



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 03:34 PM BST

PDB ID : 1W1I
Title : Crystal structure of dipeptidyl peptidase IV (DPPIV or CD26) in complex with adenosine deaminase
Authors : Weihofen, W.A.; Liu, J.; Reutter, W.; Saenger, W.; Fan, H.
Deposited on : 2004-06-22
Resolution : 3.03 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 : 2.13.1
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) : 2.13.1

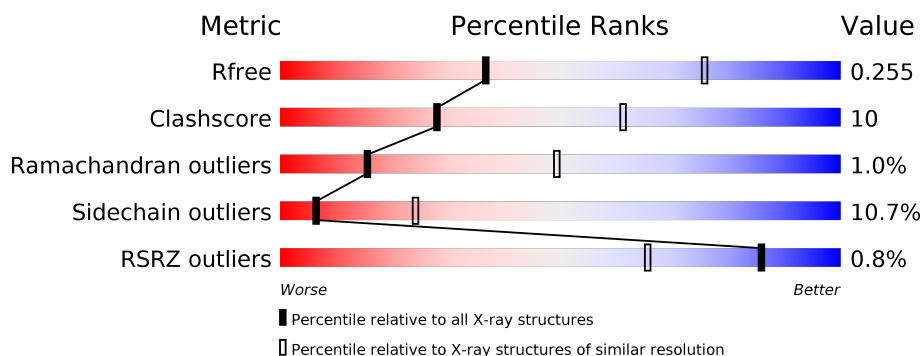
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 on 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	728	<div> <div>77%</div> <div>19%</div> <div>.</div> </div>
1	B	728	<div> <div>79%</div> <div>17%</div> <div>.</div> </div>
1	C	728	<div> <div>78%</div> <div>18%</div> <div>.</div> </div>
1	D	728	<div> <div>77%</div> <div>19%</div> <div>.</div> </div>
2	E	357	<div> <div>4%</div> <div>60%</div> <div>32%</div> <div>5%</div> <div>..</div> </div>
2	F	357	<div> <div>2%</div> <div>58%</div> <div>36%</div> <div>.</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	357	
2	H	357	
3	I	3	
3	Q	3	
4	J	2	
4	K	2	
4	N	2	
4	P	2	
4	R	2	
4	S	2	
4	U	2	
4	W	2	
4	Y	2	
5	L	4	
5	O	4	
5	T	4	
5	X	4	
6	M	2	
6	V	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
3	FUC	I	3	X	-	-	-
3	NAG	Q	2	-	-	-	X
3	FUC	Q	3	X	-	-	-
4	NAG	J	2	-	-	-	X
4	NAG	R	2	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	U	2	-	-	-	X
6	FUC	M	2	X	-	-	-
6	FUC	V	2	X	-	-	-
7	NAG	A	860	X	-	-	-
7	NAG	A	870	X	-	-	-
7	NAG	B	860	X	-	-	-
7	NAG	C	860	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 35877 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 DIPEPTIDYL PEPTIDASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	C	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	D	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			
2	F	352	Total	C	N	O	S	0	0	0
			2808	1786	472	537	13			
2	G	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			
2	H	352	Total	C	N	O	S	0	0	0
			2809	1786	473	537	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	ASP	ASN	conflict	UNP P56658
E	32	LYS	ARG	conflict	UNP P56658
E	33	ARG	LYS	conflict	UNP P56658
E	47	LEU	GLN	conflict	UNP P56658
E	57	THR	SER	conflict	UNP P56658
E	60	ASP	GLU	conflict	UNP P56658
E	77	ASP	GLU	conflict	UNP P56658
E	79	ILE	VAL	conflict	UNP P56658

Continued on next page...

Continued from previous page...

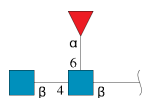
Chain	Residue	Modelled	Actual	Comment	Reference
E	199	GLN	LYS	variant	UNP P56658
E	246	THR	ALA	variant	UNP P56658
E	261	ILE	VAL	conflict	UNP P56658
E	279	ALA	PRO	conflict	UNP P56658
E	281	ILE	VAL	conflict	UNP P56658
E	313	LYS	ASN	conflict	UNP P56658
E	314	ASP	GLU	conflict	UNP P56658
E	352	ARG	GLY	variant	UNP P56658
F	8	ASP	ASN	conflict	UNP P56658
F	32	LYS	ARG	conflict	UNP P56658
F	33	ARG	LYS	conflict	UNP P56658
F	47	LEU	GLN	conflict	UNP P56658
F	57	THR	SER	conflict	UNP P56658
F	60	ASP	GLU	conflict	UNP P56658
F	77	ASP	GLU	conflict	UNP P56658
F	79	ILE	VAL	conflict	UNP P56658
F	199	GLN	LYS	variant	UNP P56658
F	246	THR	ALA	variant	UNP P56658
F	261	ILE	VAL	conflict	UNP P56658
F	279	ALA	PRO	conflict	UNP P56658
F	281	ILE	VAL	conflict	UNP P56658
F	313	LYS	ASN	conflict	UNP P56658
F	314	ASP	GLU	conflict	UNP P56658
F	352	ARG	GLY	variant	UNP P56658
G	8	ASP	ASN	conflict	UNP P56658
G	32	LYS	ARG	conflict	UNP P56658
G	33	ARG	LYS	conflict	UNP P56658
G	47	LEU	GLN	conflict	UNP P56658
G	57	THR	SER	conflict	UNP P56658
G	60	ASP	GLU	conflict	UNP P56658
G	77	ASP	GLU	conflict	UNP P56658
G	79	ILE	VAL	conflict	UNP P56658
G	199	GLN	LYS	variant	UNP P56658
G	246	THR	ALA	variant	UNP P56658
G	261	ILE	VAL	conflict	UNP P56658
G	279	ALA	PRO	conflict	UNP P56658
G	281	ILE	VAL	conflict	UNP P56658
G	313	LYS	ASN	conflict	UNP P56658
G	314	ASP	GLU	conflict	UNP P56658
G	352	ARG	GLY	variant	UNP P56658
H	8	ASP	ASN	conflict	UNP P56658
H	32	LYS	ARG	conflict	UNP P56658

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	33	ARG	LYS	conflict	UNP P56658
H	47	LEU	GLN	conflict	UNP P56658
H	57	THR	SER	conflict	UNP P56658
H	60	ASP	GLU	conflict	UNP P56658
H	77	ASP	GLU	conflict	UNP P56658
H	79	ILE	VAL	conflict	UNP P56658
H	199	GLN	LYS	variant	UNP P56658
H	246	THR	ALA	variant	UNP P56658
H	261	ILE	VAL	conflict	UNP P56658
H	279	ALA	PRO	conflict	UNP P56658
H	281	ILE	VAL	conflict	UNP P56658
H	313	LYS	ASN	conflict	UNP P56658
H	314	ASP	GLU	conflict	UNP P56658
H	352	ARG	GLY	variant	UNP P56658

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			38	22	2	14			
3	Q	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



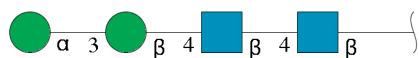
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	S	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	T	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	X	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



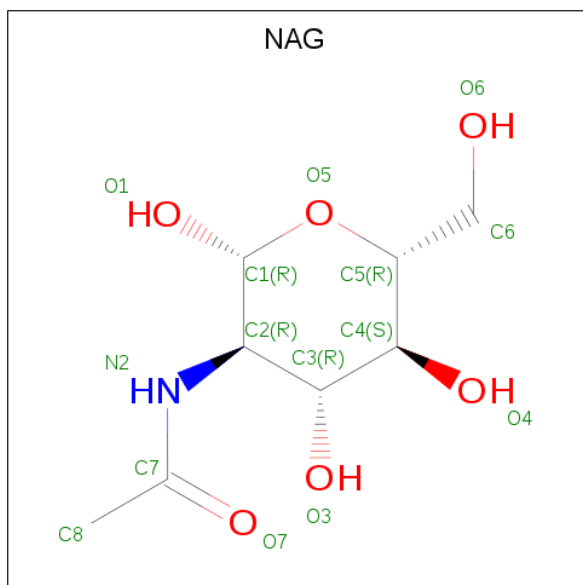
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	2	Total	C	N	O	0	0	0
			24	14	1	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	V	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

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

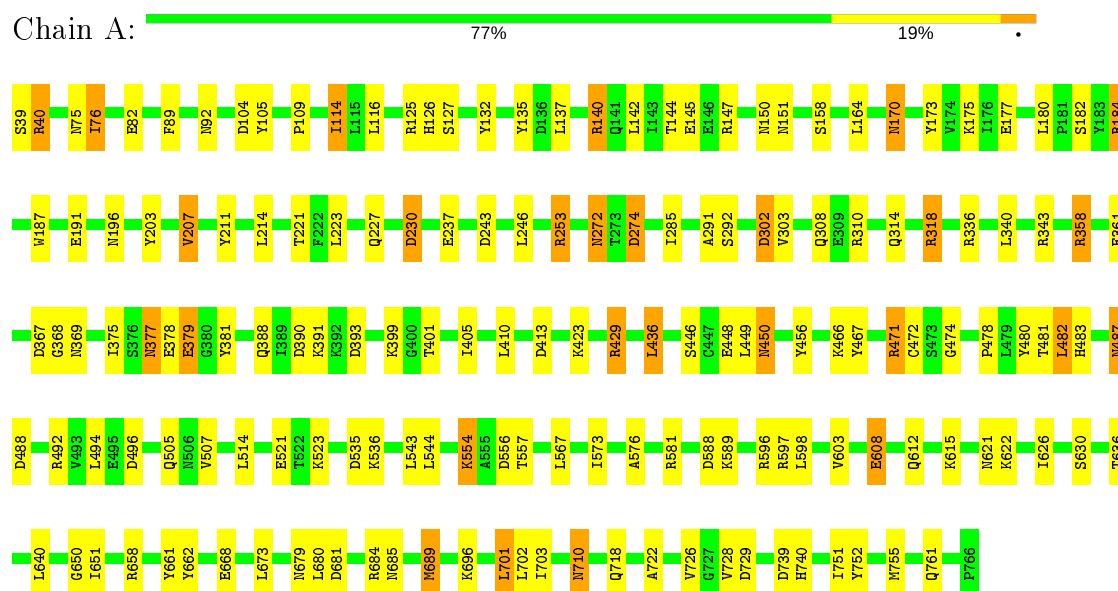
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Zn	0	0
			1	1		
8	G	1	Total	Zn	0	0
			1	1		
8	F	1	Total	Zn	0	0
			1	1		
8	E	1	Total	Zn	0	0
			1	1		

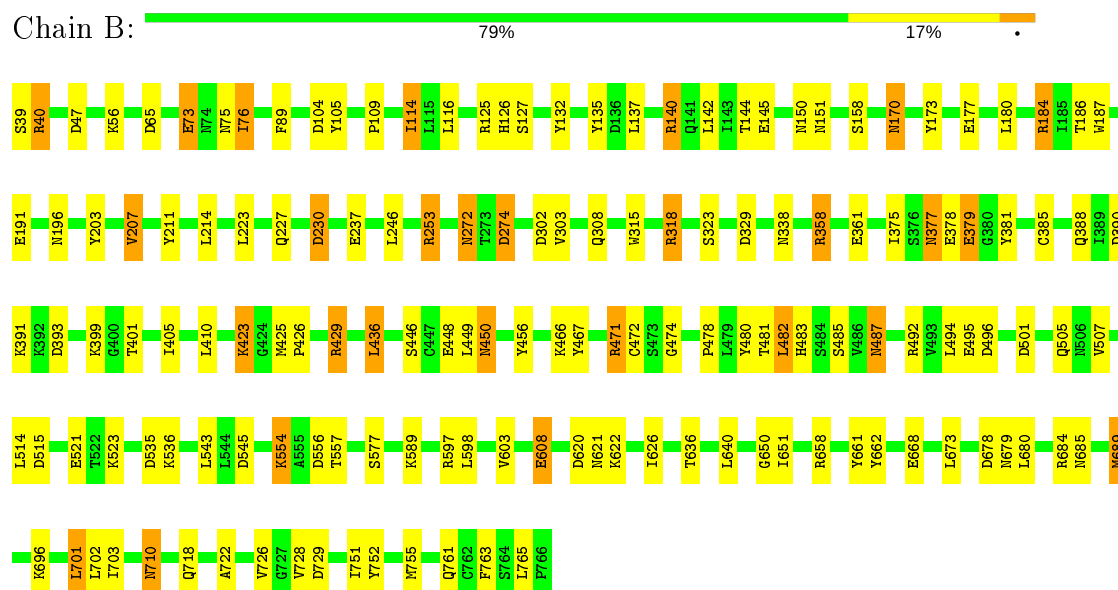
3 Residue-property plots

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.

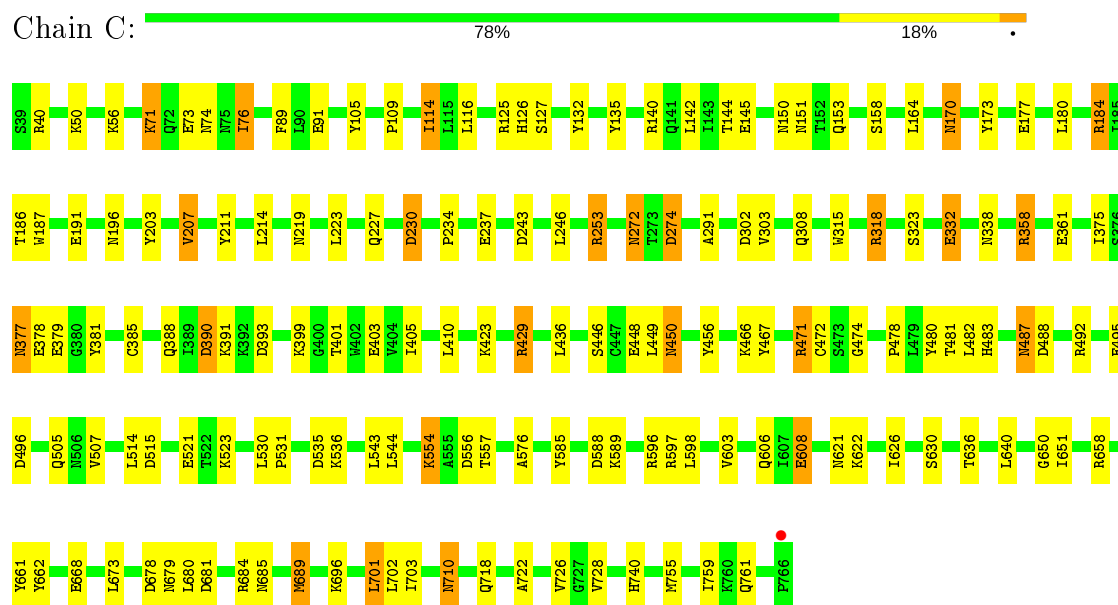
• Molecule 1: DIPEPTIDYL PEPTIDASE IV



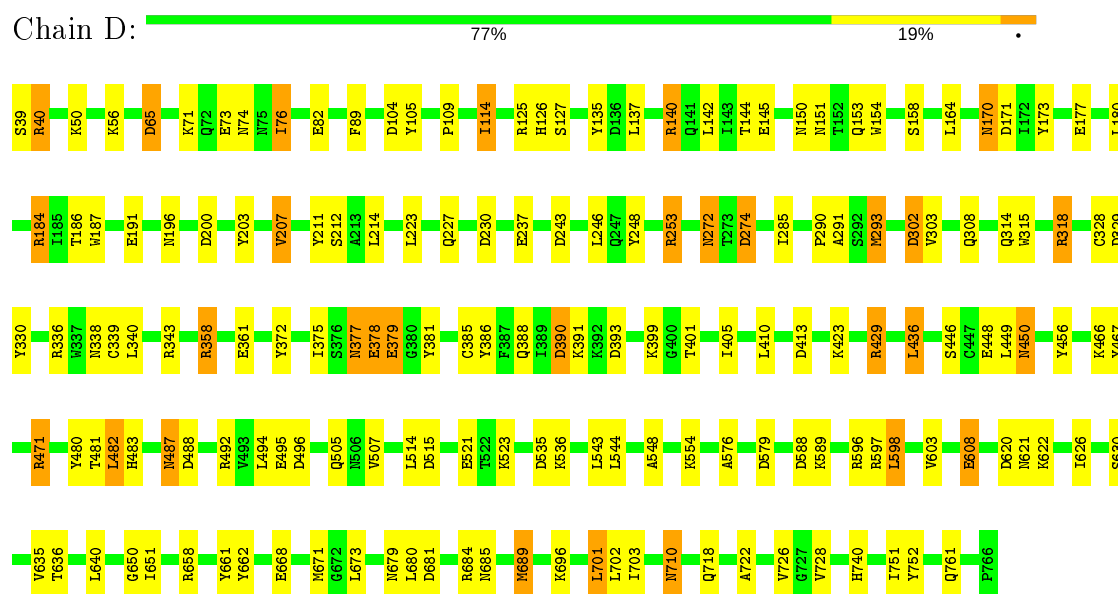
• Molecule 1: DIPEPTIDYL PEPTIDASE IV



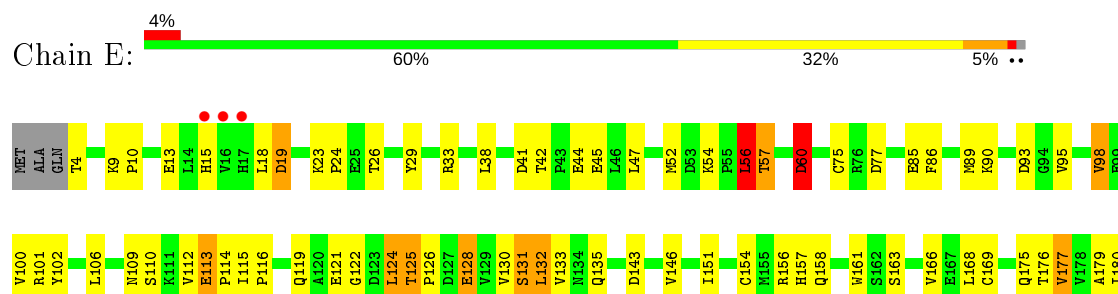
• Molecule 1: DIPEPTIDYL PEPTIDASE IV

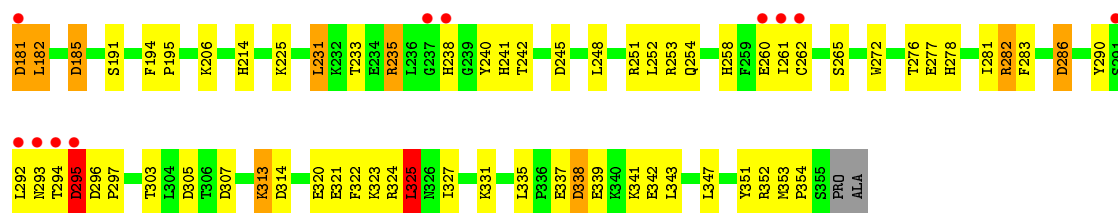


• Molecule 1: DIPEPTIDYL PEPTIDASE IV

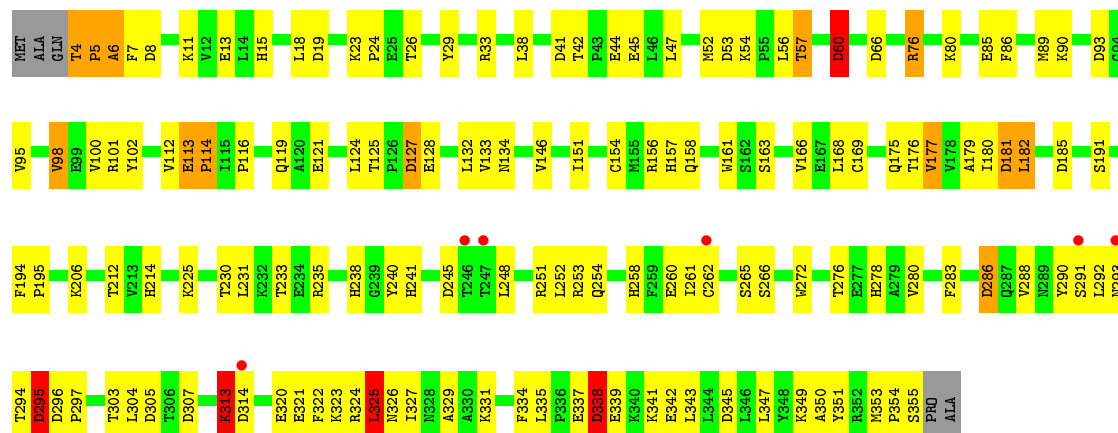


• Molecule 2: ADENOSINE DEAMINASE

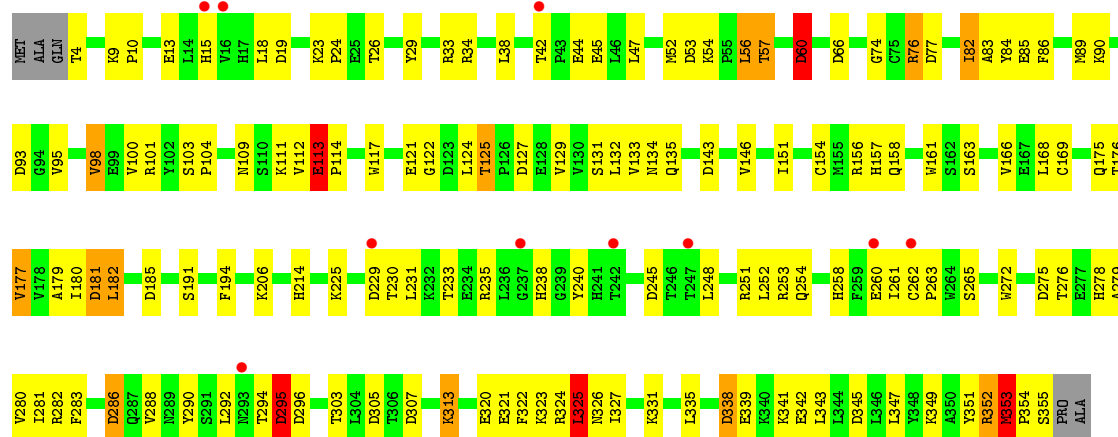




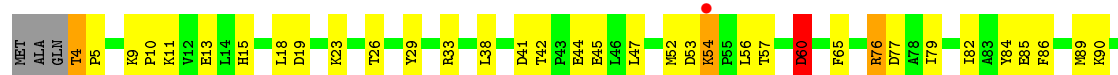
• Molecule 2: ADENOSINE DEAMINASE



• Molecule 2: ADENOSINE DEAMINASE

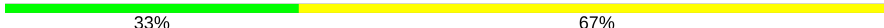


• Molecule 2: ADENOSINE DEAMINASE





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

Chain I:  33% 67%



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

Chain Q:  33% 67%



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain N:  100%



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

Chain P:  100%


MAG1
MAG2

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

Chain R:  100%

MAG1
MAG2

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

Chain S:  50% 50%


MAG1
MAG2

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

Chain U:  100%


MAG1
MAG2

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

Chain W:  50% 50%

MAG1
MAG2

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

Chain Y:  100%

MAG1
MAG2

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

Chain L:  100%

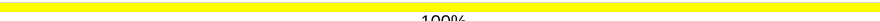
MAG1
MAG2
BMA3
MAV4

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

Chain O:  100%



NAG1
NAG2
BMA3
MAN4

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

Chain T:  100%

NAG1
NAG2
BMA3
MAN4

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

Chain X:  75%  25%

NAG1
NAG2
BMA3
MAN4

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

NAG1
FUC2

- Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%

NAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.06Å 168.50Å 236.84Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	30.00 – 3.03 29.90 – 3.03	Depositor EDS
% Data completeness (in resolution range)	85.5 (30.00-3.03) 85.5 (29.90-3.03)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.224 , 0.257 0.224 , 0.255	Depositor DCC
R_{free} test set	2048 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	35877	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/6135	0.75	15/8344 (0.2%)
1	B	0.40	0/6135	0.75	16/8344 (0.2%)
1	C	0.39	0/6135	0.76	14/8344 (0.2%)
1	D	0.40	0/6135	0.75	19/8344 (0.2%)
2	E	0.40	0/2874	0.84	16/3896 (0.4%)
2	F	0.38	0/2872	0.82	17/3891 (0.4%)
2	G	0.36	0/2874	0.83	17/3896 (0.4%)
2	H	0.36	0/2874	0.81	13/3896 (0.3%)
All	All	0.39	0/36034	0.78	127/48955 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	77	ASP	CB-CG-OD2	12.11	129.20	118.30
2	E	77	ASP	CB-CG-OD2	10.17	127.45	118.30
2	H	77	ASP	CB-CG-OD2	8.05	125.54	118.30
2	H	325	LEU	CA-CB-CG	6.80	130.95	115.30
2	F	60	ASP	CB-CG-OD2	6.67	124.30	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	337	GLU	Peptide
2	H	113	GLU	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	5963	0	5677	99	0
1	B	5963	0	5677	87	0
1	C	5963	0	5677	86	0
1	D	5963	0	5677	99	0
2	E	2809	0	2767	79	0
2	F	2808	0	2765	85	0
2	G	2809	0	2767	83	0
2	H	2809	0	2767	77	0
3	I	38	0	34	0	0
3	Q	38	0	34	1	0
4	J	28	0	25	1	0
4	K	28	0	25	3	0
4	N	28	0	25	2	0
4	P	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	1	0
4	U	28	0	25	2	0
4	W	28	0	25	2	0
4	Y	28	0	25	0	0
5	L	50	0	43	0	0
5	O	50	0	43	0	0
5	T	50	0	43	0	0
5	X	50	0	43	1	0
6	M	24	0	22	0	0
6	V	24	0	22	0	0
7	A	56	0	52	5	0
7	B	56	0	52	1	0
7	C	42	0	39	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	56	0	52	0	0
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
All	All	35877	0	34478	698	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 10.

The worst 5 of 698 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)
2:F:113:GLU:HB2	2:F:161:TRP:HE1	1.10	1.10
2:G:353:MET:HB2	2:G:354:PRO:CD	1.79	1.10
2:E:113:GLU:HB3	2:E:114:PRO:HD3	1.25	1.08
2:E:113:GLU:HB2	2:E:161:TRP:HE1	1.01	1.08
2:G:283:PHE:HD1	2:G:288:VAL:HG11	1.24	1.00

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	726/728 (100%)	674 (93%)	49 (7%)	3 (0%)	34	69
1	B	726/728 (100%)	674 (93%)	49 (7%)	3 (0%)	34	69
1	C	726/728 (100%)	670 (92%)	52 (7%)	4 (1%)	25	60
1	D	726/728 (100%)	669 (92%)	54 (7%)	3 (0%)	34	69
2	E	350/357 (98%)	320 (91%)	21 (6%)	9 (3%)	5	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	348/357 (98%)	311 (89%)	28 (8%)	9 (3%)	5	24
2	G	350/357 (98%)	318 (91%)	26 (7%)	6 (2%)	9	35
2	H	350/357 (98%)	319 (91%)	26 (7%)	5 (1%)	11	40
All	All	4302/4340 (99%)	3955 (92%)	305 (7%)	42 (1%)	15	49

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	56	LEU
2	E	113	GLU
2	E	241	HIS
2	E	338	ASP
2	F	6	ALA

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	653/653 (100%)	596 (91%)	57 (9%)	10	34
1	B	653/653 (100%)	593 (91%)	60 (9%)	9	31
1	C	653/653 (100%)	591 (90%)	62 (10%)	8	30
1	D	653/653 (100%)	591 (90%)	62 (10%)	8	30
2	E	307/310 (99%)	262 (85%)	45 (15%)	3	13
2	F	306/310 (99%)	267 (87%)	39 (13%)	4	18
2	G	307/310 (99%)	262 (85%)	45 (15%)	3	13
2	H	307/310 (99%)	265 (86%)	42 (14%)	3	15
All	All	3839/3852 (100%)	3427 (89%)	412 (11%)	6	24

5 of 412 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	184	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	621	ASN
2	H	98	VAL
1	D	230	ASP
1	D	399	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	272	ASN
1	C	710	ASN
2	G	158	GLN
1	C	338	ASN
1	C	505	GLN

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 ⓘ

44 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	$\# Z > 2$
3	NAG	I	1	1,3	14,14,15	0.63	0	17,19,21	0.95	0
3	NAG	I	2	3	14,14,15	0.53	0	17,19,21	1.53	3 (17%)
3	FUC	I	3	3	10,10,11	0.60	0	14,14,16	1.65	3 (21%)
4	NAG	J	1	1,4	14,14,15	0.55	0	17,19,21	1.18	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	2	4	14,14,15	0.60	0	17,19,21	1.99	4 (23%)
4	NAG	K	1	1,4	14,14,15	0.67	0	17,19,21	1.86	7 (41%)
4	NAG	K	2	4	14,14,15	0.56	0	17,19,21	1.71	4 (23%)
5	NAG	L	1	1,5	14,14,15	0.70	0	17,19,21	1.64	3 (17%)
5	NAG	L	2	5	14,14,15	0.79	1 (7%)	17,19,21	1.54	3 (17%)
5	BMA	L	3	5	11,11,12	0.51	0	15,15,17	2.49	6 (40%)
5	MAN	L	4	5	11,11,12	0.70	0	15,15,17	1.72	4 (26%)
6	NAG	M	1	1,6	14,14,15	0.39	0	17,19,21	2.00	2 (11%)
6	FUC	M	2	6	10,10,11	0.73	0	14,14,16	1.34	1 (7%)
4	NAG	N	1	1,4	14,14,15	0.57	0	17,19,21	1.46	4 (23%)
4	NAG	N	2	4	14,14,15	0.63	0	17,19,21	2.14	6 (35%)
5	NAG	O	1	1,5	14,14,15	0.58	0	17,19,21	2.31	6 (35%)
5	NAG	O	2	5	14,14,15	0.63	0	17,19,21	1.38	2 (11%)
5	BMA	O	3	5	11,11,12	0.62	0	15,15,17	1.69	4 (26%)
5	MAN	O	4	5	11,11,12	0.61	0	15,15,17	2.07	6 (40%)
4	NAG	P	1	1,4	14,14,15	0.81	0	17,19,21	2.38	4 (23%)
4	NAG	P	2	4	14,14,15	0.56	0	17,19,21	2.24	3 (17%)
3	NAG	Q	1	1,3	14,14,15	0.51	0	17,19,21	1.13	1 (5%)
3	NAG	Q	2	3	14,14,15	0.66	0	17,19,21	1.55	5 (29%)
3	FUC	Q	3	3	10,10,11	0.59	0	14,14,16	1.43	2 (14%)
4	NAG	R	1	1,4	14,14,15	0.80	0	17,19,21	3.03	7 (41%)
4	NAG	R	2	4	14,14,15	0.62	0	17,19,21	1.59	2 (11%)
4	NAG	S	1	1,4	14,14,15	0.57	0	17,19,21	1.32	2 (11%)
4	NAG	S	2	4	14,14,15	0.53	0	17,19,21	1.72	4 (23%)
5	NAG	T	1	1,5	14,14,15	0.61	0	17,19,21	1.96	4 (23%)
5	NAG	T	2	5	14,14,15	0.52	0	17,19,21	0.99	1 (5%)
5	BMA	T	3	5	11,11,12	0.63	0	15,15,17	1.76	4 (26%)
5	MAN	T	4	5	11,11,12	0.51	0	15,15,17	2.37	4 (26%)
4	NAG	U	1	1,4	14,14,15	0.65	0	17,19,21	3.03	9 (52%)
4	NAG	U	2	4	14,14,15	0.69	0	17,19,21	3.20	7 (41%)
6	NAG	V	1	1,6	14,14,15	0.57	0	17,19,21	1.72	4 (23%)
6	FUC	V	2	6	10,10,11	0.74	0	14,14,16	1.88	4 (28%)
4	NAG	W	1	1,4	14,14,15	0.52	0	17,19,21	1.63	4 (23%)
4	NAG	W	2	4	14,14,15	0.56	0	17,19,21	1.48	1 (5%)
5	NAG	X	1	1,5	14,14,15	0.54	0	17,19,21	1.80	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	X	2	5	14,14,15	0.59	0	17,19,21	1.28	2 (11%)
5	BMA	X	3	5	11,11,12	0.61	0	15,15,17	1.67	3 (20%)
5	MAN	X	4	5	11,11,12	0.61	0	15,15,17	0.97	0
4	NAG	Y	1	1,4	14,14,15	0.67	0	17,19,21	2.21	7 (41%)
4	NAG	Y	2	4	14,14,15	0.59	0	17,19,21	1.92	4 (23%)

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
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	FUC	I	3	3	1/1/4/5	-	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	2/2/19/22	0/1/1/1
5	MAN	L	4	5	-	1/2/19/22	0/1/1/1
6	NAG	M	1	1,6	-	2/6/23/26	0/1/1/1
6	FUC	M	2	6	1/1/4/5	-	0/1/1/1
4	NAG	N	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	N	2	4	-	4/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	4/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	MAN	O	4	5	-	2/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	FUC	Q	3	3	1/1/4/5	-	0/1/1/1
4	NAG	R	1	1,4	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	2	NAG	O5-C1	-2.05	1.40	1.43

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	2	NAG	C1-O5-C5	8.49	123.70	112.19
4	P	2	NAG	C1-O5-C5	7.43	122.26	112.19
4	U	1	NAG	C1-O5-C5	6.97	121.64	112.19
4	P	1	NAG	C2-N2-C7	6.95	132.79	122.90
5	T	4	MAN	C1-O5-C5	6.88	121.51	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	V	2	FUC	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
6	M	2	FUC	C1
3	I	3	FUC	C1
3	Q	3	FUC	C1

5 of 95 torsion outliers are listed below:

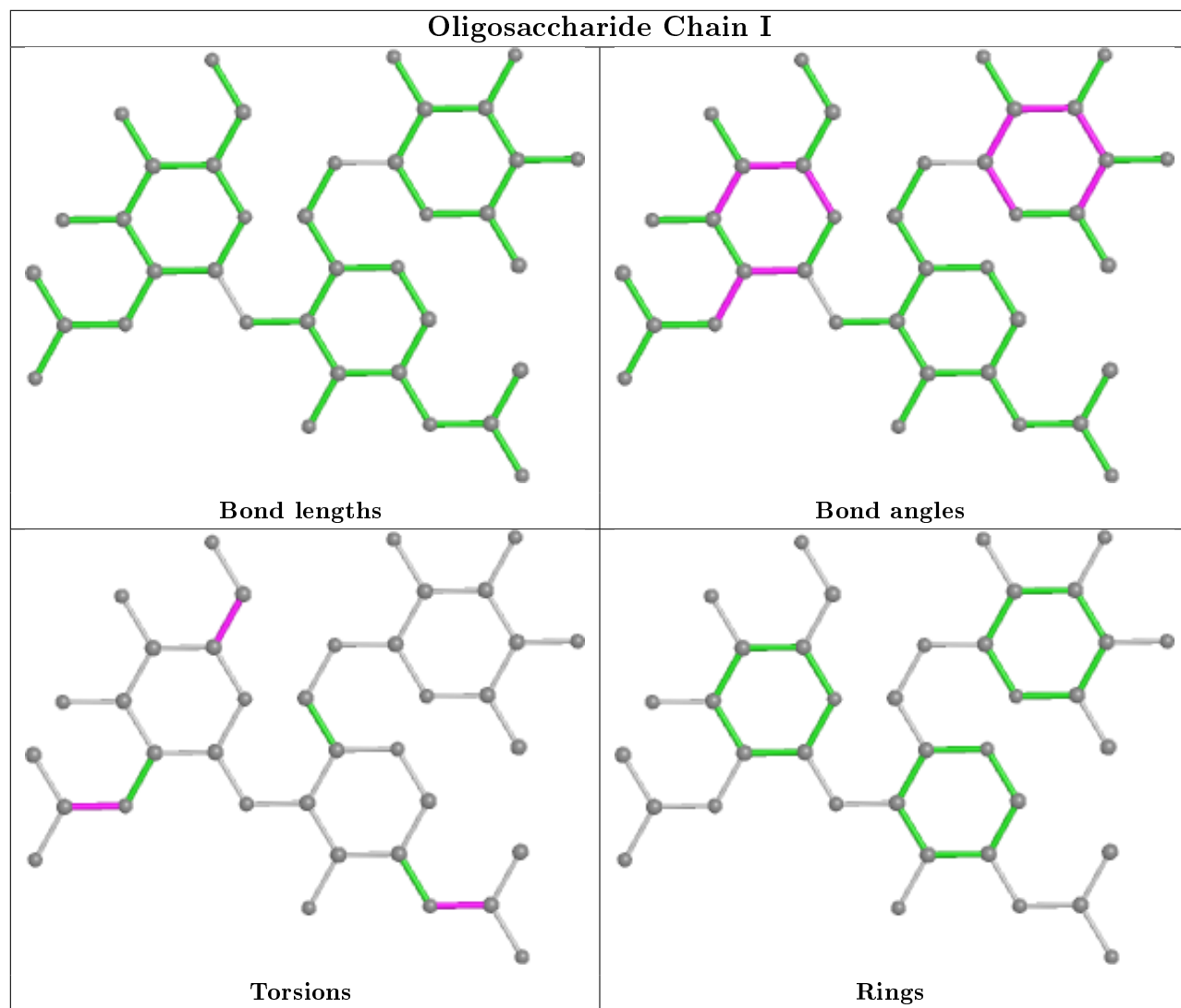
Mol	Chain	Res	Type	Atoms
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
6	V	1	NAG	C1-C2-N2-C7

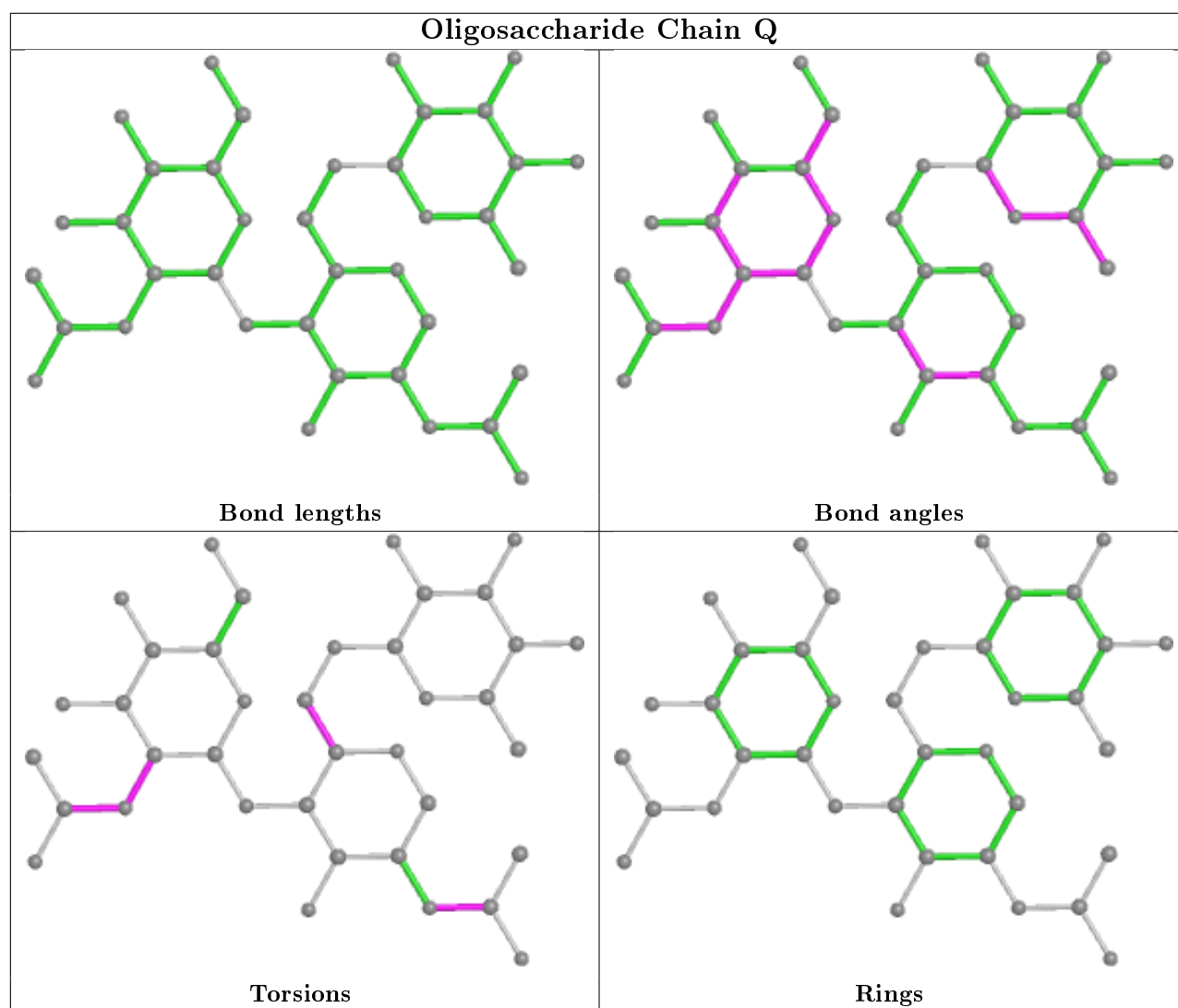
There are no ring outliers.

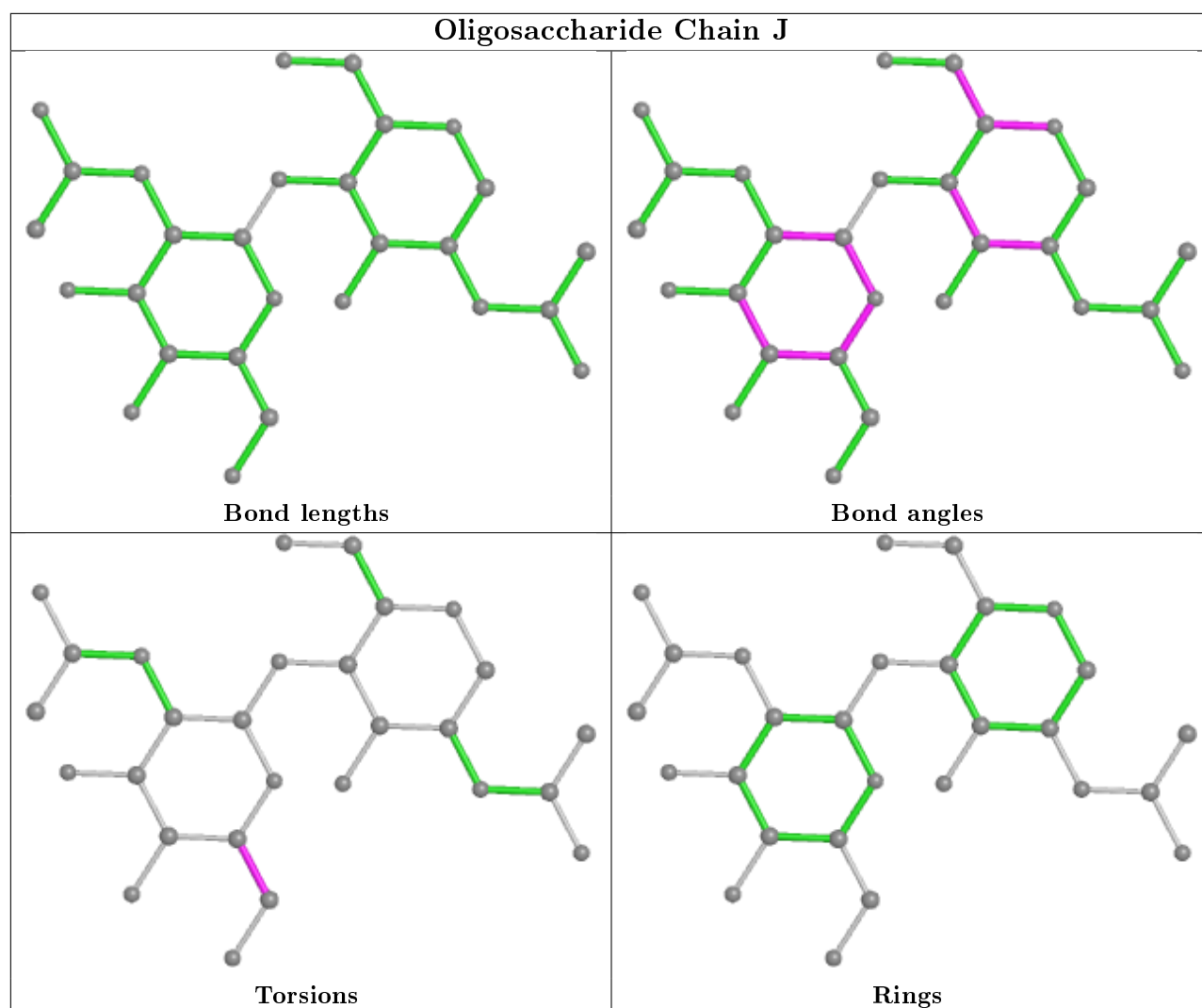
14 monomers are involved in 14 short contacts:

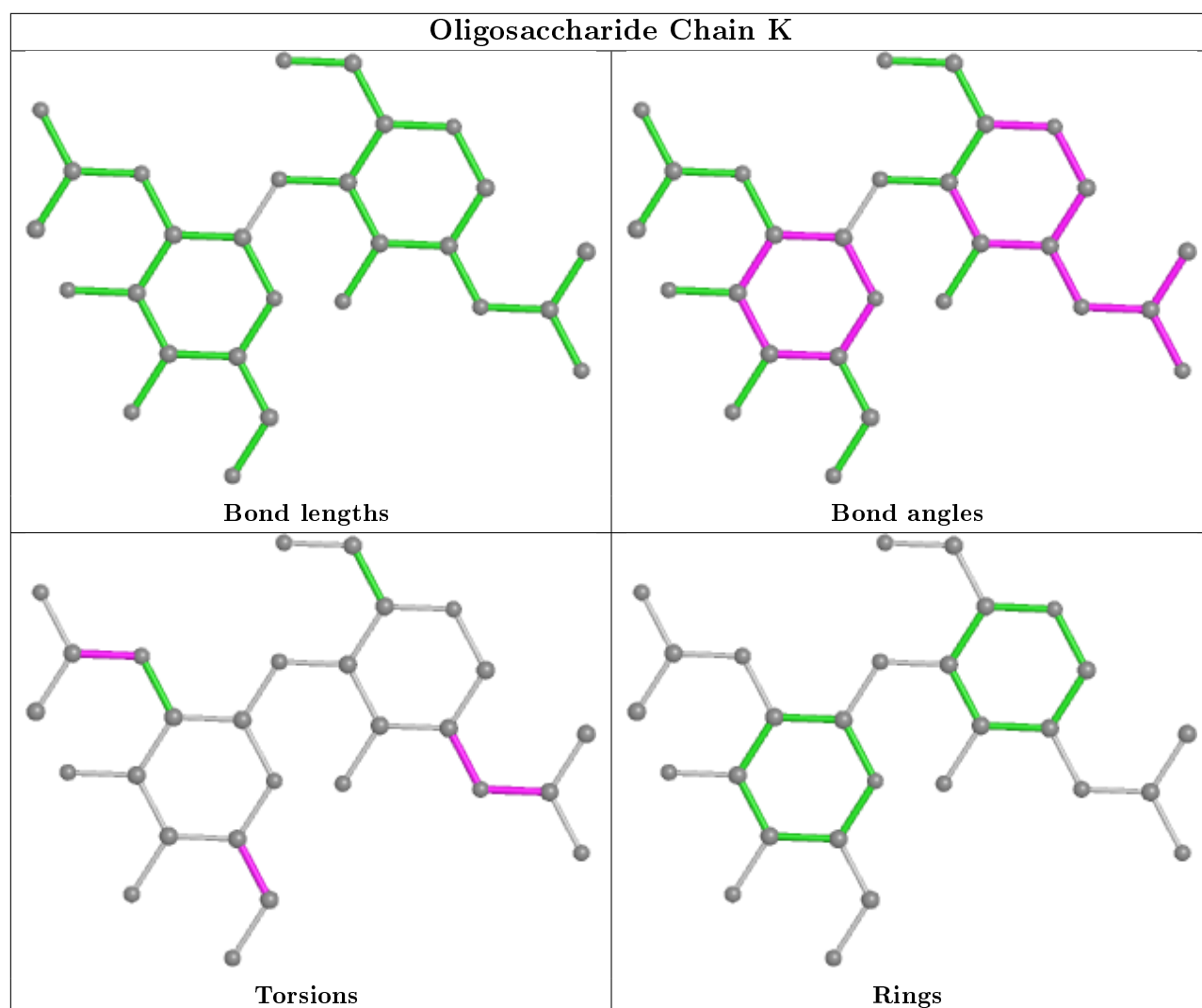
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	1	NAG	1	0
4	U	2	NAG	1	0
4	W	2	NAG	2	0
4	U	1	NAG	2	0
5	X	4	MAN	1	0
4	R	2	NAG	1	0
5	X	3	BMA	1	0
3	Q	1	NAG	1	0
4	N	1	NAG	2	0
4	N	2	NAG	1	0
4	R	1	NAG	1	0
3	Q	3	FUC	1	0
4	J	1	NAG	1	0
4	K	1	NAG	3	0

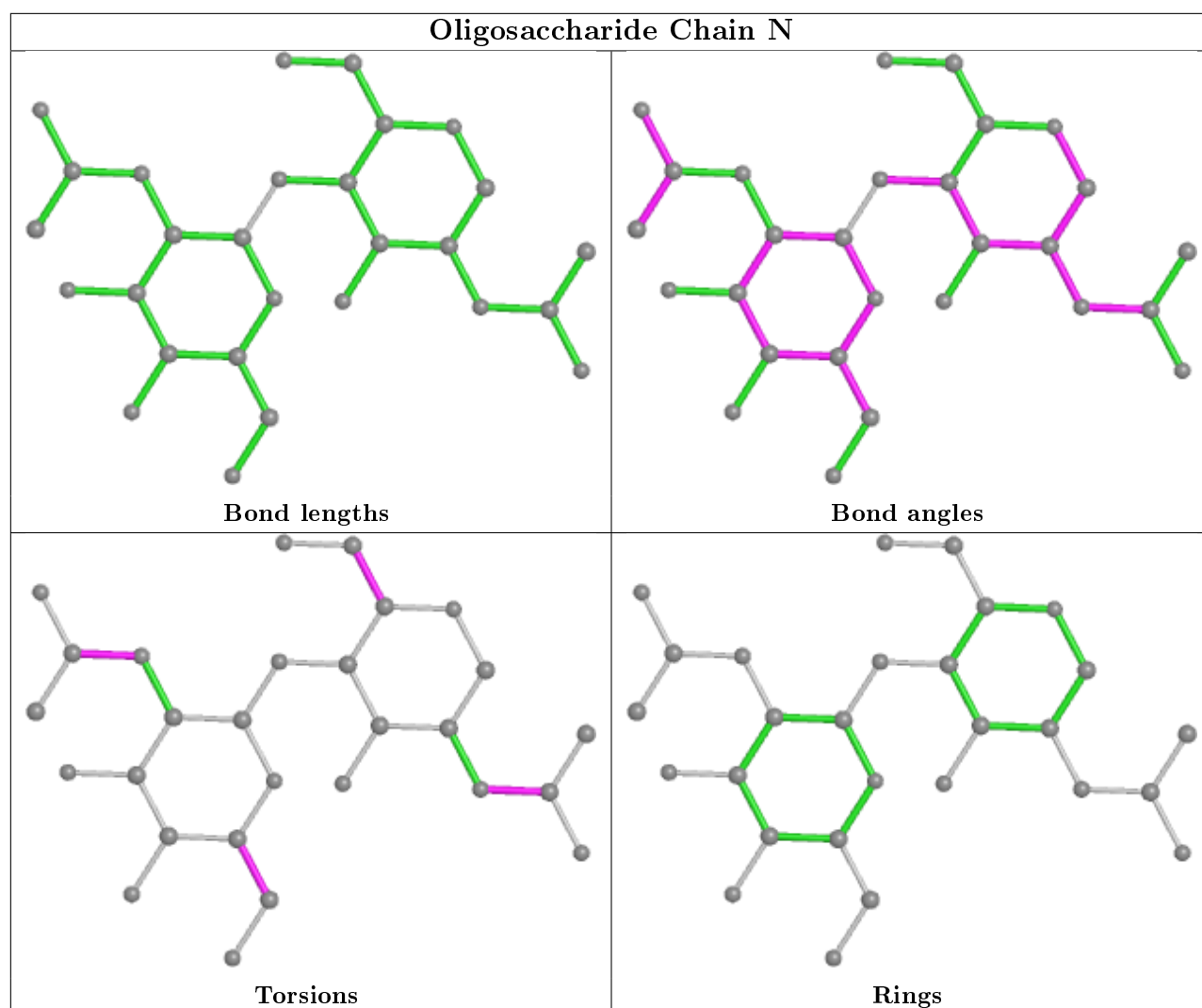
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

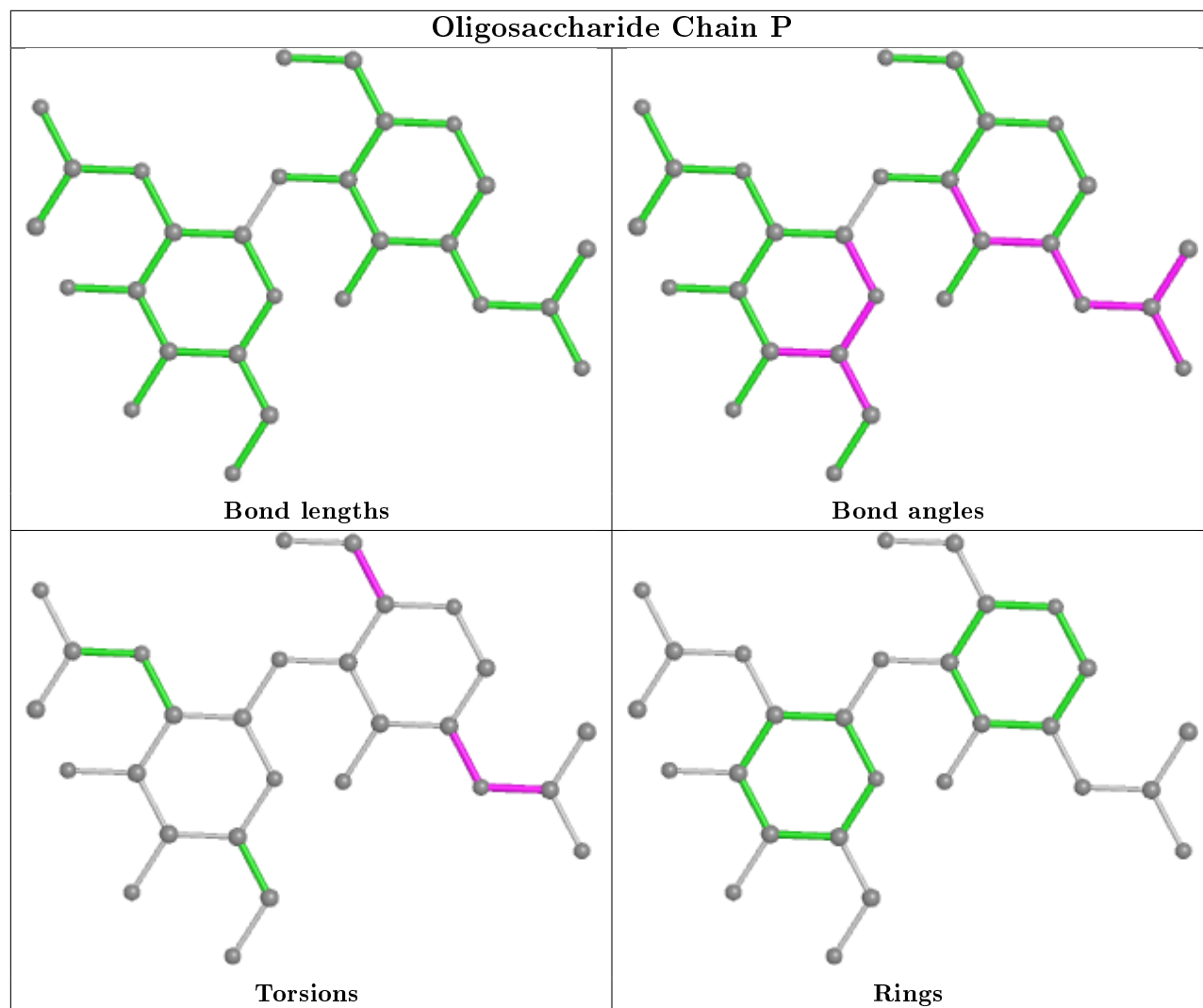


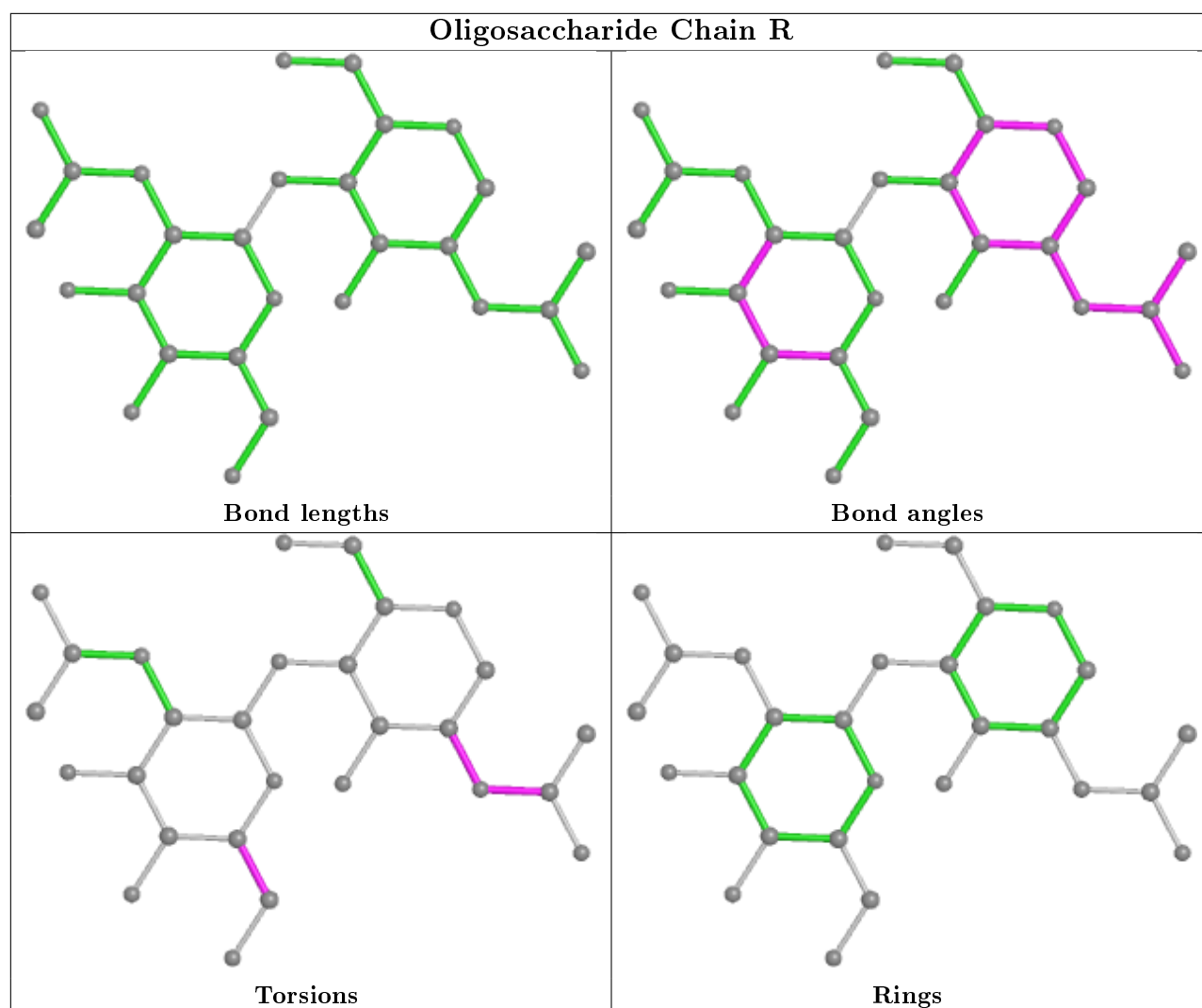


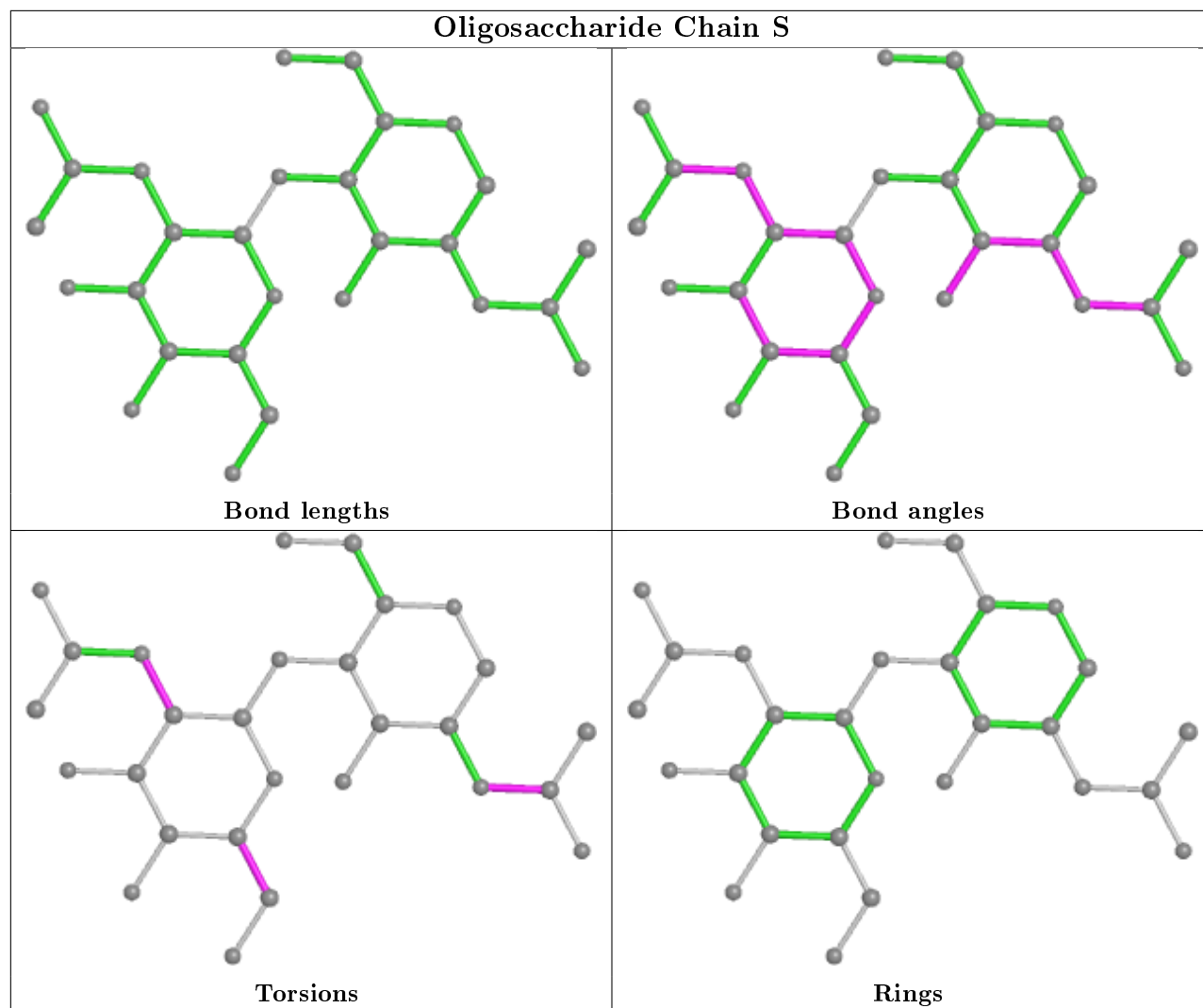


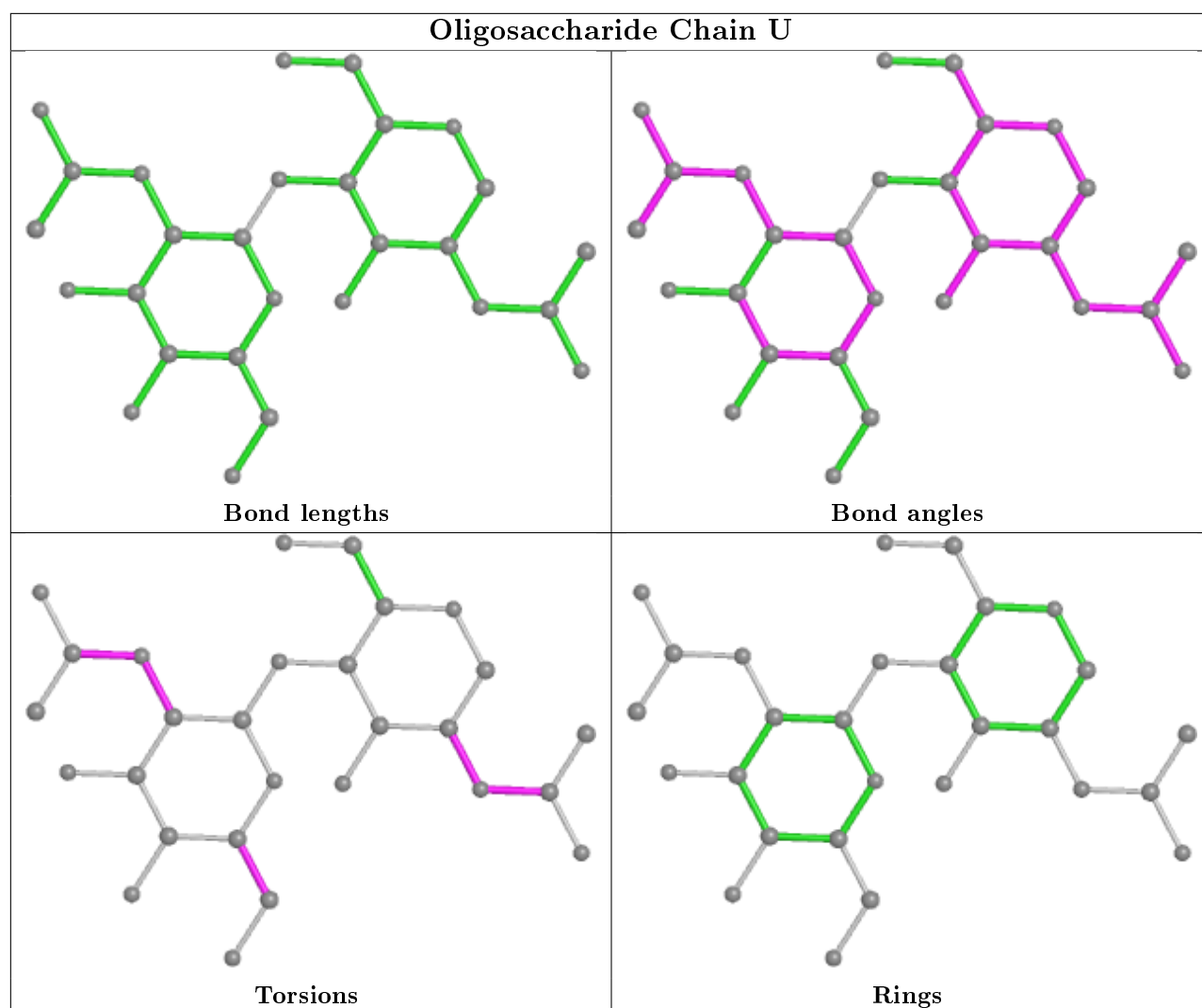


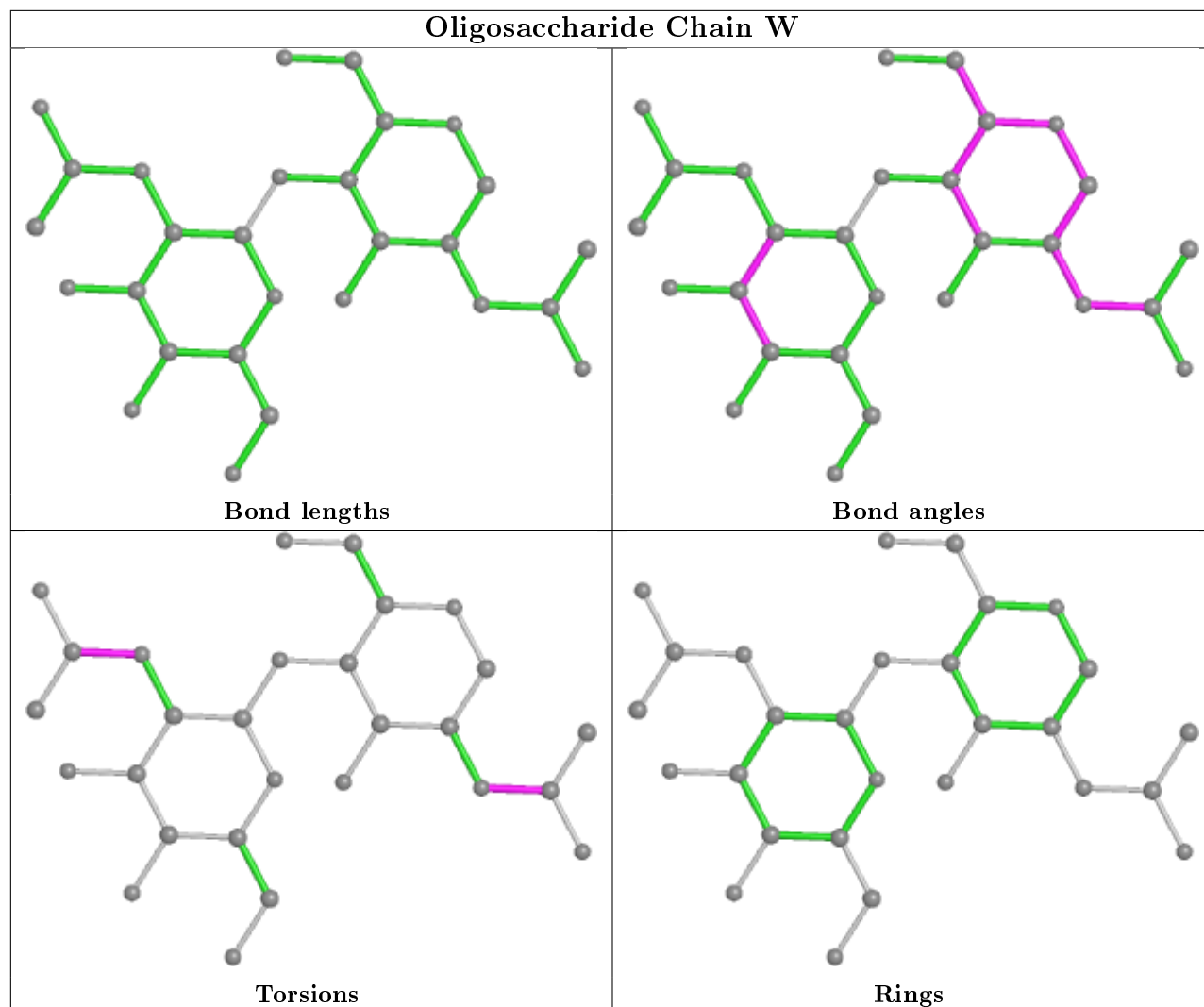


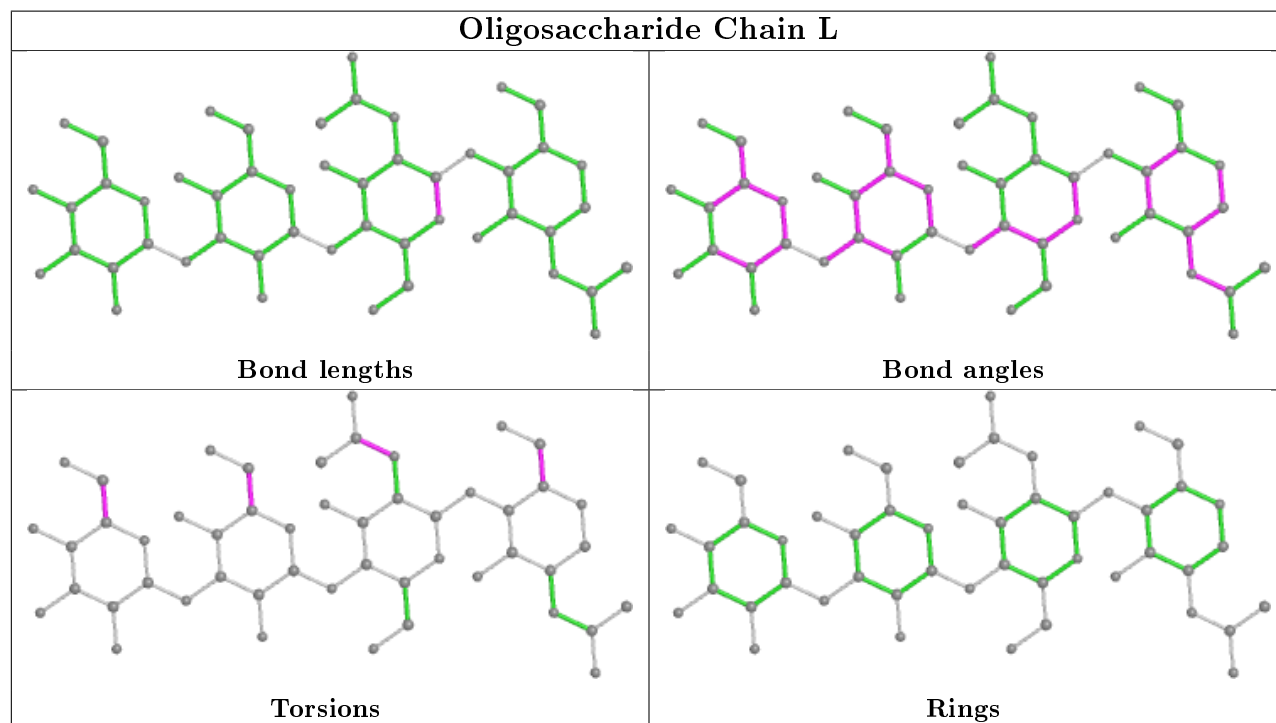
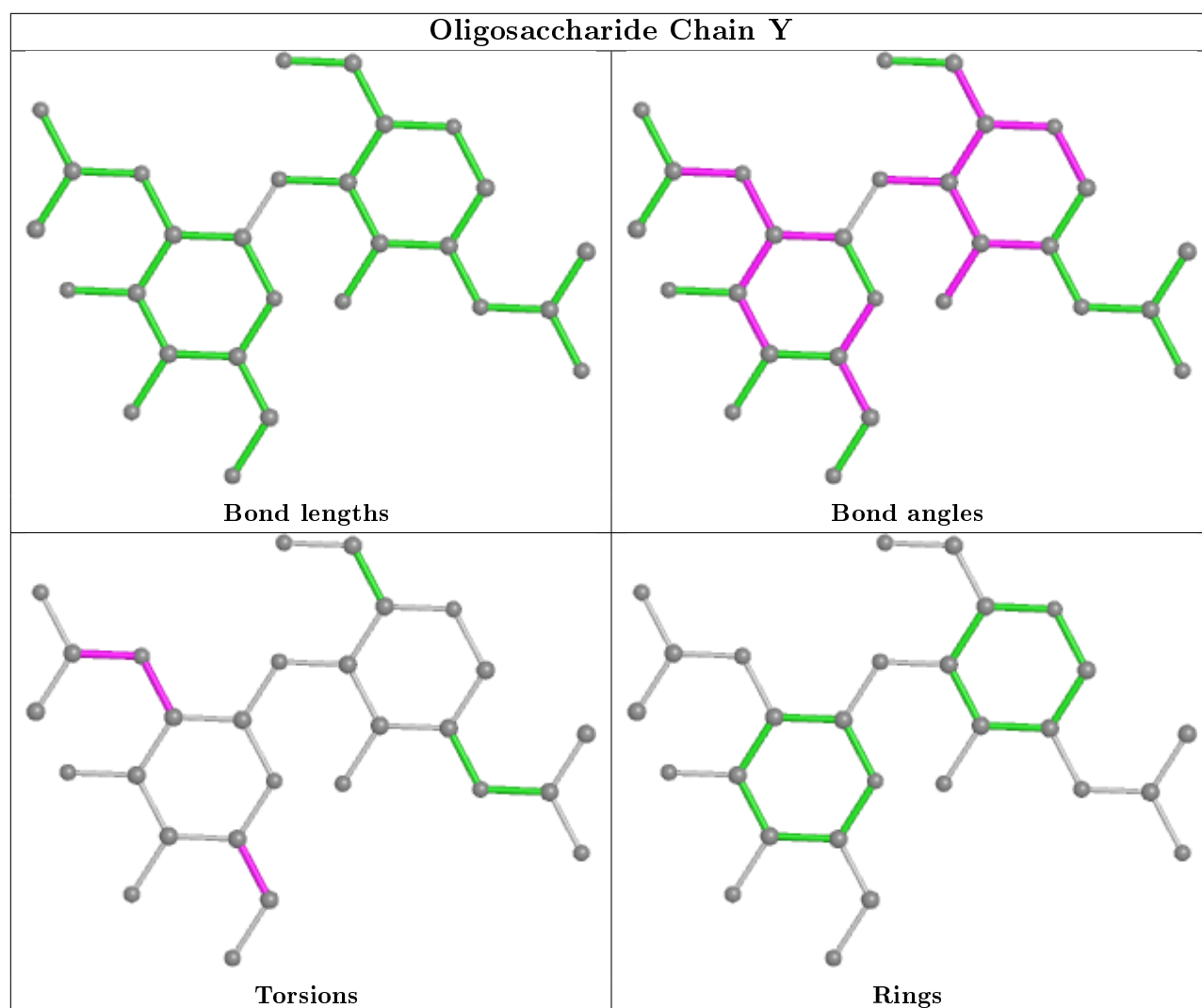




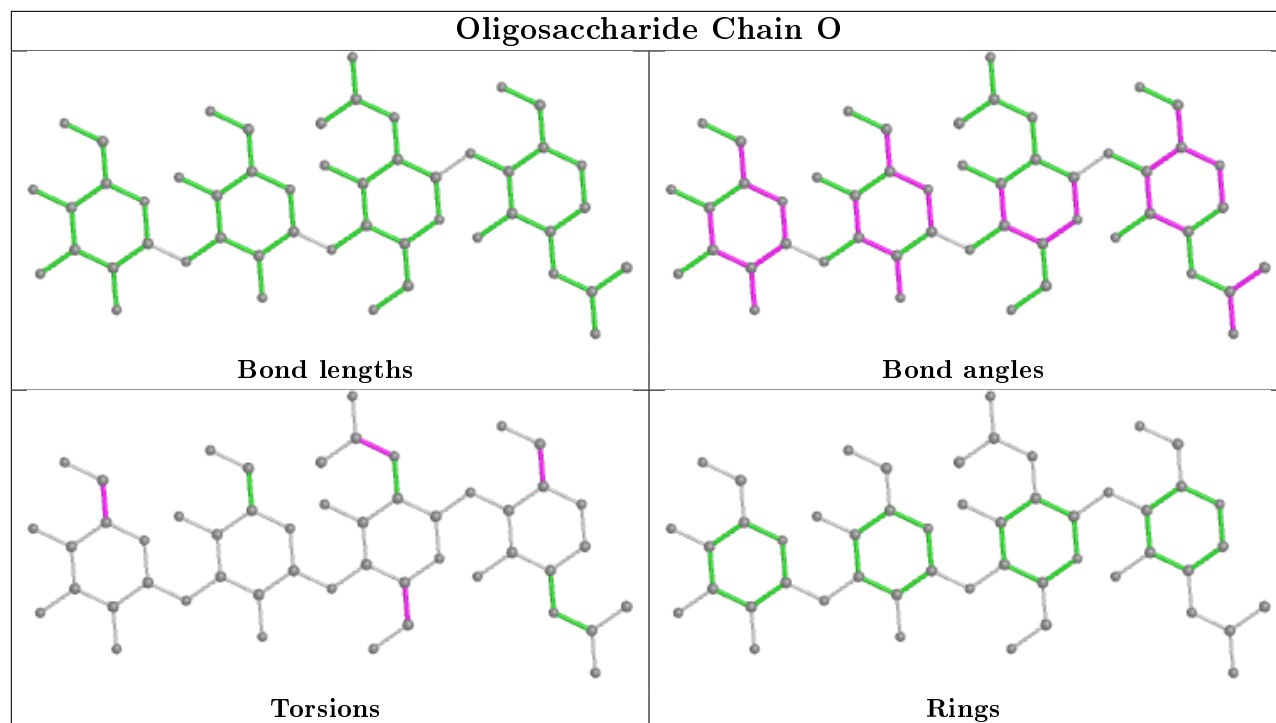




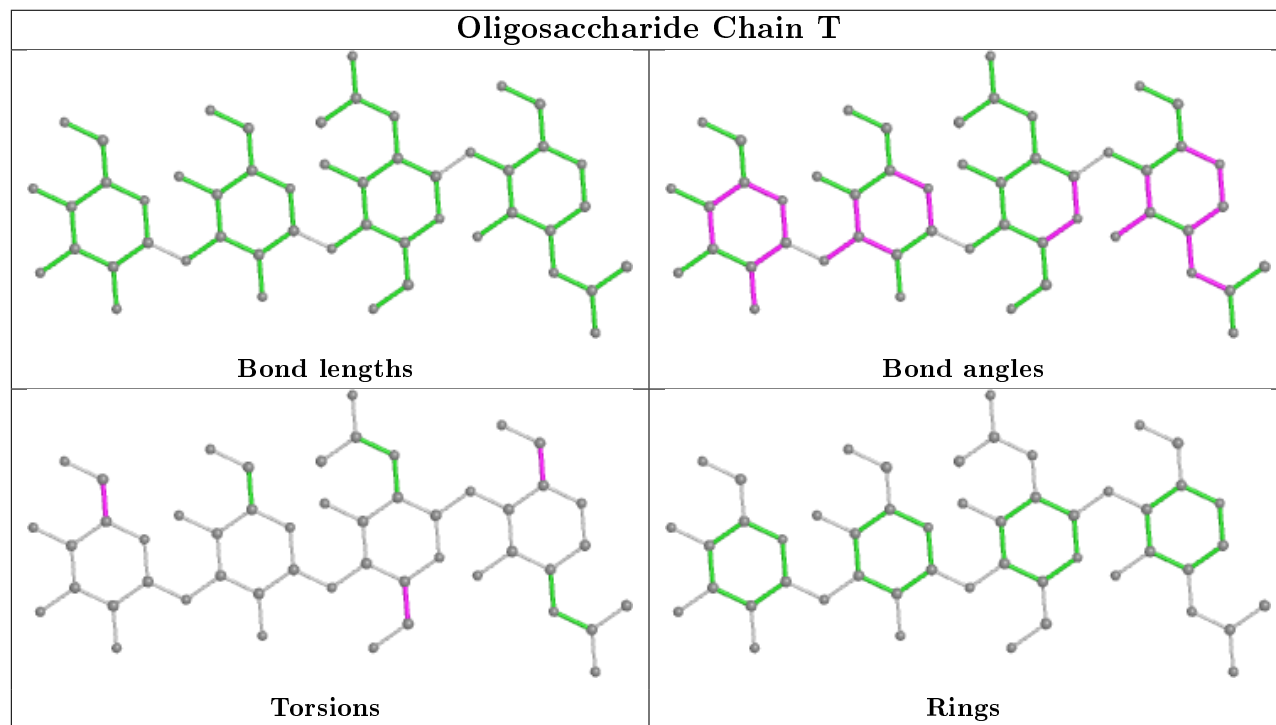


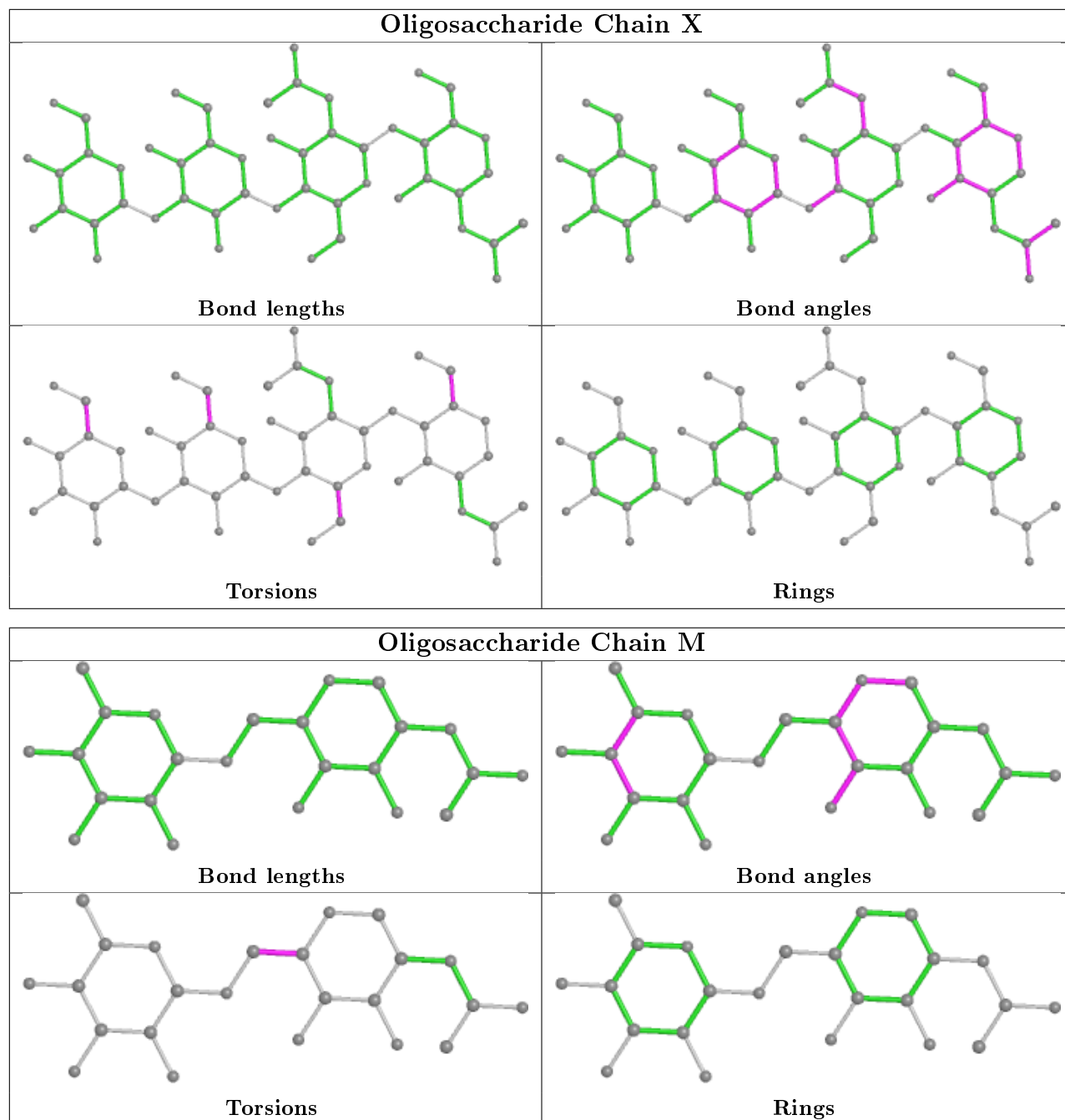


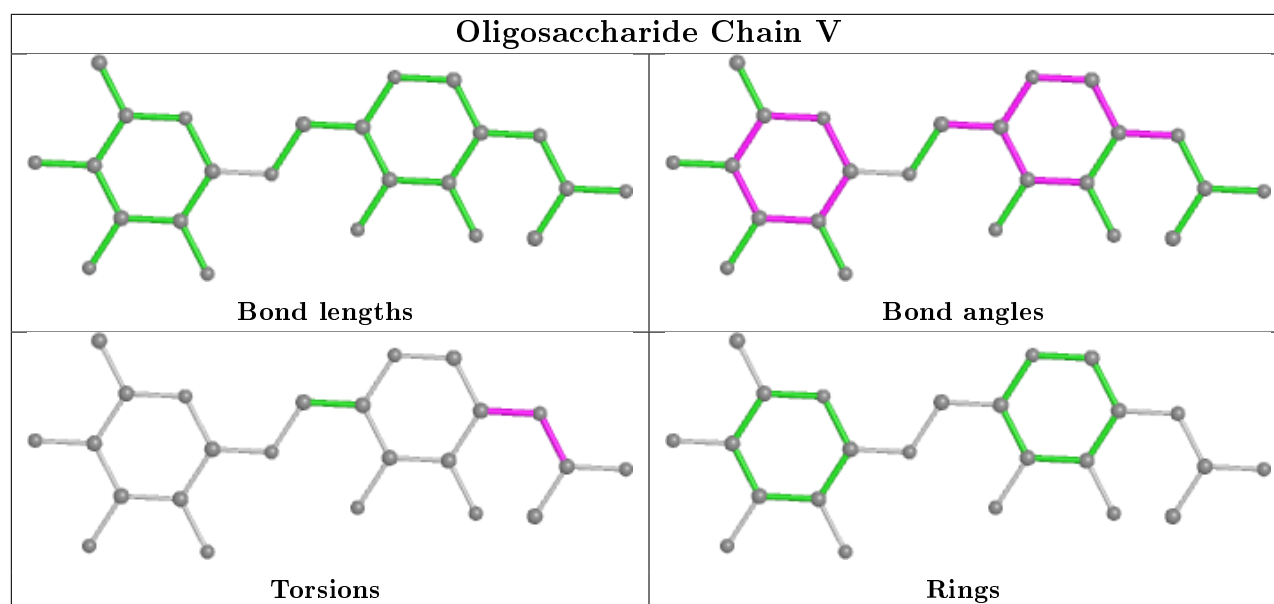
Oligosaccharide Chain O



Oligosaccharide Chain T







5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	NAG	C	860	1	14,14,15	0.77	1 (7%)	17,19,21	2.17	5 (29%)
7	NAG	C	870	1	14,14,15	0.63	0	17,19,21	2.42	4 (23%)
7	NAG	A	860	1	14,14,15	0.64	0	17,19,21	2.16	7 (41%)
7	NAG	B	860	1	14,14,15	0.64	0	17,19,21	2.02	5 (29%)
7	NAG	B	870	1	14,14,15	0.37	0	17,19,21	2.88	6 (35%)
7	NAG	B	810	1	14,14,15	0.63	0	17,19,21	2.88	6 (35%)
7	NAG	D	860	1	14,14,15	0.37	0	17,19,21	2.14	4 (23%)
7	NAG	D	840	1	14,14,15	0.74	0	17,19,21	2.40	5 (29%)
7	NAG	D	810	1	14,14,15	0.53	0	17,19,21	2.02	6 (35%)
7	NAG	B	840	1	14,14,15	0.57	0	17,19,21	2.46	5 (29%)
7	NAG	A	840	1	14,14,15	0.45	0	17,19,21	2.02	5 (29%)
7	NAG	C	840	1	14,14,15	0.46	0	17,19,21	1.91	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	870	1	14,14,15	0.46	0	17,19,21	1.56	2 (11%)
7	NAG	A	850	1	14,14,15	0.58	0	17,19,21	1.73	3 (17%)
7	NAG	D	870	1	14,14,15	0.82	0	17,19,21	1.76	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	860	1	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	C	870	1	-	3/6/23/26	0/1/1/1
7	NAG	A	860	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	B	860	1	1/1/5/7	3/6/23/26	0/1/1/1
7	NAG	B	870	1	-	4/6/23/26	0/1/1/1
7	NAG	B	810	1	-	3/6/23/26	0/1/1/1
7	NAG	D	860	1	-	4/6/23/26	0/1/1/1
7	NAG	D	840	1	-	2/6/23/26	0/1/1/1
7	NAG	D	810	1	-	2/6/23/26	0/1/1/1
7	NAG	B	840	1	-	4/6/23/26	0/1/1/1
7	NAG	A	840	1	-	2/6/23/26	0/1/1/1
7	NAG	C	840	1	-	0/6/23/26	0/1/1/1
7	NAG	A	870	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	850	1	-	0/6/23/26	0/1/1/1
7	NAG	D	870	1	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	860	NAG	C1-C2	2.21	1.55	1.52

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	870	NAG	O5-C1-C2	-7.74	99.06	111.29
7	D	840	NAG	C1-O5-C5	7.20	121.95	112.19
7	B	840	NAG	C1-O5-C5	6.69	121.25	112.19
7	B	810	NAG	C1-O5-C5	6.48	120.97	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	870	NAG	C2-N2-C7	6.15	131.67	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	860	NAG	C1
7	A	860	NAG	C1
7	B	860	NAG	C1
7	A	870	NAG	C1

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	860	NAG	C8-C7-N2-C2
7	C	860	NAG	O7-C7-N2-C2
7	C	870	NAG	C8-C7-N2-C2
7	C	870	NAG	O7-C7-N2-C2
7	A	860	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	860	NAG	1	0
7	C	870	NAG	2	0
7	A	860	NAG	3	0
7	B	870	NAG	1	0
7	A	870	NAG	2	0

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	728/728 (100%)	-0.51	0 100 100	25, 42, 71, 86	0
1	B	728/728 (100%)	-0.46	0 100 100	17, 42, 71, 86	0
1	C	728/728 (100%)	-0.49	1 (0%) 95 89	25, 43, 71, 86	0
1	D	728/728 (100%)	-0.52	0 100 100	25, 43, 71, 86	0
2	E	352/357 (98%)	0.09	14 (3%) 38 16	21, 66, 82, 88	0
2	F	352/357 (98%)	0.10	6 (1%) 70 42	40, 67, 84, 88	0
2	G	352/357 (98%)	0.00	10 (2%) 53 24	36, 67, 83, 88	0
2	H	352/357 (98%)	-0.03	2 (0%) 89 72	40, 67, 84, 88	0
All	All	4320/4340 (99%)	-0.32	33 (0%) 86 65	17, 49, 79, 88	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	293	ASN	4.0
2	E	262	CYS	3.9
2	G	293	ASN	3.4
2	E	15	HIS	3.3
2	G	247	THR	3.3

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	Q	2	14/15	0.69	0.45	90,91,92,92	0
4	NAG	J	2	14/15	0.75	0.46	78,79,80,80	0
4	NAG	R	2	14/15	0.76	0.45	78,79,80,80	0
4	NAG	U	2	14/15	0.79	0.43	67,69,71,71	0
5	MAN	O	4	11/12	0.80	0.29	48,49,50,50	0
4	NAG	Y	2	14/15	0.82	0.39	61,62,64,64	0
4	NAG	P	2	14/15	0.82	0.39	58,60,60,60	0
5	MAN	T	4	11/12	0.84	0.37	70,71,72,72	0
5	BMA	X	3	11/12	0.85	0.27	64,65,66,68	0
4	NAG	N	2	14/15	0.85	0.32	60,61,62,62	0
4	NAG	R	1	14/15	0.85	0.29	70,73,74,76	0
3	NAG	I	2	14/15	0.86	0.42	81,82,82,83	0
3	FUC	Q	3	10/11	0.86	0.43	86,86,87,87	0
6	NAG	V	1	14/15	0.87	0.29	81,83,84,86	0
5	MAN	X	4	11/12	0.87	0.31	69,69,70,71	0
6	FUC	M	2	10/11	0.87	0.28	73,74,75,75	0
5	MAN	L	4	11/12	0.87	0.24	58,59,60,61	0
4	NAG	W	2	14/15	0.88	0.33	62,65,66,66	0
6	FUC	V	2	10/11	0.88	0.32	85,86,86,86	0
4	NAG	J	1	14/15	0.88	0.23	67,70,72,75	0
6	NAG	M	1	14/15	0.89	0.25	74,75,76,76	0
3	FUC	I	3	10/11	0.89	0.40	79,80,80,80	0
5	BMA	T	3	11/12	0.89	0.27	62,64,65,68	0
4	NAG	S	2	14/15	0.89	0.36	66,68,68,69	0
4	NAG	P	1	14/15	0.90	0.25	50,53,55,56	0
4	NAG	S	1	14/15	0.90	0.28	59,61,62,64	0
4	NAG	Y	1	14/15	0.90	0.27	53,56,58,60	0
3	NAG	Q	1	14/15	0.90	0.23	82,84,86,88	0
4	NAG	W	1	14/15	0.90	0.28	58,60,61,63	0
4	NAG	K	1	14/15	0.90	0.28	57,60,62,62	0
4	NAG	K	2	14/15	0.91	0.32	62,64,66,66	0
5	NAG	L	2	14/15	0.92	0.23	52,54,54,56	0
3	NAG	I	1	14/15	0.92	0.25	74,77,80,80	0
4	NAG	U	1	14/15	0.93	0.20	54,57,60,64	0
5	NAG	X	2	14/15	0.93	0.20	55,56,59,62	0
4	NAG	N	1	14/15	0.93	0.27	55,57,58,59	0
5	NAG	L	1	14/15	0.93	0.16	42,43,46,49	0
5	NAG	T	2	14/15	0.94	0.21	52,54,57,60	0
5	NAG	O	2	14/15	0.94	0.21	35,37,38,39	0
5	BMA	O	3	11/12	0.94	0.18	41,43,45,46	0
5	BMA	L	3	11/12	0.94	0.28	56,58,58,58	0

Continued on next page...

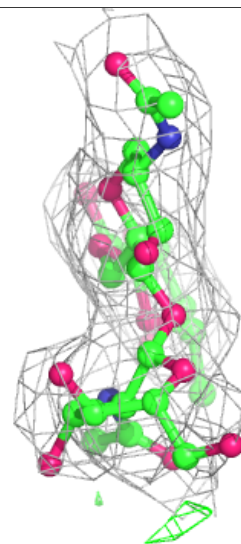
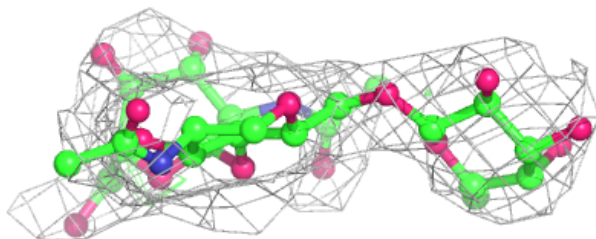
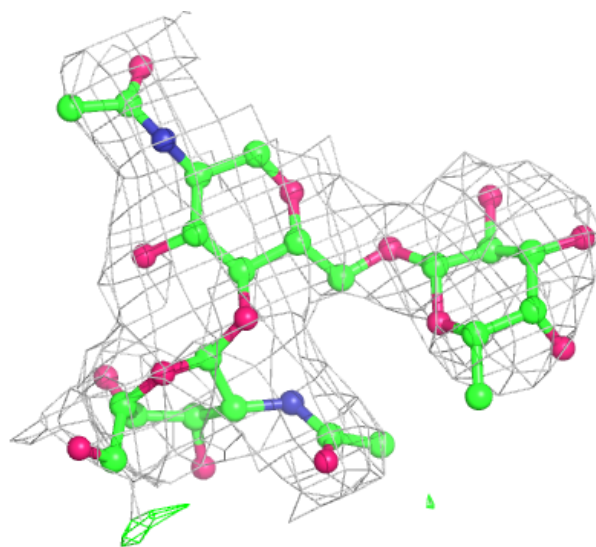
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NAG	X	1	14/15	0.94	0.18	42,45,48,52	0
5	NAG	T	1	14/15	0.95	0.12	41,42,47,49	0
5	NAG	O	1	14/15	0.97	0.15	30,31,33,33	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.

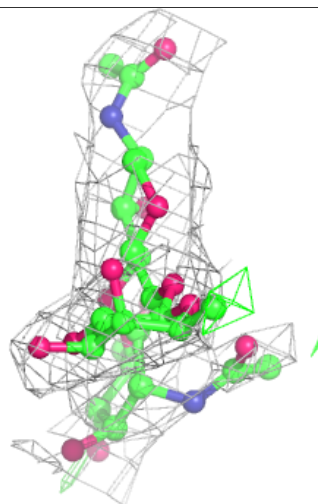
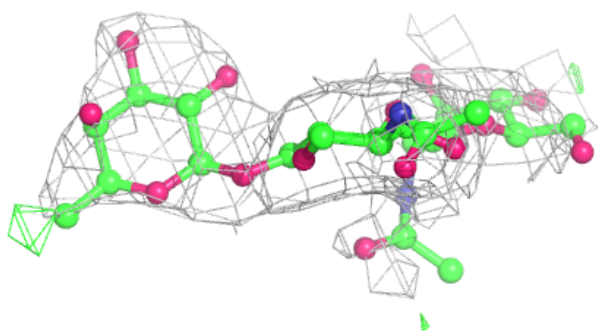
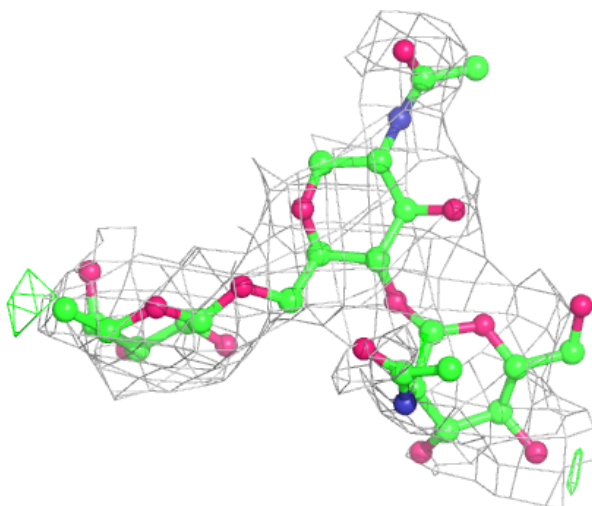
Electron density around Chain I:

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



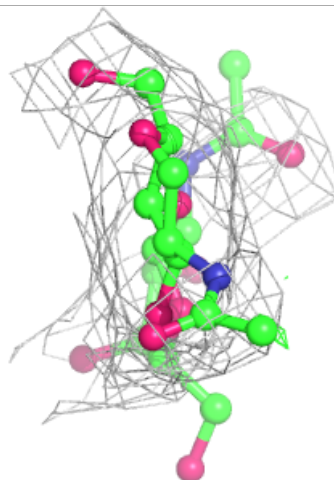
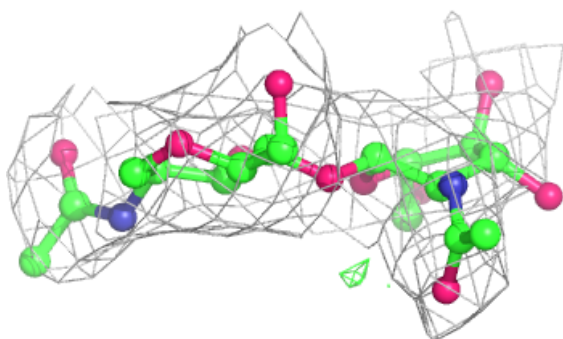
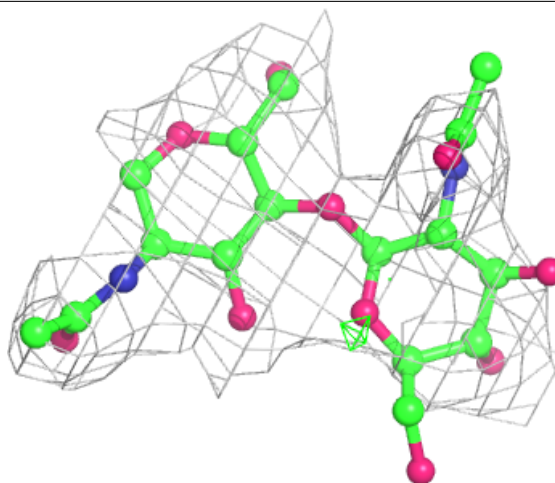
Electron density around Chain Q:

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



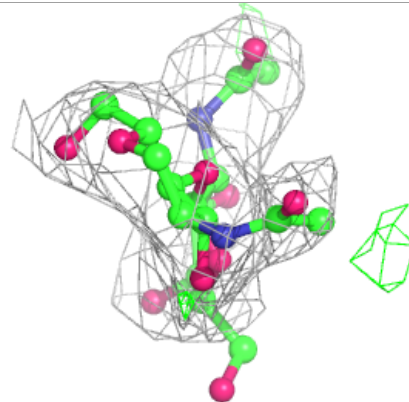
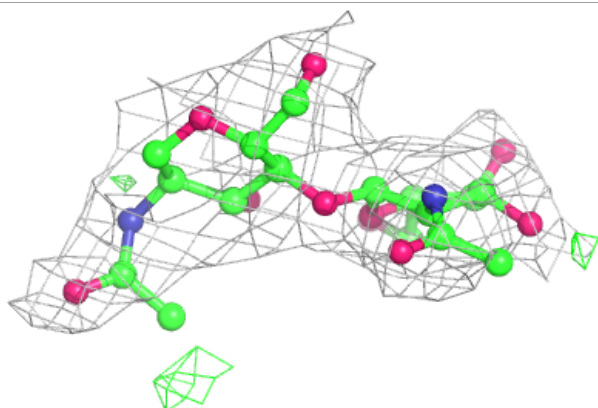
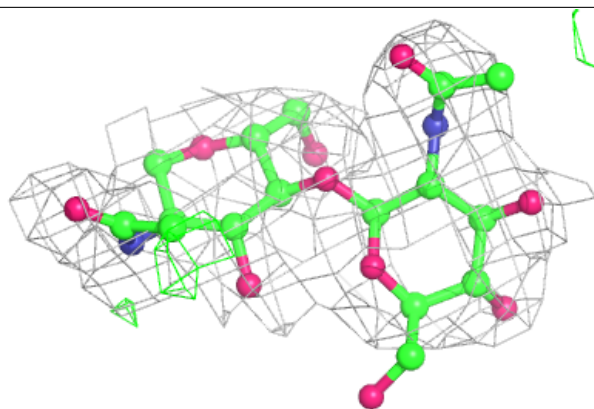
Electron density around Chain J:

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

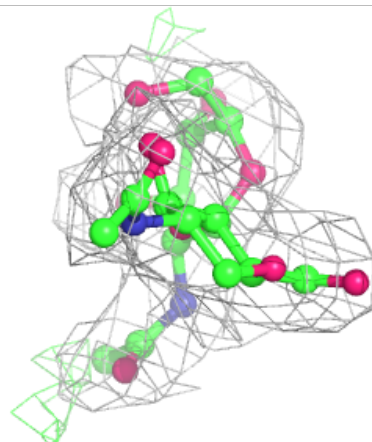
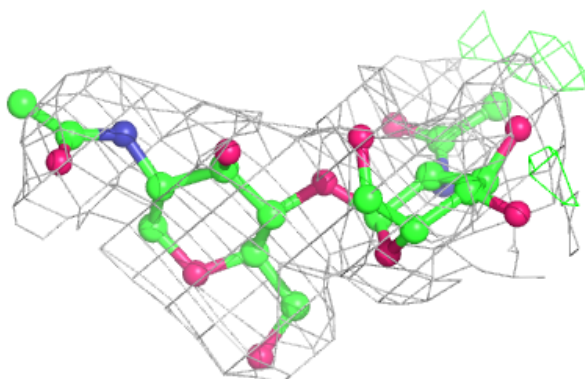
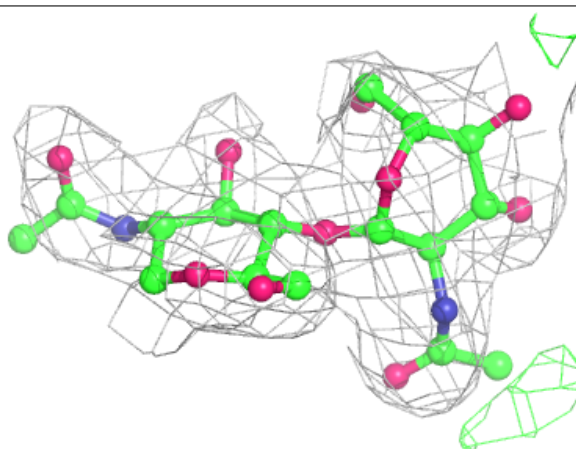


Electron density around Chain K:

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

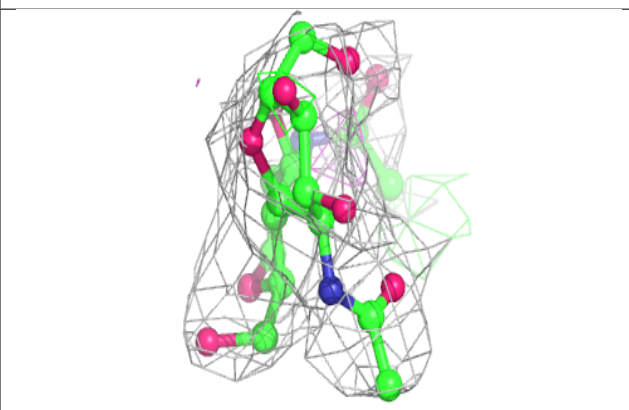
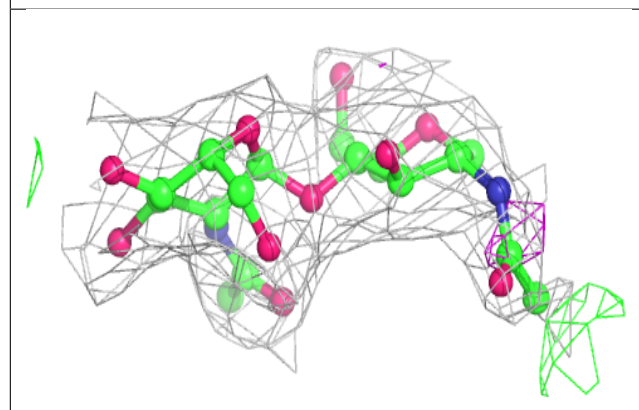
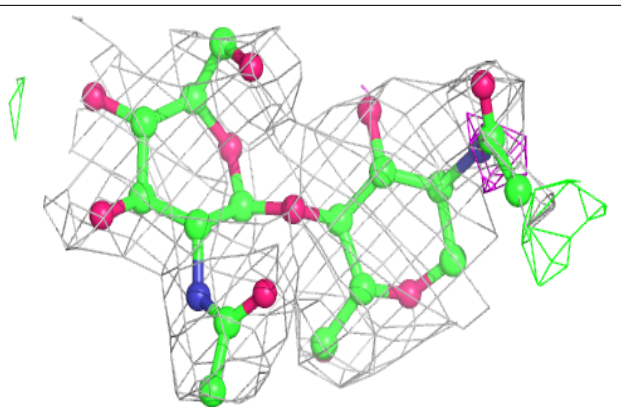
**Electron density around Chain N:**

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



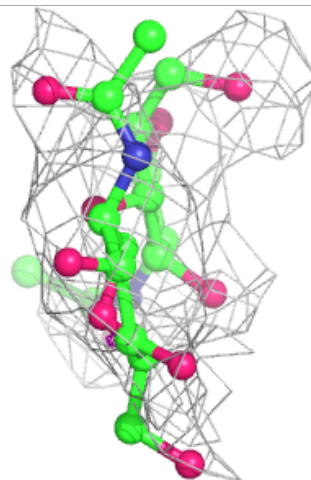
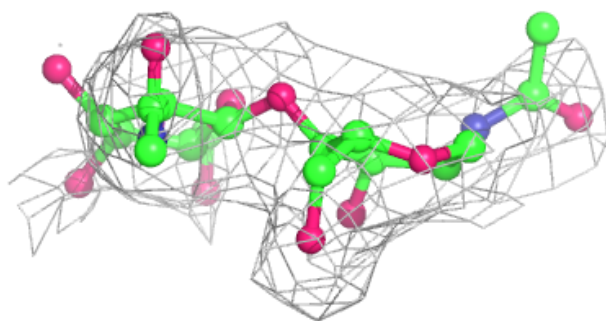
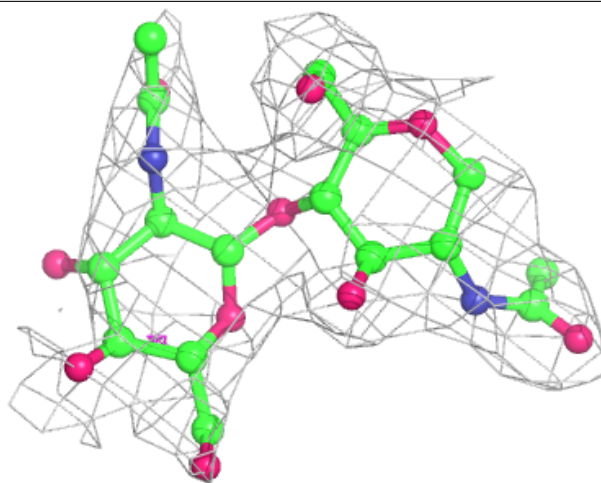
Electron density around Chain P:

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



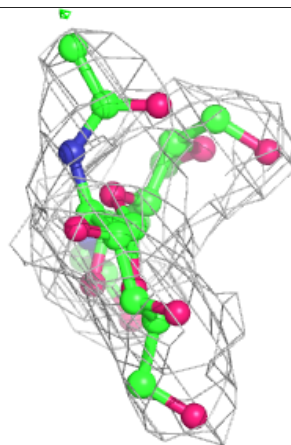
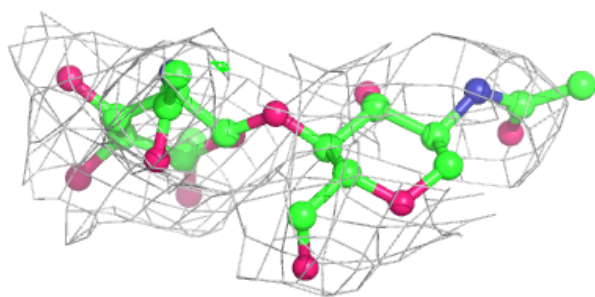
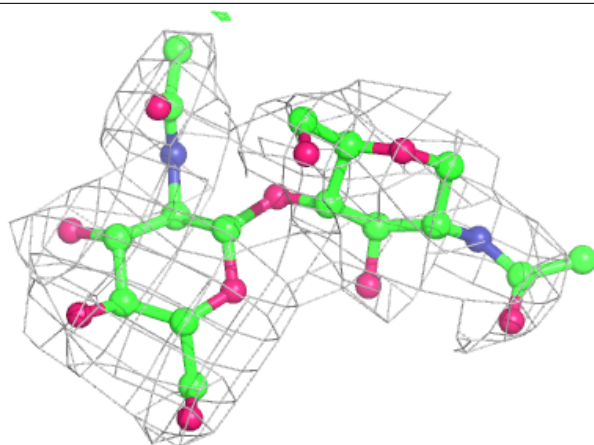
Electron density around Chain R:

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



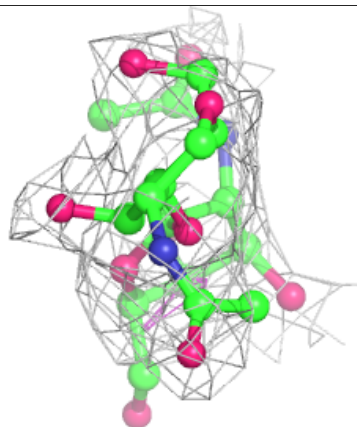
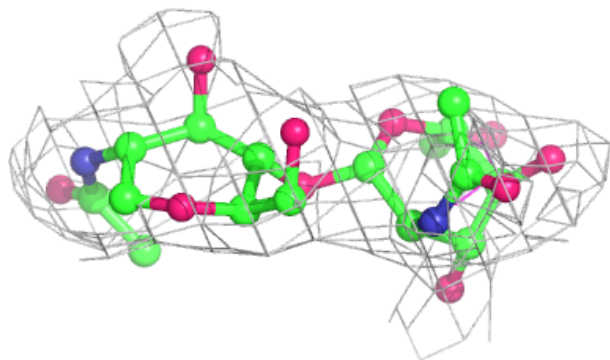
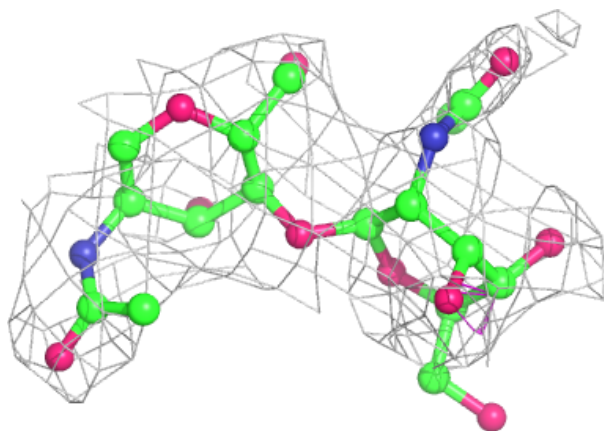
Electron density around Chain S:

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



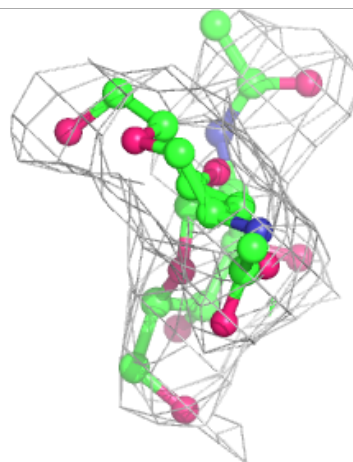
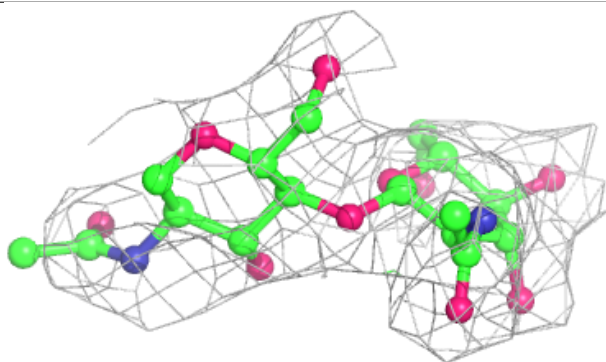
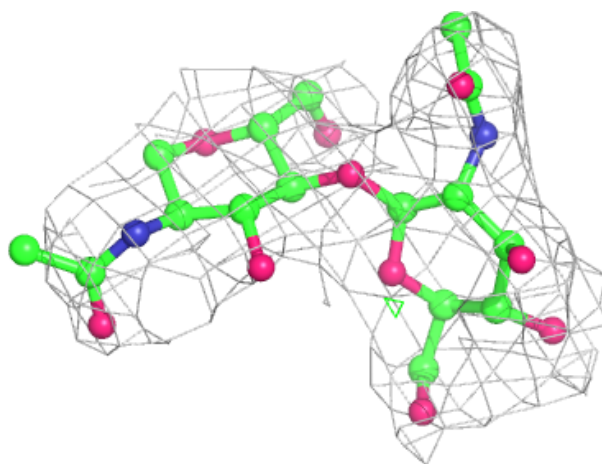
Electron density around Chain U:

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



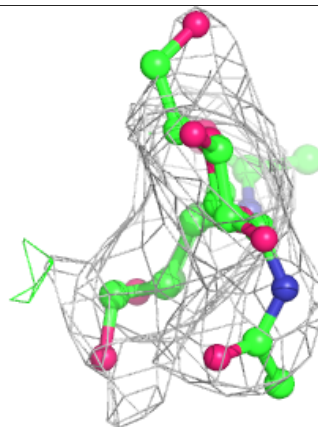
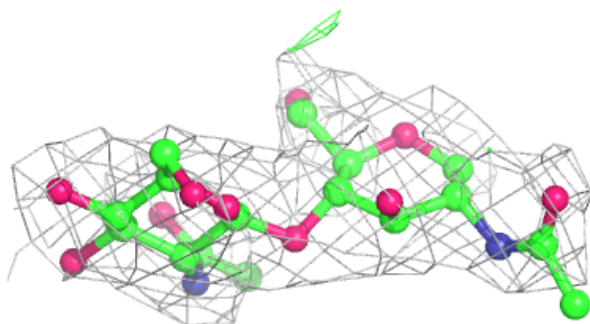
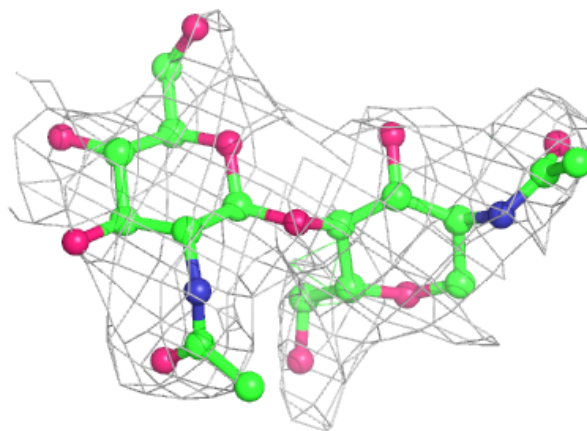
Electron density around Chain W:

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

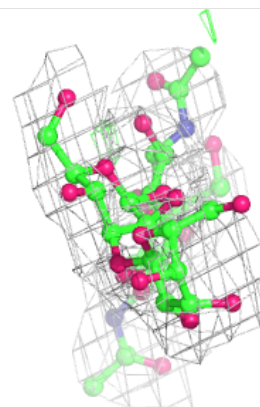
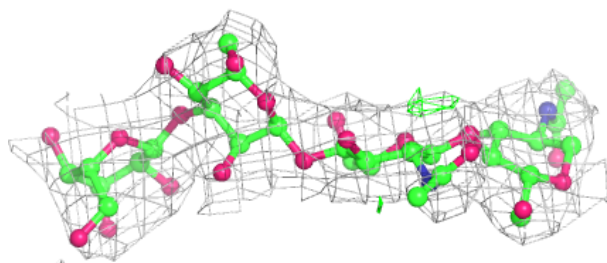
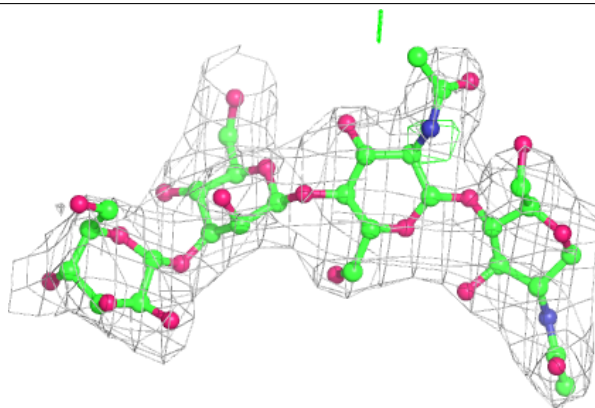


Electron density around Chain Y:

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

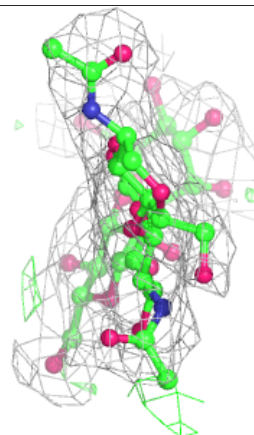
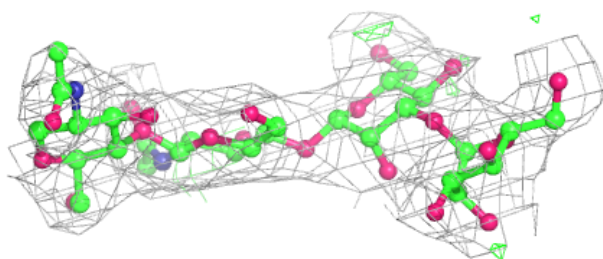
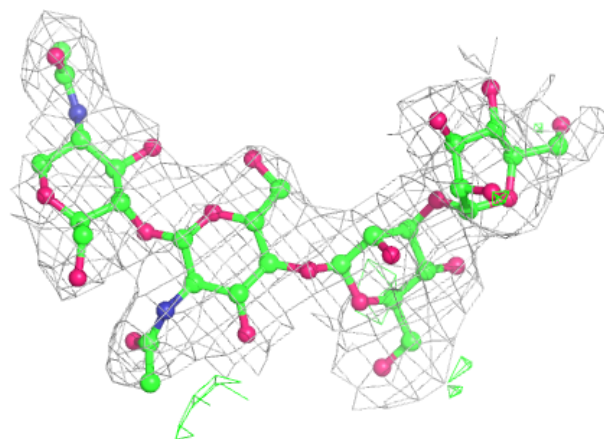
**Electron density around Chain L:**

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

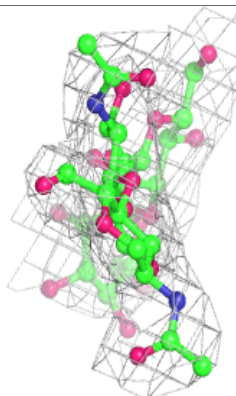
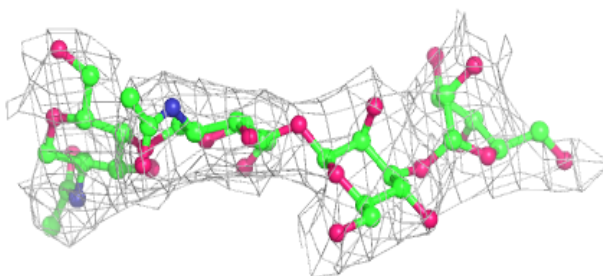
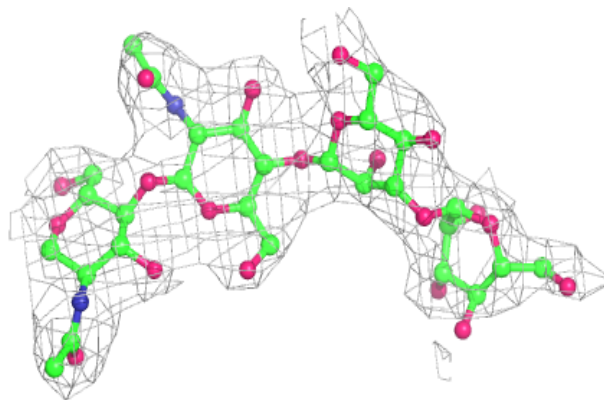


Electron density around Chain O:

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

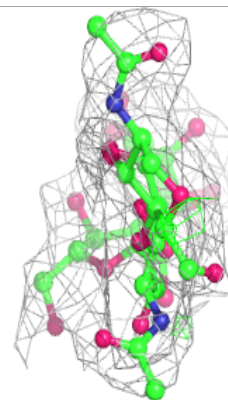
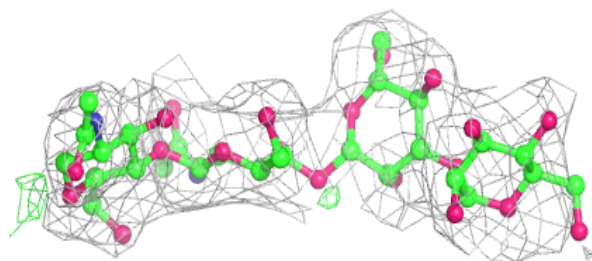
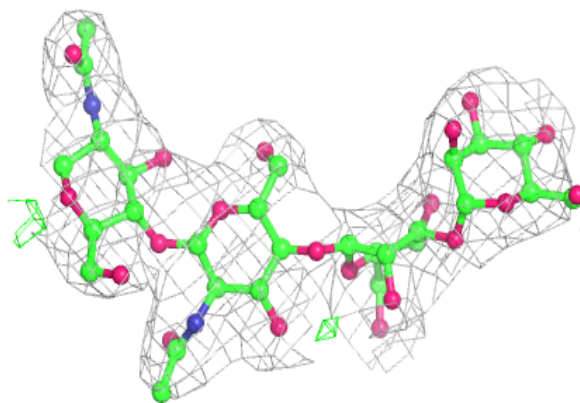
**Electron density around Chain T:**

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

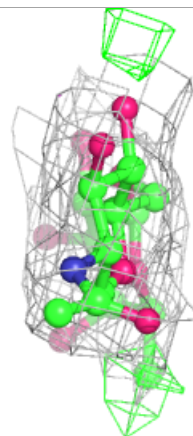
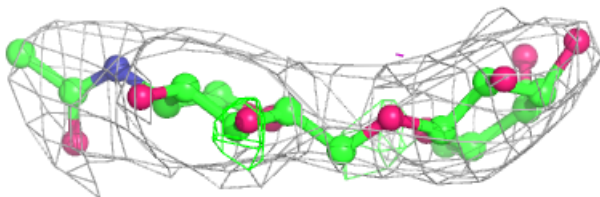
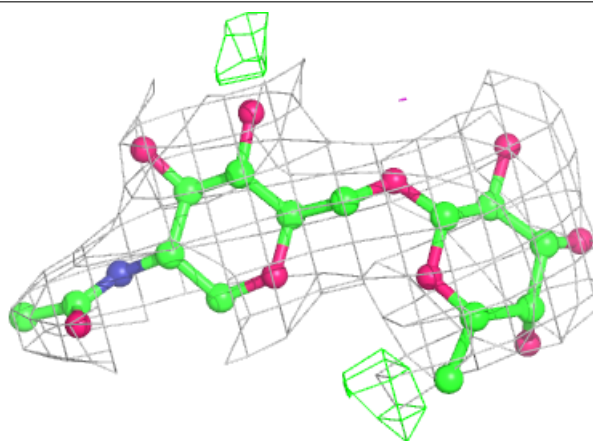


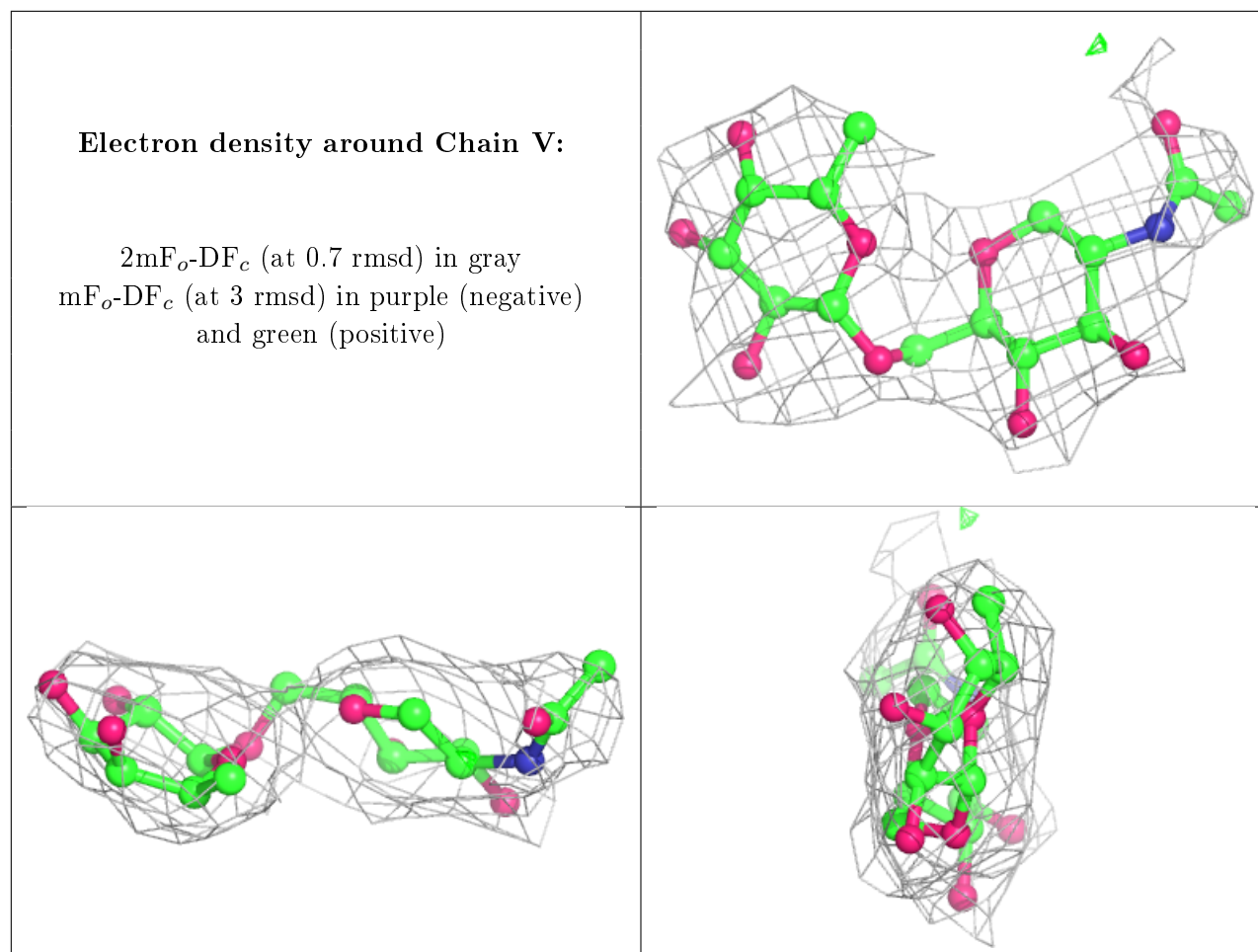
Electron density around Chain X:

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

**Electron density around Chain M:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	D	870	14/15	0.65	0.38	90,91,93,93	0
7	NAG	C	870	14/15	0.76	0.31	88,89,90,90	0
7	NAG	A	870	14/15	0.78	0.33	88,88,90,90	0
7	NAG	A	860	14/15	0.79	0.30	67,68,71,71	0
7	NAG	C	860	14/15	0.80	0.38	68,69,71,71	0
7	NAG	B	870	14/15	0.81	0.24	87,88,88,89	0
7	NAG	D	810	14/15	0.83	0.34	69,71,72,72	0
7	NAG	D	840	14/15	0.86	0.19	48,50,51,51	0
7	NAG	B	860	14/15	0.86	0.31	64,65,66,66	0
7	NAG	D	860	14/15	0.87	0.30	63,66,67,67	0
8	ZN	F	501	1/1	0.87	0.10	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NAG	B	810	14/15	0.88	0.27	64,65,66,66	0
7	NAG	B	840	14/15	0.90	0.16	46,48,49,49	0
7	NAG	A	850	14/15	0.92	0.21	52,54,57,60	0
7	NAG	C	840	14/15	0.93	0.26	51,54,55,55	0
8	ZN	H	501	1/1	0.96	0.19	58,58,58,58	0
7	NAG	A	840	14/15	0.96	0.21	48,50,50,50	0
8	ZN	G	501	1/1	0.98	0.23	58,58,58,58	0
8	ZN	E	501	1/1	0.99	0.33	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.