2	3	-	4/6/23/26	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	W	3	BMA	C1-C2	4.65	1.62	1.52
2	Q	2	NAG	O5-C1	-3.82	1.37	1.43
2	W	3	BMA	O5-C1	3.72	1.49	1.43
2	K	2	NAG	O5-C1	-3.64	1.37	1.43
2	I	3	BMA	C1-C2	3.60	1.60	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	C1-O5-C5	6.02	120.35	112.19
3	J	1	NAG	C1-O5-C5	6.02	120.34	112.19
3	R	1	NAG	C1-O5-C5	5.99	120.31	112.19
3	X	1	NAG	C1-O5-C5	5.98	120.29	112.19
3	T	1	NAG	C1-O5-C5	5.94	120.24	112.19

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	2	NAG	C4-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	U	1	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6

5 of 15 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	3	BMA	C1-C2-C3-C4-C5-O5
2	S	3	BMA	C1-C2-C3-C4-C5-O5
2	Q	3	BMA	C1-C2-C3-C4-C5-O5
2	I	3	BMA	C1-C2-C3-C4-C5-O5
2	U	3	BMA	C1-C2-C3-C4-C5-O5

30 monomers are involved in 27 short contacts:

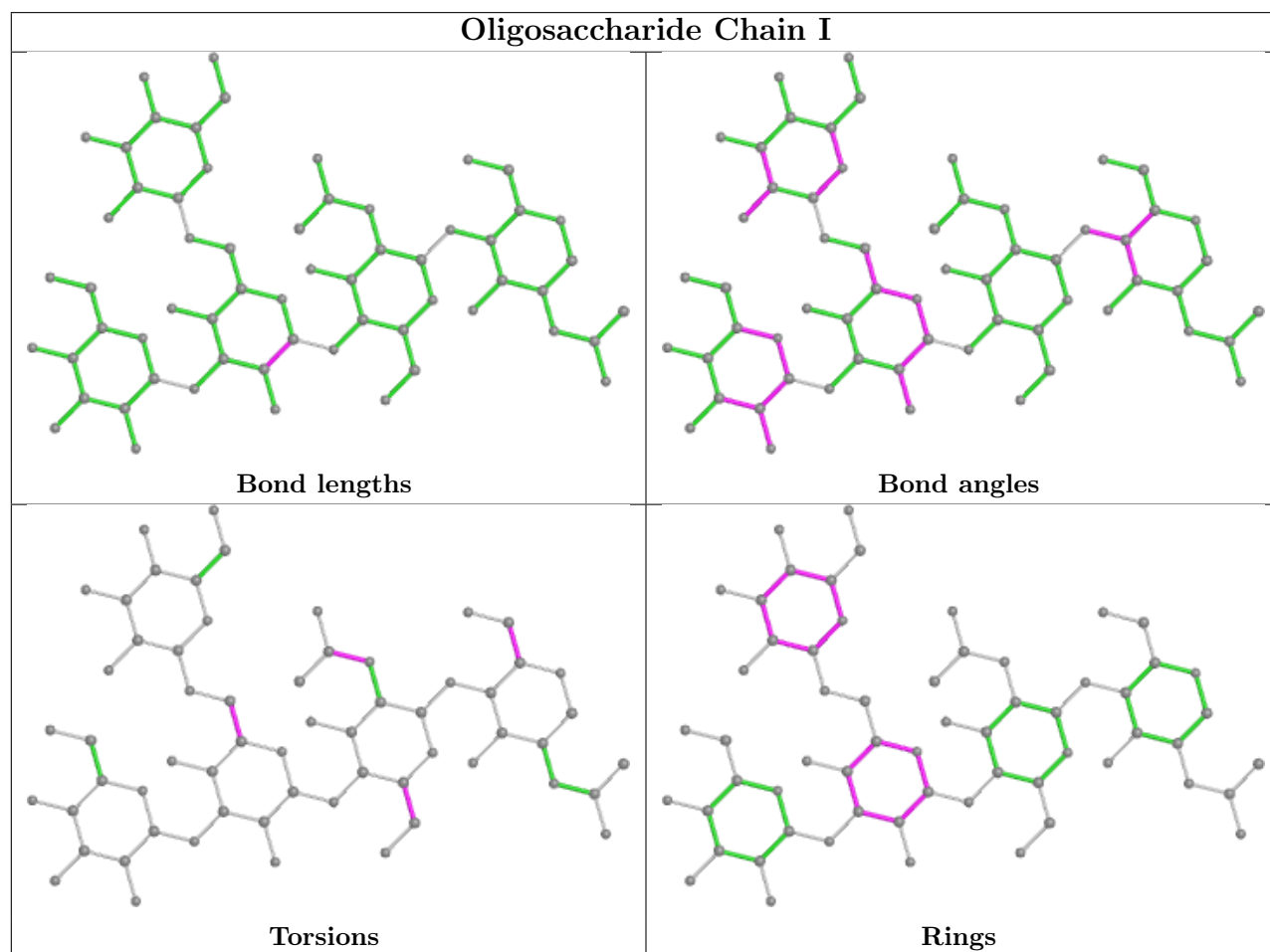
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2	NAG	1	0
3	N	1	NAG	1	0
2	K	2	NAG	2	0
2	Q	1	NAG	3	0
3	R	1	NAG	1	0
2	K	1	NAG	3	0
2	I	2	NAG	1	0
3	L	1	NAG	1	0
3	J	1	NAG	1	0
2	O	3	BMA	1	0
3	V	1	NAG	1	0
2	S	3	BMA	1	0
2	I	3	BMA	1	0
2	M	3	BMA	1	0
2	U	3	BMA	1	0
3	P	1	NAG	1	0
2	S	2	NAG	1	0
2	O	2	NAG	1	0
2	I	1	NAG	1	0
2	M	1	NAG	2	0
2	U	2	NAG	1	0
2	O	5	MAN	1	0
3	N	2	NAG	1	0
2	M	2	NAG	1	0
2	W	1	NAG	1	0
3	L	2	NAG	1	0
3	X	1	NAG	2	0

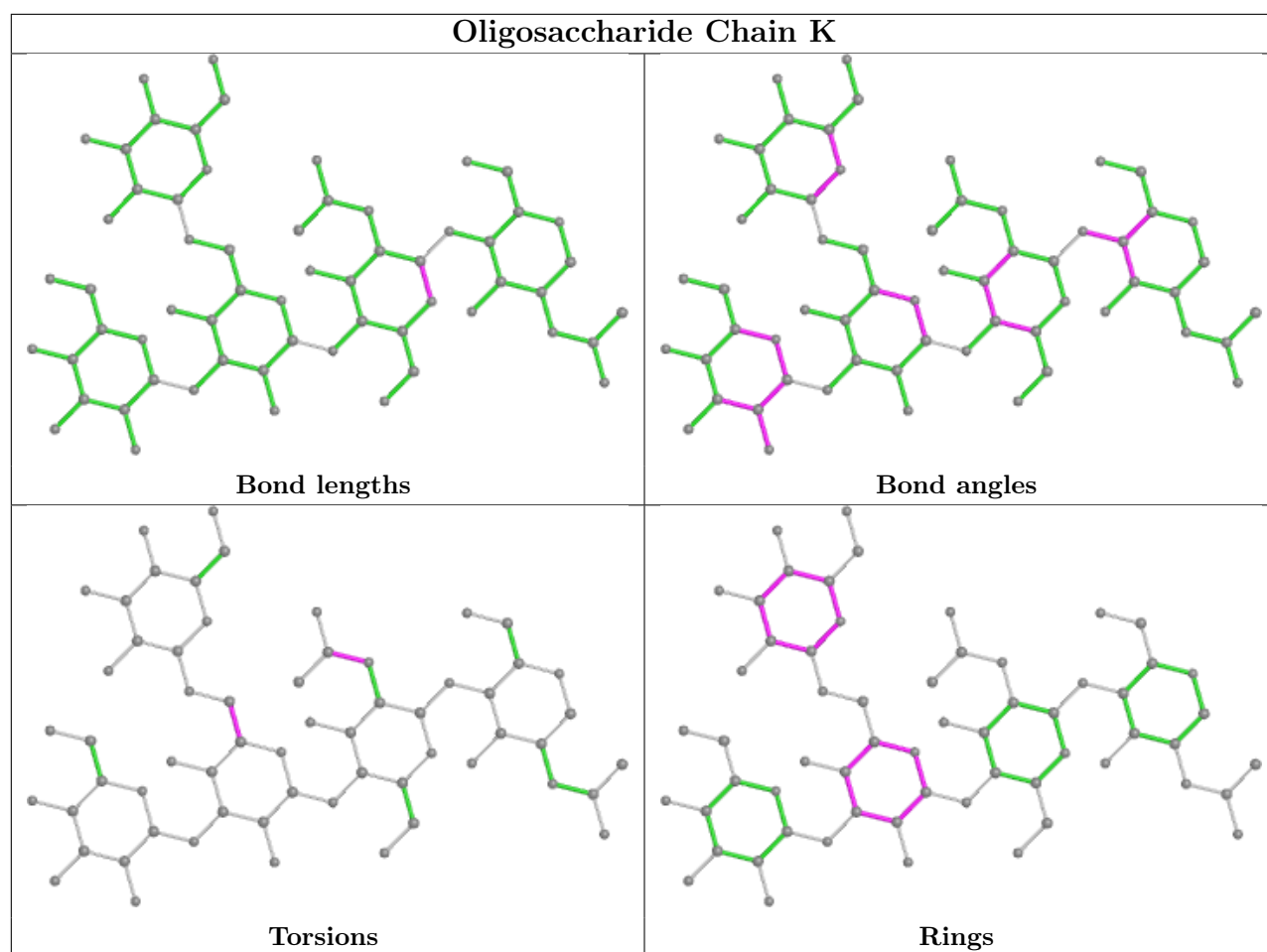
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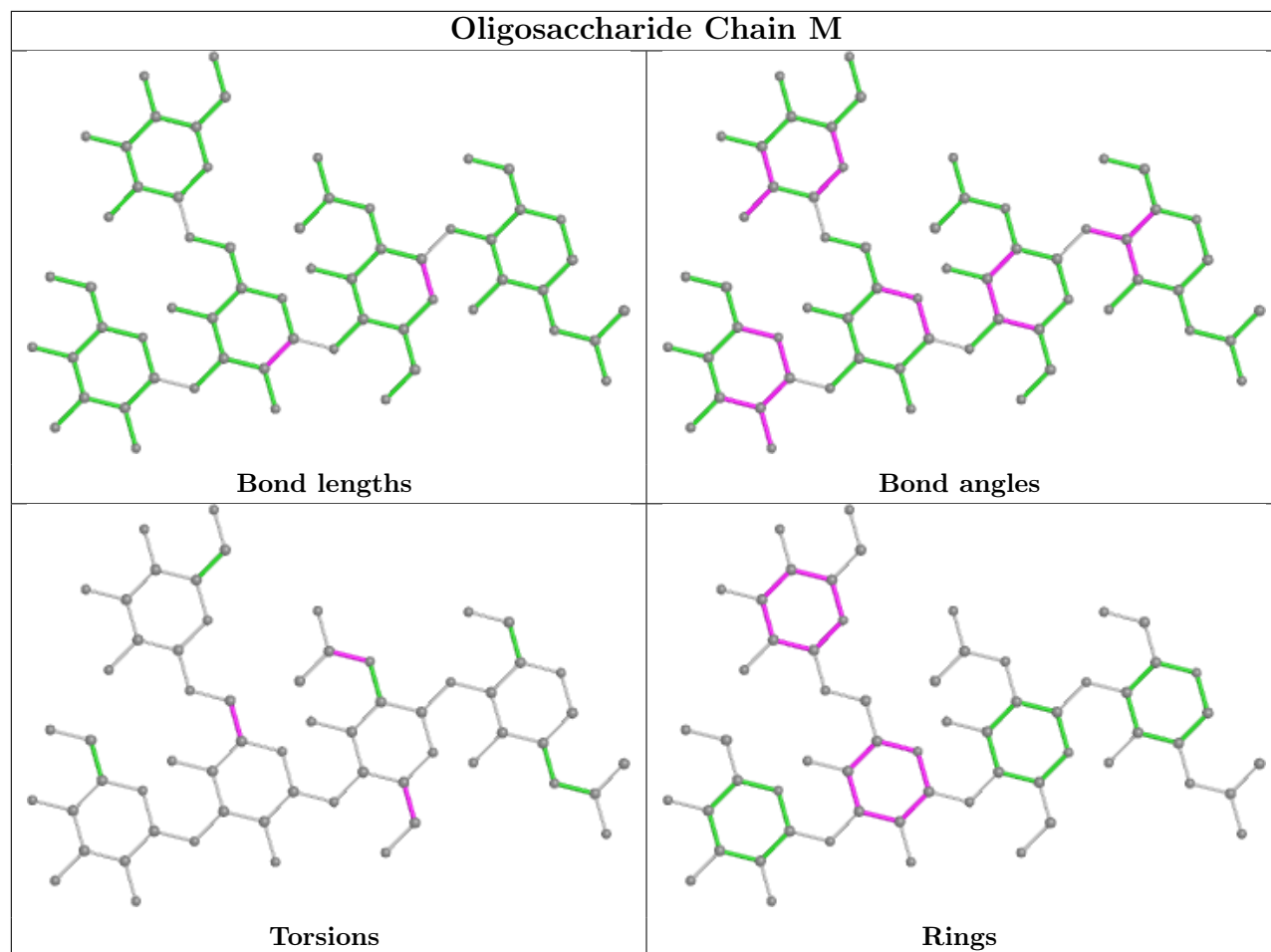
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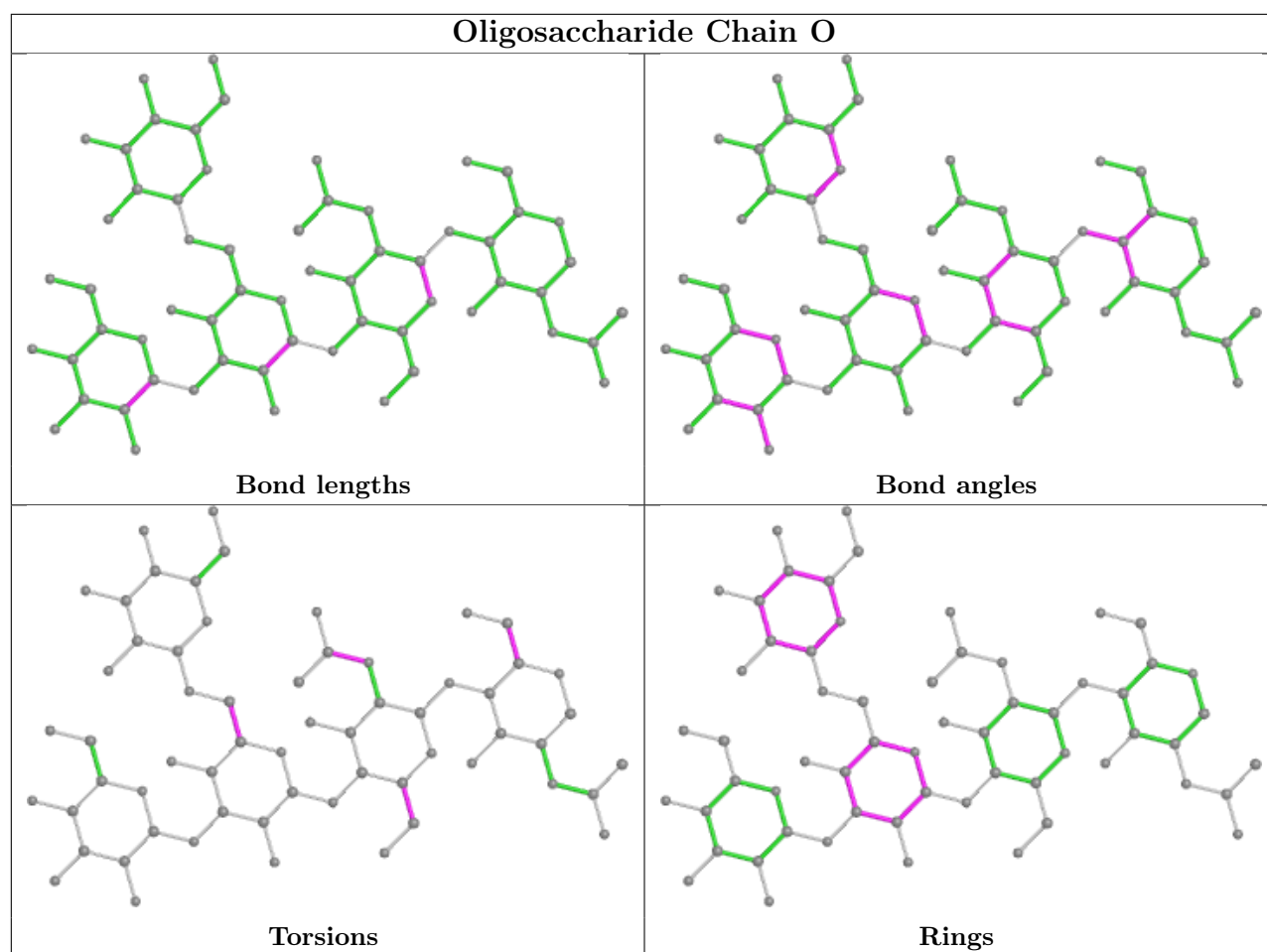
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	NAG	2	0
2	K	3	BMA	1	0
2	S	1	NAG	1	0

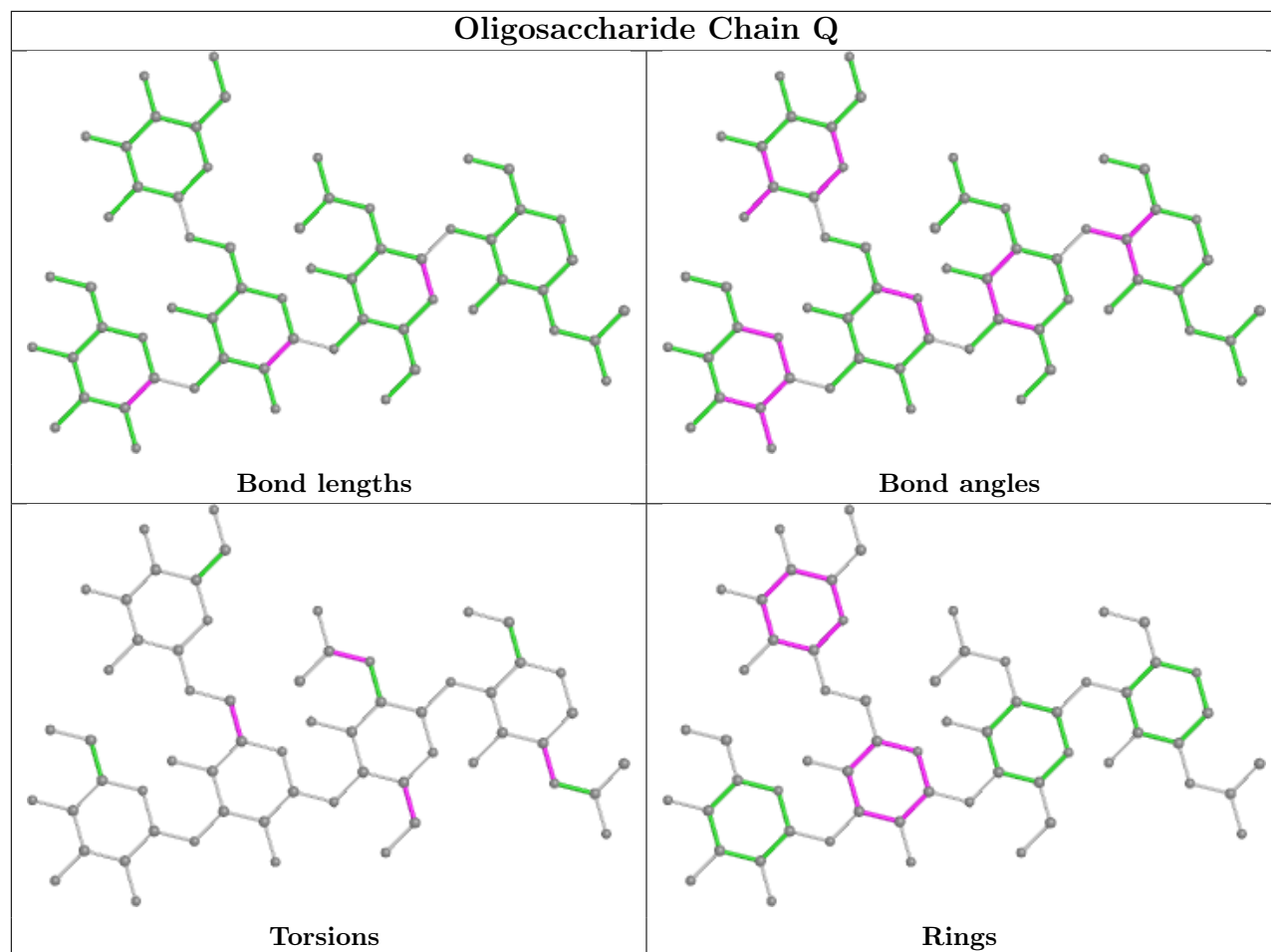
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

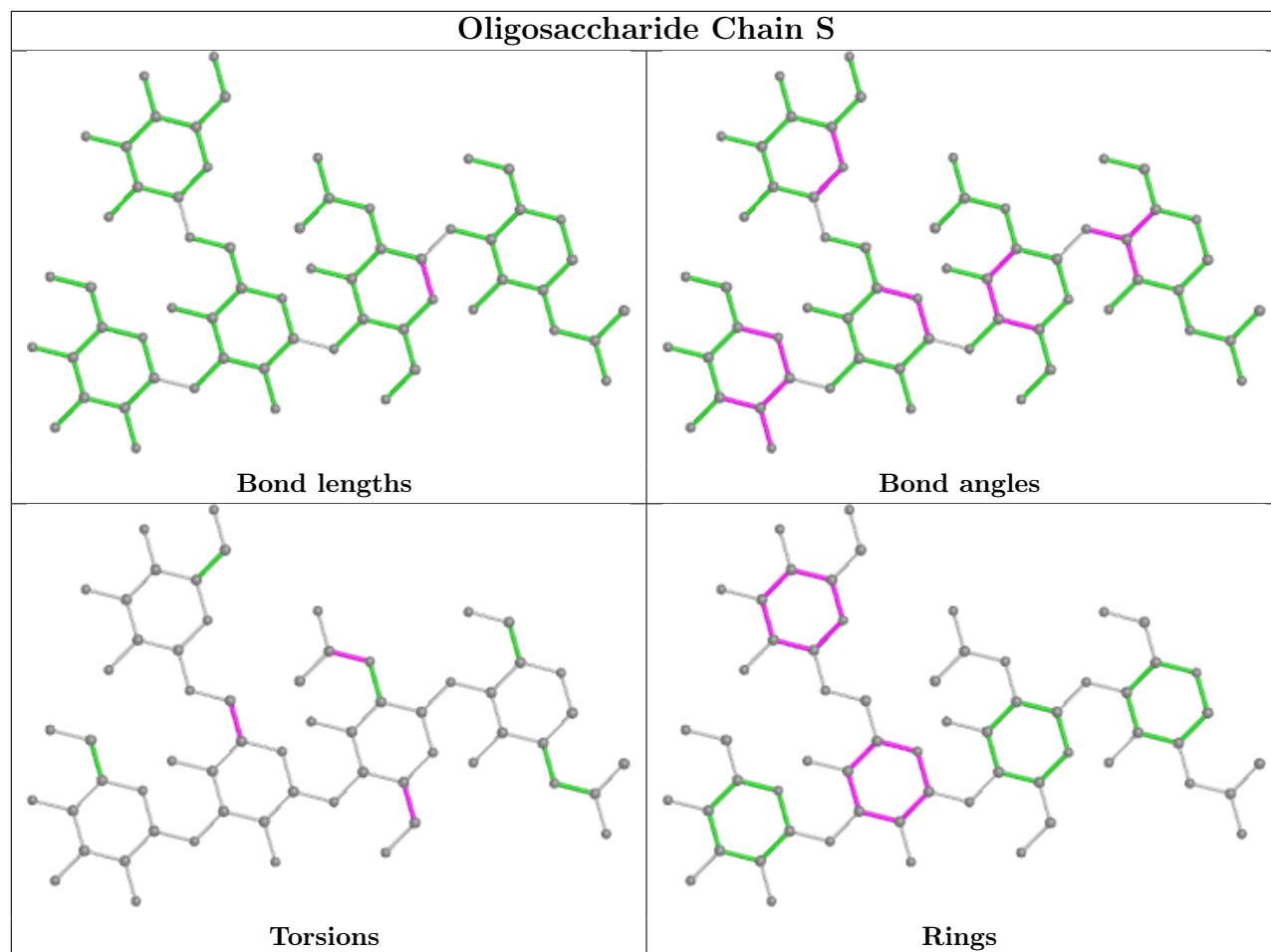


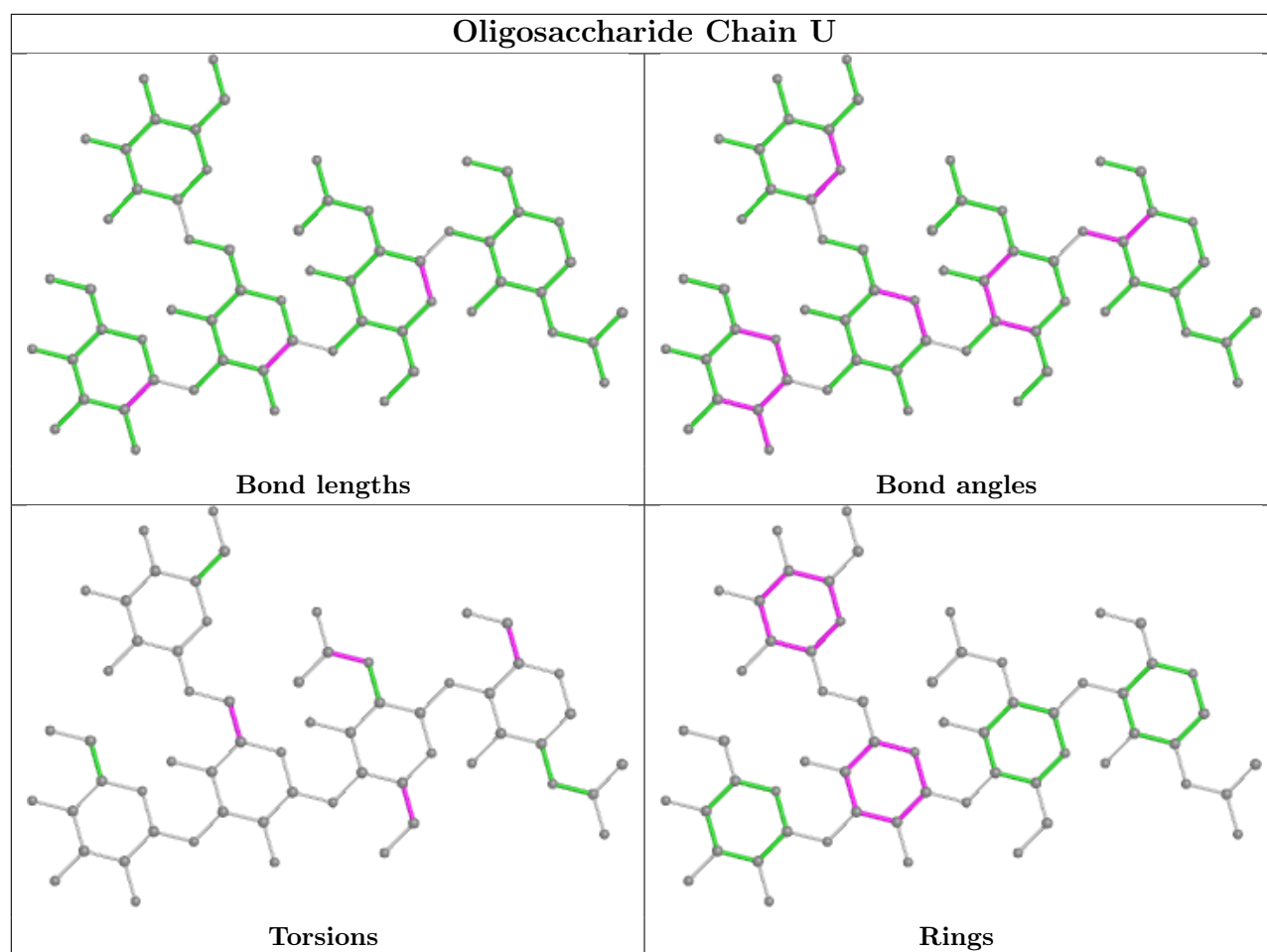


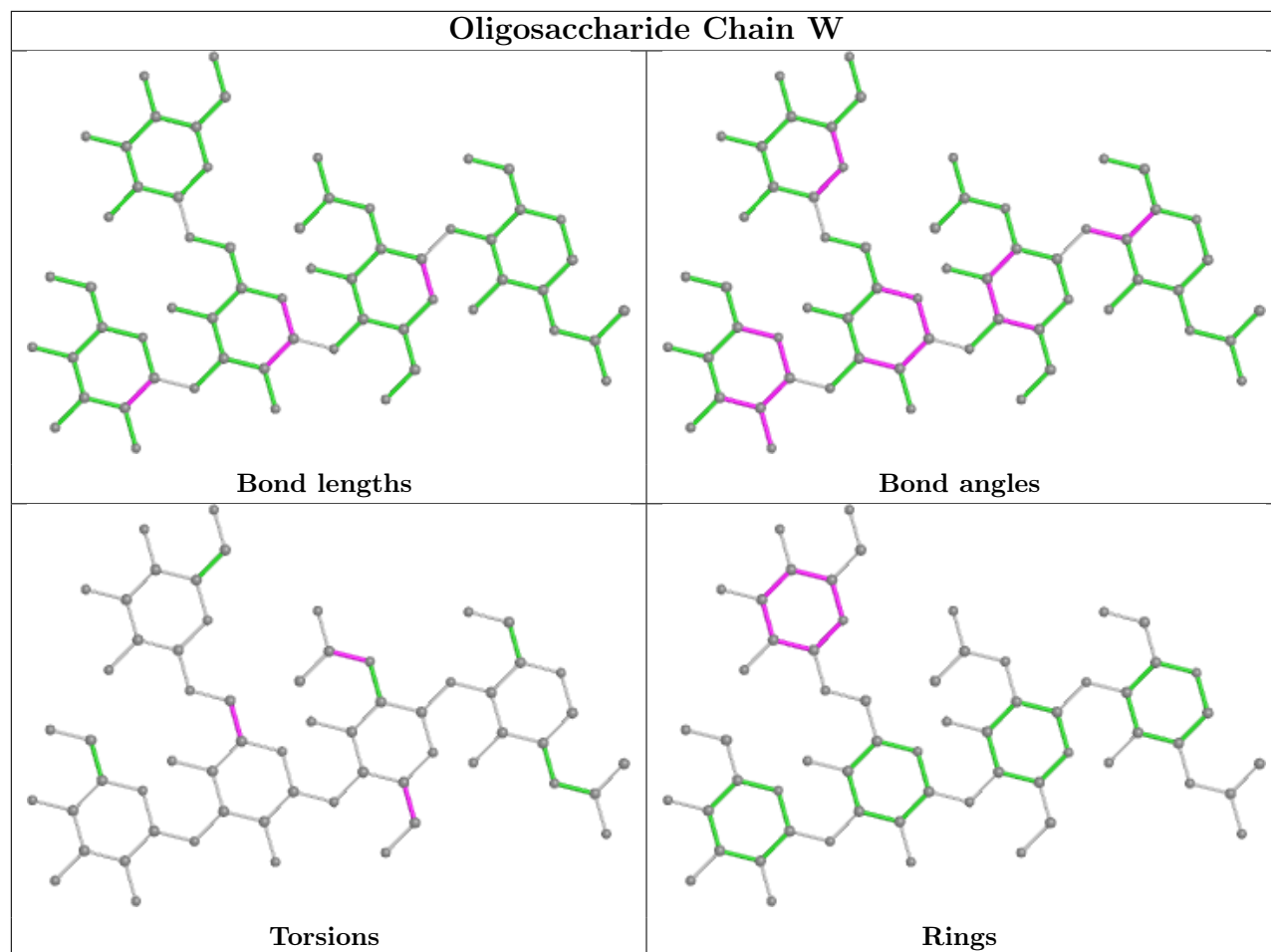


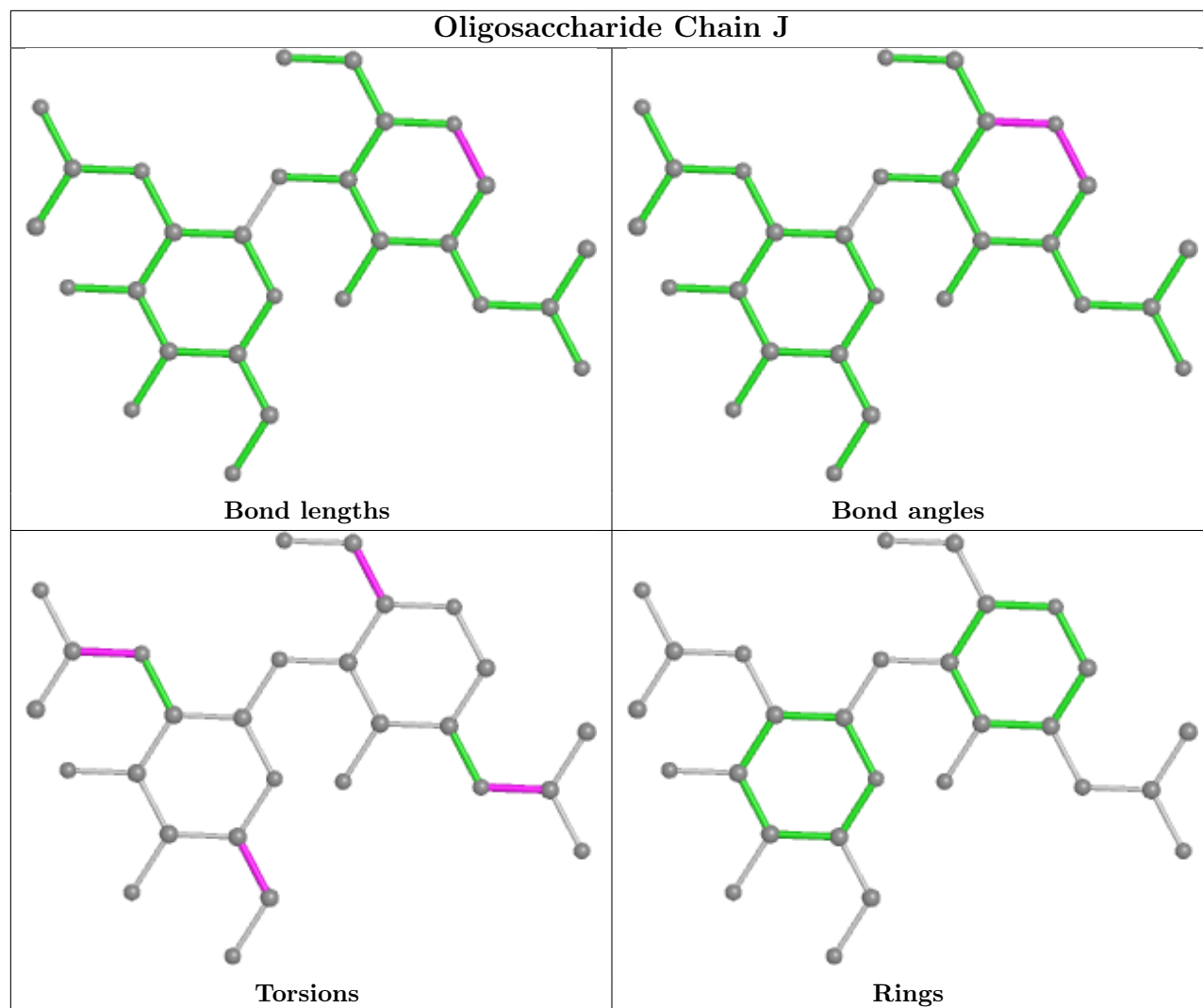


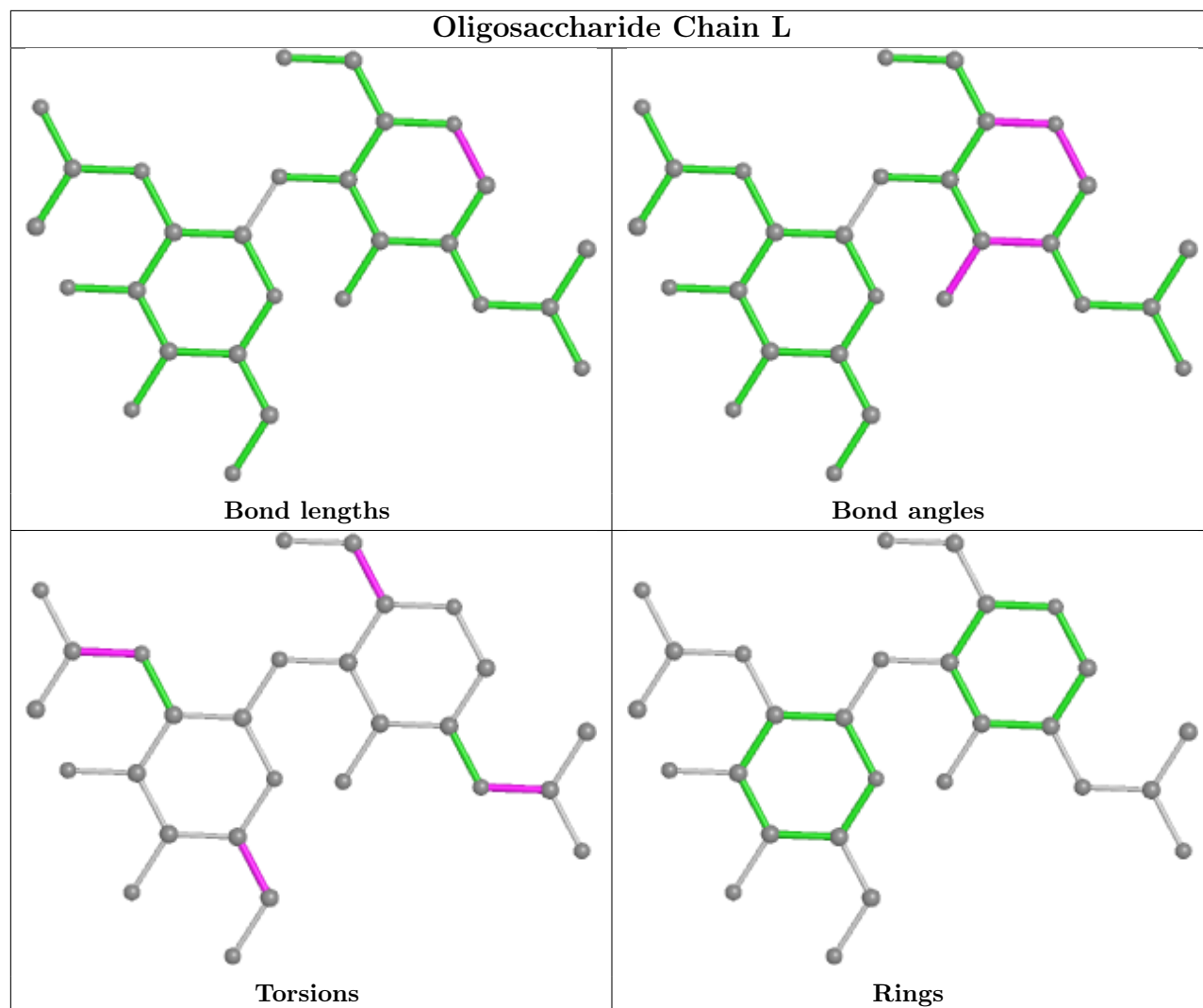


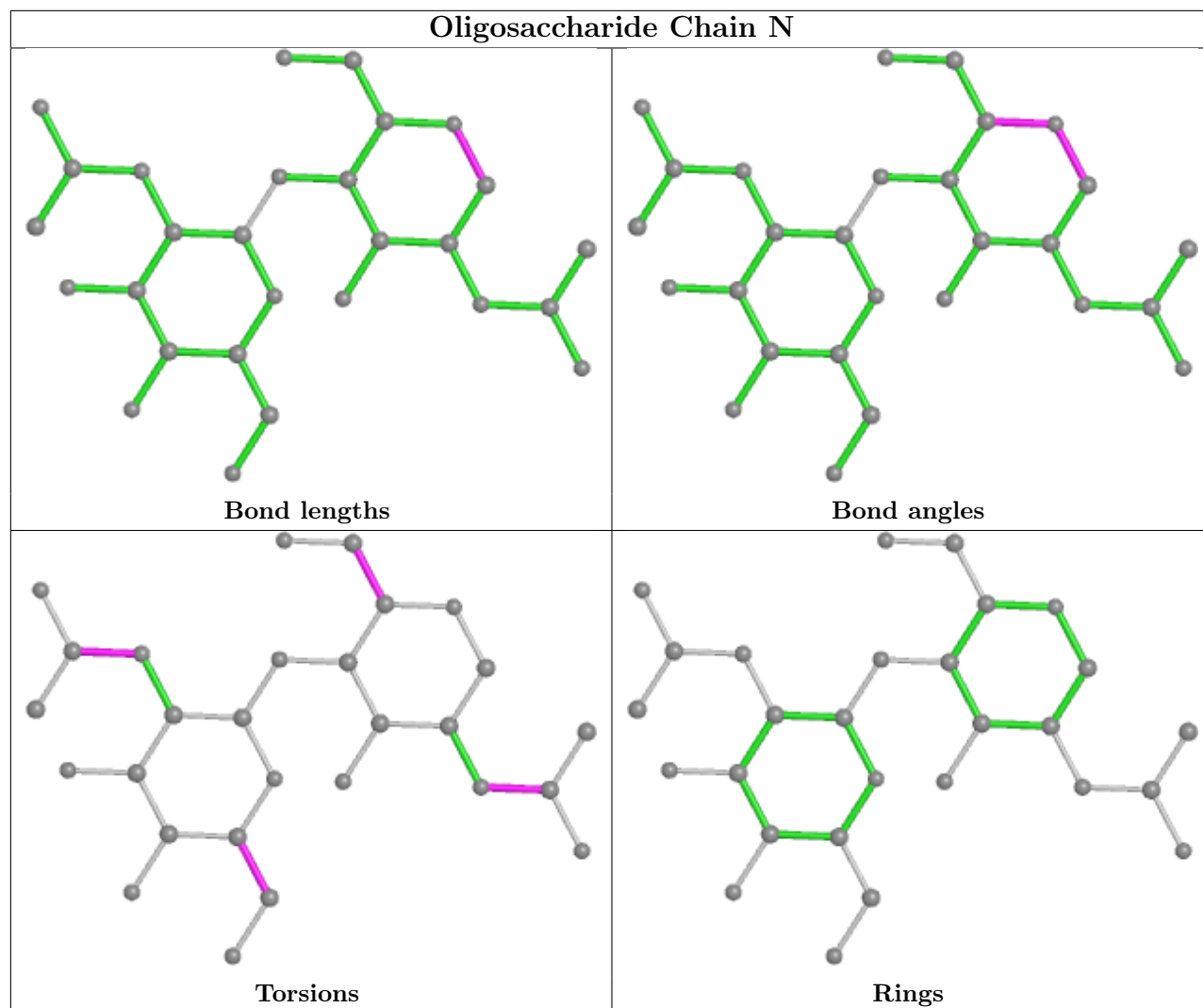


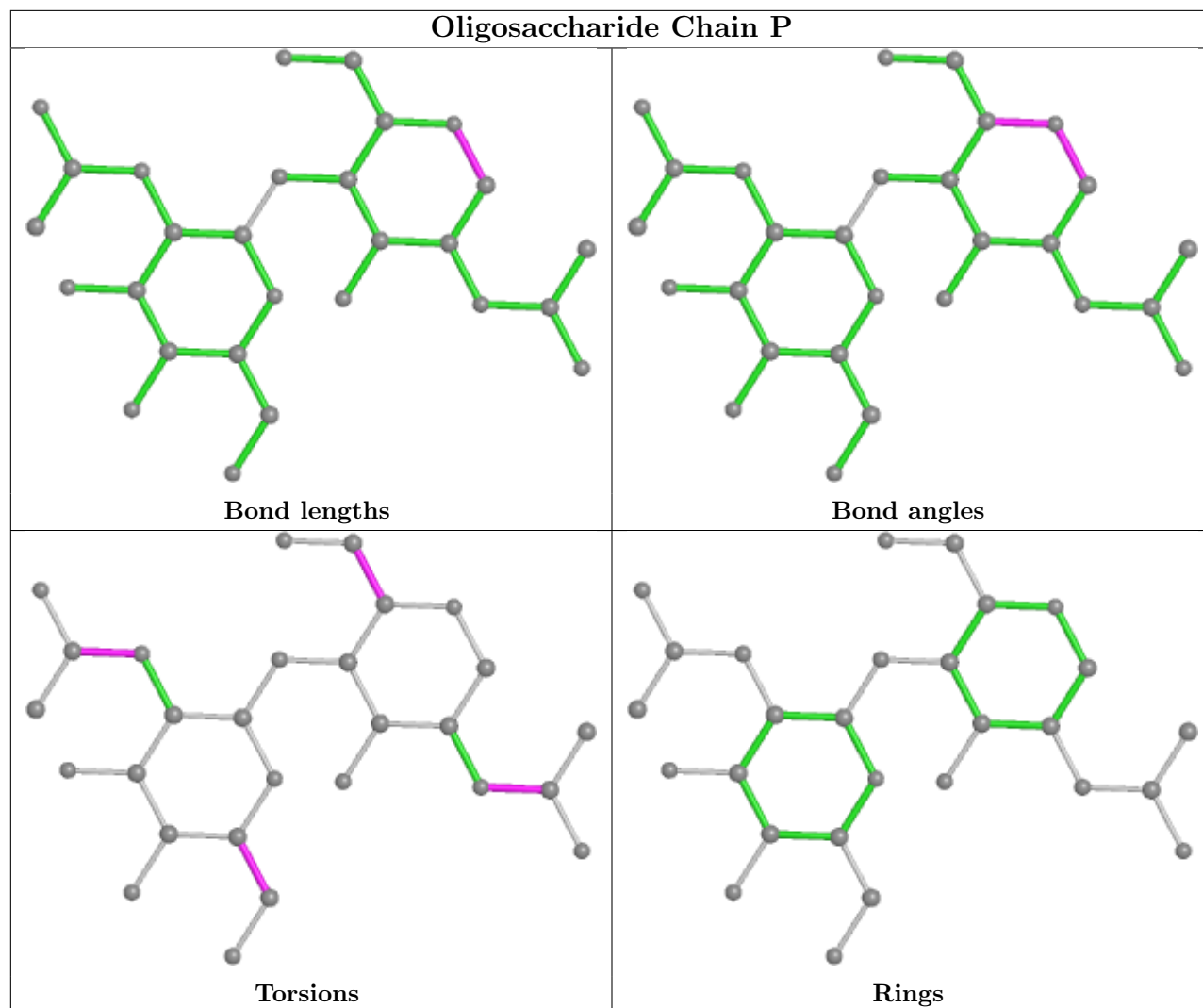


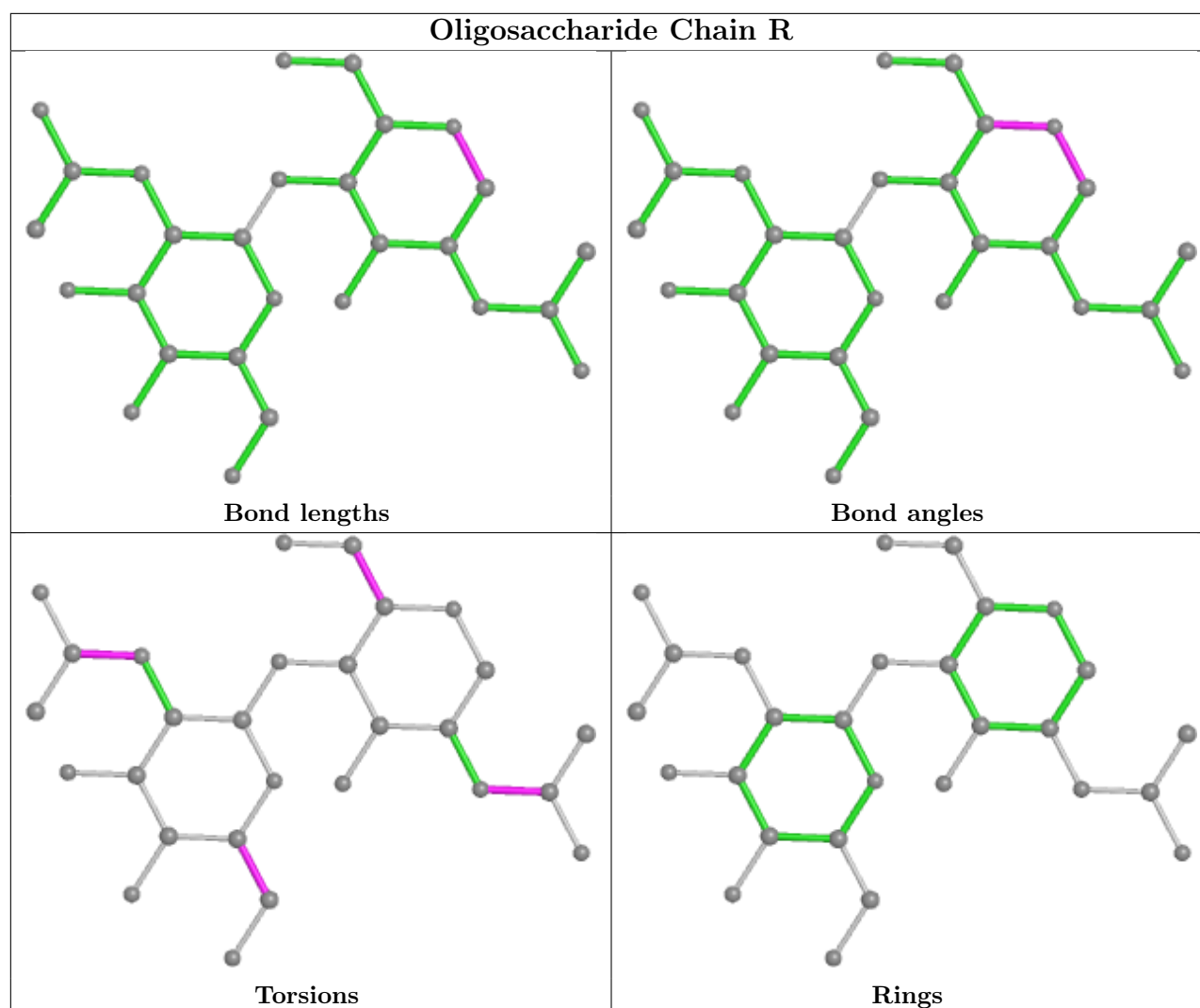


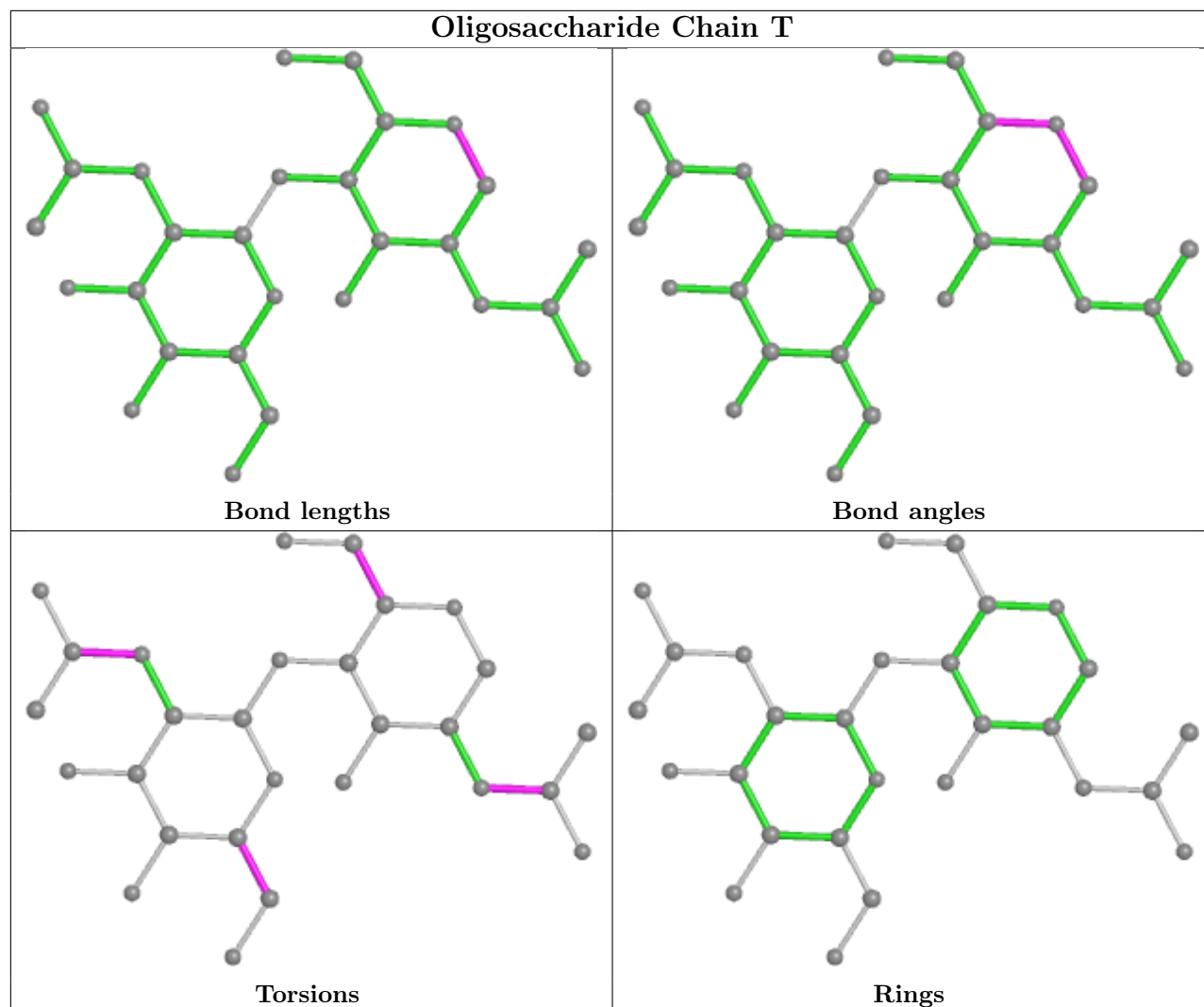


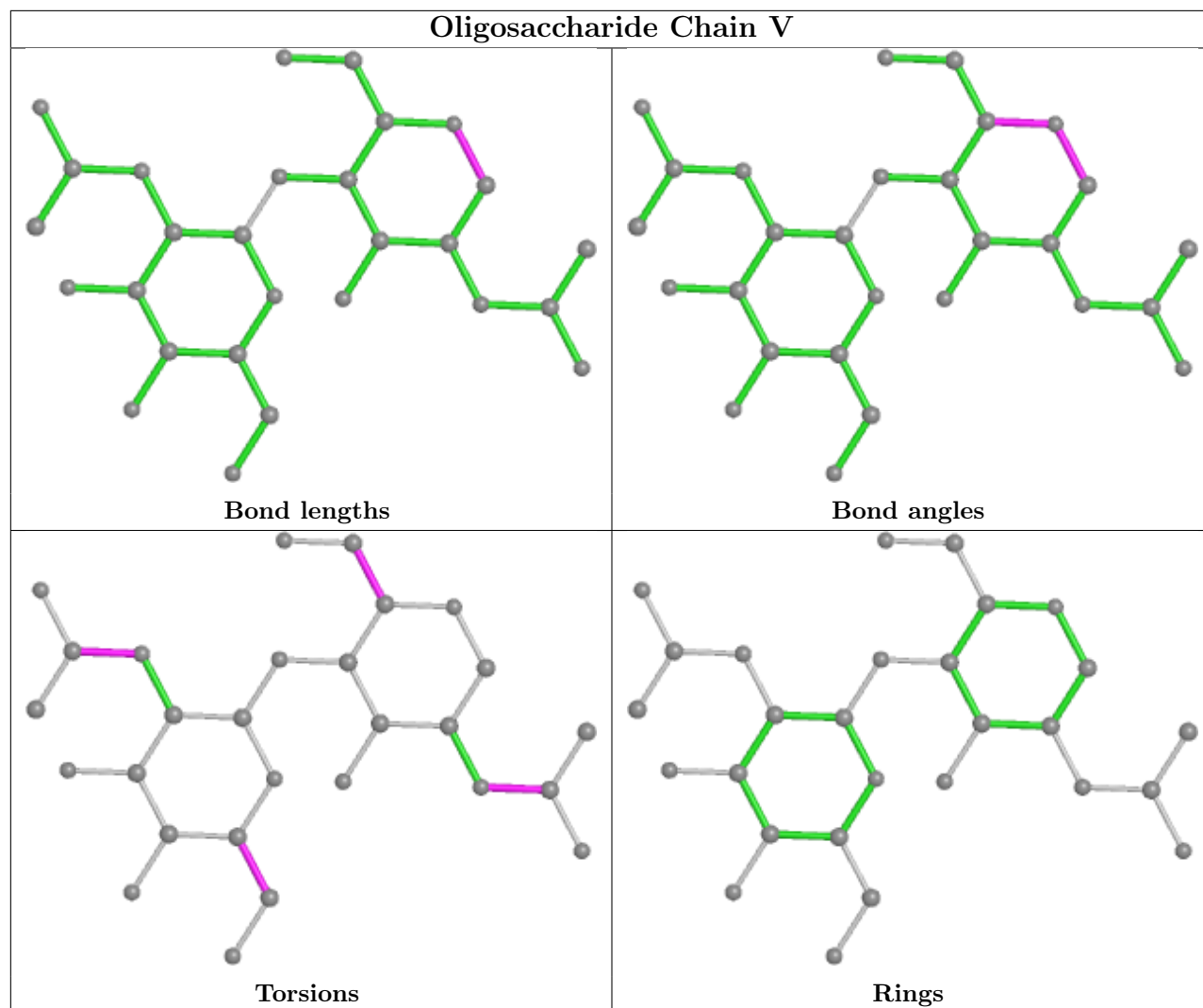


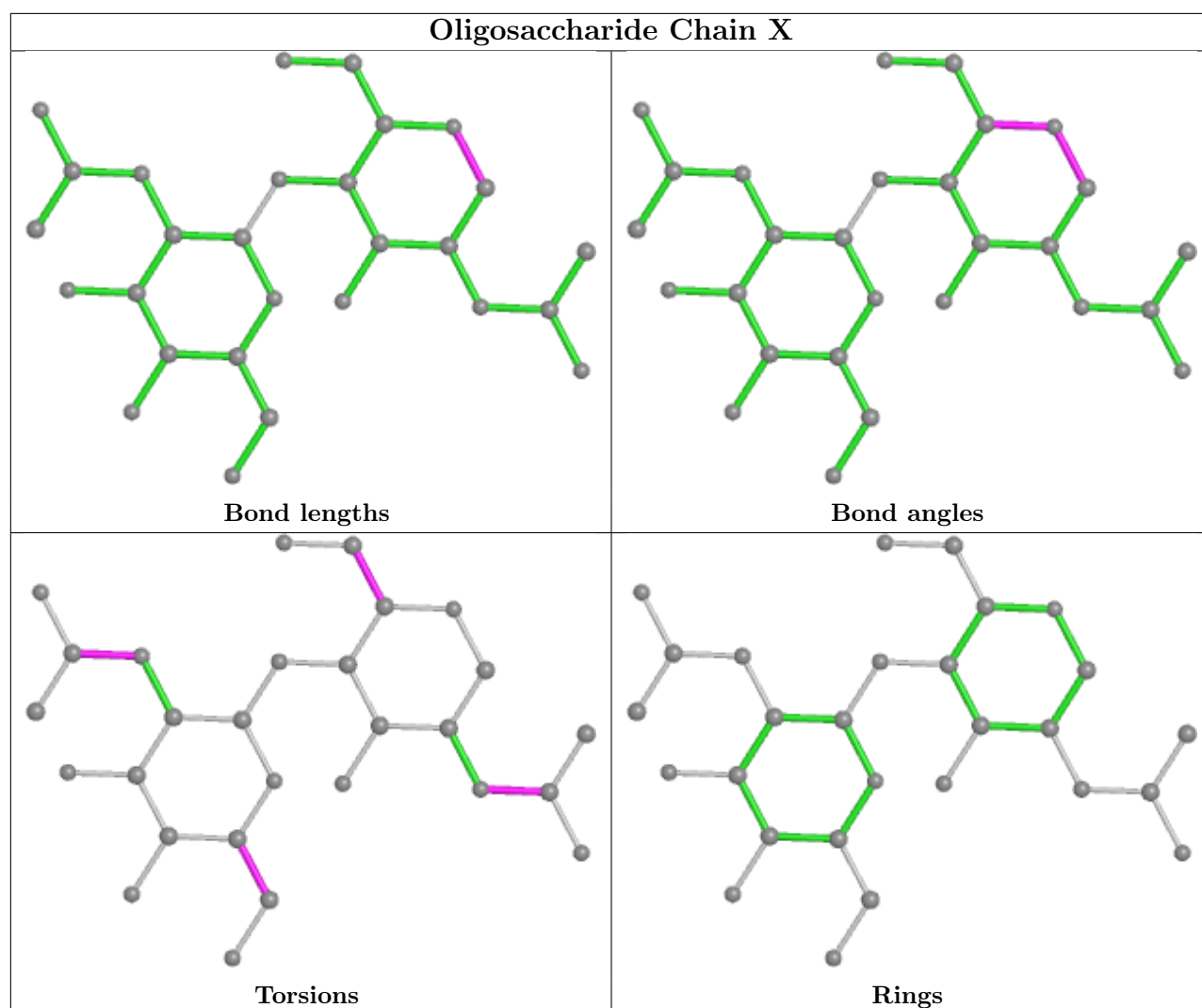












5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	G	502	1	14,14,15	0.69	0	17,19,21	1.31	2 (11%)
4	NAG	C	501	1	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	B	501	1	14,14,15	0.24	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	501	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	E	502	1	14,14,15	0.42	0	17,19,21	1.30	1 (5%)
4	NAG	D	501	1	14,14,15	0.31	0	17,19,21	0.47	0
4	NAG	F	502	1	14,14,15	0.53	0	17,19,21	1.30	1 (5%)
4	NAG	H	502	1	14,14,15	0.47	0	17,19,21	1.29	1 (5%)
4	NAG	A	501	1	14,14,15	0.32	0	17,19,21	0.44	0
4	NAG	F	501	1	14,14,15	0.28	0	17,19,21	0.45	0
4	NAG	B	502	1	14,14,15	0.59	0	17,19,21	1.27	1 (5%)
4	NAG	G	501	1	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	A	502	1	14,14,15	0.78	1 (7%)	17,19,21	1.30	1 (5%)
4	NAG	H	501	1	14,14,15	0.32	0	17,19,21	0.44	0
4	NAG	D	502	1	14,14,15	0.61	0	17,19,21	1.27	1 (5%)
4	NAG	C	502	1	14,14,15	0.96	1 (7%)	17,19,21	1.13	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
4	NAG	G	502	1	-	5/6/23/26	0/1/1/1
4	NAG	C	501	1	-	2/6/23/26	0/1/1/1
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	NAG	E	501	1	-	2/6/23/26	0/1/1/1
4	NAG	E	502	1	-	5/6/23/26	0/1/1/1
4	NAG	D	501	1	-	2/6/23/26	0/1/1/1
4	NAG	F	502	1	-	5/6/23/26	0/1/1/1
4	NAG	H	502	1	-	5/6/23/26	0/1/1/1
4	NAG	A	501	1	-	3/6/23/26	0/1/1/1
4	NAG	F	501	1	-	1/6/23/26	0/1/1/1
4	NAG	B	502	1	-	5/6/23/26	0/1/1/1
4	NAG	G	501	1	-	1/6/23/26	0/1/1/1
4	NAG	A	502	1	-	5/6/23/26	0/1/1/1
4	NAG	H	501	1	-	1/6/23/26	0/1/1/1
4	NAG	D	502	1	-	5/6/23/26	0/1/1/1
4	NAG	C	502	1	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	NAG	C1-C2	3.17	1.57	1.52
4	A	502	NAG	C1-C2	2.00	1.55	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	502	NAG	C2-N2-C7	4.40	129.17	122.90
4	G	502	NAG	C2-N2-C7	4.34	129.09	122.90
4	A	502	NAG	C2-N2-C7	4.34	129.09	122.90
4	E	502	NAG	C2-N2-C7	4.34	129.08	122.90
4	B	502	NAG	C2-N2-C7	4.28	129.00	122.90

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C4-C5-C6-O6
4	H	502	NAG	C4-C5-C6-O6
4	F	502	NAG	C4-C5-C6-O6
4	C	502	NAG	C4-C5-C6-O6
4	B	502	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	502	NAG	1	0
4	E	502	NAG	1	0
4	F	502	NAG	1	0
4	H	502	NAG	2	0
4	F	501	NAG	1	0
4	B	502	NAG	1	0
4	A	502	NAG	1	0
4	D	502	NAG	1	0
4	C	502	NAG	2	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	410/443 (92%)	-0.05	26 (6%)	20	19	5, 256, 751, 989	0
1	B	403/443 (90%)	-0.17	16 (3%)	38	34	7, 264, 660, 976	0
1	C	409/443 (92%)	-0.40	8 (1%)	65	58	133, 251, 366, 495	0
1	D	402/443 (90%)	-0.36	7 (1%)	70	62	133, 263, 431, 593	0
1	E	409/443 (92%)	-0.27	23 (5%)	24	24	8, 278, 451, 935	0
1	F	409/443 (92%)	-0.22	23 (5%)	24	24	95, 325, 691, 990	0
1	G	403/443 (90%)	-0.19	24 (5%)	21	21	136, 284, 445, 738	0
1	H	404/443 (91%)	-0.34	13 (3%)	47	41	139, 274, 391, 512	0
All	All	3249/3544 (91%)	-0.25	140 (4%)	35	32	5, 272, 517, 990	0

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	LYS	12.0
1	H	221	ALA	9.0
1	A	387	GLU	7.9
1	D	221	ALA	7.6
1	B	429	ASP	7.5

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.

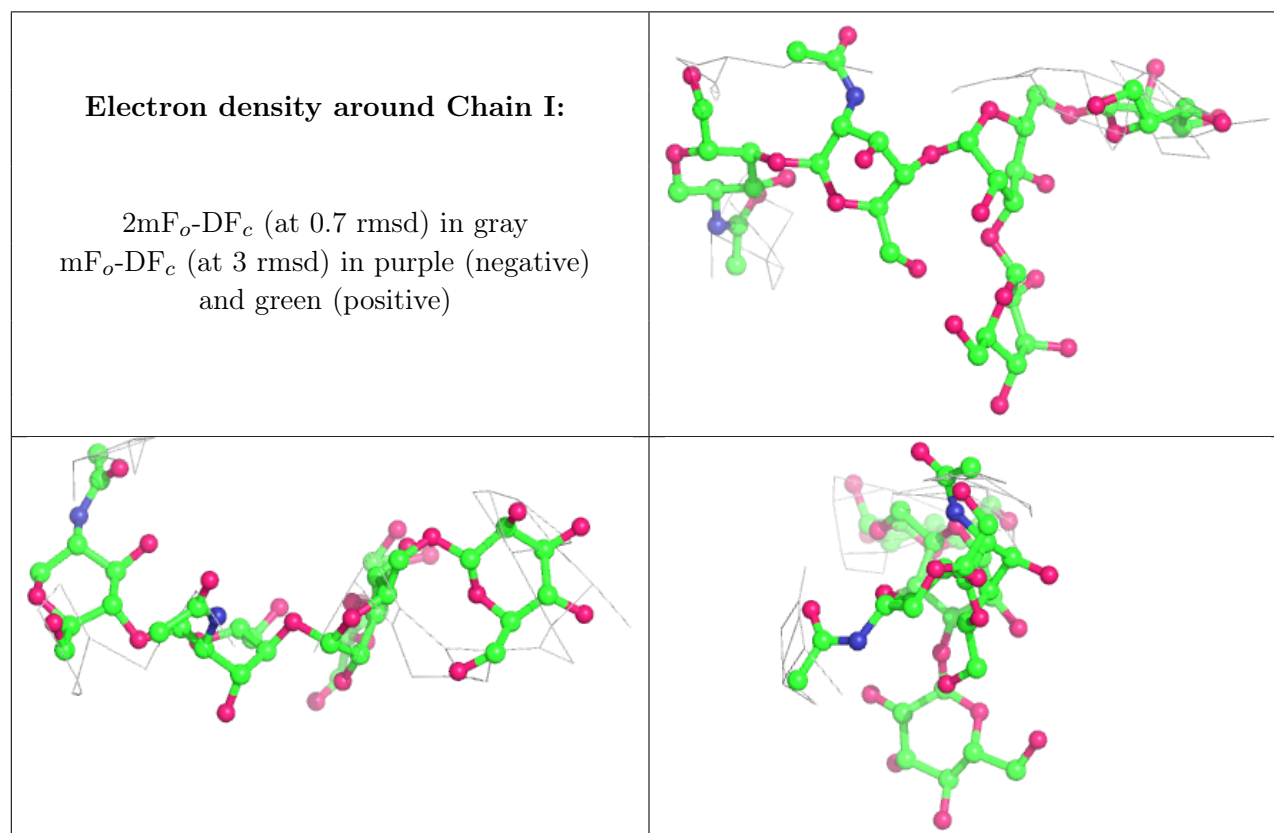
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	V	2	14/15	0.68	0.40	210,242,255,264	0
3	NAG	P	2	14/15	0.69	0.37	290,291,307,310	0
3	NAG	N	2	14/15	0.69	0.33	230,252,264,266	0
2	MAN	I	5	11/12	0.70	0.26	346,355,377,380	0
3	NAG	T	2	14/15	0.71	0.33	301,328,338,342	0
3	NAG	P	1	14/15	0.75	0.22	368,384,394,395	0
2	MAN	Q	5	11/12	0.75	0.32	284,300,328,354	0
3	NAG	T	1	14/15	0.78	0.34	330,354,369,378	0
2	MAN	O	5	11/12	0.79	0.29	246,288,309,323	0
2	MAN	Q	4	11/12	0.83	0.23	314,325,335,336	0
2	BMA	Q	3	11/12	0.83	0.13	293,329,346,353	0
3	NAG	X	2	14/15	0.83	0.39	234,247,271,274	0
2	BMA	I	3	11/12	0.84	0.22	318,324,339,349	0
3	NAG	R	2	14/15	0.84	0.42	228,244,264,268	0
2	BMA	K	3	11/12	0.85	0.18	250,278,294,301	0
3	NAG	N	1	14/15	0.85	0.31	257,261,271,272	0
2	NAG	W	2	14/15	0.86	0.16	285,304,326,328	0
2	NAG	W	1	14/15	0.86	0.19	368,404,415,416	0
2	MAN	K	5	11/12	0.87	0.20	276,293,310,317	0
2	NAG	U	1	14/15	0.89	0.19	223,235,263,263	0
2	MAN	K	4	11/12	0.89	0.26	247,258,269,298	0
2	MAN	O	4	11/12	0.89	0.22	232,250,254,258	0
2	BMA	S	3	11/12	0.89	0.22	280,293,297,300	0
2	NAG	K	1	14/15	0.90	0.15	244,255,271,271	0
3	NAG	J	1	14/15	0.90	0.23	196,210,273,274	0
3	NAG	J	2	14/15	0.90	0.28	231,244,257,260	0
2	NAG	M	1	14/15	0.90	0.20	319,328,355,357	0
3	NAG	V	1	14/15	0.90	0.24	217,233,269,279	0
2	BMA	M	3	11/12	0.90	0.21	290,322,334,344	0
2	MAN	M	5	11/12	0.90	0.23	285,293,314,322	0
2	MAN	W	4	11/12	0.91	0.18	293,313,344,345	0
3	NAG	R	1	14/15	0.91	0.24	247,254,263,264	0
2	NAG	Q	1	14/15	0.91	0.22	261,273,293,294	0
2	MAN	I	4	11/12	0.91	0.37	210,233,302,305	0
2	NAG	I	1	14/15	0.92	0.20	247,255,264,277	0
2	NAG	I	2	14/15	0.92	0.23	271,293,303,305	0
2	MAN	S	5	11/12	0.93	0.21	265,272,282,291	0
2	NAG	K	2	14/15	0.93	0.14	285,294,310,310	0
2	MAN	S	4	11/12	0.93	0.37	235,244,286,286	0
2	BMA	O	3	11/12	0.94	0.11	275,276,313,330	0
2	MAN	W	5	11/12	0.94	0.16	296,299,312,315	0

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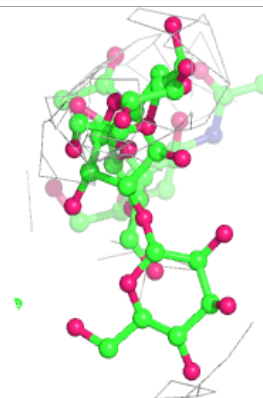
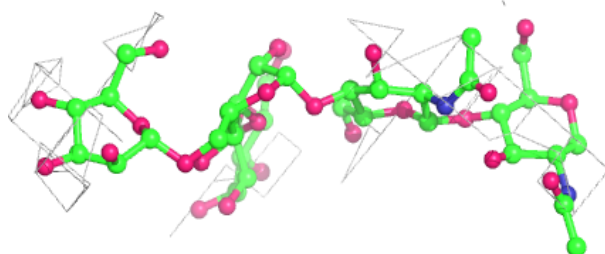
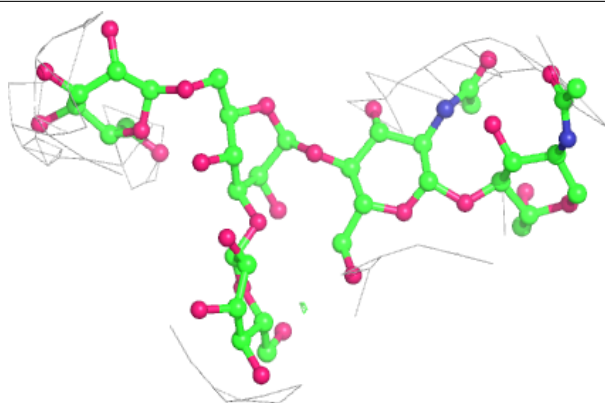
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MAN	M	4	11/12	0.94	0.40	236,263,312,315	0
2	NAG	M	2	14/15	0.94	0.20	302,315,339,349	0
3	NAG	L	2	14/15	0.94	0.43	240,249,275,277	0
2	NAG	S	2	14/15	0.94	0.21	245,250,266,271	0
2	NAG	O	1	14/15	0.94	0.15	291,292,292,314	0
2	BMA	W	3	11/12	0.94	0.11	305,321,343,363	0
2	MAN	U	5	11/12	0.95	0.20	317,330,367,371	0
2	NAG	S	1	14/15	0.95	0.18	249,264,288,291	0
3	NAG	L	1	14/15	0.95	0.27	180,236,255,271	0
2	NAG	O	2	14/15	0.96	0.13	275,280,286,293	0
2	NAG	U	2	14/15	0.96	0.23	217,237,275,308	0
2	MAN	U	4	11/12	0.96	0.22	259,264,273,275	0
3	NAG	X	1	14/15	0.96	0.18	281,290,302,305	0
2	NAG	Q	2	14/15	0.96	0.16	267,277,307,327	0
2	BMA	U	3	11/12	0.97	0.21	288,300,306,312	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.

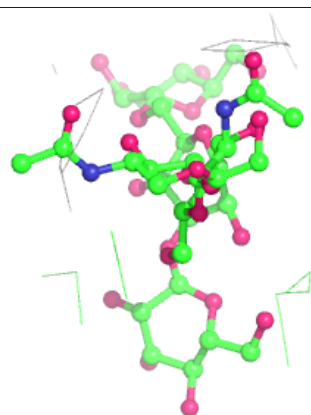
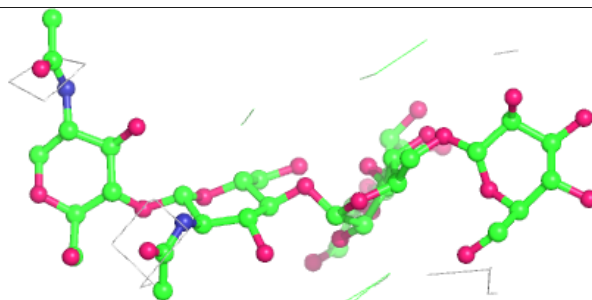
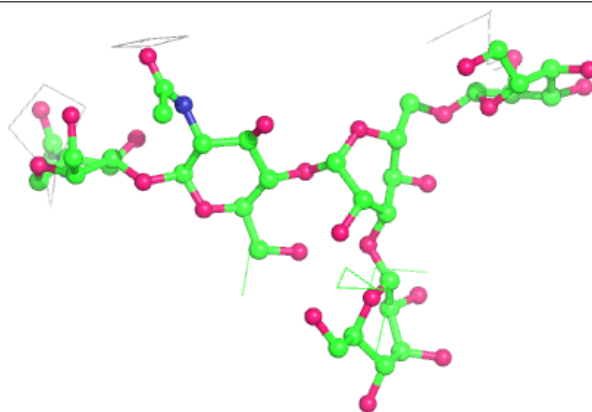


Electron density around Chain K:

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

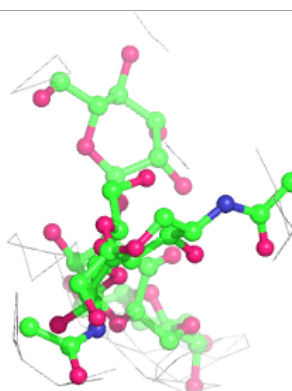
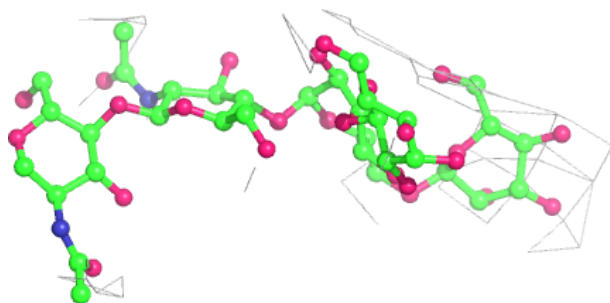
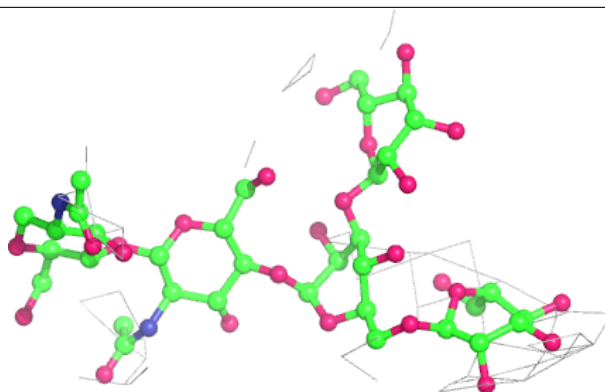
**Electron density around Chain M:**

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

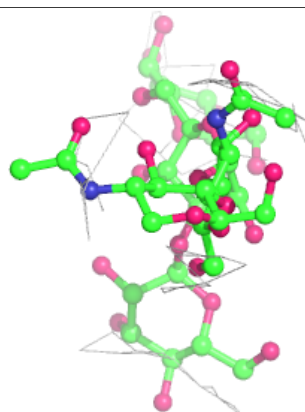
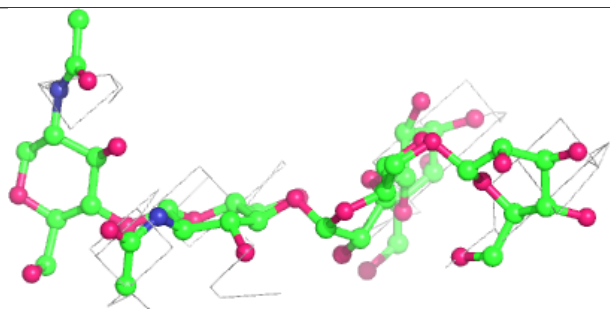
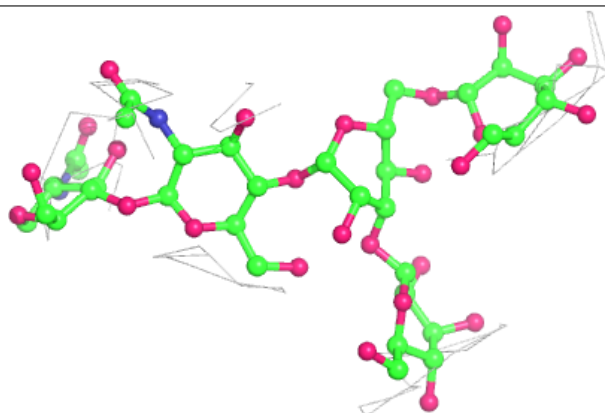


Electron density around Chain O:

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

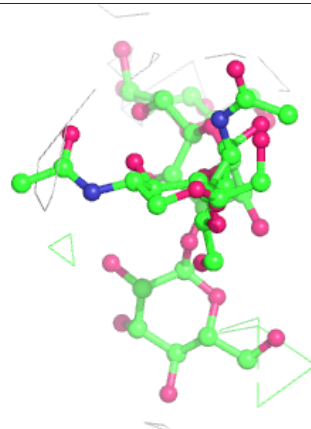
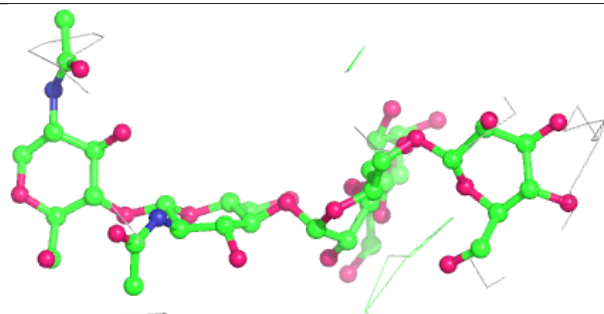
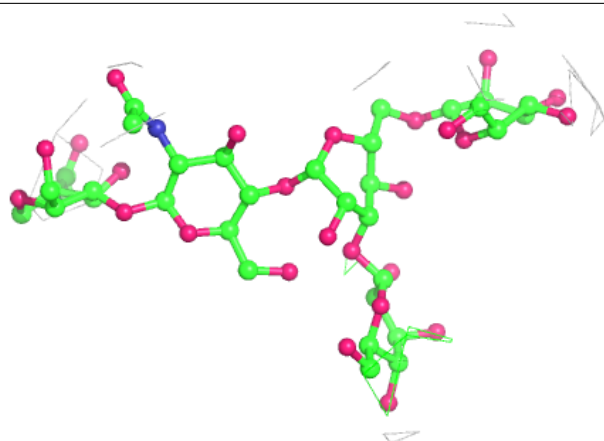
**Electron density around Chain Q:**

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

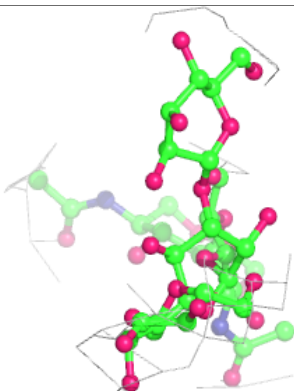
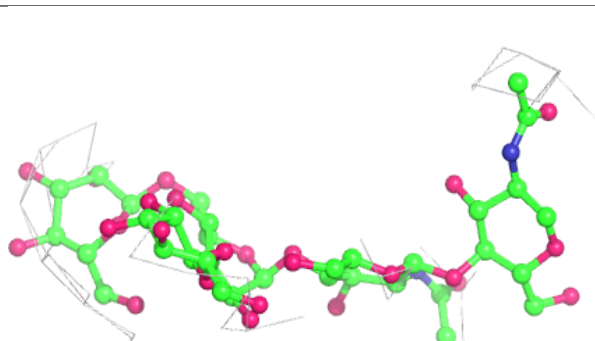
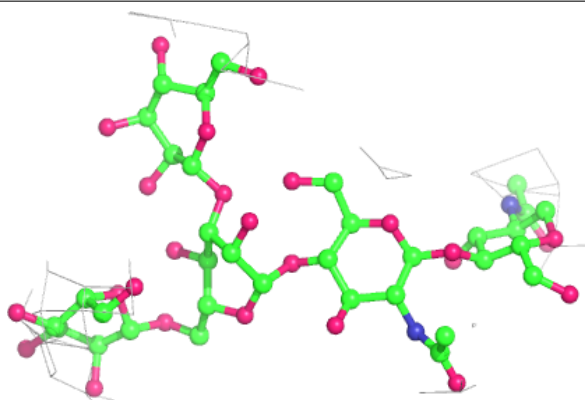


Electron density around Chain S:

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

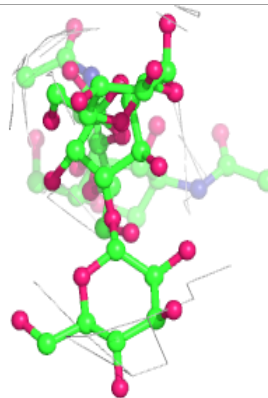
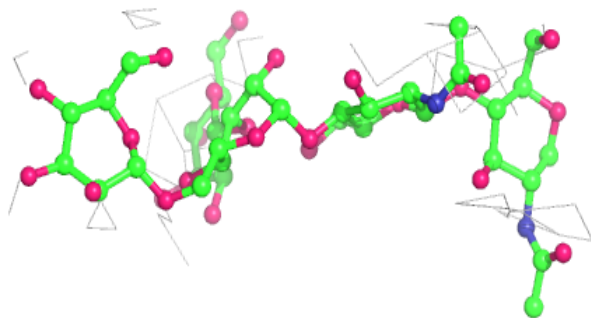
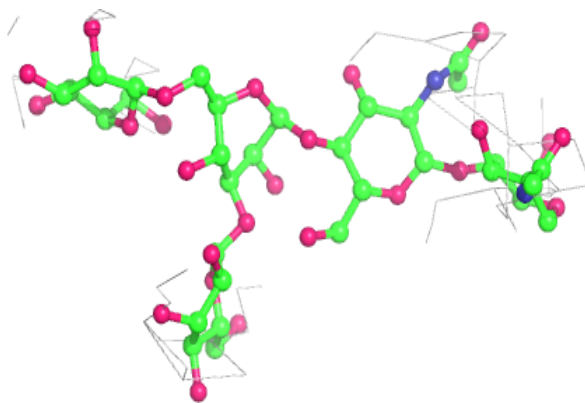
**Electron density around Chain U:**

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



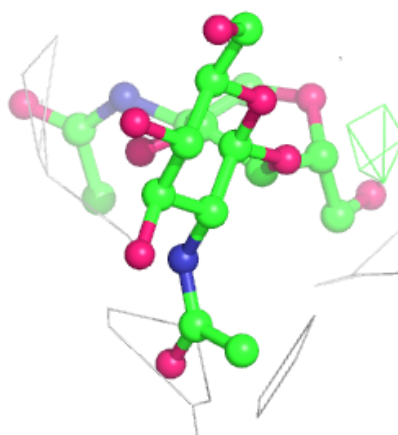
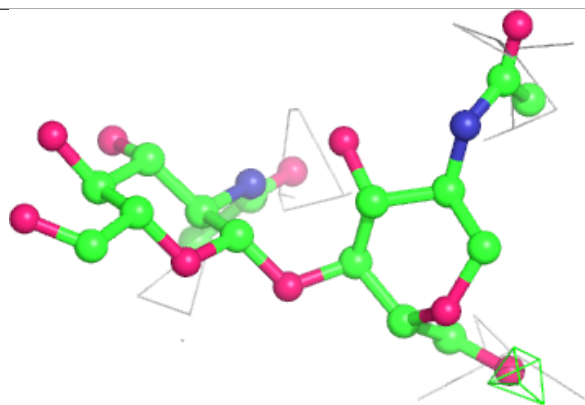
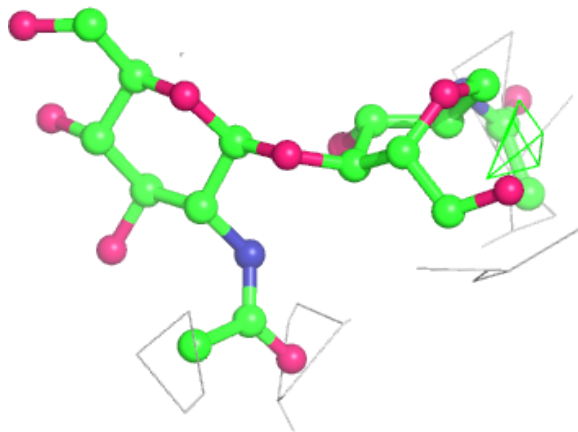
Electron density around Chain W:

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



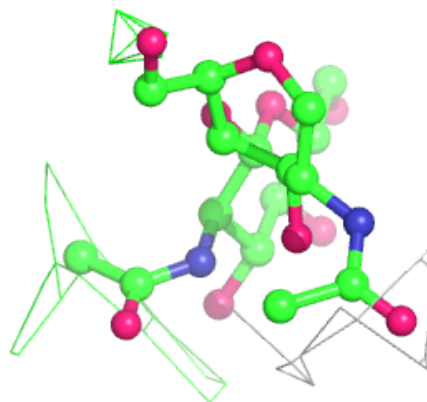
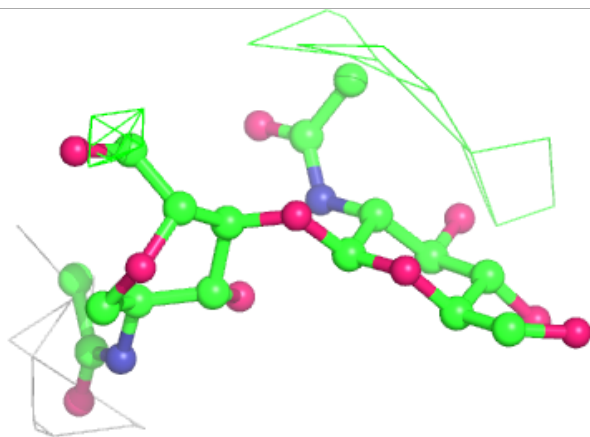
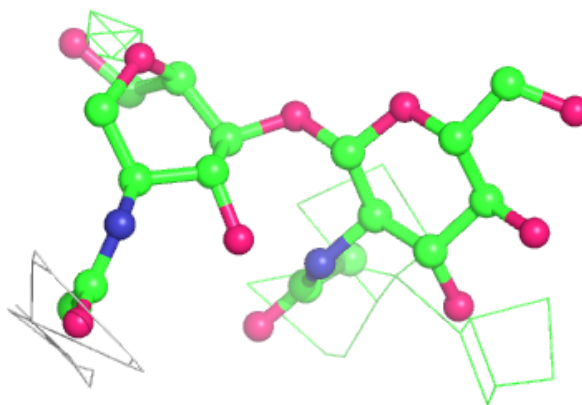
Electron density around Chain J:

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



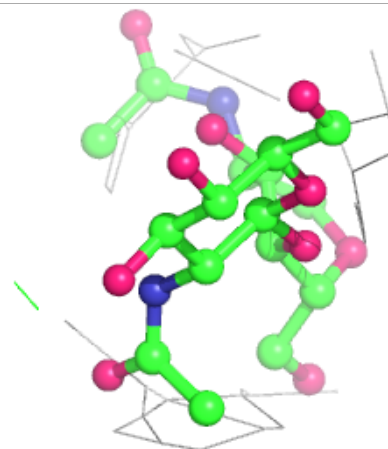
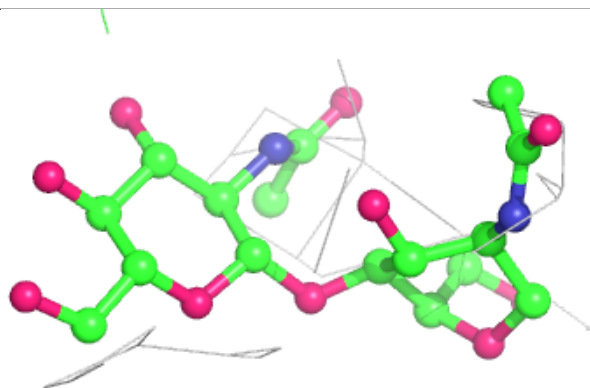
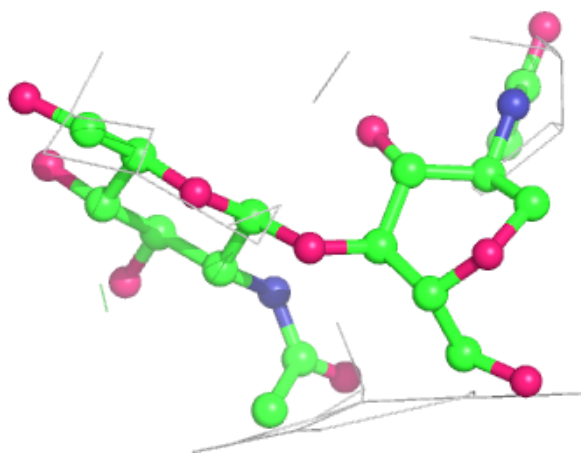
Electron density around Chain L:

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



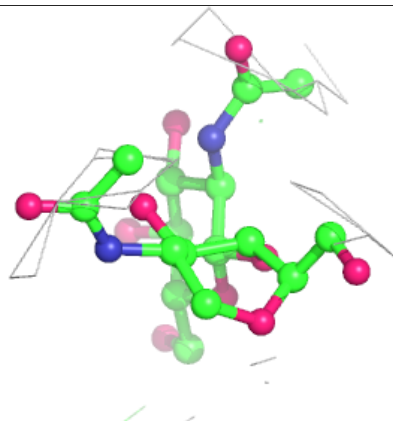
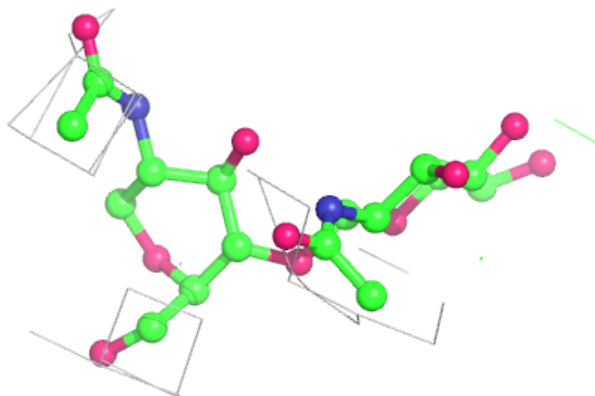
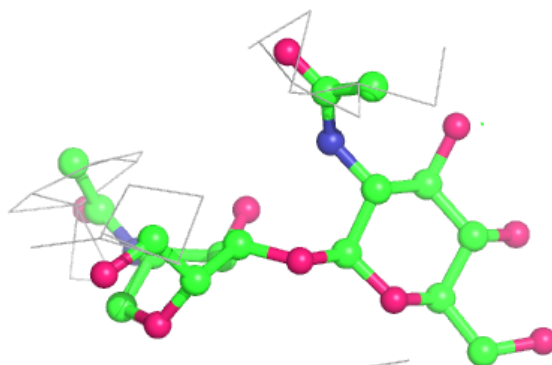
Electron density around Chain N:

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



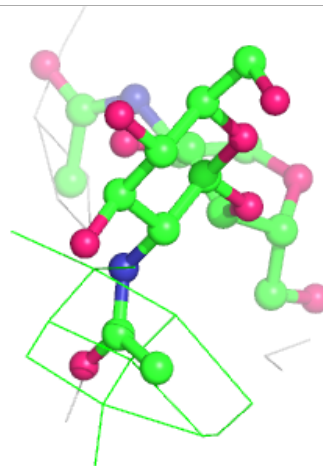
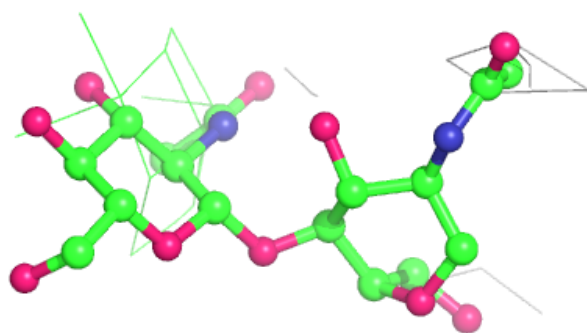
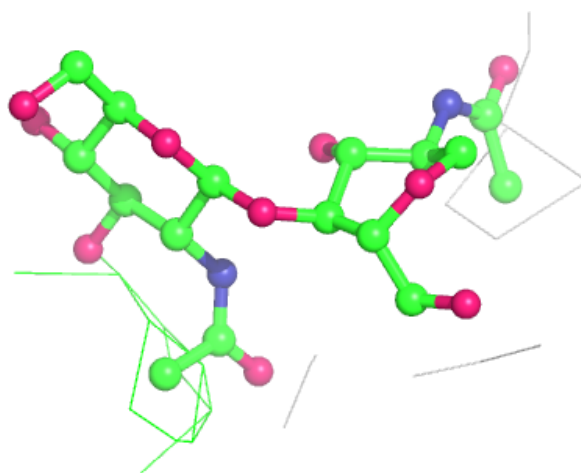
Electron density around Chain P:

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



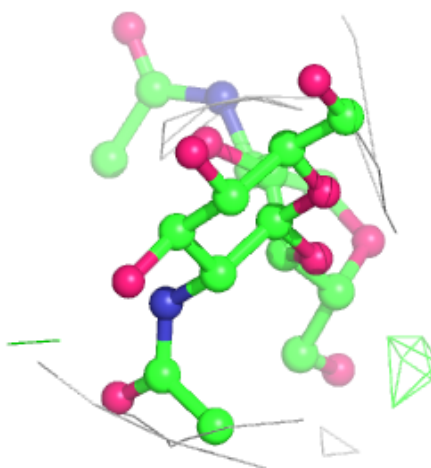
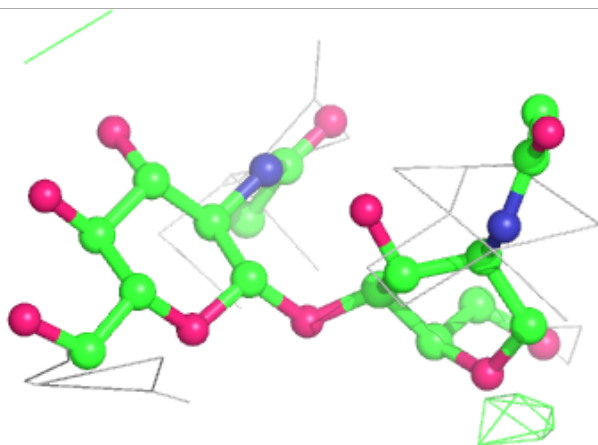
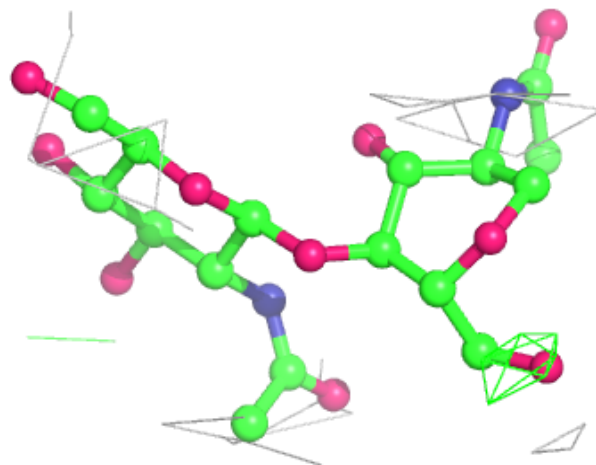
Electron density around Chain R:

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



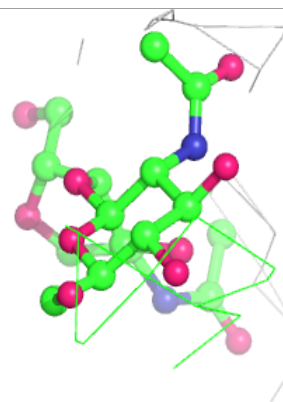
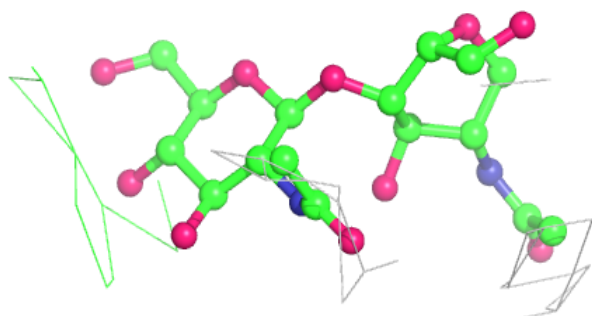
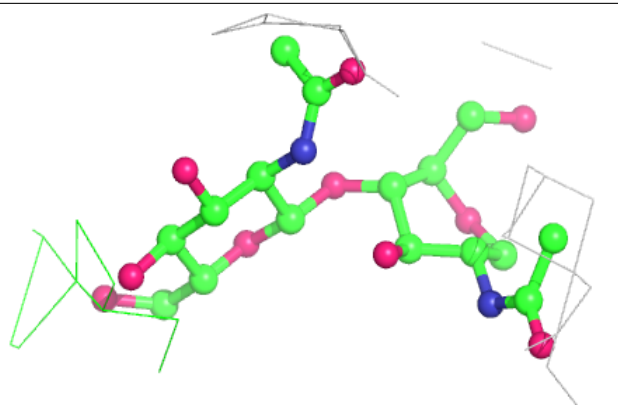
Electron density around Chain T:

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

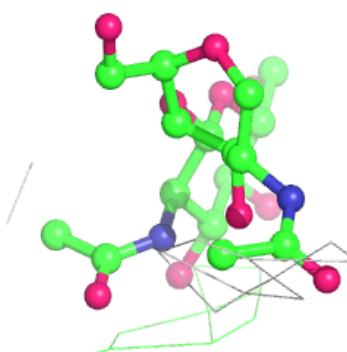
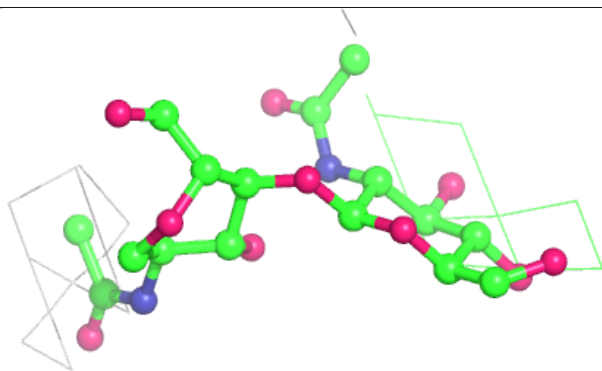
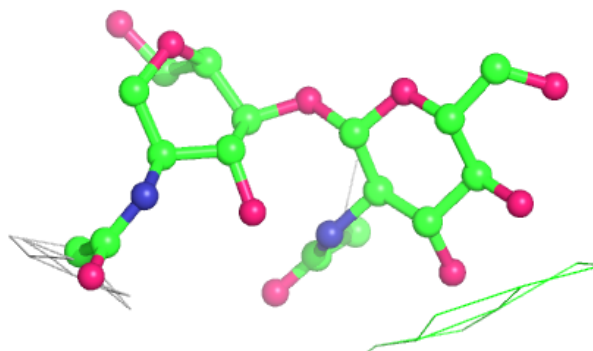


Electron density around Chain V:

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

**Electron density around Chain X:**

$2mF_o-DF_c$ (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
4	NAG	D	502	14/15	0.19	0.29	294,305,310,311	0
4	NAG	A	502	14/15	0.45	0.46	272,294,342,358	0
4	NAG	F	502	14/15	0.58	0.29	384,389,395,415	0
4	NAG	G	502	14/15	0.58	1.12	630,644,655,665	0
4	NAG	E	502	14/15	0.67	0.60	310,323,336,360	0
4	NAG	C	502	14/15	0.71	0.33	210,235,284,296	0
4	NAG	H	502	14/15	0.75	0.25	213,222,243,245	0
4	NAG	B	502	14/15	0.76	0.38	153,182,198,201	0
4	NAG	C	501	14/15	0.76	0.29	252,277,314,324	0
4	NAG	F	501	14/15	0.82	0.27	277,290,329,330	0
4	NAG	H	501	14/15	0.84	0.23	262,266,287,289	0
4	NAG	B	501	14/15	0.84	0.26	260,281,311,311	0
4	NAG	G	501	14/15	0.87	0.21	215,242,272,289	0
4	NAG	E	501	14/15	0.88	0.25	246,251,269,287	0
4	NAG	D	501	14/15	0.89	0.32	254,302,315,317	0
4	NAG	A	501	14/15	0.90	0.24	251,253,283,303	0

6.5 Other polymers

There are no such residues in this entry.