



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2024 – 10:25 AM EST

PDB ID : 5FFO
Title : Integrin alpha V beta 6 in complex with pro-TGF-beta
Authors : Dong, X.; Zhao, B.; Springer, T.A.
Deposited on : 2015-12-18
Resolution : 3.49 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

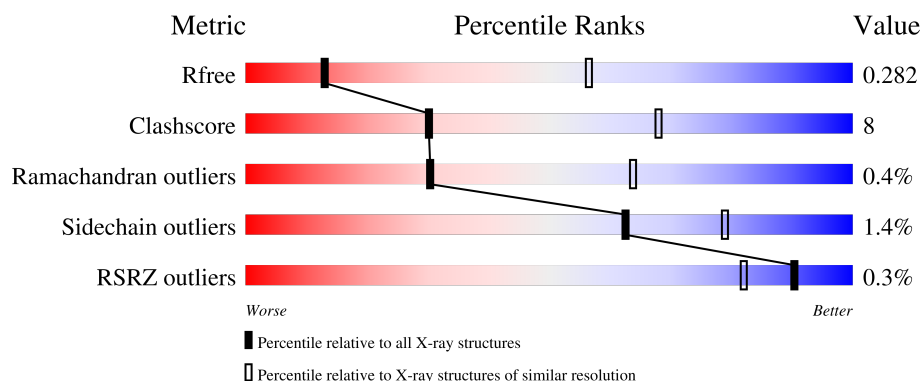
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




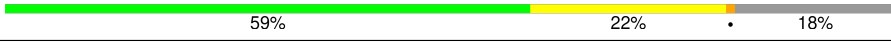

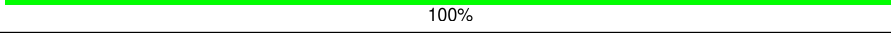
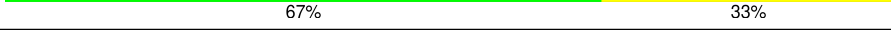
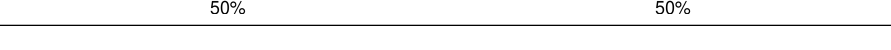
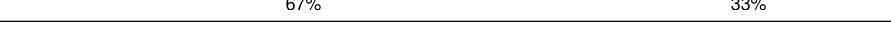
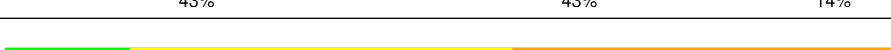

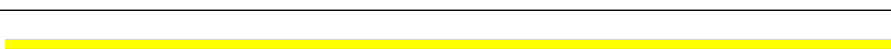

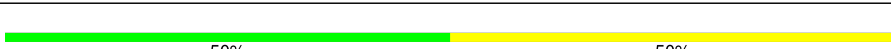





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	601	<div> <div>80%</div> <div>18%</div> <div>•</div> </div>
1	E	601	<div> <div>%</div> <div>82%</div> <div>16%</div> <div>•</div> </div>
2	B	257	<div> <div>68%</div> <div>26%</div> <div>6%</div> </div>
2	F	257	<div> <div>72%</div> <div>23%</div> <div>6%</div> </div>
3	C	363	<div> <div>%</div> <div>62%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	363	% 
3	G	363	
3	H	363	
4	I	3	
4	P	3	
5	J	6	
5	Q	6	
6	K	7	
6	R	7	
7	L	4	
7	S	4	
8	M	2	
8	T	2	
9	N	4	
9	O	4	
9	U	4	
10	V	6	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 23786 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4570	2898	776	875	21			
1	E	587	Total	C	N	O	S	0	0	0
			4547	2880	772	874	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	conflict	UNP P06756
A	597	THR	CYS	conflict	UNP P06756
A	599	GLY	-	expression tag	UNP P06756
A	600	LEU	-	expression tag	UNP P06756
A	601	GLU	-	expression tag	UNP P06756
E	400	GLY	-	insertion	UNP P06756
E	401	CYS	MET	conflict	UNP P06756
E	597	THR	CYS	conflict	UNP P06756
E	599	GLY	-	expression tag	UNP P06756
E	600	LEU	-	expression tag	UNP P06756
E	601	GLU	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1891	1210	302	368	11			
2	F	242	Total	C	N	O	S	0	0	0
			1891	1210	302	368	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	270	CYS	ILE	conflict	UNP P18564
B	362	HIS	-	expression tag	UNP P18564
B	363	HIS	-	expression tag	UNP P18564
B	364	HIS	-	expression tag	UNP P18564
B	365	HIS	-	expression tag	UNP P18564
B	366	HIS	-	expression tag	UNP P18564
B	367	HIS	-	expression tag	UNP P18564
F	270	CYS	ILE	conflict	UNP P18564
F	362	HIS	-	expression tag	UNP P18564
F	363	HIS	-	expression tag	UNP P18564
F	364	HIS	-	expression tag	UNP P18564
F	365	HIS	-	expression tag	UNP P18564
F	366	HIS	-	expression tag	UNP P18564
F	367	HIS	-	expression tag	UNP P18564

- Molecule 3 is a protein called Transforming growth factor beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	305	Total	C	N	O	S	0	0	0
			2445	1555	434	439	17			
3	D	322	Total	C	N	O	S	0	0	0
			2590	1650	457	466	17			
3	G	297	Total	C	N	O	S	0	0	0
			2399	1529	425	429	16			
3	H	325	Total	C	N	O	S	0	0	0
			2612	1660	465	471	16			

There are 32 discrepancies between the modelled and reference sequences:

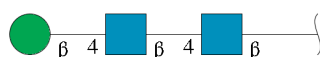
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P01137
C	0	PRO	-	expression tag	UNP P01137
C	1	LEU	-	expression tag	UNP P01137
C	2	SER	-	expression tag	UNP P01137
C	3	THR	-	expression tag	UNP P01137
C	4	SER	-	expression tag	UNP P01137
C	107	GLN	ASN	conflict	UNP P01137
C	147	GLN	ASN	conflict	UNP P01137
D	-1	GLY	-	expression tag	UNP P01137
D	0	PRO	-	expression tag	UNP P01137
D	1	LEU	-	expression tag	UNP P01137
D	2	SER	-	expression tag	UNP P01137
D	3	THR	-	expression tag	UNP P01137

Continued on next page...

Continued from previous page...

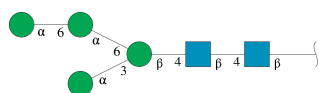
Chain	Residue	Modelled	Actual	Comment	Reference
D	4	SER	-	expression tag	UNP P01137
D	107	GLN	ASN	conflict	UNP P01137
D	147	GLN	ASN	conflict	UNP P01137
G	-1	GLY	-	expression tag	UNP P01137
G	0	PRO	-	expression tag	UNP P01137
G	1	LEU	-	expression tag	UNP P01137
G	2	SER	-	expression tag	UNP P01137
G	3	THR	-	expression tag	UNP P01137
G	4	SER	-	expression tag	UNP P01137
G	107	GLN	ASN	conflict	UNP P01137
G	147	GLN	ASN	conflict	UNP P01137
H	-1	GLY	-	expression tag	UNP P01137
H	0	PRO	-	expression tag	UNP P01137
H	1	LEU	-	expression tag	UNP P01137
H	2	SER	-	expression tag	UNP P01137
H	3	THR	-	expression tag	UNP P01137
H	4	SER	-	expression tag	UNP P01137
H	107	GLN	ASN	conflict	UNP P01137
H	147	GLN	ASN	conflict	UNP P01137

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



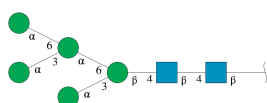
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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	J	6	Total	C	N	O	0	0	0
			72	40	2	30			
5	Q	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
6	K	7	Total	C	N	O	0	0	0
			83	46	2	35			
6	R	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



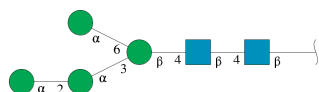
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	T	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 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
9	N	4	Total	C	N	O	0	0	0
			50	28	2	20			
9	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
9	U	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



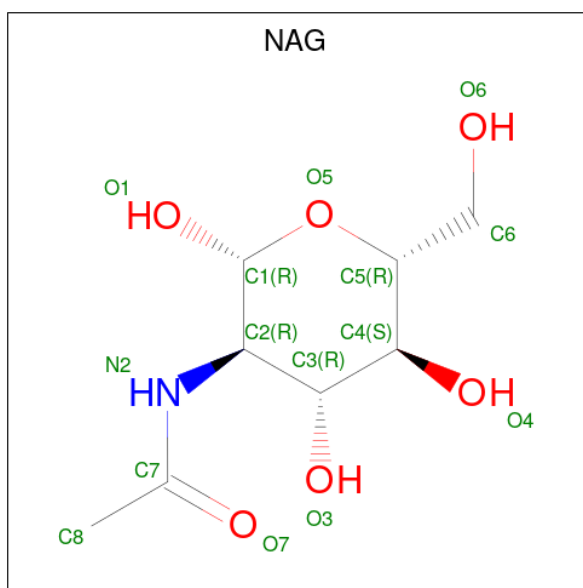
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	V	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total	Ca	0	0
			4	4		
11	E	4	Total	Ca	0	0
			4	4		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula: $C_8H_{15}NO_6$).



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

- Molecule 13 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	3	Total	Mn	0	0
			3	3		
13	F	3	Total	Mn	0	0
			3	3		

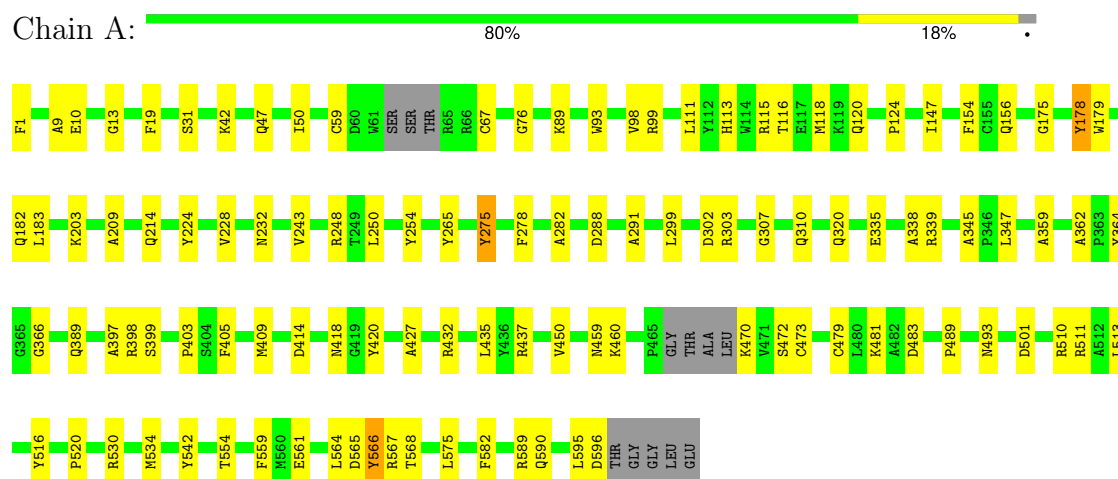
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	3	Total	O	0	0
			3	3		
14	F	2	Total	O	0	0
			2	2		

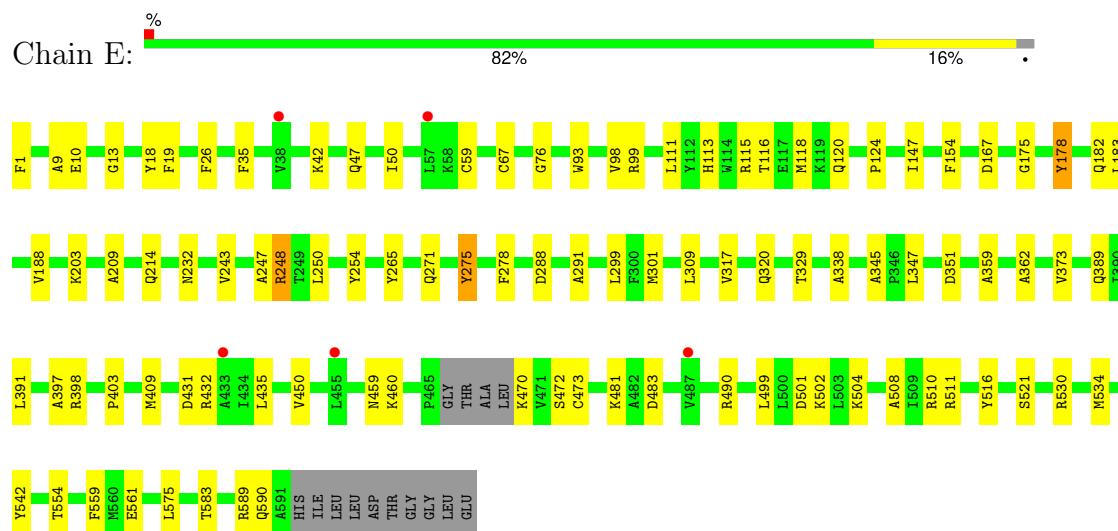
3 Residue-property plots [i](#)

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

• Molecule 1: Integrin alpha-V

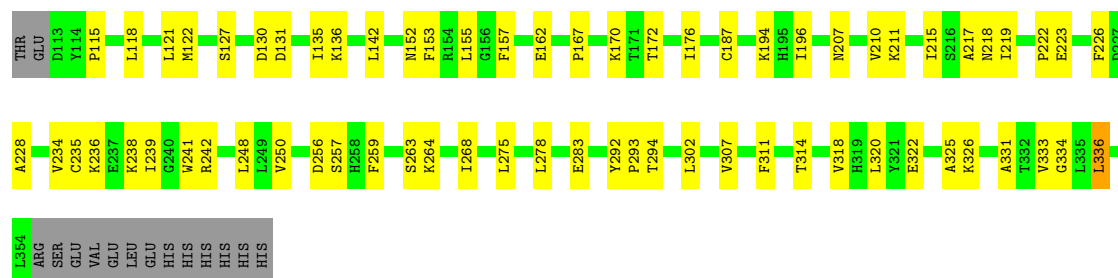


• Molecule 1: Integrin alpha-V



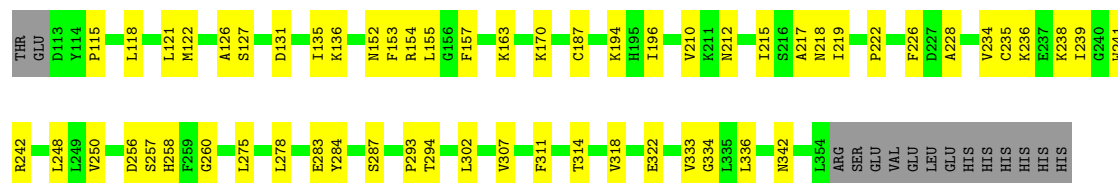
• Molecule 2: Integrin beta-6





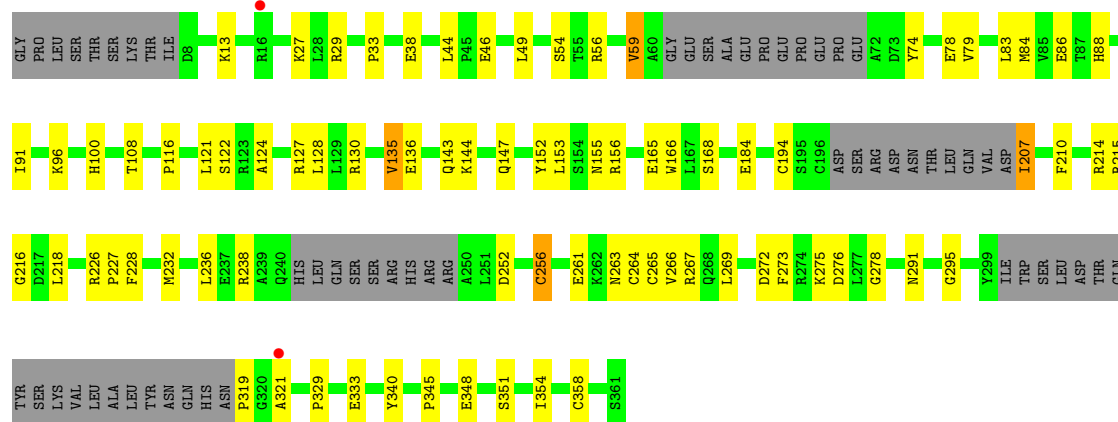
• Molecule 2: Integrin beta-6

Chain F: 72% 23% 6%



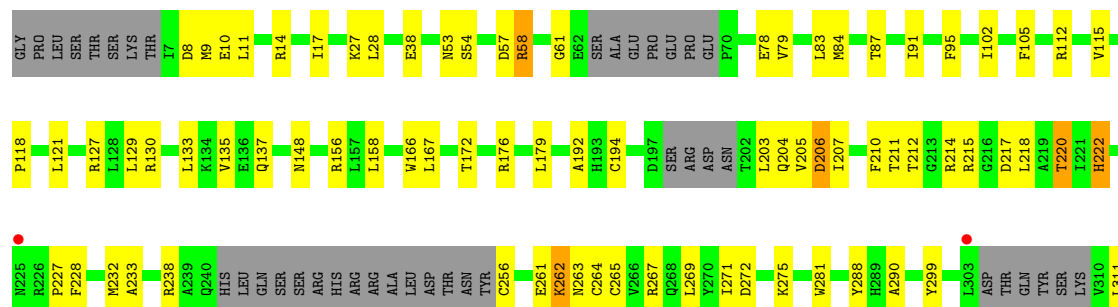
• Molecule 3: Transforming growth factor beta-1

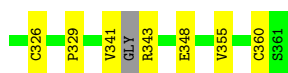
Chain C: 62% 21% 16%



• Molecule 3: Transforming growth factor beta-1

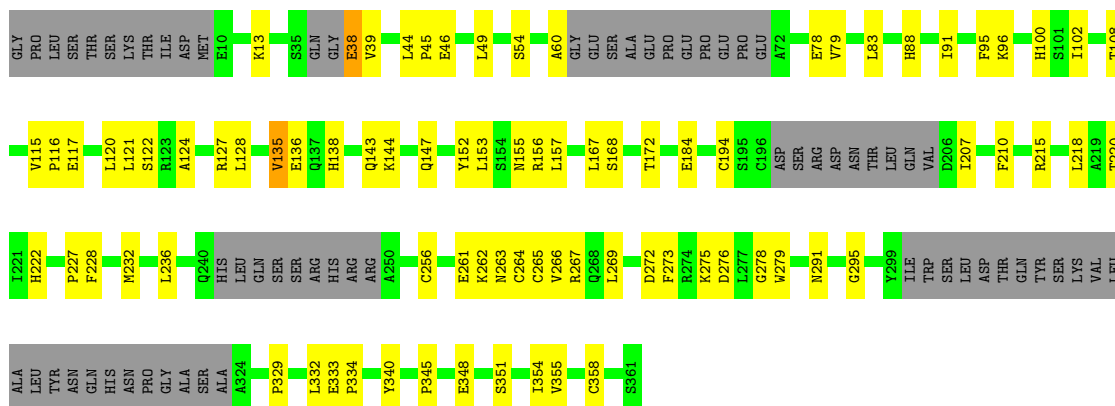
Chain D: 65% 22% 11%





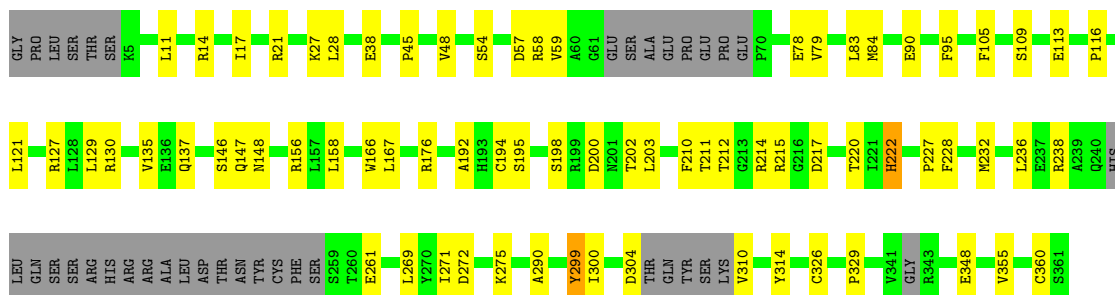
- Molecule 3: Transforming growth factor beta-1

Chain G: 59% 22% 18%



- Molecule 3: Transforming growth factor beta-1

Chain H: 69% 20% 10%



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

Chain I: 100%




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

Chain P: 67% 33%




- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[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

ido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%



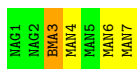
- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  67% 33%



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 K:  43% 43% 14%



- Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 R:  14% 43% 43%



- Molecule 7: 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 L:  50% 50%



- Molecule 7: 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:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



- Molecule 9: 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 N:  50% 50%



- Molecule 9: 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:  75% 25%




- Molecule 9: 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 U:  50% 50%



- Molecule 10: alpha-D-mannopyranose-(1-2)-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 V:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 91.44Å 131.03Å 89.98° 86.25° 89.85°	Depositor
Resolution (Å)	45.72 – 3.49 45.72 – 3.49	Depositor EDS
% Data completeness (in resolution range)	94.4 (45.72-3.49) 94.0 (45.72-3.49)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.224 , 0.277 0.228 , 0.282	Depositor DCC
R_{free} test set	1058 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	124.4	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 240.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.286 for -h,k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	23786	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: BMA, MN, NAG, MAN, CA

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	0.29	0/4672	0.49	1/6321 (0.0%)
1	E	0.28	0/4649	0.48	0/6291
2	B	0.35	0/1930	0.50	0/2618
2	F	0.32	1/1930 (0.1%)	0.44	0/2618
3	C	0.35	2/2501 (0.1%)	0.47	1/3381 (0.0%)
3	D	0.45	5/2650 (0.2%)	0.51	0/3585
3	G	0.37	2/2454 (0.1%)	0.45	0/3317
3	H	0.45	4/2672 (0.1%)	0.52	0/3616
All	All	0.35	14/23458 (0.1%)	0.48	2/31747 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	38	GLU	CG-CD	8.88	1.65	1.51
3	D	38	GLU	CG-CD	8.35	1.64	1.51
3	C	38	GLU	CG-CD	8.05	1.64	1.51
3	H	148	ASN	CB-CG	7.88	1.69	1.51
3	H	38	GLU	CB-CG	7.88	1.67	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	LEU	CA-CB-CG	7.55	132.66	115.30
3	C	319	PRO	N-CA-CB	5.96	110.45	103.30

There are no chirality outliers.

There are no planarity outliers.

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	4570	0	4414	74	0
1	E	4547	0	4388	60	0
2	B	1891	0	1866	48	0
2	F	1891	0	1866	33	0
3	C	2445	0	2435	51	0
3	D	2590	0	2580	55	0
3	G	2399	0	2394	52	0
3	H	2612	0	2608	45	0
4	I	39	0	34	0	0
4	P	39	0	34	0	0
5	J	72	0	61	5	0
5	Q	72	0	61	4	0
6	K	83	0	70	1	0
6	R	83	0	70	2	0
7	L	50	0	43	0	0
7	S	50	0	43	2	0
8	M	28	0	25	0	0
8	T	28	0	25	1	0
9	N	50	0	43	1	0
9	O	50	0	43	0	0
9	U	50	0	43	0	0
10	V	72	0	61	0	0
11	A	4	0	0	0	0
11	E	4	0	0	0	0
12	A	14	0	13	0	0
12	B	14	0	13	0	0
12	E	14	0	13	0	0
12	F	14	0	13	0	0
13	B	3	0	0	0	0
13	F	3	0	0	0	0
14	B	3	0	0	0	0
14	F	2	0	0	0	0
All	All	23786	0	23259	391	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 8.

The worst 5 of 391 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:HE	2:B:320:LEU:HD12	1.35	0.92
1:A:460:LYS:HB3	1:A:470:LYS:HB3	1.63	0.80
1:E:502:LYS:HE2	8:T:1:NAG:H81	1.65	0.79
3:C:100:HIS:HA	3:C:210:PHE:HB2	1.68	0.75
3:C:261:GLU:HG3	3:C:263:ASN:H	1.51	0.74

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	583/601 (97%)	548 (94%)	34 (6%)	1 (0%)	44	75
1	E	583/601 (97%)	552 (95%)	31 (5%)	0	100	100
2	B	240/257 (93%)	217 (90%)	23 (10%)	0	100	100
2	F	240/257 (93%)	218 (91%)	22 (9%)	0	100	100
3	C	295/363 (81%)	263 (89%)	30 (10%)	2 (1%)	19	53
3	D	310/363 (85%)	272 (88%)	35 (11%)	3 (1%)	13	46
3	G	285/363 (78%)	254 (89%)	28 (10%)	3 (1%)	12	45
3	H	315/363 (87%)	273 (87%)	39 (12%)	3 (1%)	13	46
All	All	2851/3168 (90%)	2597 (91%)	242 (8%)	12 (0%)	30	64

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	135	VAL
3	G	135	VAL
1	A	566	TYR
3	H	135	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	202	THR

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	483/491 (98%)	478 (99%)	5 (1%)	73	84
1	E	481/491 (98%)	475 (99%)	6 (1%)	67	82
2	B	215/230 (94%)	213 (99%)	2 (1%)	75	86
2	F	215/230 (94%)	213 (99%)	2 (1%)	75	86
3	C	268/323 (83%)	265 (99%)	3 (1%)	70	83
3	D	286/323 (88%)	278 (97%)	8 (3%)	38	65
3	G	265/323 (82%)	262 (99%)	3 (1%)	70	83
3	H	288/323 (89%)	281 (98%)	7 (2%)	44	68
All	All	2501/2734 (92%)	2465 (99%)	36 (1%)	62	79

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	256	CYS
3	H	314	TYR
3	H	95	PHE
3	H	198	SER
3	D	220	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	342	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 ⓘ

62 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	I	1	4,1	14,14,15	0.44	0	17,19,21	0.47	0
4	NAG	I	2	4	14,14,15	0.28	0	17,19,21	0.51	0
4	BMA	I	3	4	11,11,12	0.53	0	15,15,17	0.88	0
5	NAG	J	1	1,5	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	J	2	5	14,14,15	0.43	0	17,19,21	0.47	0
5	BMA	J	3	5	11,11,12	1.02	0	15,15,17	1.15	2 (13%)
5	MAN	J	4	5	11,11,12	0.77	0	15,15,17	1.27	2 (13%)
5	MAN	J	5	5	11,11,12	0.85	1 (9%)	15,15,17	1.10	2 (13%)
5	MAN	J	6	5	11,11,12	1.01	1 (9%)	15,15,17	1.02	1 (6%)
6	NAG	K	1	6,1	14,14,15	0.56	0	17,19,21	0.51	0
6	NAG	K	2	6	14,14,15	0.33	0	17,19,21	0.47	0
6	BMA	K	3	6	11,11,12	0.72	0	15,15,17	1.14	1 (6%)
6	MAN	K	4	6	11,11,12	1.15	2 (18%)	15,15,17	1.91	3 (20%)
6	MAN	K	5	6	11,11,12	0.77	0	15,15,17	0.81	0
6	MAN	K	6	6	11,11,12	0.78	0	15,15,17	1.02	2 (13%)
6	MAN	K	7	6	11,11,12	0.68	0	15,15,17	0.99	1 (6%)
7	NAG	L	1	1,7	14,14,15	0.22	0	17,19,21	0.39	0
7	NAG	L	2	7	14,14,15	0.29	0	17,19,21	0.46	0
7	BMA	L	3	7	11,11,12	0.70	0	15,15,17	1.15	1 (6%)
7	MAN	L	4	7	11,11,12	0.75	1 (9%)	15,15,17	1.26	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	M	1	1,8	14,14,15	0.42	0	17,19,21	0.48	0
8	NAG	M	2	8	14,14,15	0.38	0	17,19,21	0.49	0
9	NAG	N	1	3,9	14,14,15	0.41	0	17,19,21	0.43	0
9	NAG	N	2	9	14,14,15	0.38	0	17,19,21	0.59	0
9	BMA	N	3	9	11,11,12	0.58	0	15,15,17	0.81	0
9	MAN	N	4	9	11,11,12	0.85	0	15,15,17	1.02	1 (6%)
9	NAG	O	1	3,9	14,14,15	0.39	0	17,19,21	0.57	0
9	NAG	O	2	9	14,14,15	0.33	0	17,19,21	0.35	0
9	BMA	O	3	9	11,11,12	0.55	0	15,15,17	0.86	0
9	MAN	O	4	9	11,11,12	0.56	0	15,15,17	1.06	2 (13%)
4	NAG	P	1	4,1	14,14,15	0.34	0	17,19,21	0.47	0
4	NAG	P	2	4	14,14,15	0.50	0	17,19,21	0.59	0
4	BMA	P	3	4	11,11,12	0.63	0	15,15,17	0.99	1 (6%)
5	NAG	Q	1	1,5	14,14,15	0.31	0	17,19,21	0.45	0
5	NAG	Q	2	5	14,14,15	0.43	0	17,19,21	0.49	0
5	BMA	Q	3	5	11,11,12	1.03	0	15,15,17	1.14	2 (13%)
5	MAN	Q	4	5	11,11,12	0.79	0	15,15,17	1.25	2 (13%)
5	MAN	Q	5	5	11,11,12	0.76	0	15,15,17	1.06	1 (6%)
5	MAN	Q	6	5	11,11,12	1.04	1 (9%)	15,15,17	1.02	1 (6%)
6	NAG	R	1	6,1	14,14,15	0.61	1 (7%)	17,19,21	0.55	0
6	NAG	R	2	6	14,14,15	0.29	0	17,19,21	0.42	0
6	BMA	R	3	6	11,11,12	0.65	0	15,15,17	1.10	1 (6%)
6	MAN	R	4	6	11,11,12	1.20	2 (18%)	15,15,17	1.94	3 (20%)
6	MAN	R	5	6	11,11,12	0.82	1 (9%)	15,15,17	0.82	1 (6%)
6	MAN	R	6	6	11,11,12	0.91	0	15,15,17	1.06	2 (13%)
6	MAN	R	7	6	11,11,12	0.67	0	15,15,17	0.98	2 (13%)
7	NAG	S	1	1,7	14,14,15	0.23	0	17,19,21	0.39	0
7	NAG	S	2	7	14,14,15	0.23	0	17,19,21	0.46	0
7	BMA	S	3	7	11,11,12	0.81	0	15,15,17	1.17	1 (6%)
7	MAN	S	4	7	11,11,12	0.74	0	15,15,17	1.37	2 (13%)
8	NAG	T	1	1,8	14,14,15	0.55	0	17,19,21	0.37	0
8	NAG	T	2	8	14,14,15	0.34	0	17,19,21	0.45	0
9	NAG	U	1	3,9	14,14,15	0.51	0	17,19,21	0.59	0
9	NAG	U	2	9	14,14,15	0.35	0	17,19,21	0.63	0
9	BMA	U	3	9	11,11,12	1.21	2 (18%)	15,15,17	1.15	1 (6%)
9	MAN	U	4	9	11,11,12	1.14	1 (9%)	15,15,17	1.52	3 (20%)
10	NAG	V	1	3,10	14,14,15	0.33	0	17,19,21	0.64	0
10	NAG	V	2	10	14,14,15	0.38	0	17,19,21	0.43	0
10	BMA	V	3	10	11,11,12	1.31	1 (9%)	15,15,17	1.19	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	V	4	10	11,11,12	1.56	2 (18%)	15,15,17	1.34	2 (13%)
10	MAN	V	5	10	11,11,12	0.69	0	15,15,17	0.97	2 (13%)
10	MAN	V	6	10	11,11,12	0.88	1 (9%)	15,15,17	1.17	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	BMA	I	3	4	-	2/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	1/2/19/22	0/1/1/1
5	MAN	J	5	5	-	2/2/19/22	0/1/1/1
5	MAN	J	6	5	-	2/2/19/22	0/1/1/1
6	NAG	K	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	3/6/23/26	0/1/1/1
6	BMA	K	3	6	-	2/2/19/22	0/1/1/1
6	MAN	K	4	6	-	1/2/19/22	0/1/1/1
6	MAN	K	5	6	-	0/2/19/22	0/1/1/1
6	MAN	K	6	6	-	0/2/19/22	0/1/1/1
6	MAN	K	7	6	-	0/2/19/22	0/1/1/1
7	NAG	L	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/23/26	0/1/1/1
7	BMA	L	3	7	-	1/2/19/22	0/1/1/1
7	MAN	L	4	7	-	0/2/19/22	1/1/1/1
8	NAG	M	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
9	NAG	N	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	N	2	9	-	2/6/23/26	0/1/1/1
9	BMA	N	3	9	-	0/2/19/22	0/1/1/1
9	MAN	N	4	9	-	2/2/19/22	0/1/1/1
9	NAG	O	1	3,9	-	4/6/23/26	0/1/1/1
9	NAG	O	2	9	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BMA	O	3	9	-	2/2/19/22	0/1/1/1
9	MAN	O	4	9	-	0/2/19/22	0/1/1/1
4	NAG	P	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	BMA	P	3	4	-	2/2/19/22	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	0/2/19/22	0/1/1/1
5	MAN	Q	4	5	-	1/2/19/22	0/1/1/1
5	MAN	Q	5	5	-	2/2/19/22	0/1/1/1
5	MAN	Q	6	5	-	2/2/19/22	0/1/1/1
6	NAG	R	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	3/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1
6	MAN	R	5	6	-	0/2/19/22	0/1/1/1
6	MAN	R	6	6	-	0/2/19/22	0/1/1/1
6	MAN	R	7	6	-	0/2/19/22	0/1/1/1
7	NAG	S	1	1,7	-	4/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
8	NAG	T	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	2/6/23/26	0/1/1/1
9	NAG	U	1	3,9	-	1/6/23/26	0/1/1/1
9	NAG	U	2	9	-	2/6/23/26	0/1/1/1
9	BMA	U	3	9	-	0/2/19/22	0/1/1/1
9	MAN	U	4	9	-	2/2/19/22	0/1/1/1
10	NAG	V	1	3,10	-	4/6/23/26	0/1/1/1
10	NAG	V	2	10	-	2/6/23/26	0/1/1/1
10	BMA	V	3	10	-	2/2/19/22	0/1/1/1
10	MAN	V	4	10	-	2/2/19/22	0/1/1/1
10	MAN	V	5	10	-	1/2/19/22	0/1/1/1
10	MAN	V	6	10	-	2/2/19/22	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	4	MAN	C1-C2	3.64	1.60	1.52
10	V	4	MAN	C2-C3	3.59	1.58	1.52
6	R	4	MAN	C2-C3	2.59	1.56	1.52
10	V	3	BMA	C4-C5	2.58	1.58	1.53
5	J	6	MAN	C1-C2	2.53	1.58	1.52

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	4	MAN	C1-O5-C5	4.67	118.45	112.19
6	K	4	MAN	C1-O5-C5	4.44	118.13	112.19
7	S	4	MAN	C1-O5-C5	4.07	117.64	112.19
6	R	4	MAN	C1-C2-C3	3.82	115.21	109.64
6	K	4	MAN	C1-C2-C3	3.78	115.14	109.64

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	O	3	BMA	O5-C5-C6-O6
8	M	2	NAG	O5-C5-C6-O6
10	V	3	BMA	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	4	MAN	C1-C2-C3-C4-C5-O5

17 monomers are involved in 16 short contacts:

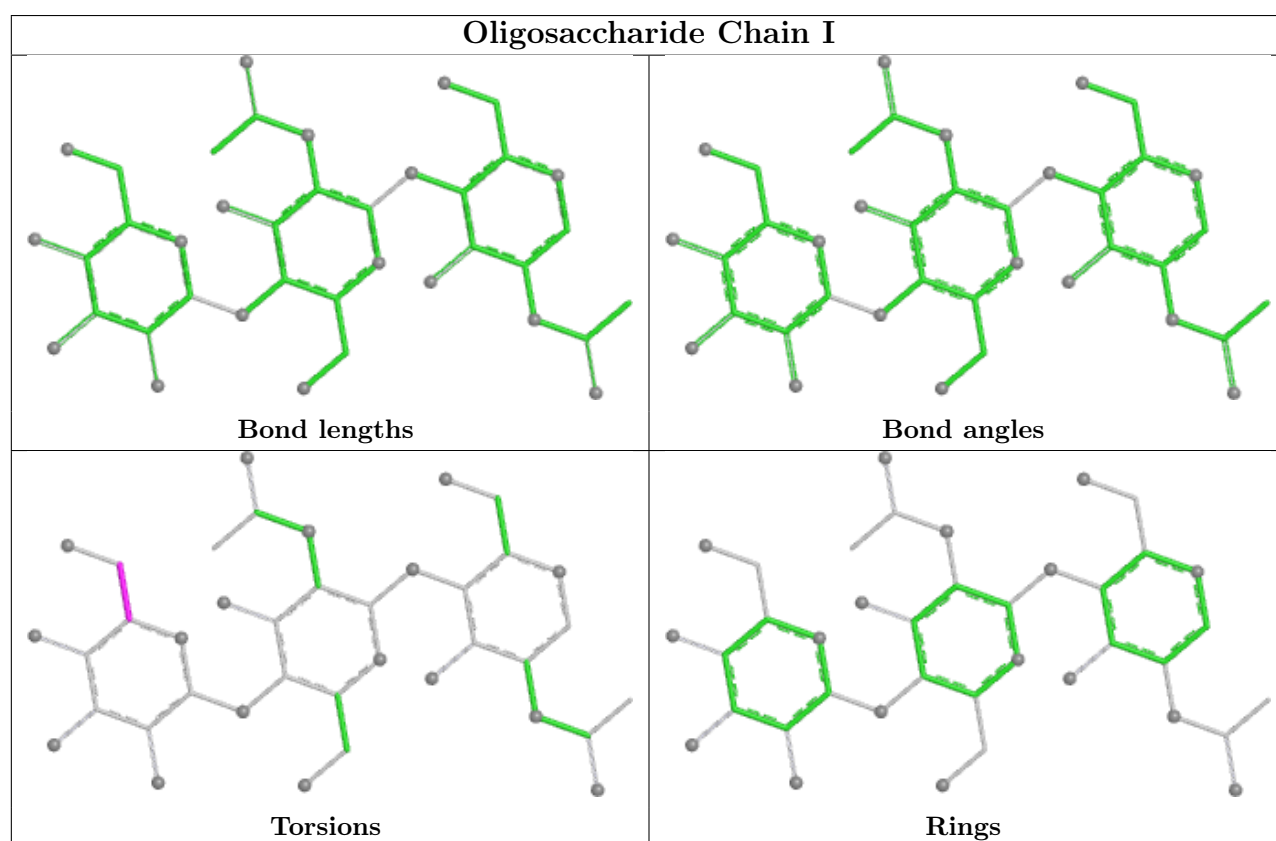
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	S	1	NAG	2	0
9	N	1	NAG	1	0
6	R	6	MAN	1	0
5	J	3	BMA	1	0
5	Q	2	NAG	3	0
5	Q	1	NAG	1	0
7	S	2	NAG	2	0
6	K	3	BMA	1	0
8	T	1	NAG	1	0

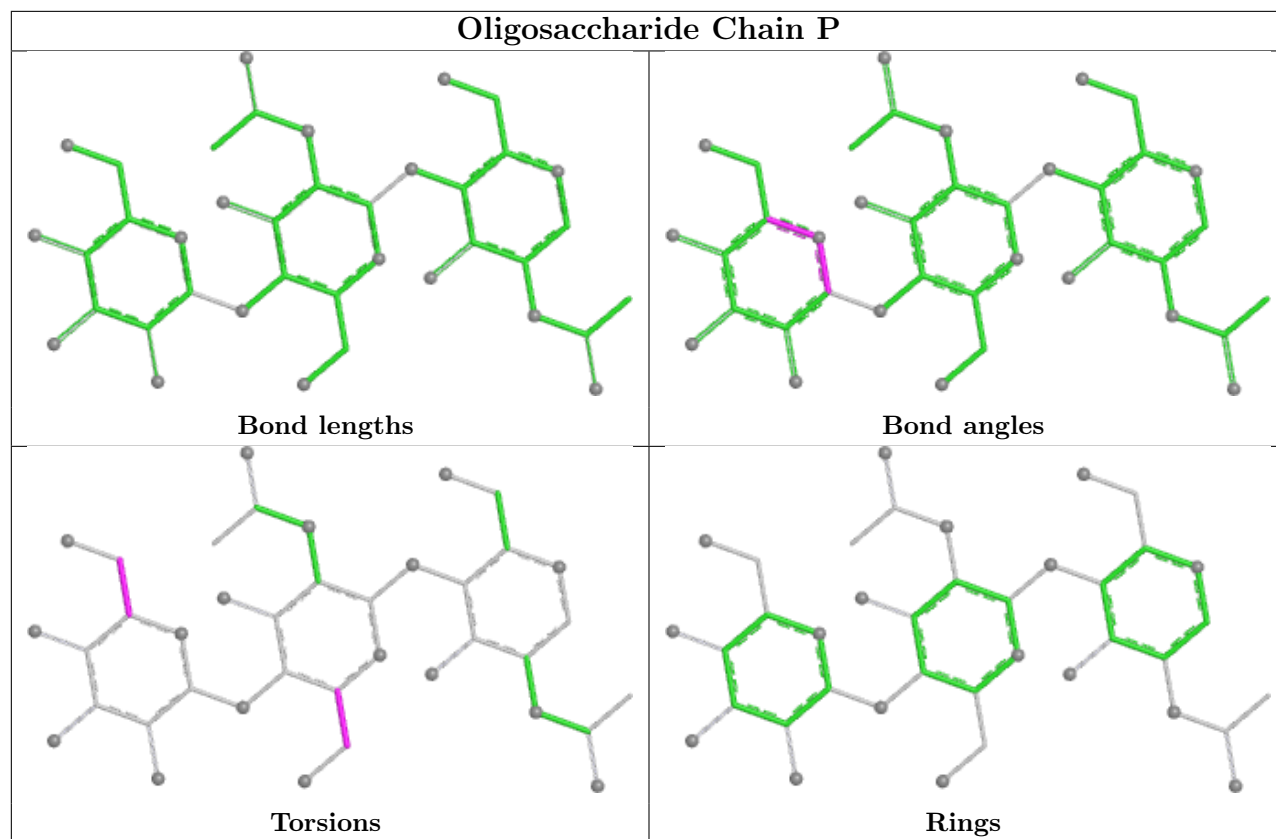
Continued on next page...

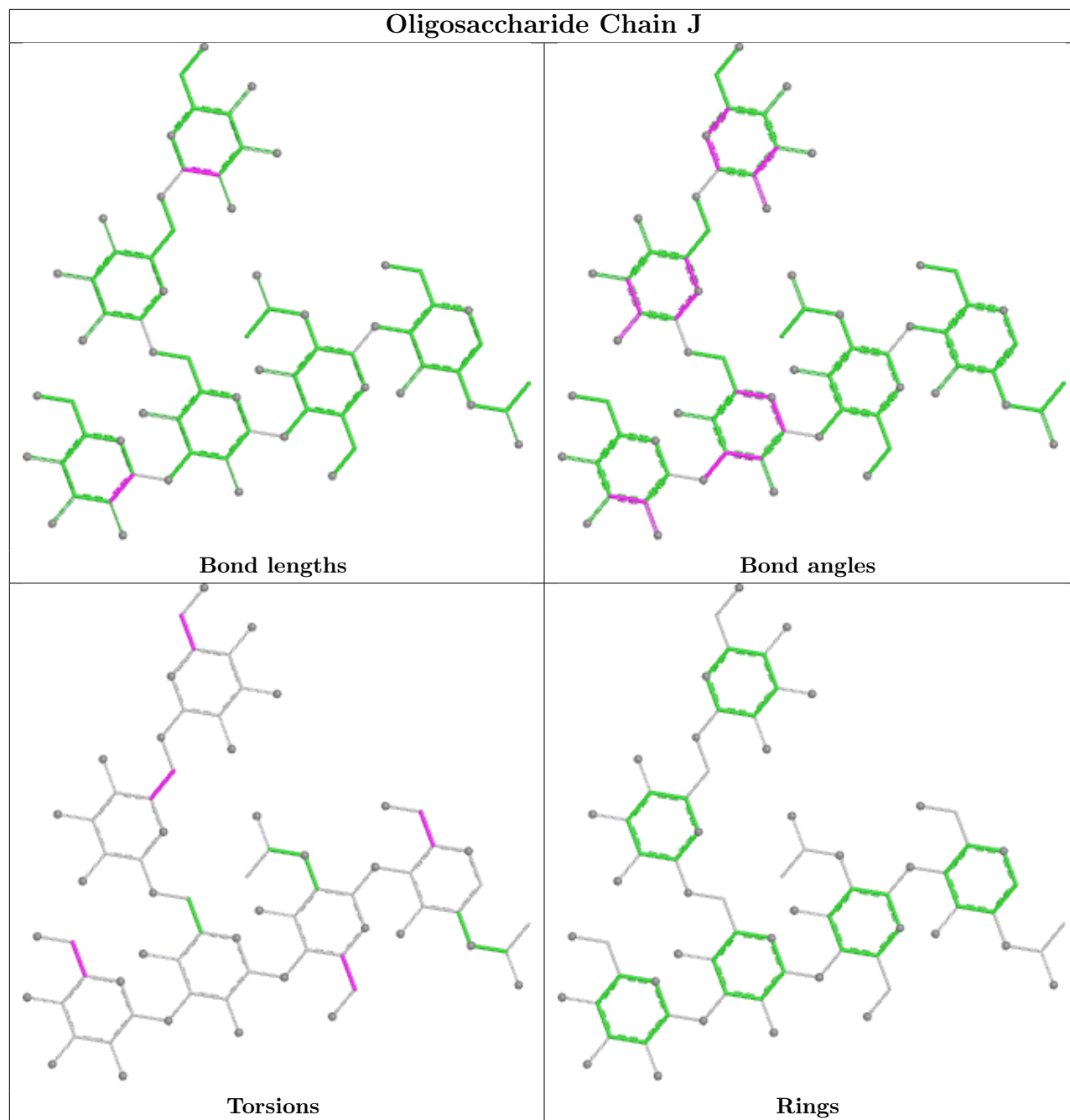
Continued from previous page...

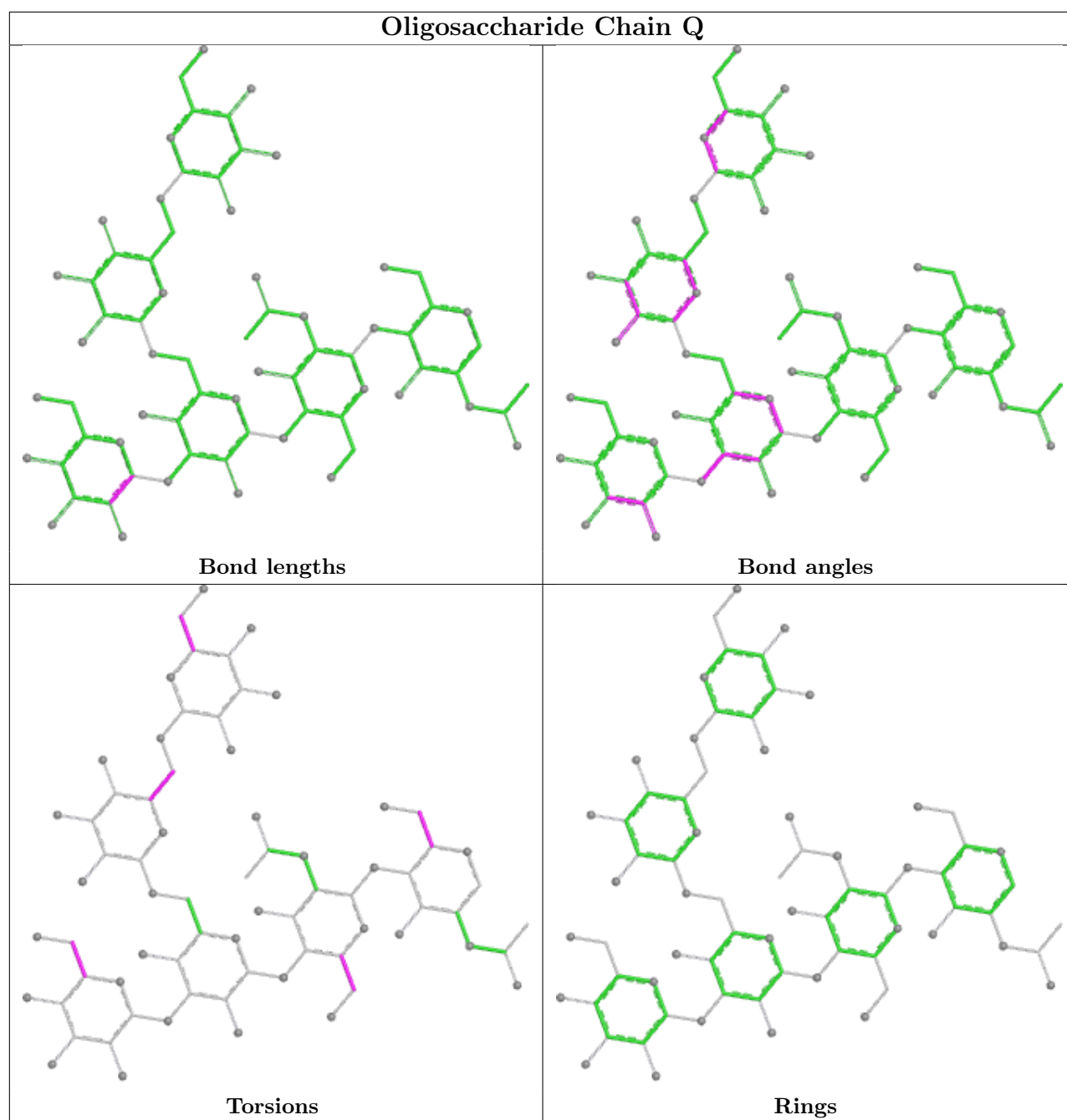
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	3	BMA	1	0
5	J	5	MAN	2	0
5	J	1	NAG	1	0
6	R	4	MAN	1	0
5	Q	5	MAN	1	0
5	J	4	MAN	1	0
5	J	2	NAG	3	0
5	Q	3	BMA	1	0

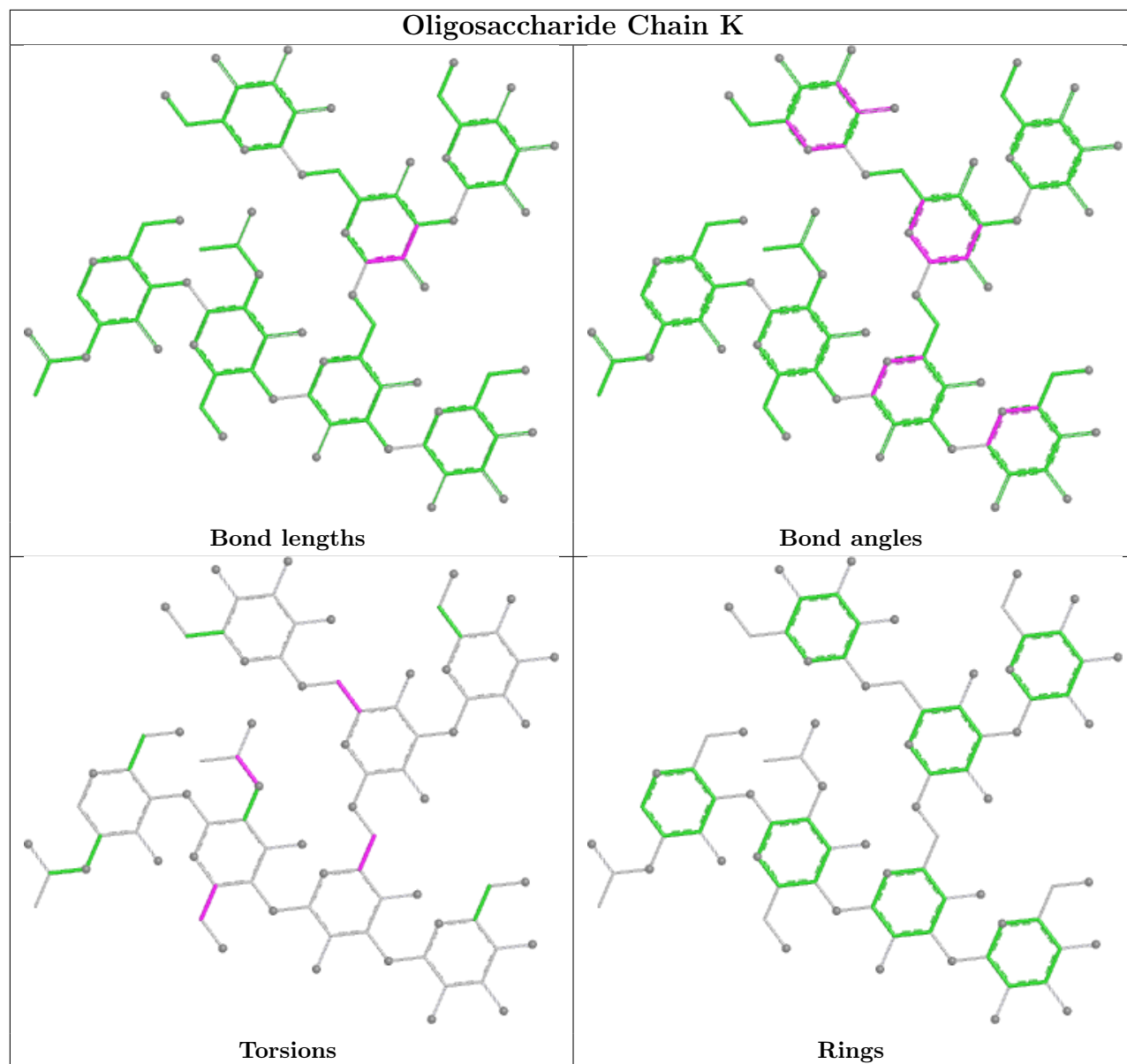
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

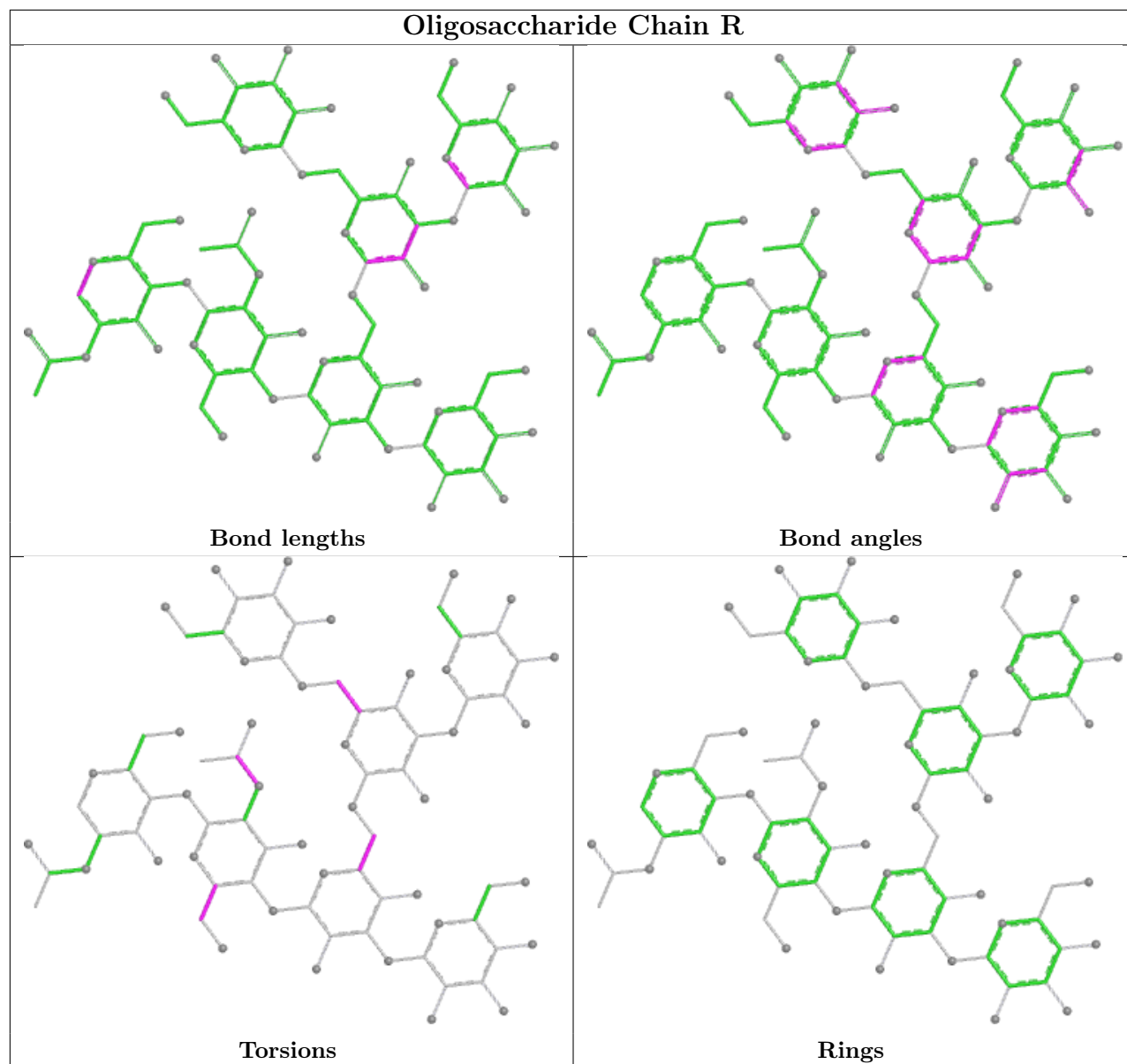


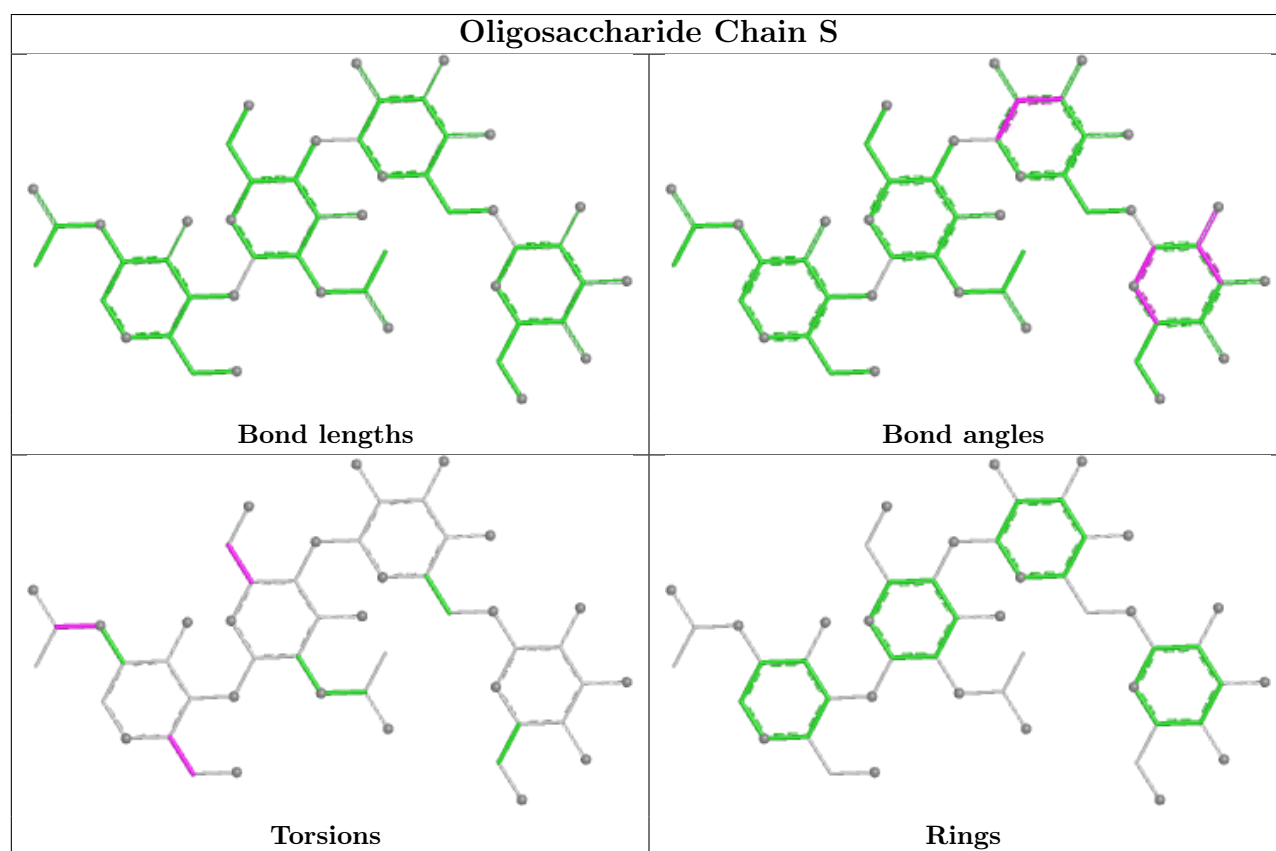
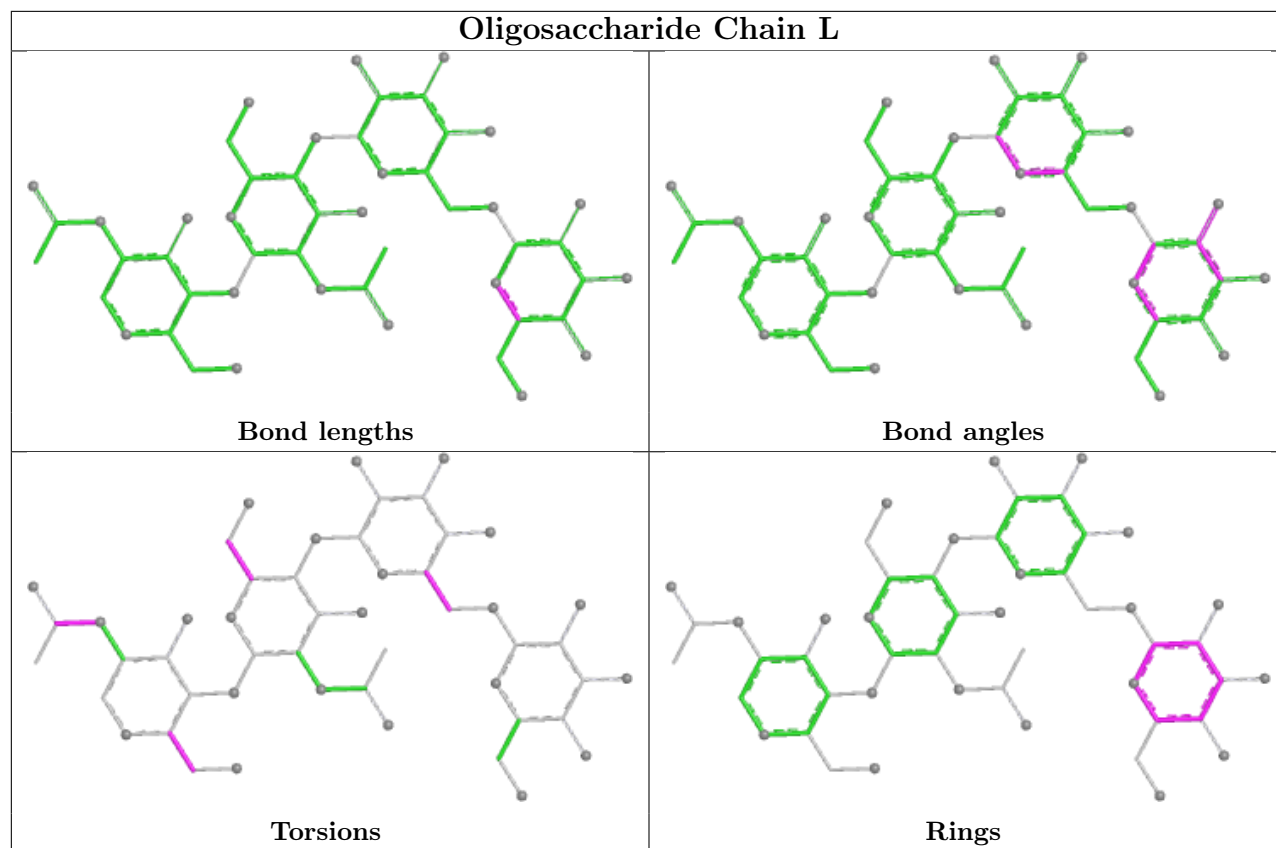


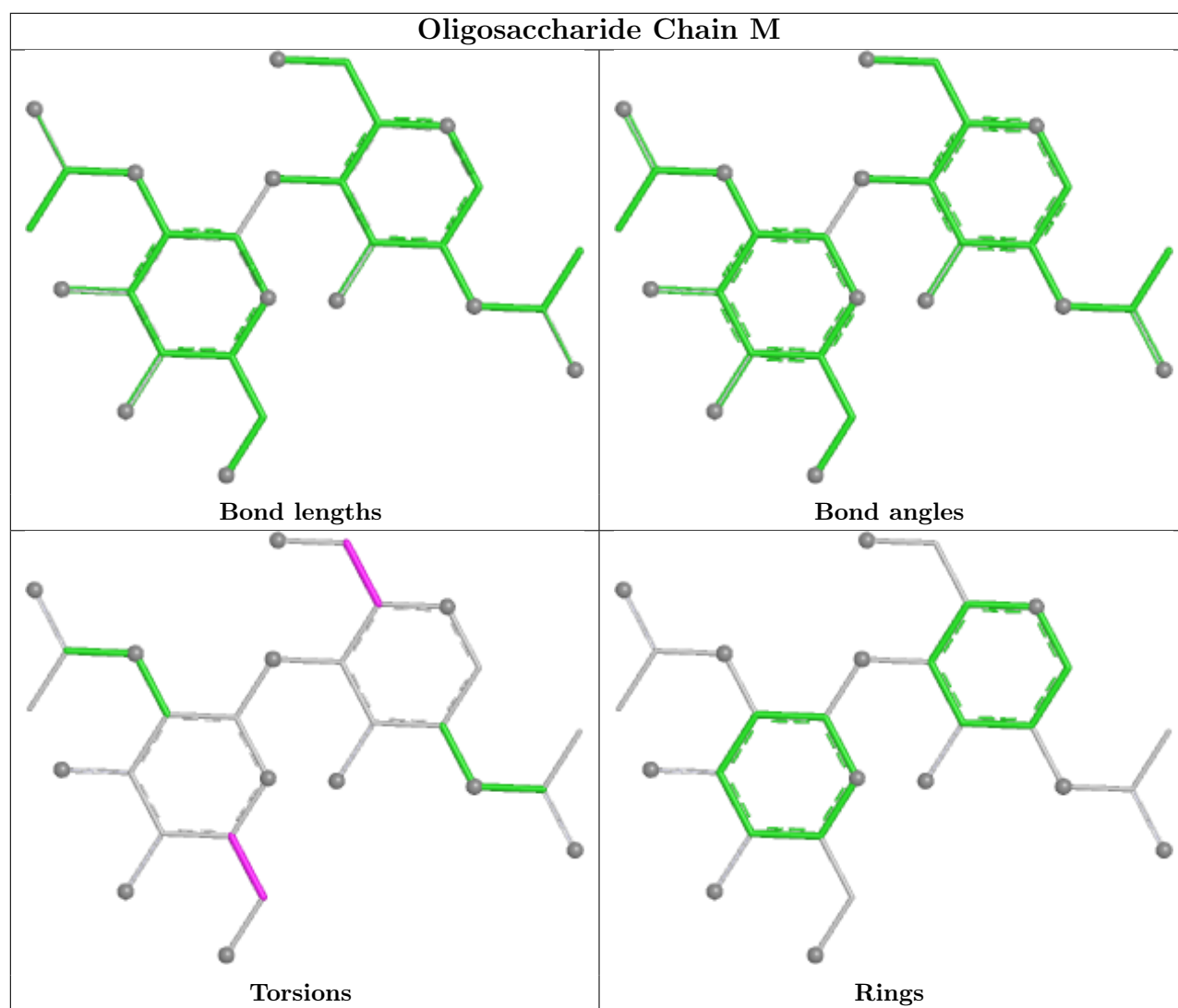


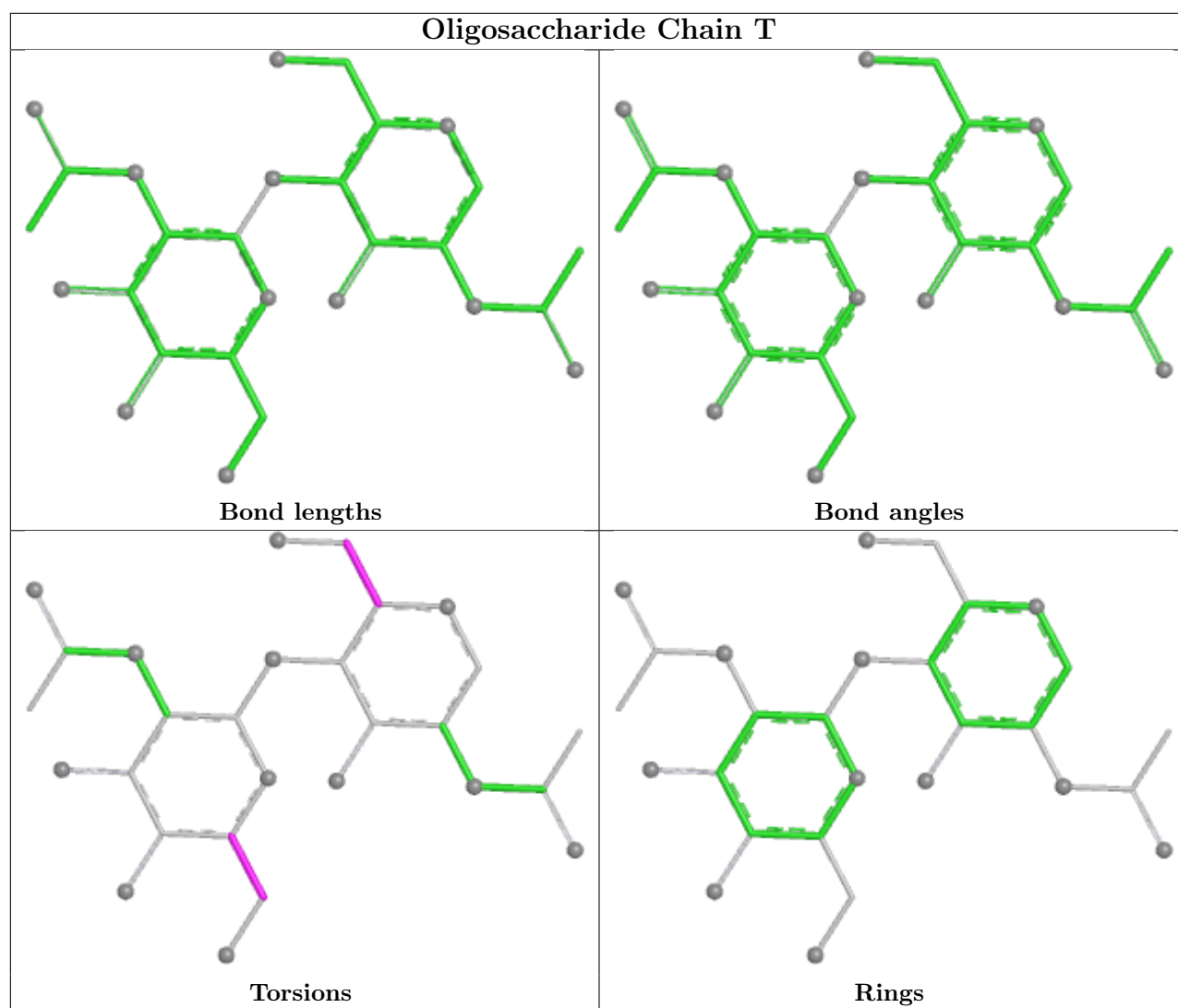


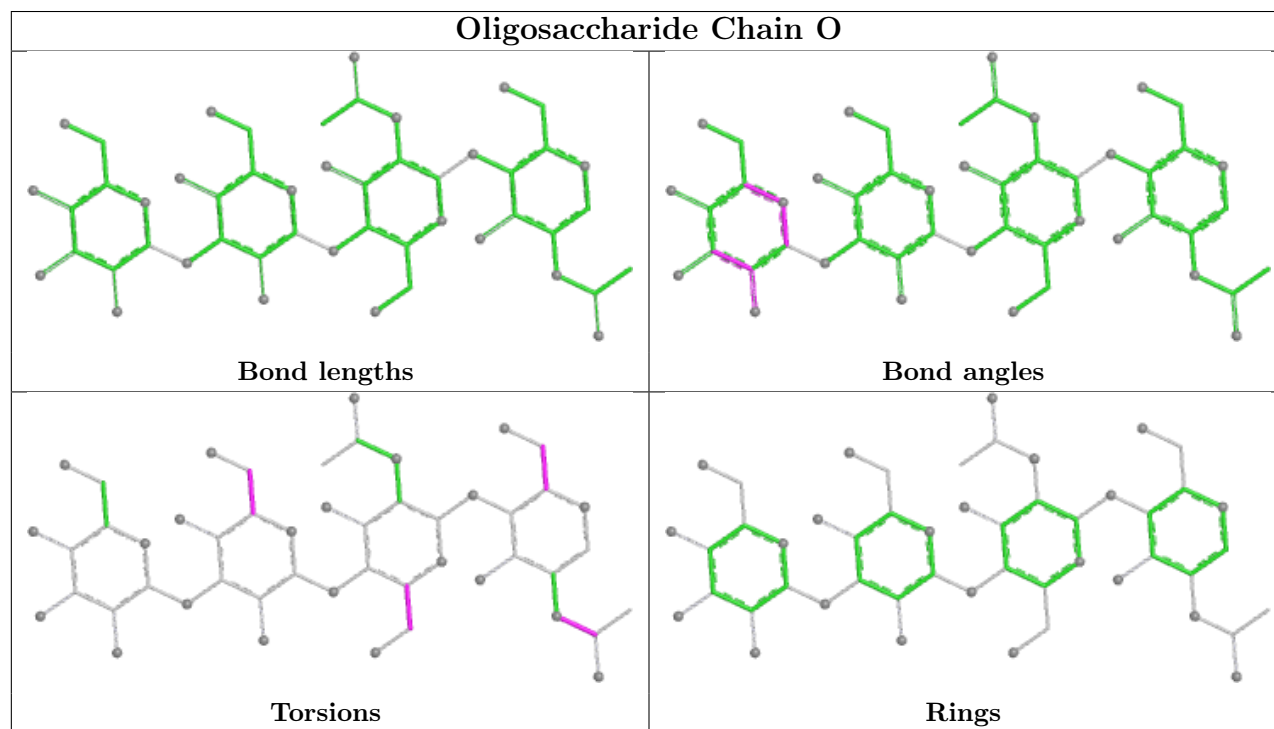
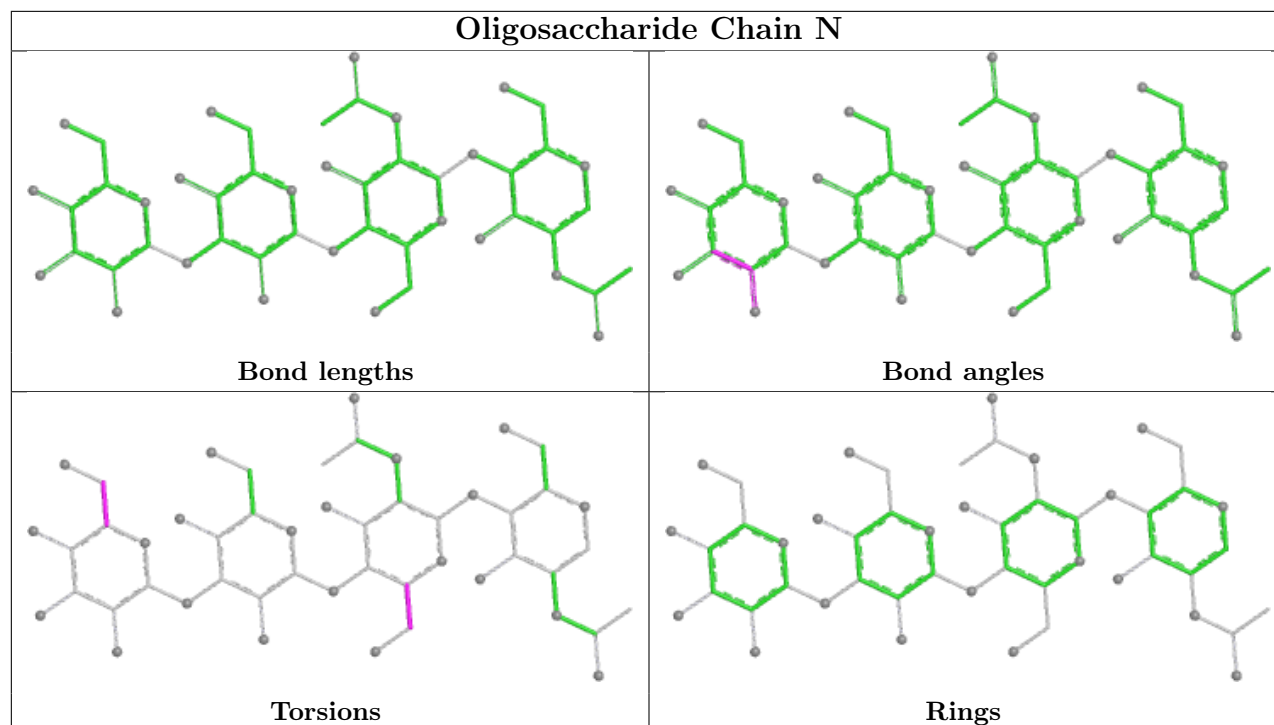




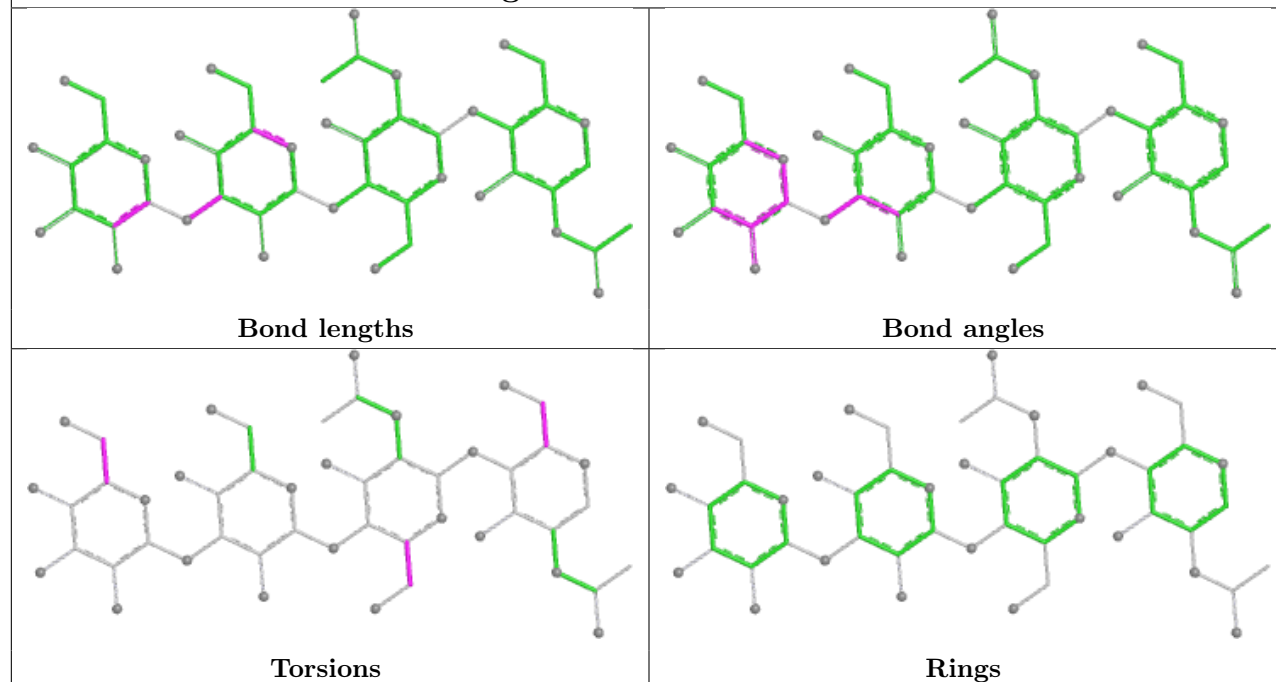




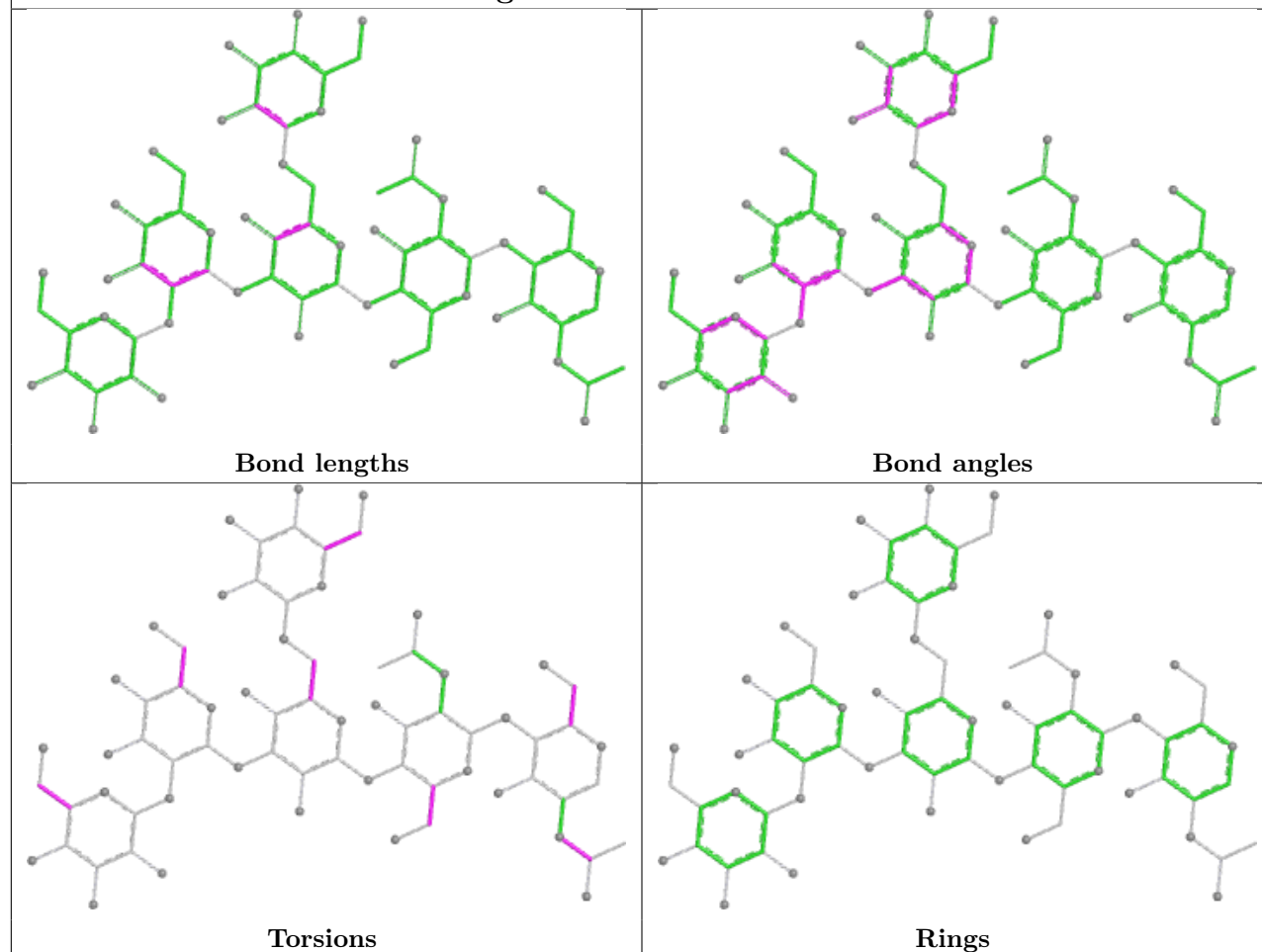




Oligosaccharide Chain U



Oligosaccharide Chain V



5.6 Ligand geometry

Of 18 ligands modelled in this entry, 14 are monoatomic - leaving 4 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	$\# Z > 2$
12	NAG	F	2004	2	14,14,15	0.22	0	17,19,21	0.34	0
12	NAG	B	2004	2	14,14,15	0.35	0	17,19,21	0.39	0
12	NAG	A	2025	1	14,14,15	0.58	0	17,19,21	0.40	0
12	NAG	E	2025	1	14,14,15	0.66	0	17,19,21	0.40	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
12	NAG	F	2004	2	-	2/6/23/26	0/1/1/1
12	NAG	B	2004	2	-	1/6/23/26	0/1/1/1
12	NAG	A	2025	1	-	2/6/23/26	0/1/1/1
12	NAG	E	2025	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	2004	NAG	O5-C5-C6-O6
12	A	2025	NAG	C4-C5-C6-O6
12	A	2025	NAG	O5-C5-C6-O6
12	B	2004	NAG	O5-C5-C6-O6
12	F	2004	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	589/601 (98%)	-0.70	0 100 100	133, 206, 281, 311	0
1	E	587/601 (97%)	-0.90	5 (0%) 81 64	139, 222, 286, 333	0
2	B	242/257 (94%)	-0.76	0 100 100	63, 146, 259, 309	0
2	F	242/257 (94%)	-0.95	0 100 100	171, 224, 261, 287	0
3	C	305/363 (84%)	-0.86	2 (0%) 84 69	159, 243, 294, 338	0
3	D	322/363 (88%)	-1.04	2 (0%) 85 72	158, 225, 274, 300	0
3	G	297/363 (81%)	-0.98	0 100 100	127, 227, 284, 315	0
3	H	325/363 (89%)	-1.01	0 100 100	133, 202, 256, 273	0
All	All	2909/3168 (91%)	-0.88	9 (0%) 90 82	63, 219, 280, 338	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	38	VAL	3.5
1	E	487	VAL	3.5
1	E	455	LEU	3.5
3	D	303	LEU	2.7
3	C	321	ALA	2.4

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
8	NAG	M	2	14/15	0.91	0.05	189,242,281,286	0
6	MAN	K	4	11/12	0.92	0.06	187,214,265,277	0
4	BMA	P	3	11/12	0.92	0.06	195,223,230,231	0
9	BMA	U	3	11/12	0.93	0.04	207,247,255,268	0
10	MAN	V	5	11/12	0.93	0.07	182,265,283,288	0
5	MAN	J	6	11/12	0.94	0.04	144,256,279,288	0
9	MAN	N	4	11/12	0.94	0.05	206,239,263,266	0
6	MAN	R	5	11/12	0.94	0.07	216,259,290,308	0
10	BMA	V	3	11/12	0.94	0.05	204,259,281,282	0
7	NAG	S	2	14/15	0.94	0.06	251,293,309,313	0
6	MAN	K	7	11/12	0.95	0.05	167,197,224,249	0
6	MAN	R	4	11/12	0.95	0.04	205,229,252,264	0
9	NAG	O	1	14/15	0.95	0.09	193,229,252,259	0
6	NAG	K	1	14/15	0.95	0.06	157,208,243,252	0
7	NAG	S	1	14/15	0.95	0.06	255,303,326,328	0
10	MAN	V	4	11/12	0.95	0.08	241,259,269,273	0
5	MAN	Q	5	11/12	0.95	0.06	170,229,254,263	0
10	MAN	V	6	11/12	0.95	0.05	227,249,268,271	0
5	NAG	J	1	14/15	0.96	0.09	188,238,257,265	0
5	MAN	Q	6	11/12	0.96	0.05	228,253,286,286	0
7	MAN	S	4	11/12	0.96	0.04	260,296,321,322	0
5	NAG	J	2	14/15	0.96	0.05	251,285,298,299	0
8	NAG	T	1	14/15	0.96	0.06	256,296,331,332	0
9	NAG	N	2	14/15	0.96	0.05	257,291,310,311	0
5	BMA	J	3	11/12	0.96	0.05	242,283,305,308	0
5	MAN	J	4	11/12	0.96	0.06	238,258,280,291	0
9	NAG	O	2	14/15	0.96	0.07	188,213,241,242	0
9	BMA	O	3	11/12	0.96	0.06	193,230,238,242	0
9	MAN	O	4	11/12	0.96	0.07	156,208,226,234	0
9	NAG	U	2	14/15	0.96	0.05	202,251,281,284	0
4	BMA	I	3	11/12	0.96	0.07	181,242,253,260	0
9	MAN	U	4	11/12	0.96	0.04	210,251,267,270	0
5	BMA	Q	3	11/12	0.96	0.04	260,279,289,294	0
6	MAN	R	6	11/12	0.96	0.08	236,241,265,267	0
7	BMA	L	3	11/12	0.96	0.05	279,294,313,321	0
7	MAN	L	4	11/12	0.96	0.05	223,243,287,291	0
9	BMA	N	3	11/12	0.97	0.06	246,266,287,288	0
6	MAN	R	7	11/12	0.97	0.04	208,229,241,241	0
6	NAG	K	2	14/15	0.97	0.06	165,185,197,203	0
4	NAG	I	2	14/15	0.97	0.08	194,225,238,255	0
6	MAN	K	5	11/12	0.97	0.11	257,283,289,293	0

Continued on next page...

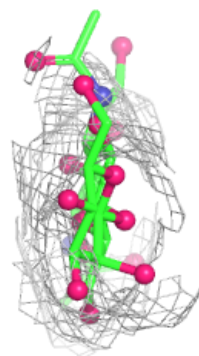
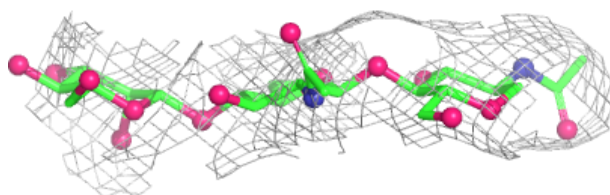
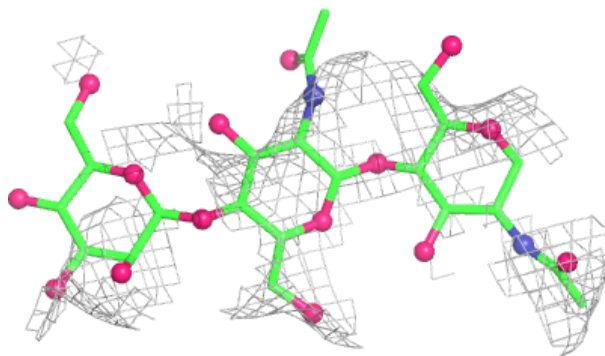
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MAN	Q	4	11/12	0.97	0.07	224,281,298,305	0
9	NAG	U	1	14/15	0.97	0.04	231,270,278,279	0
7	BMA	S	3	11/12	0.97	0.05	268,283,319,345	0
6	NAG	R	1	14/15	0.97	0.06	157,187,255,258	0
8	NAG	M	1	14/15	0.97	0.04	170,256,290,295	0
4	NAG	P	2	14/15	0.97	0.05	181,186,204,214	0
5	NAG	Q	1	14/15	0.97	0.08	210,229,277,283	0
8	NAG	T	2	14/15	0.97	0.04	251,324,342,342	0
5	NAG	Q	2	14/15	0.97	0.04	223,250,271,275	0
7	NAG	L	2	14/15	0.98	0.07	253,281,301,303	0
4	NAG	I	1	14/15	0.98	0.07	155,202,243,244	0
4	NAG	P	1	14/15	0.98	0.04	157,203,222,230	0
10	NAG	V	2	14/15	0.98	0.05	215,238,266,275	0
5	MAN	J	5	11/12	0.98	0.06	210,237,246,247	0
6	BMA	K	3	11/12	0.98	0.04	117,192,216,216	0
9	NAG	N	1	14/15	0.98	0.03	181,240,272,278	0
7	NAG	L	1	14/15	0.98	0.10	239,291,308,308	0
6	BMA	R	3	11/12	0.99	0.04	190,205,228,232	0
6	MAN	K	6	11/12	0.99	0.10	210,220,237,246	0
10	NAG	V	1	14/15	0.99	0.08	178,216,248,264	0
6	NAG	R	2	14/15	0.99	0.06	156,199,262,266	0

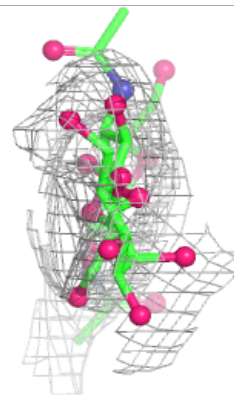
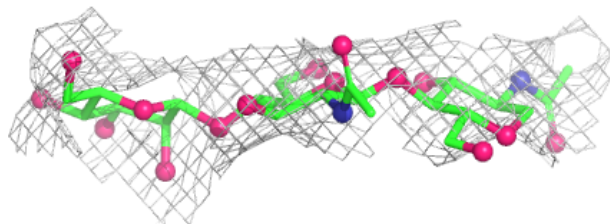
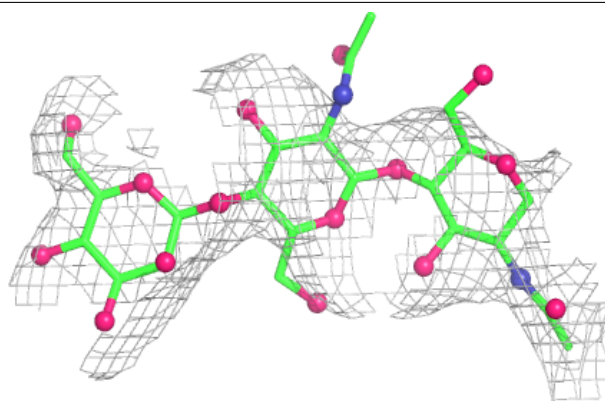
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

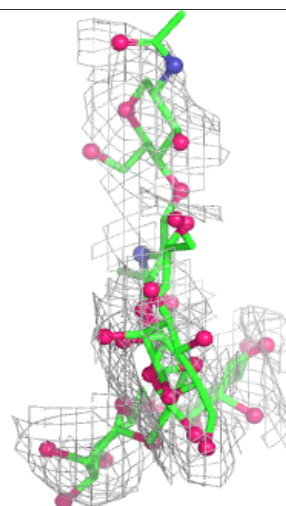
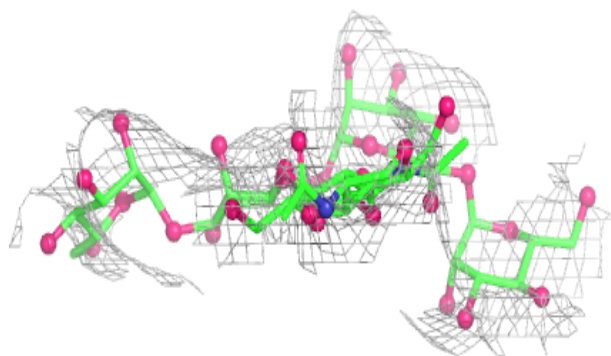
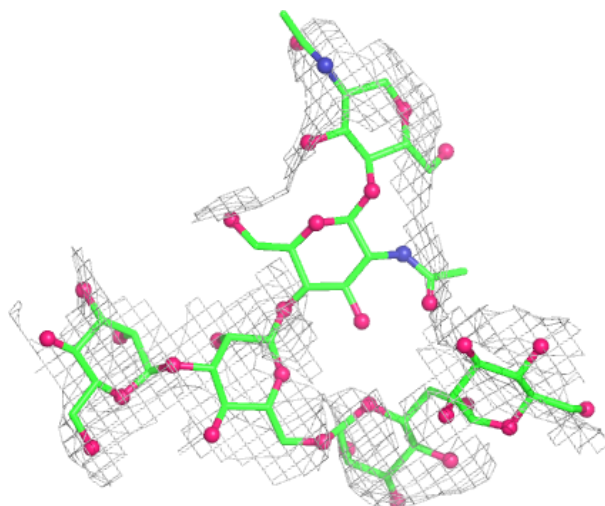
**Electron density around Chain P:**

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



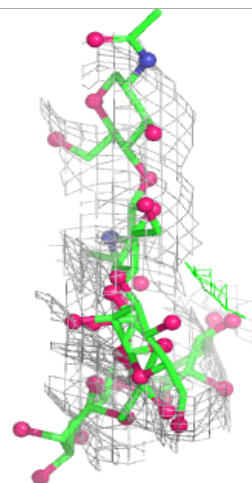
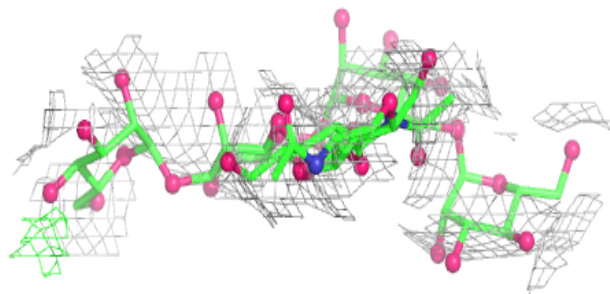
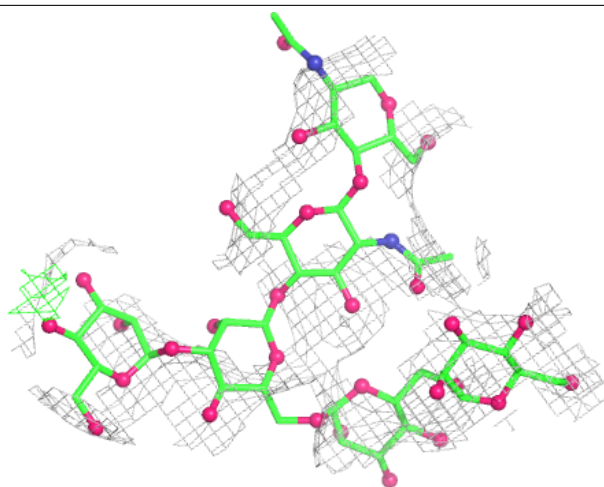
Electron density around Chain J:

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



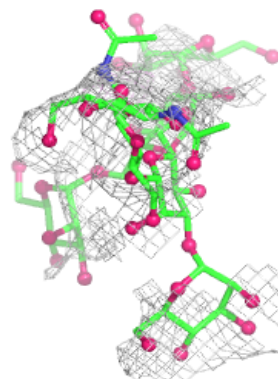
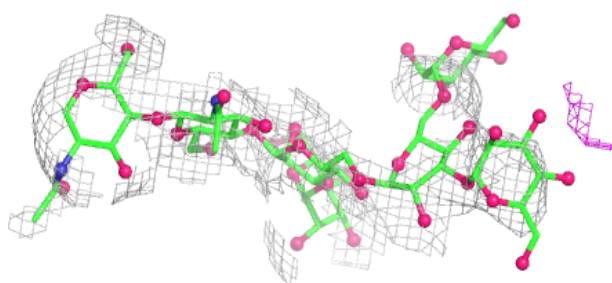
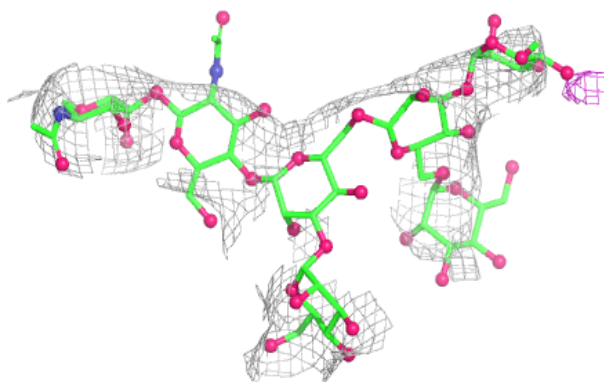
Electron density around Chain Q:

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

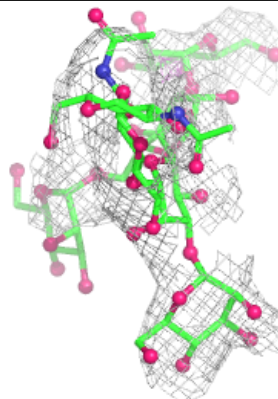
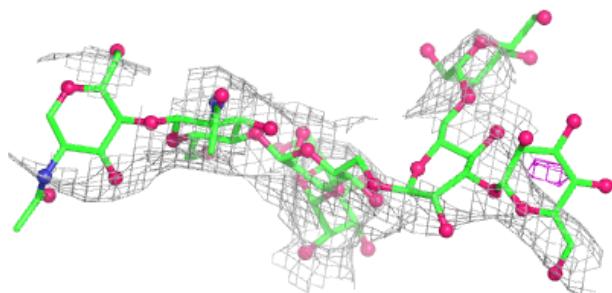
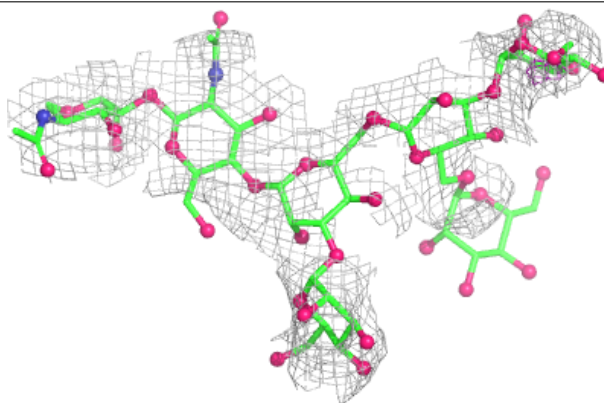


Electron density around Chain K:

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

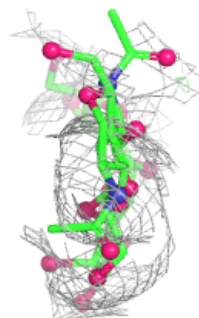
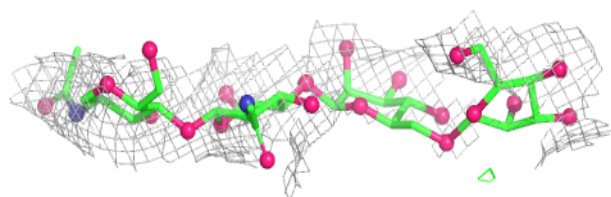
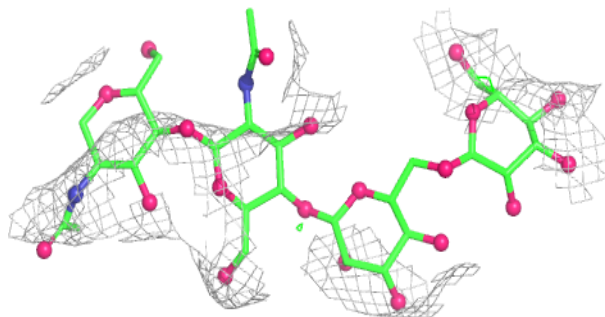
**Electron density around Chain R:**

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

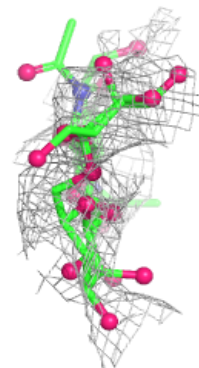
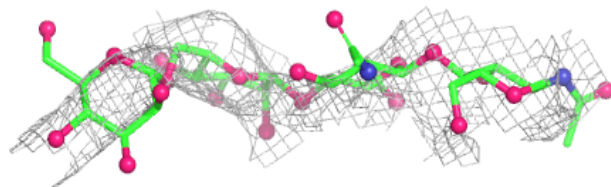
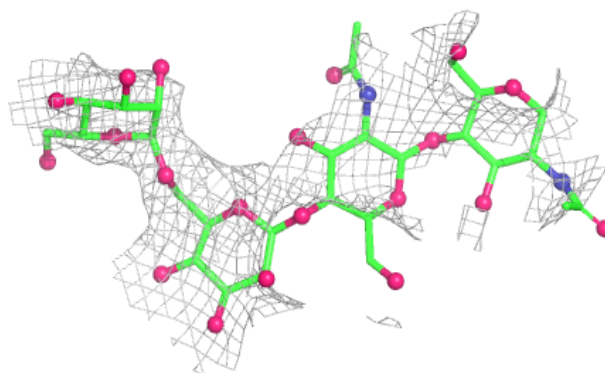


Electron density around Chain L:

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

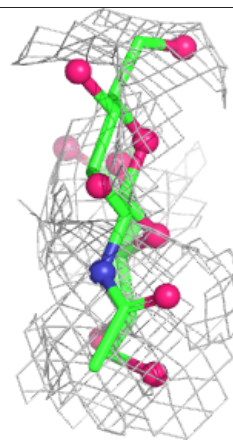
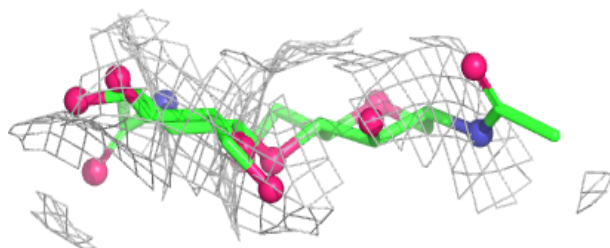
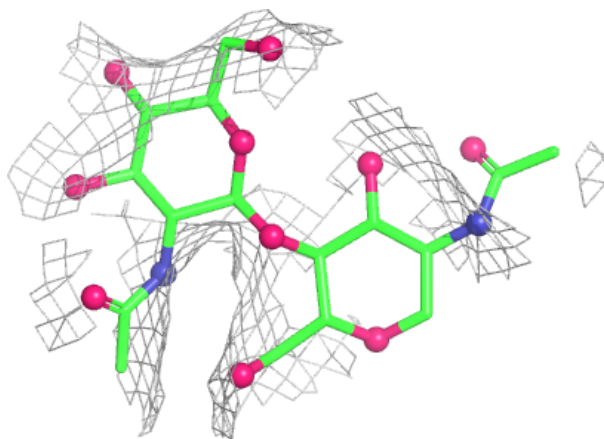
**Electron density around Chain S:**

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



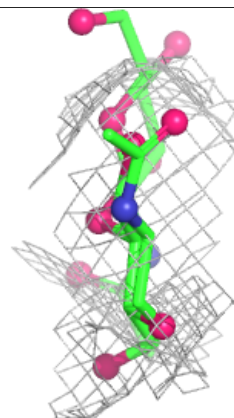
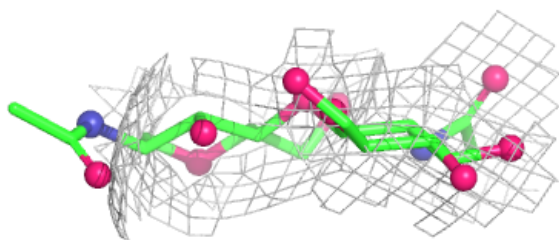
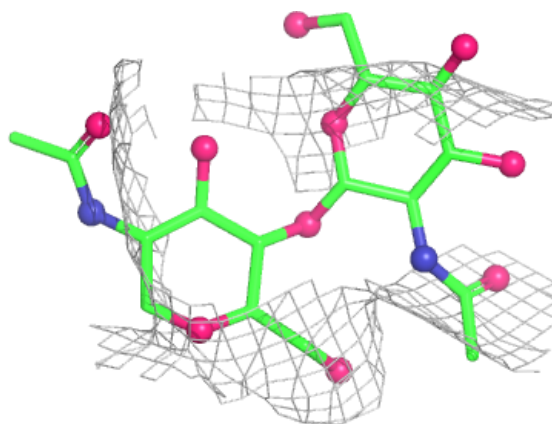
Electron density around Chain M:

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

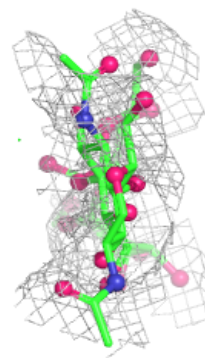
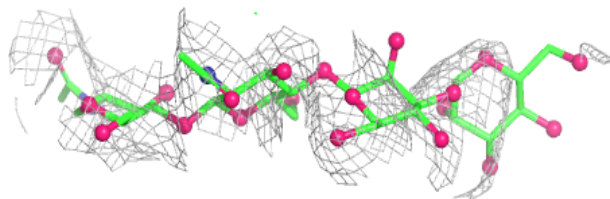
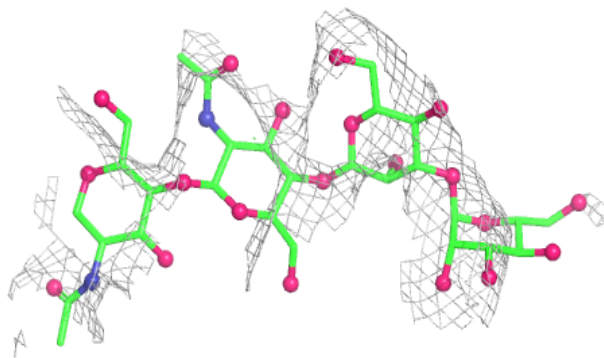


Electron density around Chain T:

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

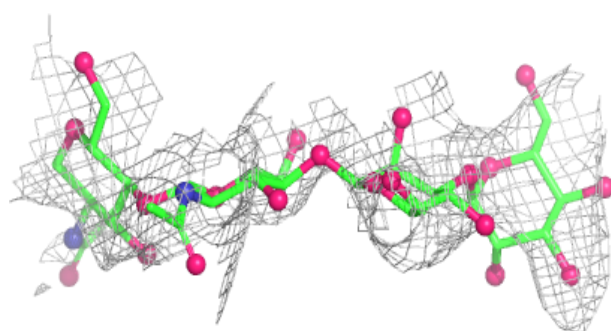
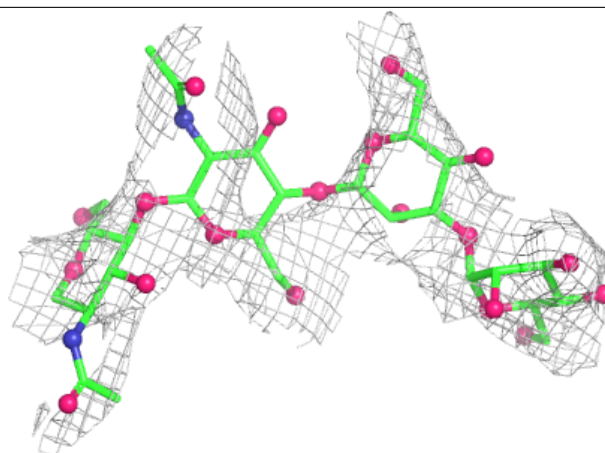
**Electron density around Chain N:**

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

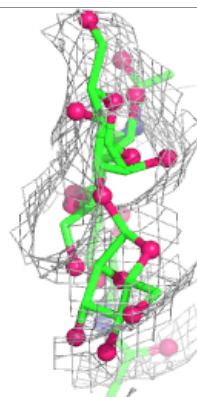
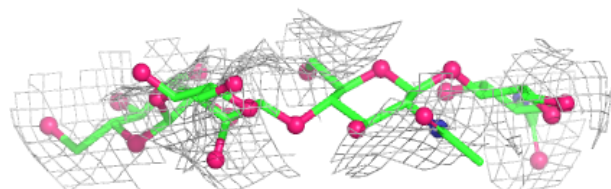
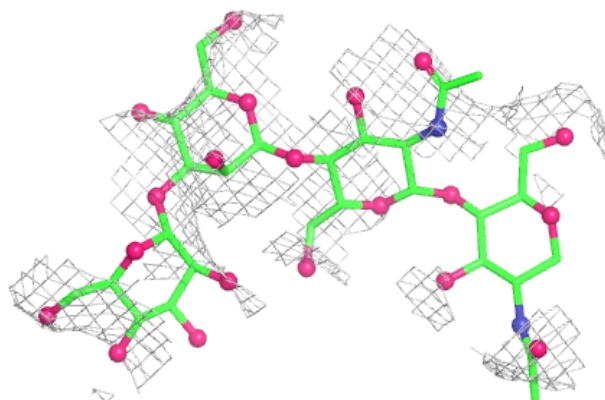


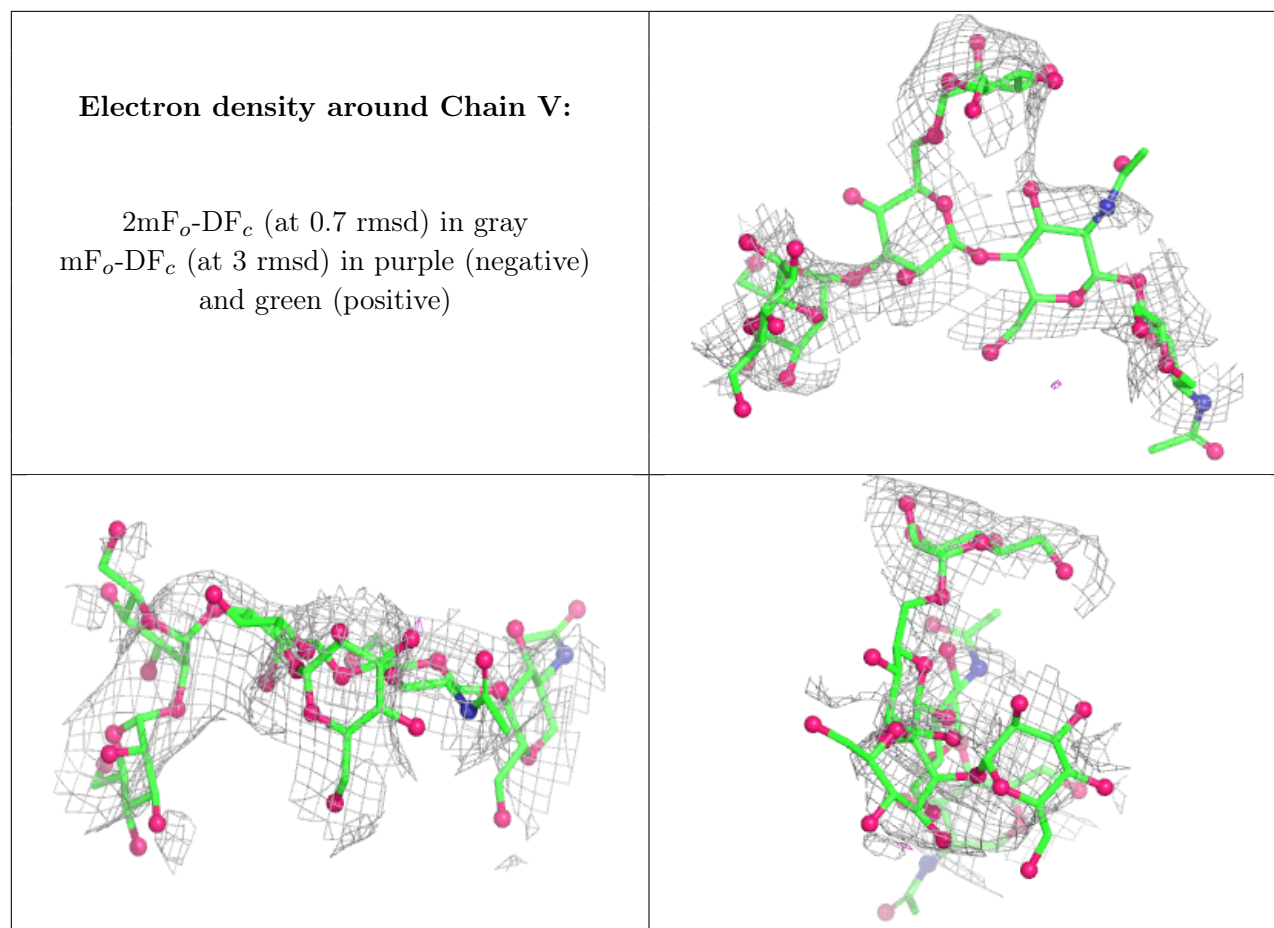
Electron density around Chain O:

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

**Electron density around Chain U:**

$2mF_o-DF_c$ (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
12	NAG	F	2004	14/15	0.93	0.06	258,270,279,284	0
12	NAG	A	2025	14/15	0.94	0.07	280,323,340,345	0
12	NAG	B	2004	14/15	0.95	0.07	234,258,269,269	0
12	NAG	E	2025	14/15	0.98	0.07	223,252,285,293	0
11	CA	A	2001	1/1	0.98	0.06	189,189,189,189	0
11	CA	E	2004	1/1	0.99	0.02	225,225,225,225	0
11	CA	A	2002	1/1	0.99	0.04	222,222,222,222	0
11	CA	A	2003	1/1	0.99	0.04	199,199,199,199	0
11	CA	E	2002	1/1	0.99	0.03	256,256,256,256	0
11	CA	E	2003	1/1	0.99	0.04	219,219,219,219	0
13	MN	B	2001	1/1	0.99	0.03	181,181,181,181	0
13	MN	F	2001	1/1	0.99	0.05	217,217,217,217	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	CA	E	2001	1/1	1.00	0.02	218,218,218,218	0
13	MN	B	2002	1/1	1.00	0.02	110,110,110,110	0
13	MN	B	2003	1/1	1.00	0.02	144,144,144,144	0
11	CA	A	2004	1/1	1.00	0.02	155,155,155,155	0
13	MN	F	2002	1/1	1.00	0.02	233,233,233,233	0
13	MN	F	2003	1/1	1.00	0.02	213,213,213,213	0

6.5 Other polymers [i](#)

There are no such residues in this entry.