



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2020 – 06:22 PM BST

PDB ID : 3ALA
Title : Crystal structure of vascular adhesion protein-1 in space group C2
Authors : Ernberg, K.E.; McGrath, A.P.; Guss, J.M.
Deposited on : 2010-07-29
Resolution : 2.90 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

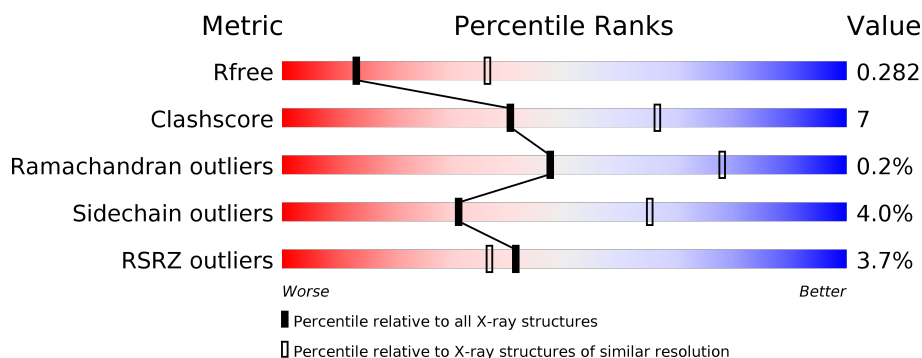
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	748	<div> <div>81%</div> <div>11% • 6%</div> </div>
1	B	748	<div> <div>80%</div> <div>13% • 6%</div> </div>
1	C	748	<div> <div>80%</div> <div>13% • 5%</div> </div>
1	D	748	<div> <div>%</div> <div>83%</div> <div>11% • 5%</div> </div>
1	E	748	<div> <div>%</div> <div>78%</div> <div>15% • 6%</div> </div>
1	F	748	<div> <div>7%</div> <div>72%</div> <div>20% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	748	
2	H	3	
2	K	3	
2	M	3	
2	P	3	
2	S	3	
2	V	3	
2	Y	3	
3	I	2	
3	N	2	
3	Q	2	
3	T	2	
3	W	2	
3	Z	2	
4	J	2	
4	O	2	
4	R	2	
4	U	2	
4	X	2	
5	L	3	
6	a	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
2	BMA	P	3	X	-	-	-
3	NAG	Z	1	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	Z	2	-	-	-	X
4	NAG	J	1	X	-	-	-
4	FUL	O	2	X	-	-	-
4	NAG	R	1	X	-	-	-
4	NAG	U	1	X	-	-	-
5	NAG	L	1	X	-	-	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 39103 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 Membrane primary amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	705	Total	C	N	O	S	0	3	0
			5494	3539	927	1007	21			
1	B	705	Total	C	N	O	S	0	2	0
			5488	3532	935	1000	21			
1	C	709	Total	C	N	O	S	0	2	0
			5498	3546	927	1004	21			
1	D	711	Total	C	N	O	S	0	1	0
			5510	3546	935	1007	22			
1	E	702	Total	C	N	O	S	0	0	0
			5423	3496	914	992	21			
1	F	701	Total	C	N	O	S	0	3	0
			5390	3460	916	993	21			
1	G	706	Total	C	N	O	S	8	1	0
			5392	3470	907	994	21			

There are 119 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ASP	-	expression tag	UNP Q16853
A	17	ILE	-	expression tag	UNP Q16853
A	18	VAL	-	expression tag	UNP Q16853
A	19	ASP	-	expression tag	UNP Q16853
A	20	TYR	-	expression tag	UNP Q16853
A	21	LYS	-	expression tag	UNP Q16853
A	22	ASP	-	expression tag	UNP Q16853
A	23	ASP	-	expression tag	UNP Q16853
A	24	ASP	-	expression tag	UNP Q16853
A	25	ASP	-	expression tag	UNP Q16853
A	26	LYS	-	expression tag	UNP Q16853
A	27	GLU	-	expression tag	UNP Q16853
A	28	ASN	-	expression tag	UNP Q16853
A	29	LEU	-	expression tag	UNP Q16853
A	30	TYR	-	expression tag	UNP Q16853

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Chain	Residue	Modelled	Actual	Comment	Reference
A	31	PHE	-	expression tag	UNP Q16853
A	32	GLN	-	expression tag	UNP Q16853
B	16	ASP	-	expression tag	UNP Q16853
B	17	ILE	-	expression tag	UNP Q16853
B	18	VAL	-	expression tag	UNP Q16853
B	19	ASP	-	expression tag	UNP Q16853
B	20	TYR	-	expression tag	UNP Q16853
B	21	LYS	-	expression tag	UNP Q16853
B	22	ASP	-	expression tag	UNP Q16853
B	23	ASP	-	expression tag	UNP Q16853
B	24	ASP	-	expression tag	UNP Q16853
B	25	ASP	-	expression tag	UNP Q16853
B	26	LYS	-	expression tag	UNP Q16853
B	27	GLU	-	expression tag	UNP Q16853
B	28	ASN	-	expression tag	UNP Q16853
B	29	LEU	-	expression tag	UNP Q16853
B	30	TYR	-	expression tag	UNP Q16853
B	31	PHE	-	expression tag	UNP Q16853
B	32	GLN	-	expression tag	UNP Q16853
C	16	ASP	-	expression tag	UNP Q16853
C	17	ILE	-	expression tag	UNP Q16853
C	18	VAL	-	expression tag	UNP Q16853
C	19	ASP	-	expression tag	UNP Q16853
C	20	TYR	-	expression tag	UNP Q16853
C	21	LYS	-	expression tag	UNP Q16853
C	22	ASP	-	expression tag	UNP Q16853
C	23	ASP	-	expression tag	UNP Q16853
C	24	ASP	-	expression tag	UNP Q16853
C	25	ASP	-	expression tag	UNP Q16853
C	26	LYS	-	expression tag	UNP Q16853
C	27	GLU	-	expression tag	UNP Q16853
C	28	ASN	-	expression tag	UNP Q16853
C	29	LEU	-	expression tag	UNP Q16853
C	30	TYR	-	expression tag	UNP Q16853
C	31	PHE	-	expression tag	UNP Q16853
C	32	GLN	-	expression tag	UNP Q16853
D	16	ASP	-	expression tag	UNP Q16853
D	17	ILE	-	expression tag	UNP Q16853
D	18	VAL	-	expression tag	UNP Q16853
D	19	ASP	-	expression tag	UNP Q16853
D	20	TYR	-	expression tag	UNP Q16853
D	21	LYS	-	expression tag	UNP Q16853

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Chain	Residue	Modelled	Actual	Comment	Reference
D	22	ASP	-	expression tag	UNP Q16853
D	23	ASP	-	expression tag	UNP Q16853
D	24	ASP	-	expression tag	UNP Q16853
D	25	ASP	-	expression tag	UNP Q16853
D	26	LYS	-	expression tag	UNP Q16853
D	27	GLU	-	expression tag	UNP Q16853
D	28	ASN	-	expression tag	UNP Q16853
D	29	LEU	-	expression tag	UNP Q16853
D	30	TYR	-	expression tag	UNP Q16853
D	31	PHE	-	expression tag	UNP Q16853
D	32	GLN	-	expression tag	UNP Q16853
E	16	ASP	-	expression tag	UNP Q16853
E	17	ILE	-	expression tag	UNP Q16853
E	18	VAL	-	expression tag	UNP Q16853
E	19	ASP	-	expression tag	UNP Q16853
E	20	TYR	-	expression tag	UNP Q16853
E	21	LYS	-	expression tag	UNP Q16853
E	22	ASP	-	expression tag	UNP Q16853
E	23	ASP	-	expression tag	UNP Q16853
E	24	ASP	-	expression tag	UNP Q16853
E	25	ASP	-	expression tag	UNP Q16853
E	26	LYS	-	expression tag	UNP Q16853
E	27	GLU	-	expression tag	UNP Q16853
E	28	ASN	-	expression tag	UNP Q16853
E	29	LEU	-	expression tag	UNP Q16853
E	30	TYR	-	expression tag	UNP Q16853
E	31	PHE	-	expression tag	UNP Q16853
E	32	GLN	-	expression tag	UNP Q16853
F	16	ASP	-	expression tag	UNP Q16853
F	17	ILE	-	expression tag	UNP Q16853
F	18	VAL	-	expression tag	UNP Q16853
F	19	ASP	-	expression tag	UNP Q16853
F	20	TYR	-	expression tag	UNP Q16853
F	21	LYS	-	expression tag	UNP Q16853
F	22	ASP	-	expression tag	UNP Q16853
F	23	ASP	-	expression tag	UNP Q16853
F	24	ASP	-	expression tag	UNP Q16853
F	25	ASP	-	expression tag	UNP Q16853
F	26	LYS	-	expression tag	UNP Q16853
F	27	GLU	-	expression tag	UNP Q16853
F	28	ASN	-	expression tag	UNP Q16853
F	29	LEU	-	expression tag	UNP Q16853

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	TYR	-	expression tag	UNP Q16853
F	31	PHE	-	expression tag	UNP Q16853
F	32	GLN	-	expression tag	UNP Q16853
G	16	ASP	-	expression tag	UNP Q16853
G	17	ILE	-	expression tag	UNP Q16853
G	18	VAL	-	expression tag	UNP Q16853
G	19	ASP	-	expression tag	UNP Q16853
G	20	TYR	-	expression tag	UNP Q16853
G	21	LYS	-	expression tag	UNP Q16853
G	22	ASP	-	expression tag	UNP Q16853
G	23	ASP	-	expression tag	UNP Q16853
G	24	ASP	-	expression tag	UNP Q16853
G	25	ASP	-	expression tag	UNP Q16853
G	26	LYS	-	expression tag	UNP Q16853
G	27	GLU	-	expression tag	UNP Q16853
G	28	ASN	-	expression tag	UNP Q16853
G	29	LEU	-	expression tag	UNP Q16853
G	30	TYR	-	expression tag	UNP Q16853
G	31	PHE	-	expression tag	UNP Q16853
G	32	GLN	-	expression tag	UNP Q16853

- Molecule 2 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
2	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	P	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	S	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	V	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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



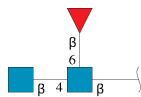
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	W	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	O	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	R	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	U	2	Total	C	N	O	0	0	0
			24	14	1	9			
4	X	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- 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	a	2	Total	C	N	O	0	0	0
			24	14	1	9			

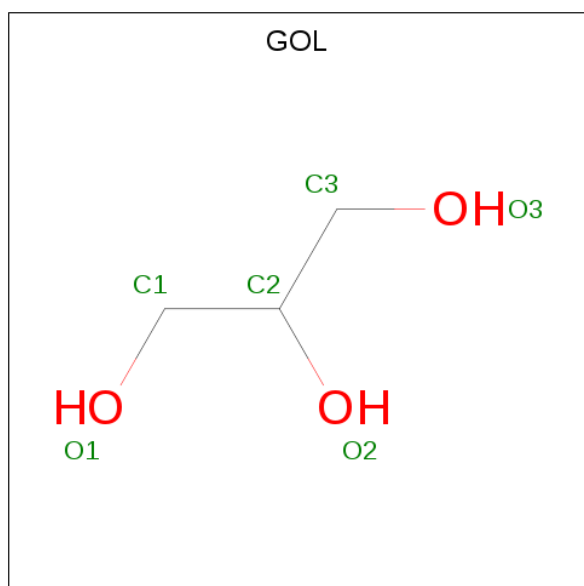
- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Cu	0	0
			1	1		
7	D	1	Total	Cu	0	0
			1	1		
7	E	1	Total	Cu	0	0
			1	1		
7	B	1	Total	Cu	0	0
			1	1		
7	C	1	Total	Cu	0	0
			1	1		
7	A	1	Total	Cu	0	0
			1	1		
7	F	1	Total	Cu	0	0
			1	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

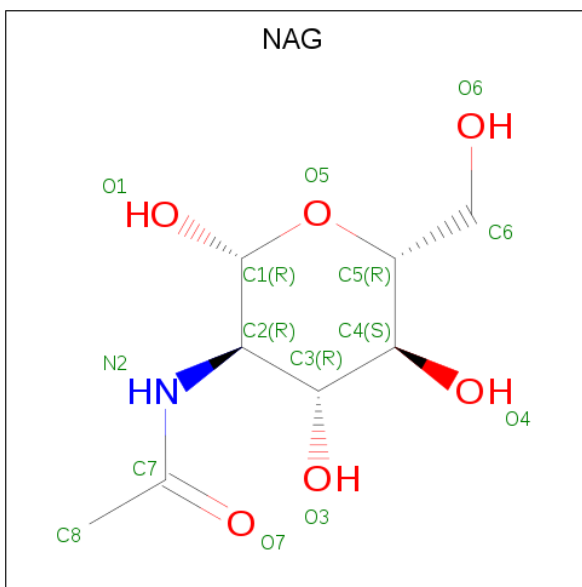
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	G	2	Total Ca 2 2	0	0
8	D	2	Total Ca 2 2	0	0
8	E	2	Total Ca 2 2	0	0
8	B	2	Total Ca 2 2	0	0
8	C	2	Total Ca 2 2	0	0
8	A	2	Total Ca 2 2	0	0
8	F	2	Total Ca 2 2	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

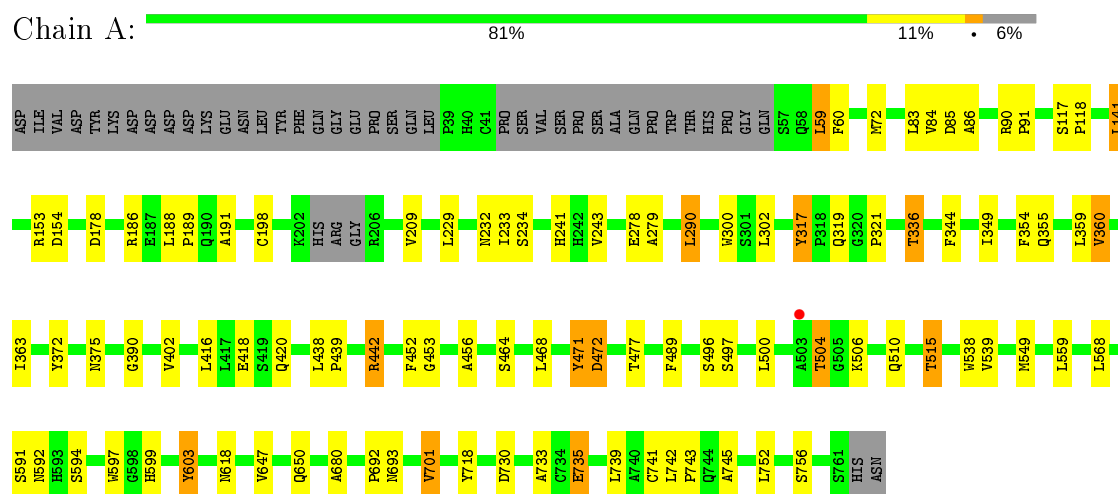
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	49	Total	O	0	0
			49	49		
11	B	47	Total	O	0	0
			47	47		
11	C	33	Total	O	0	0
			33	33		
11	D	40	Total	O	0	0
			40	40		
11	E	23	Total	O	0	0
			23	23		
11	F	23	Total	O	0	0
			23	23		
11	G	15	Total	O	0	0
			15	15		

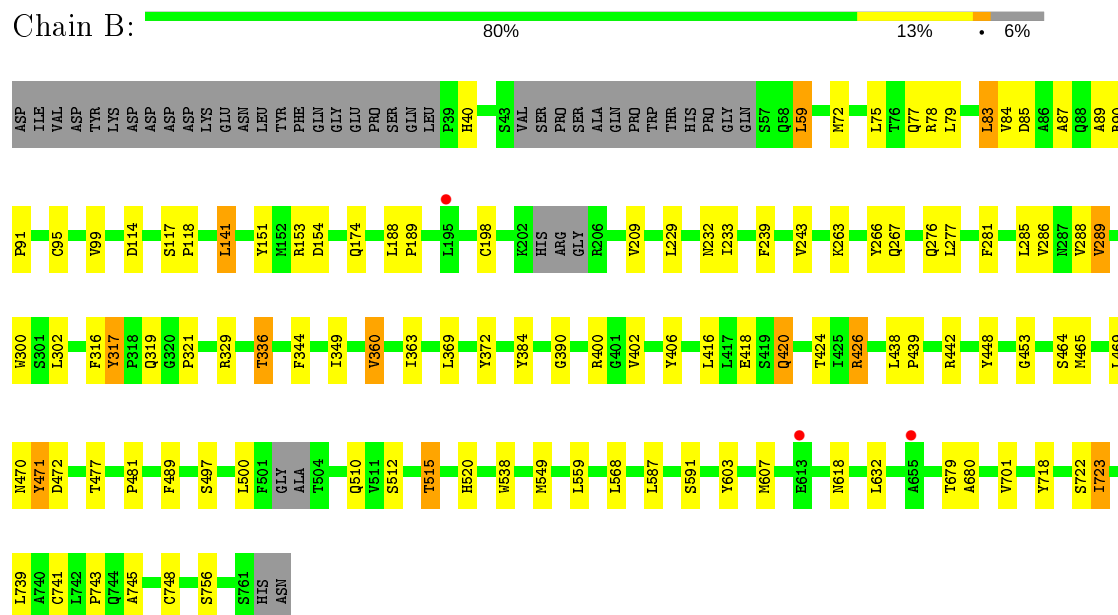
3 Residue-property plots

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: Membrane primary amine oxidase

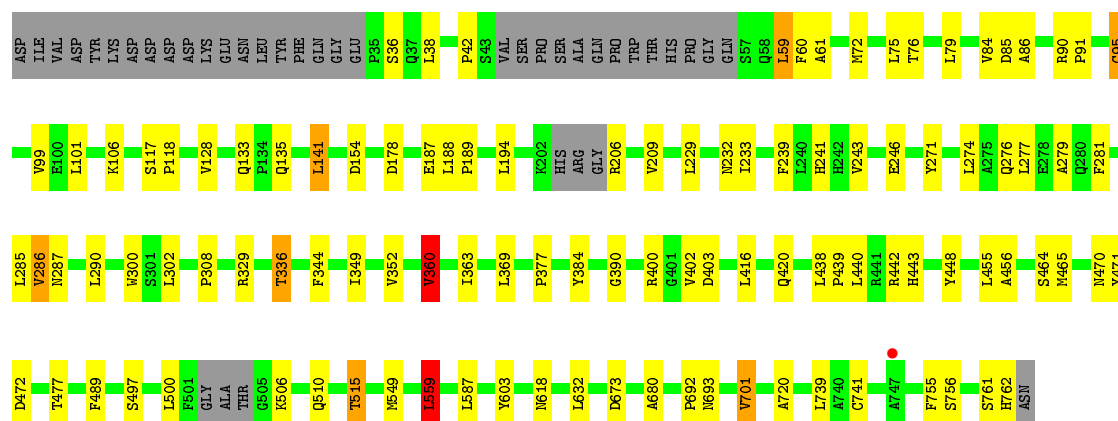


- Molecule 1: Membrane primary amine oxidase




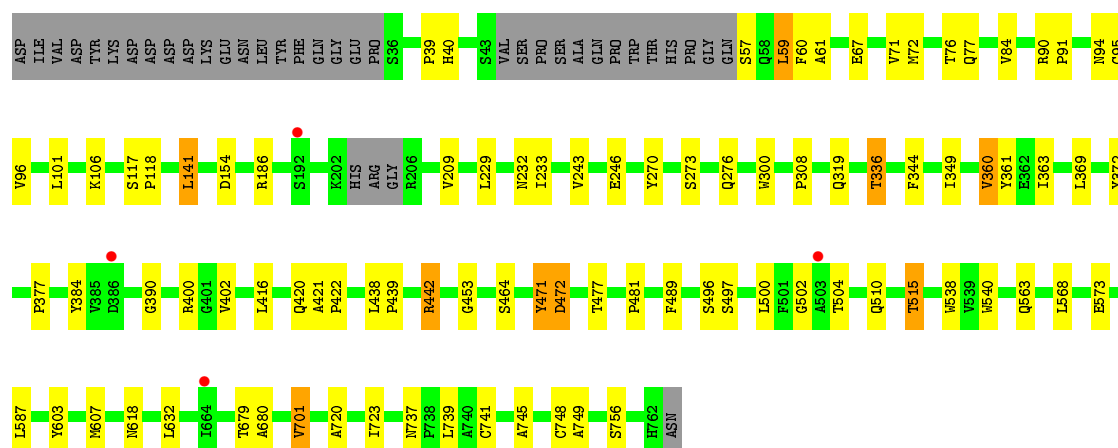
- Molecule 1: Membrane primary amine oxidase

Chain C:  80% 13% • 5%




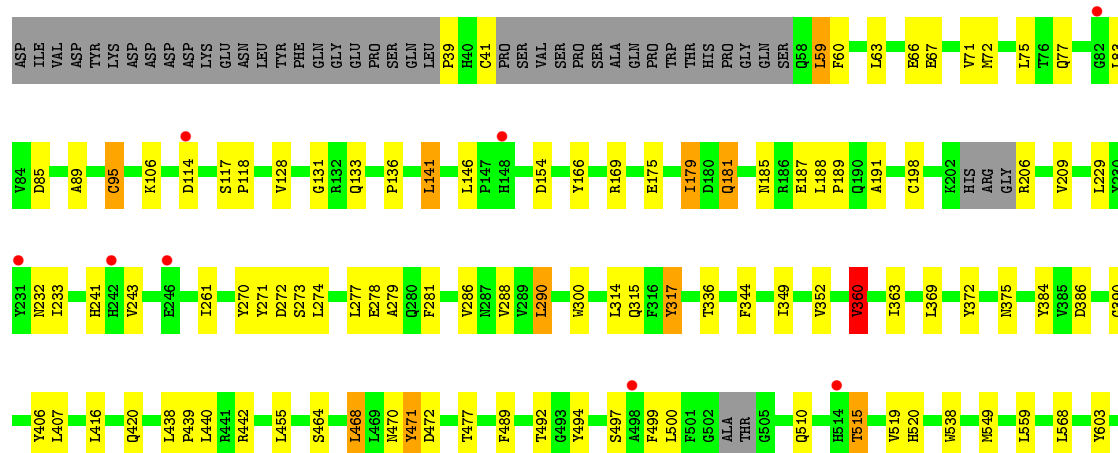
• Molecule 1: Membrane primary amine oxidase

Chain D:  83% 11% • 5%



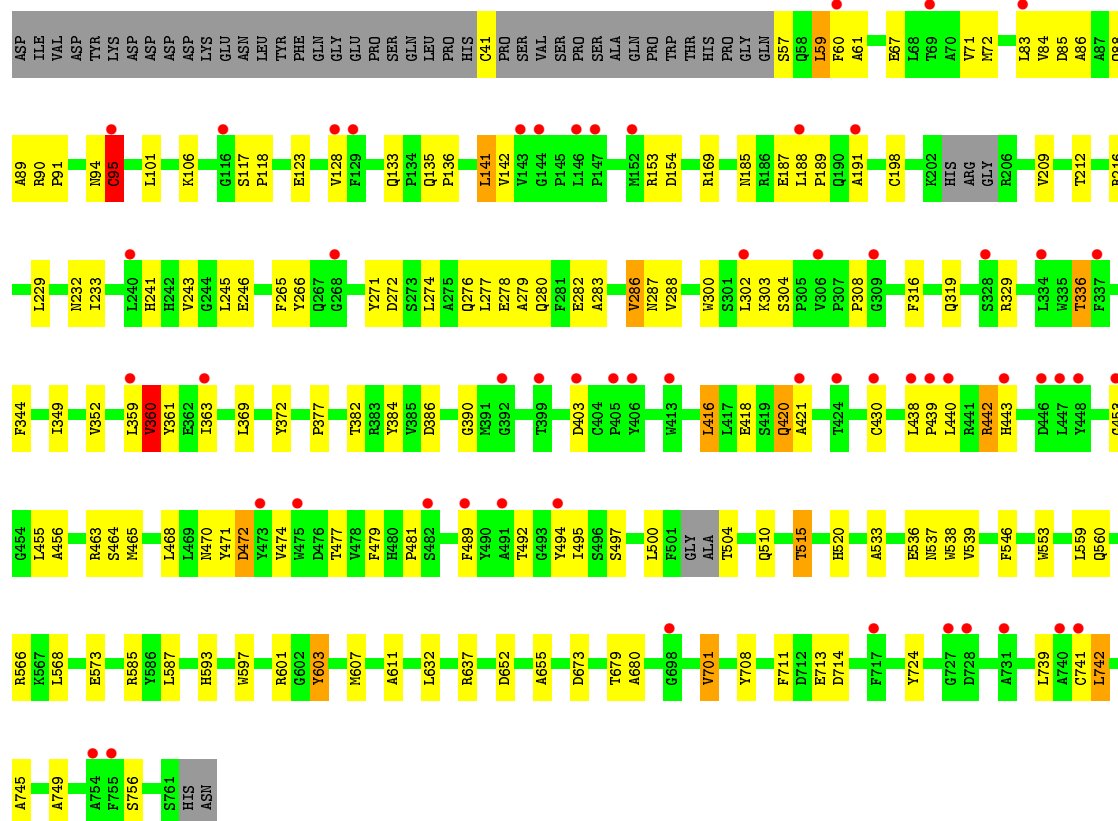
• Molecule 1: Membrane primary amine oxidase

Chain E:  78% 15% • 6%

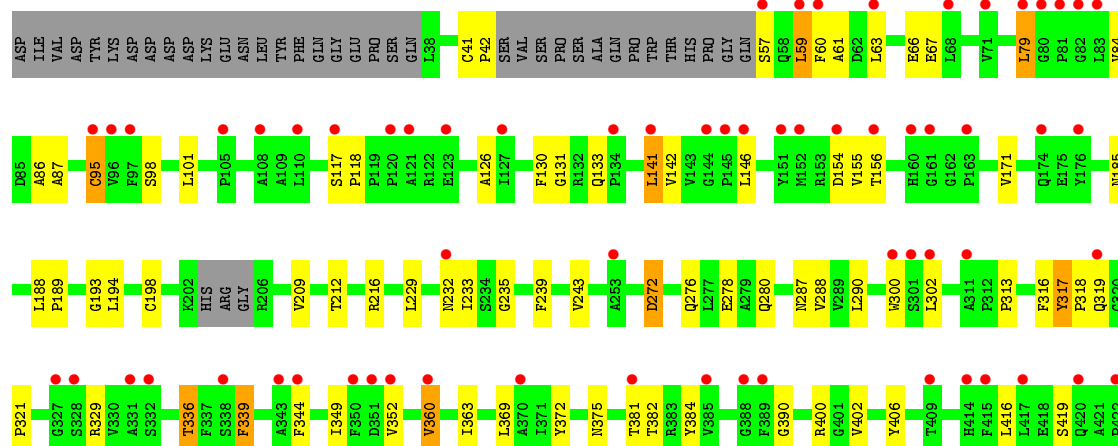
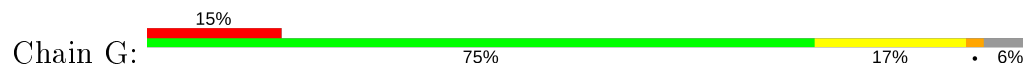


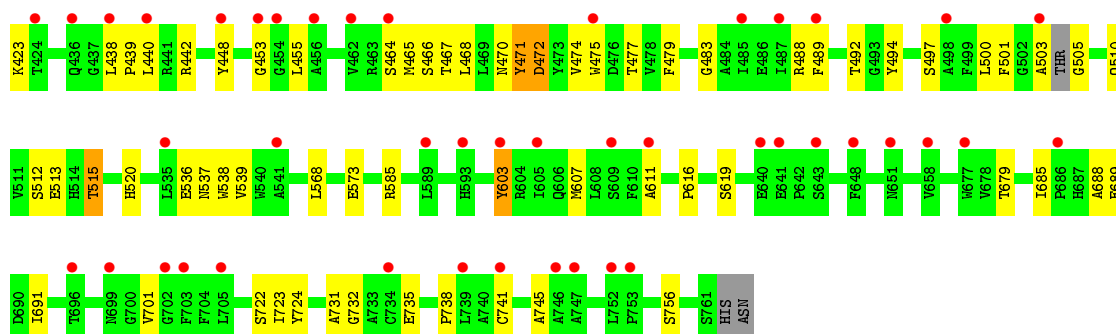


- Molecule 1: Membrane primary amine oxidase



- Molecule 1: Membrane primary amine oxidase





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

Chain H: 100%



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

Chain K: 100%



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

Chain M: 67% 33%



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

Chain P: 33% 67%



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

Chain S: 67% 33%



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

Chain V:  100%

NAG1
NAG2
BNA3

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

Chain Y:  33% 67%

NAG1
NAG2
BNA3

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

Chain I:  50% 50%

NAG1
NAG2

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

Chain N:  50% 50%

NAG1
NAG2

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

Chain Q:  50% 50%

NAG1
NAG2

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

Chain T:  50% 50%

NAG1
NAG2

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

Chain W:  50% 50%

MAG1
MAG2

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

Chain Z:  100%

MAG1
MAG2

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

Chain J:  100%

MAG1
FUL2

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

Chain O:  100%

MAG1
FUL2

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

Chain R:  100%

MAG1
FUL2

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

Chain U:  100%

MAG1
FUL2

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

Chain X:  50% 50%

MAG1
FUL2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

HA61
HA62
FOL3

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

Chain a:

100%

HA61
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	394.47Å 115.83Å 179.29Å 90.00° 112.34° 90.00°	Depositor
Resolution (Å)	110.40 – 2.90 110.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.3 (110.40-2.90) 98.3 (110.40-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.250 , 0.286 0.249 , 0.282	Depositor DCC
R_{free} test set	8187 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	39103	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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: GOL, BMA, NAG, CA, FUC, TPQ, FUL, CU

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	0.76	1/5660 (0.0%)	0.72	2/7728 (0.0%)
1	B	0.76	2/5653 (0.0%)	0.73	2/7716 (0.0%)
1	C	0.70	2/5665 (0.0%)	0.71	1/7737 (0.0%)
1	D	0.69	0/5672	0.72	2/7746 (0.0%)
1	E	0.70	1/5582 (0.0%)	0.72	2/7622 (0.0%)
1	F	0.83	1/5551 (0.0%)	0.76	1/7583 (0.0%)
1	G	0.85	0/5553	0.77	1/7590 (0.0%)
All	All	0.76	7/39336 (0.0%)	0.73	11/53722 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	430	CYS	CB-SG	-8.73	1.67	1.82
1	B	95	CYS	CB-SG	-7.45	1.69	1.82
1	C	95	CYS	CB-SG	-7.08	1.70	1.82
1	A	360	VAL	CB-CG1	-6.40	1.39	1.52
1	E	95	CYS	CB-SG	-5.80	1.72	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	701	VAL	CG1-CB-CG2	9.11	125.48	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	VAL	CG1-CB-CG2	6.69	121.61	110.90
1	D	360	VAL	CG1-CB-CG2	6.38	121.11	110.90
1	C	559	LEU	CB-CG-CD1	6.27	121.66	111.00
1	B	426	ARG	NE-CZ-NH1	6.23	123.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	95	CYS	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	5494	0	5167	65	0
1	B	5488	0	5174	79	0
1	C	5498	0	5157	77	0
1	D	5510	0	5162	61	0
1	E	5423	0	5067	82	0
1	F	5390	0	4995	125	0
1	G	5392	0	4980	110	0
2	H	39	0	34	0	0
2	K	39	0	34	0	0
2	M	39	0	34	3	0
2	P	39	0	34	5	0
2	S	39	0	34	2	0
2	V	39	0	34	0	0
2	Y	39	0	34	4	0
3	I	28	0	25	1	0
3	N	28	0	25	6	0
3	Q	28	0	25	3	0
3	T	28	0	25	6	0
3	W	28	0	25	1	0
3	Z	28	0	25	0	0
4	J	24	0	22	0	0
4	O	24	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	24	0	22	0	0
4	U	24	0	22	0	0
4	X	24	0	22	1	0
5	L	38	0	34	0	0
6	a	24	0	22	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
8	G	2	0	0	0	0
9	A	6	0	8	0	0
10	B	14	0	13	4	0
10	D	14	0	13	0	0
11	A	49	0	0	0	0
11	B	47	0	0	1	0
11	C	33	0	0	0	0
11	D	40	0	0	0	0
11	E	23	0	0	0	0
11	F	23	0	0	0	0
11	G	15	0	0	3	0
All	All	39103	0	36290	544	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 7.

The worst 5 of 544 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:C:232:ASN:ND2	3:N:1:NAG:H83	1.56	1.20
1:C:232:ASN:HD22	3:N:1:NAG:H83	0.90	1.06
1:E:206:ARG:O	3:T:1:NAG:H81	1.58	1.03
1:D:72:MET:HE1	1:D:416:LEU:HD11	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ASN:HD22	3:Q:1:NAG:H83	1.19	1.01

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	701/748 (94%)	660 (94%)	40 (6%)	1 (0%)	51	82
1	B	698/748 (93%)	653 (94%)	44 (6%)	1 (0%)	51	82
1	C	702/748 (94%)	659 (94%)	40 (6%)	3 (0%)	34	66
1	D	705/748 (94%)	666 (94%)	38 (5%)	1 (0%)	51	82
1	E	693/748 (93%)	655 (94%)	35 (5%)	3 (0%)	34	66
1	F	696/748 (93%)	658 (94%)	37 (5%)	1 (0%)	51	82
1	G	698/748 (93%)	650 (93%)	47 (7%)	1 (0%)	51	82
All	All	4893/5236 (93%)	4601 (94%)	281 (6%)	11 (0%)	47	78

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	618	ASN
1	G	87	ALA
1	C	618	ASN
1	C	279	ALA
1	E	272	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	568/625 (91%)	545 (96%)	23 (4%)	31	65
1	B	569/625 (91%)	549 (96%)	20 (4%)	36	70
1	C	565/625 (90%)	546 (97%)	19 (3%)	37	71
1	D	567/625 (91%)	546 (96%)	21 (4%)	34	68
1	E	555/625 (89%)	533 (96%)	22 (4%)	31	65
1	F	549/625 (88%)	524 (95%)	25 (5%)	27	60
1	G	545/625 (87%)	519 (95%)	26 (5%)	25	58
All	All	3918/4375 (90%)	3762 (96%)	156 (4%)	31	65

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	442	ARG
1	E	141	LEU
1	G	416	LEU
1	D	472	ASP
1	D	701	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	319	GLN
1	D	563	GLN
1	F	319	GLN
1	C	693	ASN
1	G	319	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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$
1	TPQ	C	471	1	13,14,15	1.47	2 (15%)	15,19,21	1.79	4 (26%)
1	TPQ	E	471	1	13,14,15	1.69	2 (15%)	15,19,21	2.37	5 (33%)
1	TPQ	B	471	1	13,14,15	1.44	2 (15%)	15,19,21	2.44	3 (20%)
1	TPQ	G	471	1	13,14,15	1.50	2 (15%)	15,19,21	2.22	3 (20%)
1	TPQ	D	471	1	13,14,15	1.44	1 (7%)	15,19,21	1.54	2 (13%)
1	TPQ	F	471	1	13,14,15	1.73	4 (30%)	15,19,21	1.42	3 (20%)
1	TPQ	A	471	1	13,14,15	1.43	2 (15%)	15,19,21	2.02	3 (20%)

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
1	TPQ	C	471	1	-	3/5/22/24	0/1/1/1
1	TPQ	E	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	B	471	1	-	2/5/22/24	0/1/1/1
1	TPQ	G	471	1	-	2/5/22/24	0/1/1/1
1	TPQ	D	471	1	-	2/5/22/24	0/1/1/1
1	TPQ	F	471	1	-	4/5/22/24	0/1/1/1
1	TPQ	A	471	1	-	3/5/22/24	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	471	TPQ	O4-C4	-3.96	1.23	1.34
1	C	471	TPQ	O4-C4	-3.83	1.24	1.34
1	A	471	TPQ	O4-C4	-3.79	1.24	1.34
1	E	471	TPQ	O4-C4	-3.65	1.24	1.34
1	B	471	TPQ	O4-C4	-3.48	1.25	1.34

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	TPQ	C6-C1-C2	6.98	124.00	118.64
1	E	471	TPQ	C6-C1-C2	6.10	123.33	118.64
1	G	471	TPQ	C6-C1-C2	5.80	123.10	118.64
1	E	471	TPQ	CB-CA-C	-5.35	101.43	111.47
1	C	471	TPQ	C6-C1-C2	5.01	122.49	118.64

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	471	TPQ	N-CA-CB-C1
1	C	471	TPQ	C-CA-CB-C1
1	E	471	TPQ	N-CA-CB-C1
1	E	471	TPQ	O-C-CA-CB
1	B	471	TPQ	N-CA-CB-C1

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	471	TPQ	2	0
1	B	471	TPQ	1	0
1	G	471	TPQ	2	0
1	D	471	TPQ	1	0
1	A	471	TPQ	1	0

5.5 Carbohydrates

48 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	H	1	1,2	14,14,15	0.71	0	17,19,21	2.12	2 (11%)
2	NAG	H	2	2	14,14,15	0.78	1 (7%)	17,19,21	1.57	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	H	3	2	11,11,12	0.99	0	15,15,17	2.35	7 (46%)
3	NAG	I	1	1,3	14,14,15	1.00	1 (7%)	17,19,21	2.75	5 (29%)
3	NAG	I	2	3	14,14,15	0.82	1 (7%)	17,19,21	1.02	0
4	NAG	J	1	1,4	14,14,15	2.37	3 (21%)	17,19,21	2.91	10 (58%)
4	FUL	J	2	4	10,10,11	1.54	2 (20%)	14,14,16	1.95	5 (35%)
2	NAG	K	1	1,2	14,14,15	0.73	0	17,19,21	2.24	4 (23%)
2	NAG	K	2	2	14,14,15	0.75	0	17,19,21	2.60	6 (35%)
2	BMA	K	3	2	11,11,12	1.09	1 (9%)	15,15,17	1.96	5 (33%)
5	NAG	L	1	1,5	14,14,15	0.77	0	17,19,21	2.12	4 (23%)
5	NAG	L	2	5	14,14,15	0.66	0	17,19,21	1.49	4 (23%)
5	FUL	L	3	5	10,10,11	1.94	3 (30%)	14,14,16	2.16	5 (35%)
2	NAG	M	1	1,2	14,14,15	1.04	1 (7%)	17,19,21	1.96	6 (35%)
2	NAG	M	2	2	14,14,15	0.94	1 (7%)	17,19,21	2.58	6 (35%)
2	BMA	M	3	2	11,11,12	1.19	1 (9%)	15,15,17	1.85	6 (40%)
3	NAG	N	1	1,3	14,14,15	0.72	0	17,19,21	1.69	4 (23%)
3	NAG	N	2	3	14,14,15	0.90	1 (7%)	17,19,21	2.97	6 (35%)
4	NAG	O	1	1,4	14,14,15	1.57	4 (28%)	17,19,21	1.86	4 (23%)
4	FUL	O	2	4	10,10,11	1.03	0	14,14,16	1.85	4 (28%)
2	NAG	P	1	1,2	14,14,15	1.05	1 (7%)	17,19,21	2.49	4 (23%)
2	NAG	P	2	2	14,14,15	0.52	0	17,19,21	2.02	5 (29%)
2	BMA	P	3	2	11,11,12	0.87	0	15,15,17	3.00	3 (20%)
3	NAG	Q	1	1,3	14,14,15	0.84	0	17,19,21	2.17	6 (35%)
3	NAG	Q	2	3	14,14,15	0.93	1 (7%)	17,19,21	1.48	3 (17%)
4	NAG	R	1	1,4	14,14,15	1.37	2 (14%)	17,19,21	1.72	5 (29%)
4	FUL	R	2	4	10,10,11	2.50	6 (60%)	14,14,16	2.10	7 (50%)
2	NAG	S	1	1,2	14,14,15	0.54	0	17,19,21	2.65	8 (47%)
2	NAG	S	2	2	14,14,15	0.59	0	17,19,21	1.22	2 (11%)
2	BMA	S	3	2	11,11,12	0.74	0	15,15,17	1.01	1 (6%)
3	NAG	T	1	1,3	14,14,15	0.55	0	17,19,21	1.65	2 (11%)
3	NAG	T	2	3	14,14,15	0.78	0	17,19,21	1.38	3 (17%)
4	NAG	U	1	1,4	14,14,15	1.39	2 (14%)	17,19,21	2.86	4 (23%)
4	FUL	U	2	4	10,10,11	1.88	2 (20%)	14,14,16	1.95	4 (28%)
2	NAG	V	1	1,2	14,14,15	0.84	1 (7%)	17,19,21	1.88	2 (11%)
2	NAG	V	2	2	14,14,15	0.76	0	17,19,21	2.41	4 (23%)
2	BMA	V	3	2	11,11,12	1.04	1 (9%)	15,15,17	1.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	W	1	1,3	14,14,15	0.58	0	17,19,21	2.02	6 (35%)
3	NAG	W	2	3	14,14,15	0.82	1 (7%)	17,19,21	2.23	4 (23%)
4	NAG	X	1	1,4	14,14,15	1.11	1 (7%)	17,19,21	3.61	5 (29%)
4	FUL	X	2	4	10,10,11	1.24	1 (10%)	14,14,16	2.77	5 (35%)
2	NAG	Y	1	1,2	14,14,15	0.70	0	17,19,21	2.31	3 (17%)
2	NAG	Y	2	2	14,14,15	0.70	0	17,19,21	1.73	3 (17%)
2	BMA	Y	3	2	11,11,12	0.76	0	15,15,17	1.82	2 (13%)
3	NAG	Z	1	1,3	14,14,15	0.59	0	17,19,21	2.43	7 (41%)
3	NAG	Z	2	3	14,14,15	0.58	0	17,19,21	1.08	2 (11%)
6	NAG	a	1	1,6	14,14,15	1.10	1 (7%)	17,19,21	2.19	5 (29%)
6	FUC	a	2	6	10,10,11	2.15	3 (30%)	14,14,16	1.51	3 (21%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	P	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	3/6/23/26	0/1/1/1
2	BMA	P	3	2	1/1/4/5	2/2/19/22	0/1/1/1
3	NAG	Q	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
4	NAG	R	1	1,4	1/1/5/7	4/6/23/26	0/1/1/1
4	FUL	R	2	4	-	-	0/1/1/1
2	NAG	S	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	BMA	S	3	2	-	2/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
4	NAG	U	1	1,4	1/1/5/7	1/6/23/26	0/1/1/1
4	FUL	U	2	4	-	-	0/1/1/1
2	NAG	V	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	V	2	2	-	2/6/23/26	0/1/1/1
2	BMA	V	3	2	-	1/2/19/22	0/1/1/1
3	NAG	W	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	2/6/23/26	0/1/1/1
4	FUL	X	2	4	-	-	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	BMA	Y	3	2	-	2/2/19/22	0/1/1/1
3	NAG	Z	1	1,3	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	4/6/23/26	0/1/1/1
6	FUC	a	2	6	-	-	0/1/1/1

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	1	NAG	O5-C1	7.04	1.55	1.43
6	a	2	FUC	O5-C1	5.01	1.51	1.43
4	R	2	FUL	O5-C1	4.56	1.51	1.43
4	U	2	FUL	O5-C1	4.52	1.50	1.43
5	L	3	FUL	O5-C1	4.48	1.50	1.43

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	1	NAG	O5-C5-C6	-12.87	87.03	107.20
2	P	3	BMA	C1-C2-C3	-8.80	98.85	109.67
3	N	2	NAG	C1-O5-C5	8.69	123.96	112.19
3	I	1	NAG	C1-C2-N2	-8.42	96.10	110.49
2	H	1	NAG	C1-O5-C5	7.30	122.08	112.19

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1	NAG	C1
4	U	1	NAG	C1
4	J	1	NAG	C1
4	R	1	NAG	C1
4	O	2	FUL	C1

5 of 79 torsion outliers are listed below:

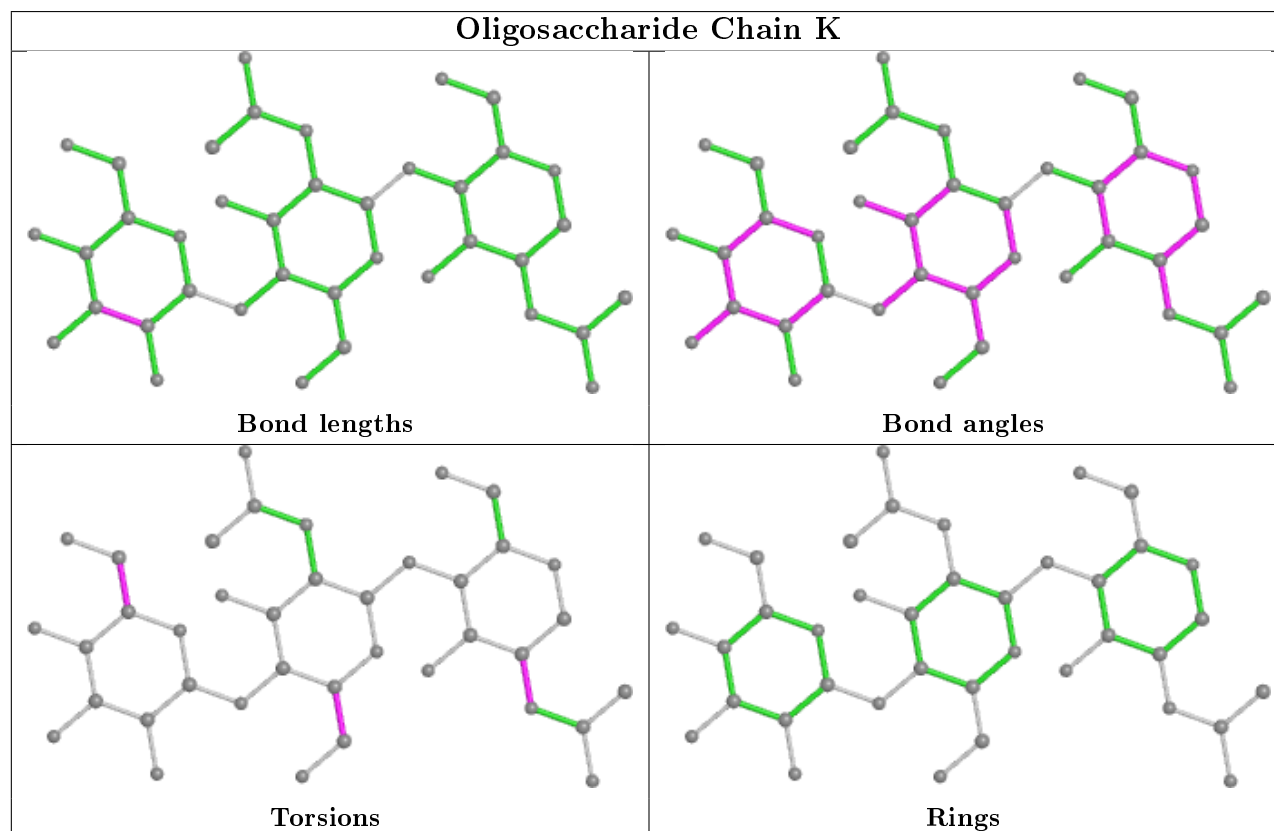
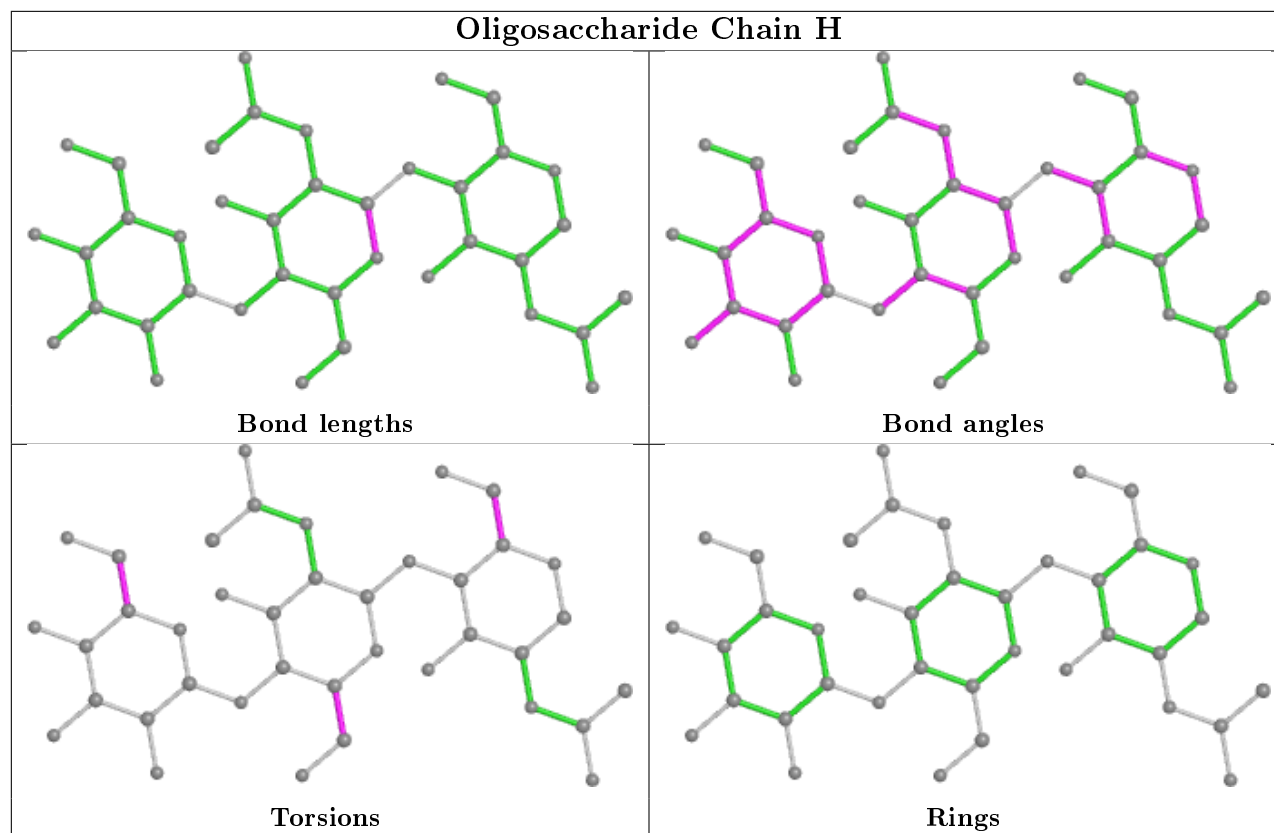
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C3-C2-N2-C7
2	P	2	NAG	C3-C2-N2-C7
4	R	1	NAG	O5-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6

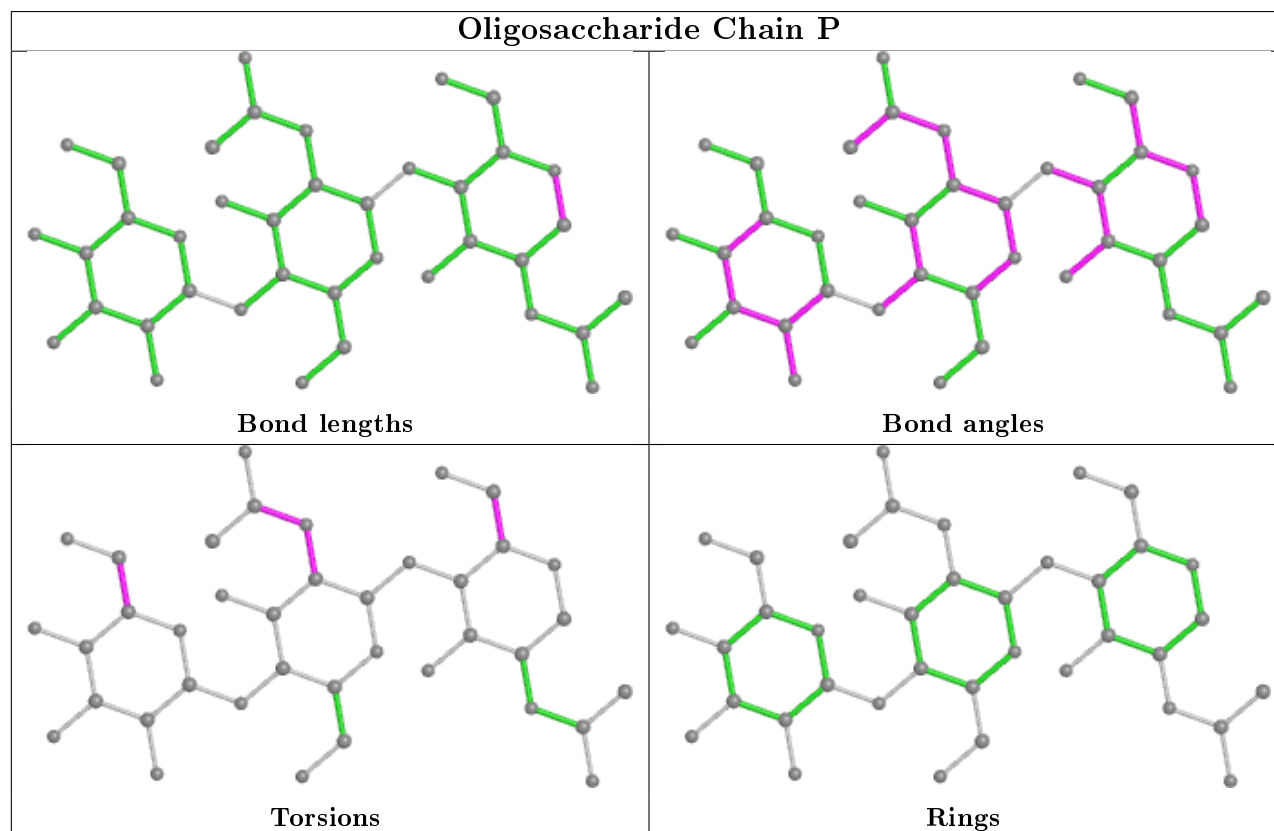
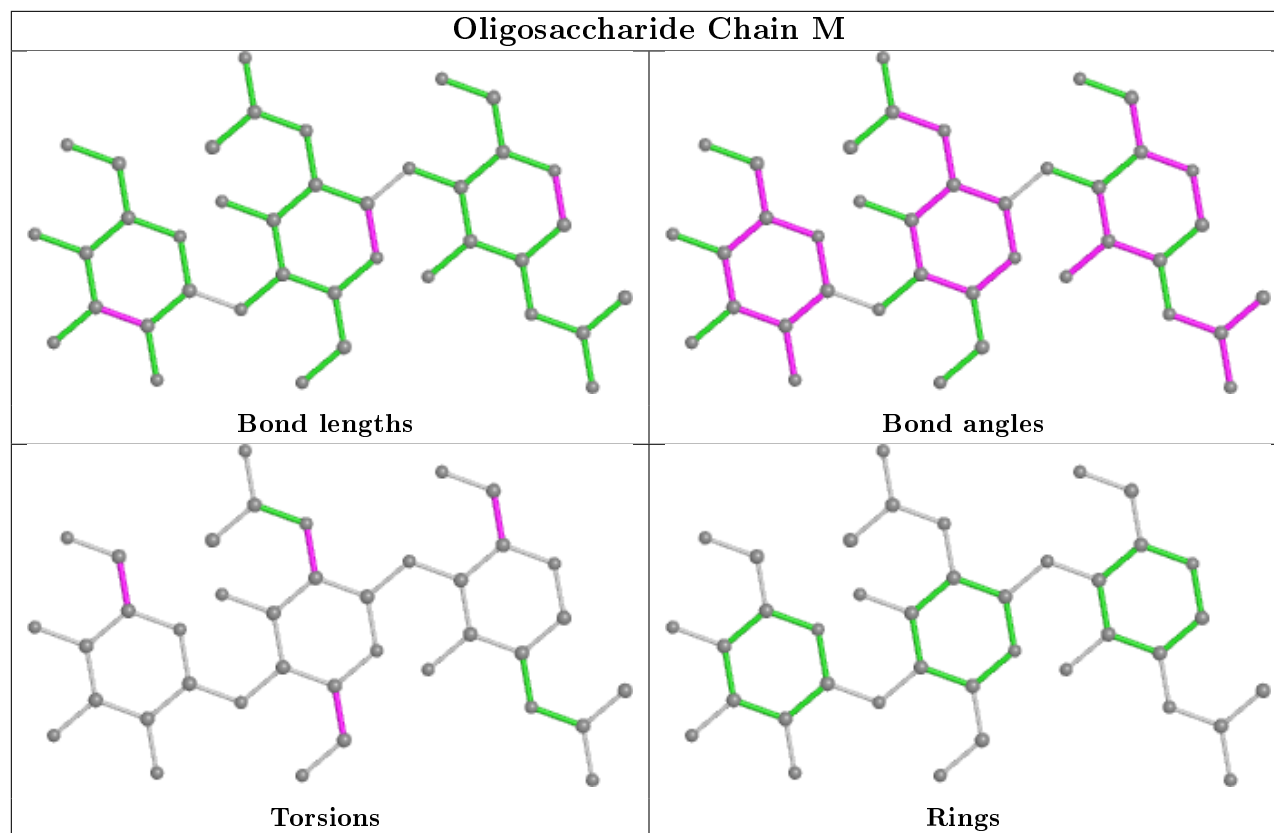
There are no ring outliers.

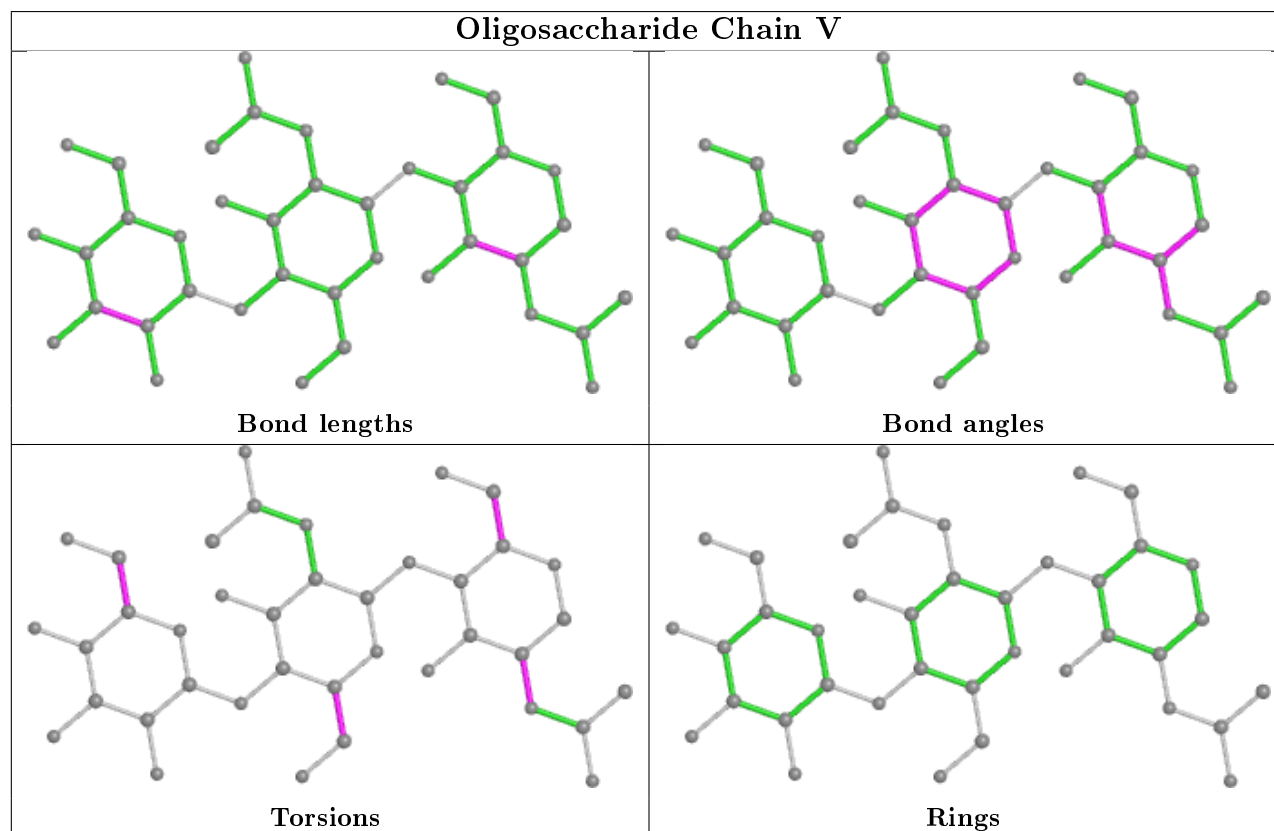
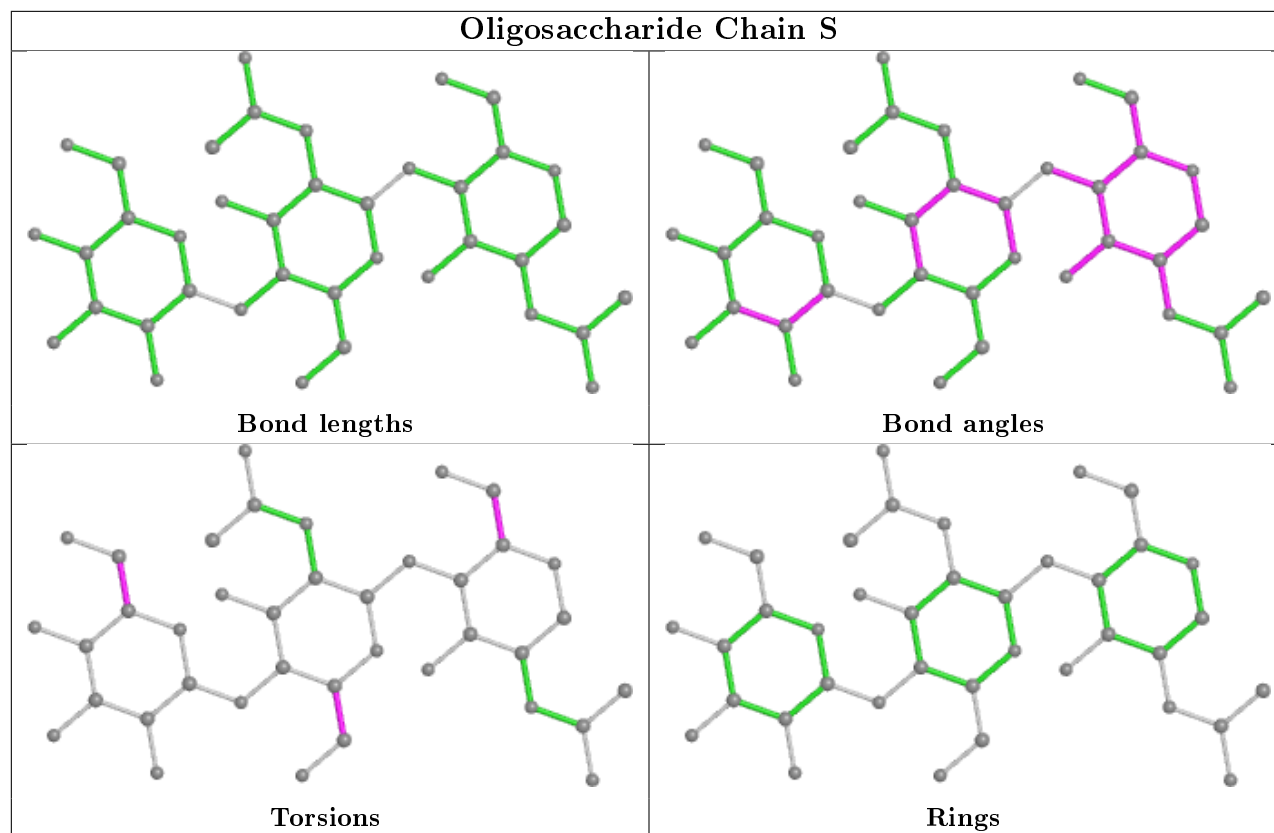
12 monomers are involved in 32 short contacts:

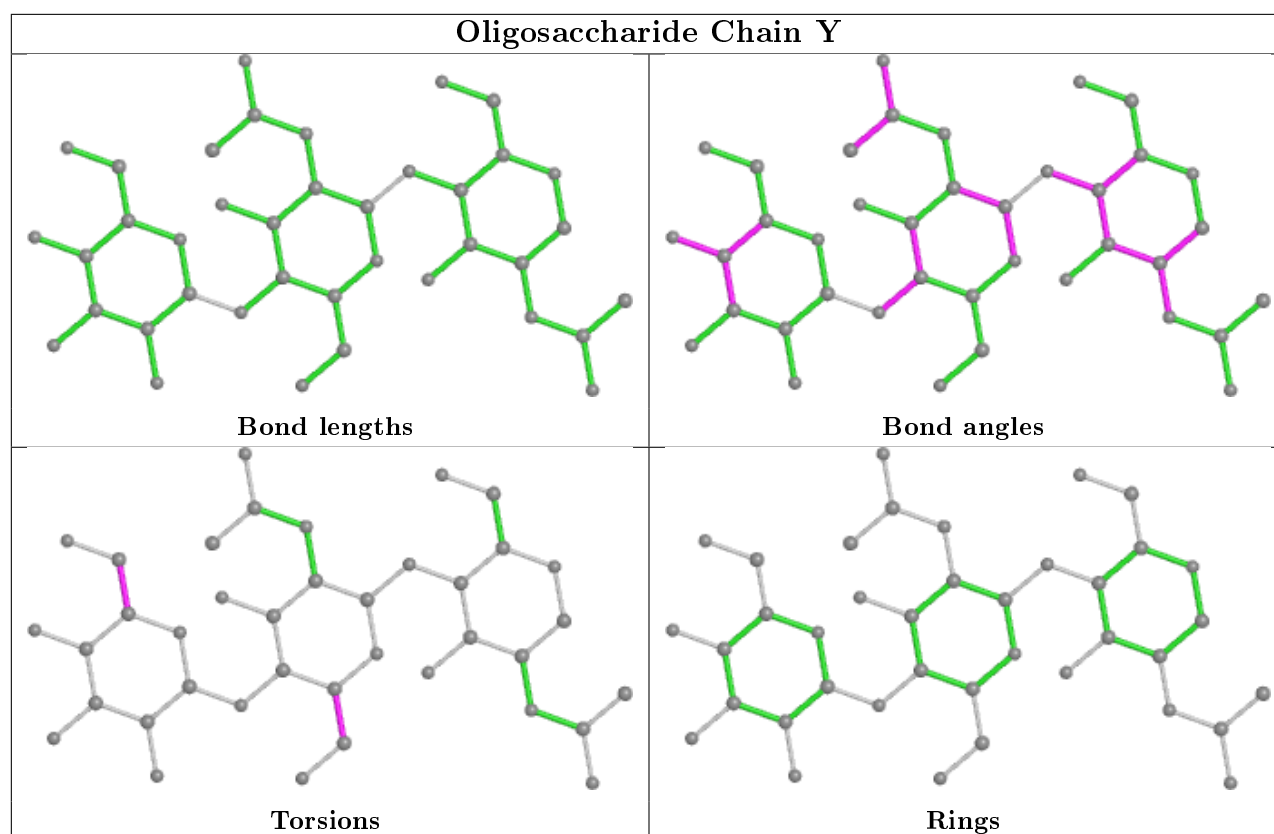
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	W	1	NAG	1	0
3	T	1	NAG	6	0
2	Y	1	NAG	1	0
2	P	2	NAG	5	0
3	I	1	NAG	1	0
3	Q	1	NAG	3	0
4	X	1	NAG	1	0
3	N	1	NAG	6	0
2	S	1	NAG	2	0
2	P	3	BMA	1	0
2	Y	2	NAG	3	0
2	M	1	NAG	3	0

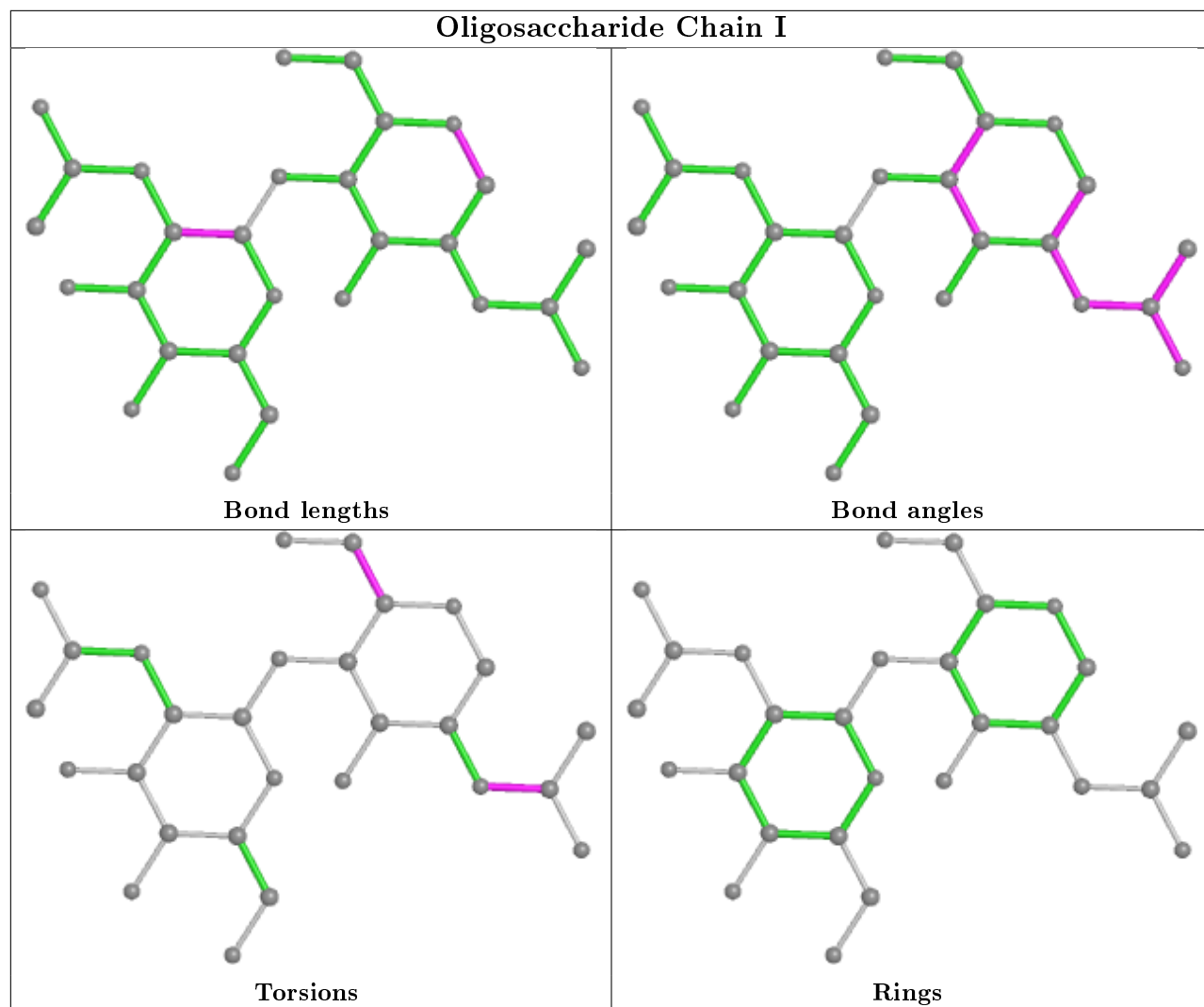
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

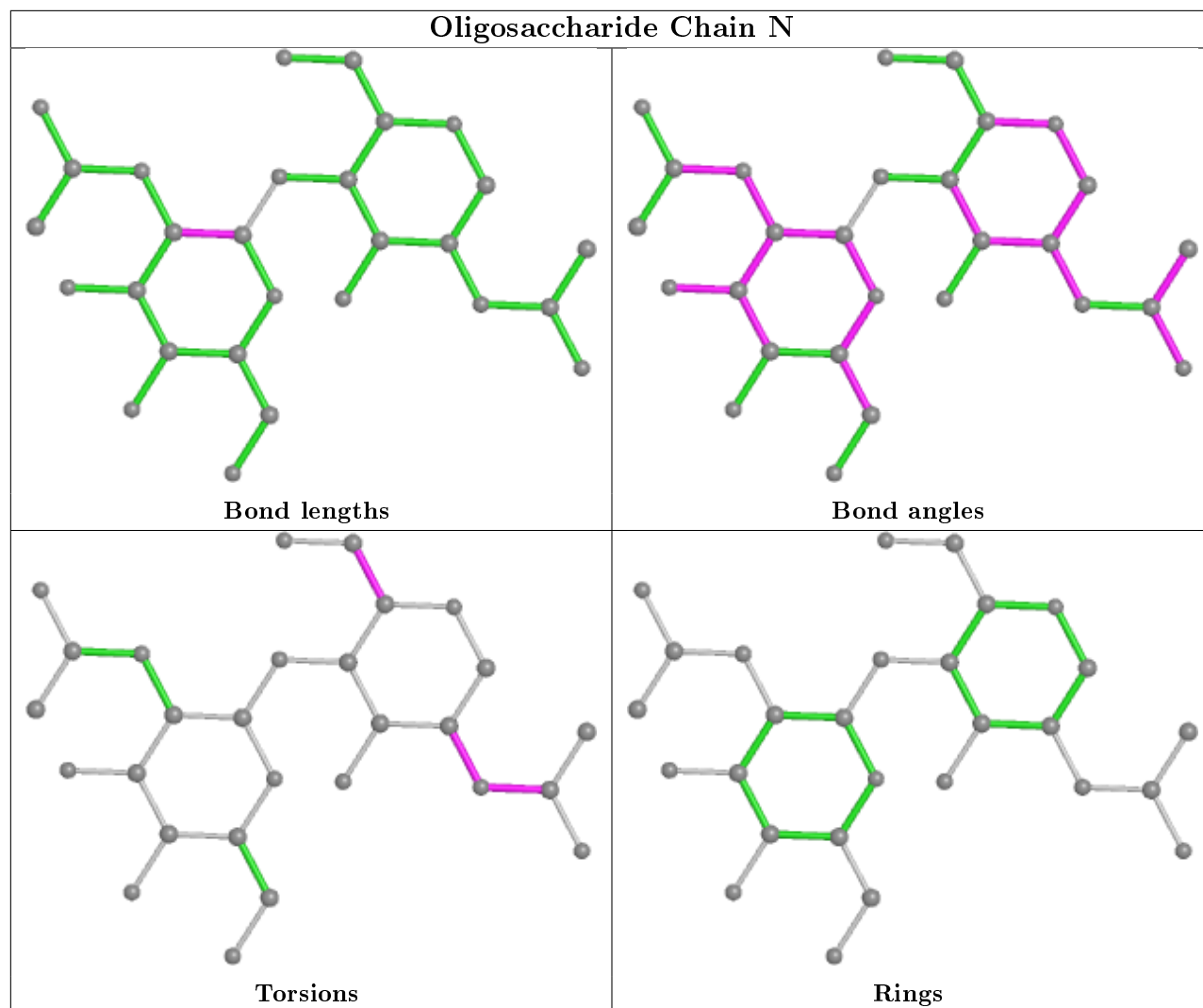


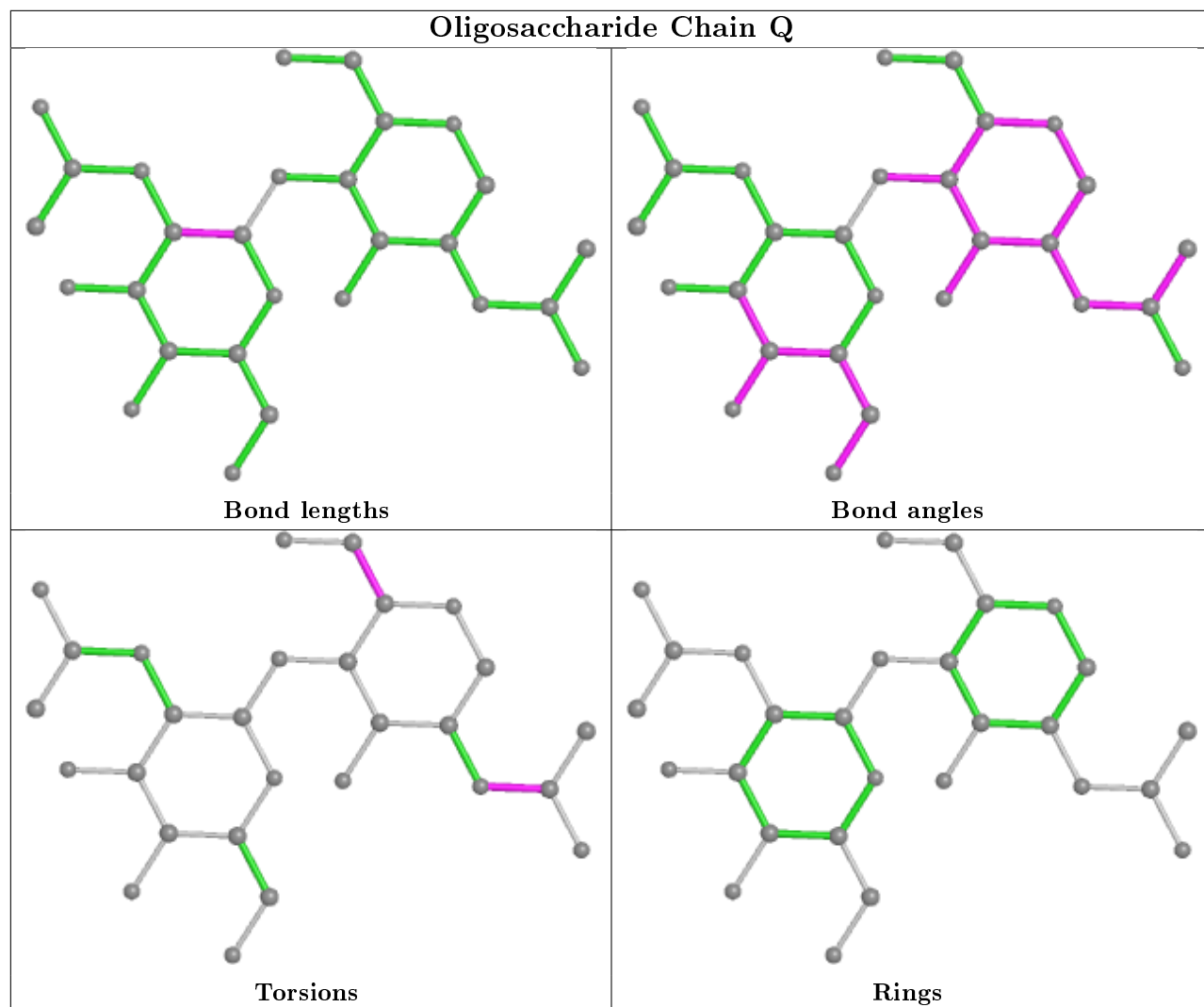


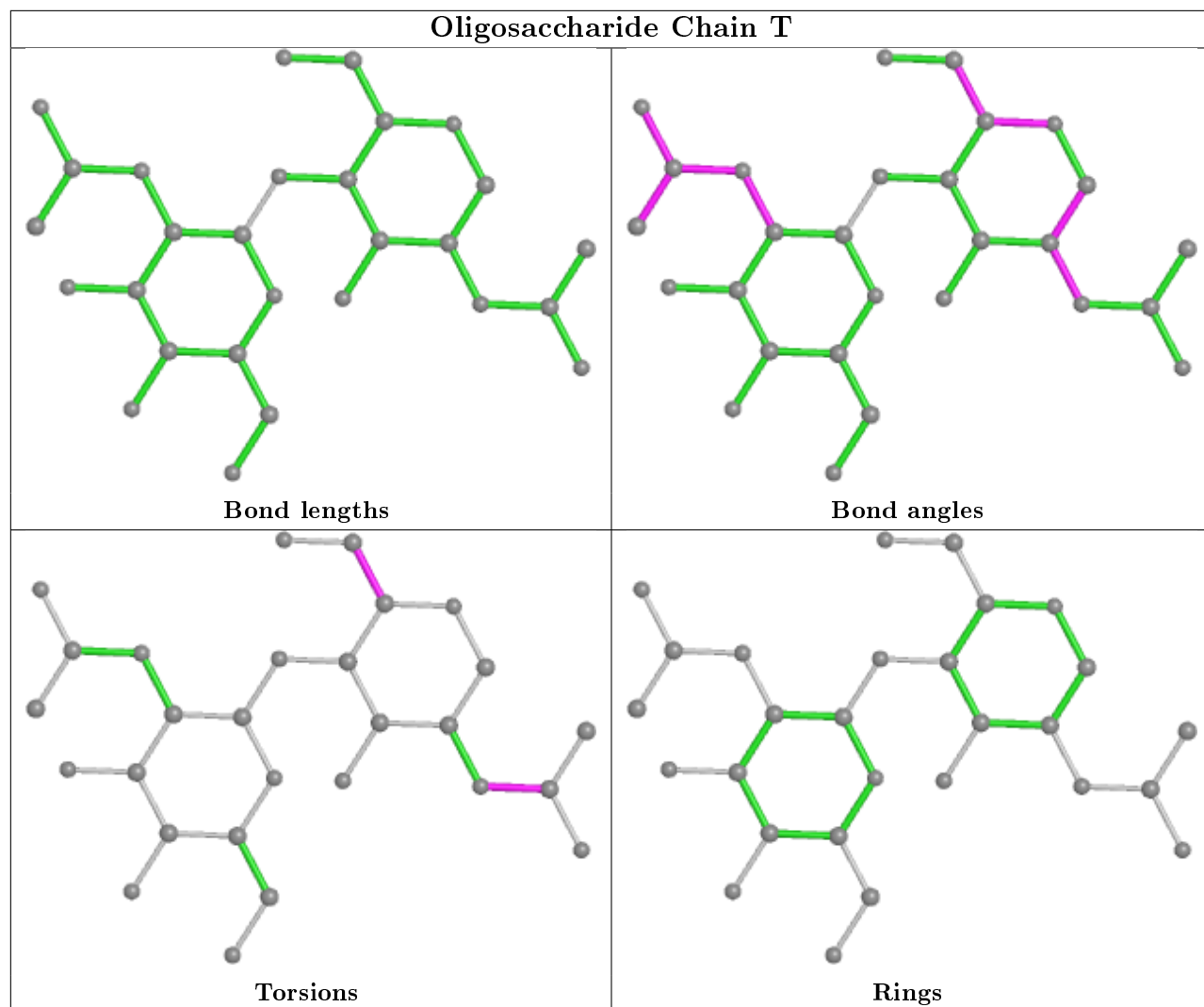


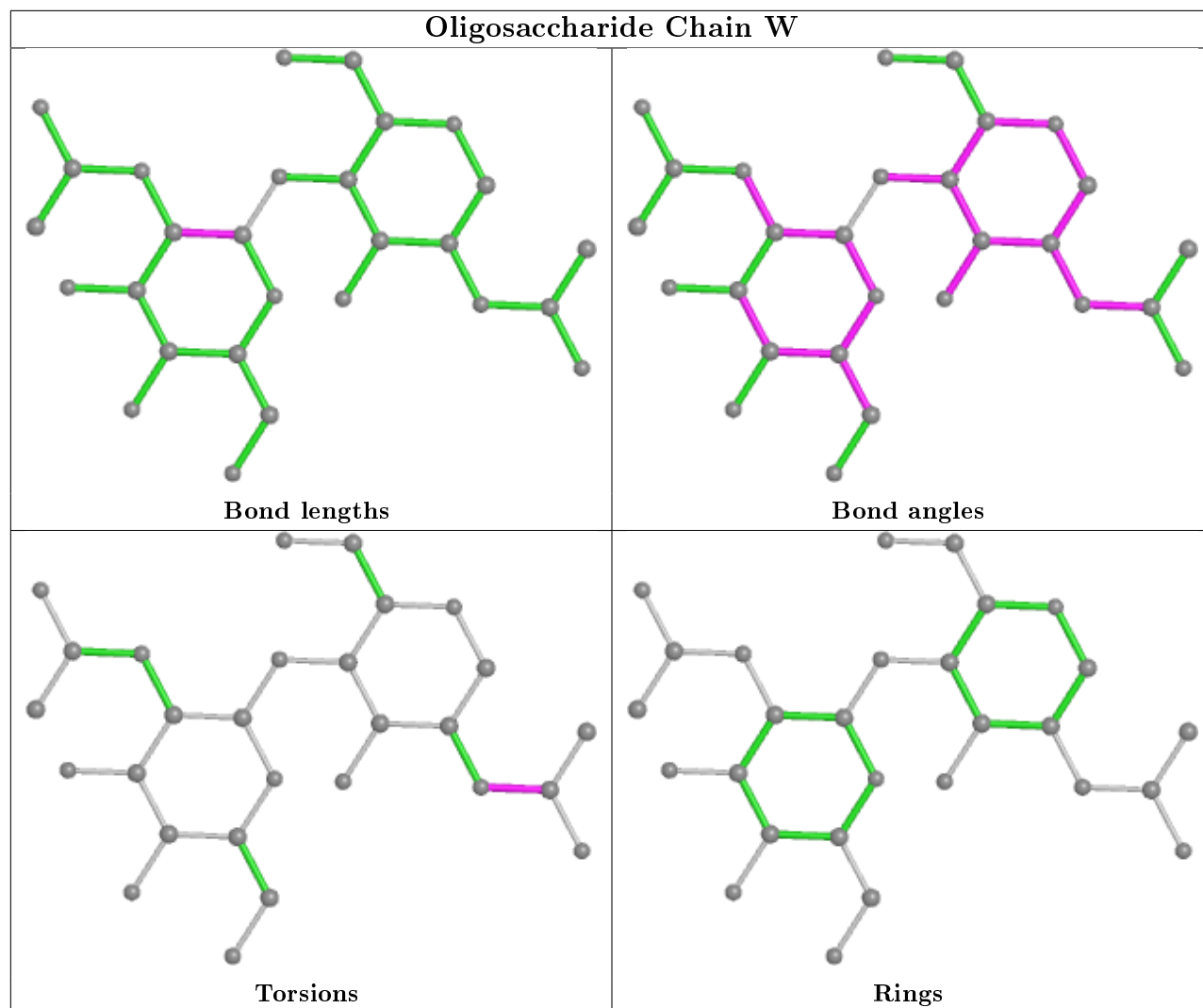


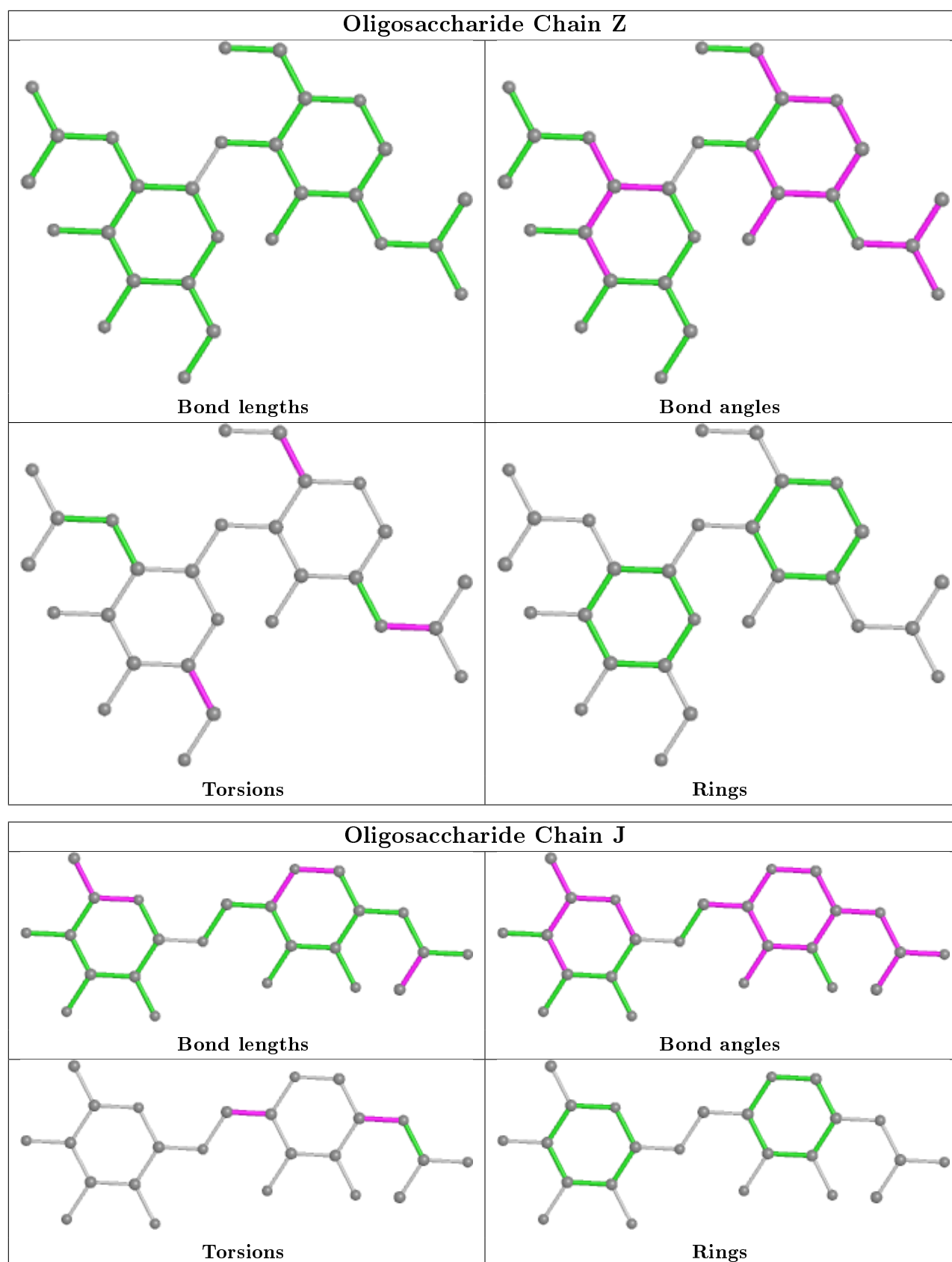


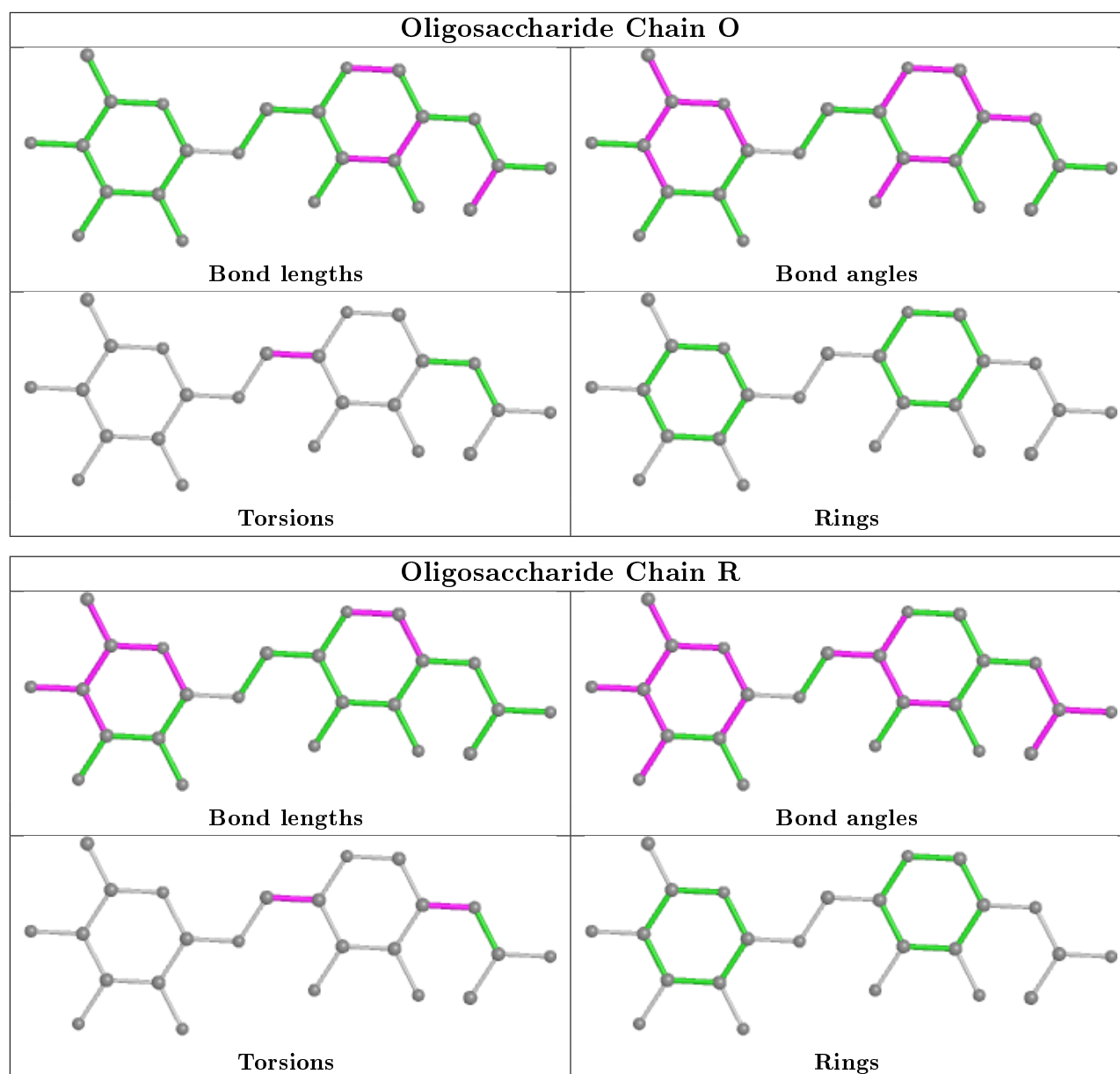


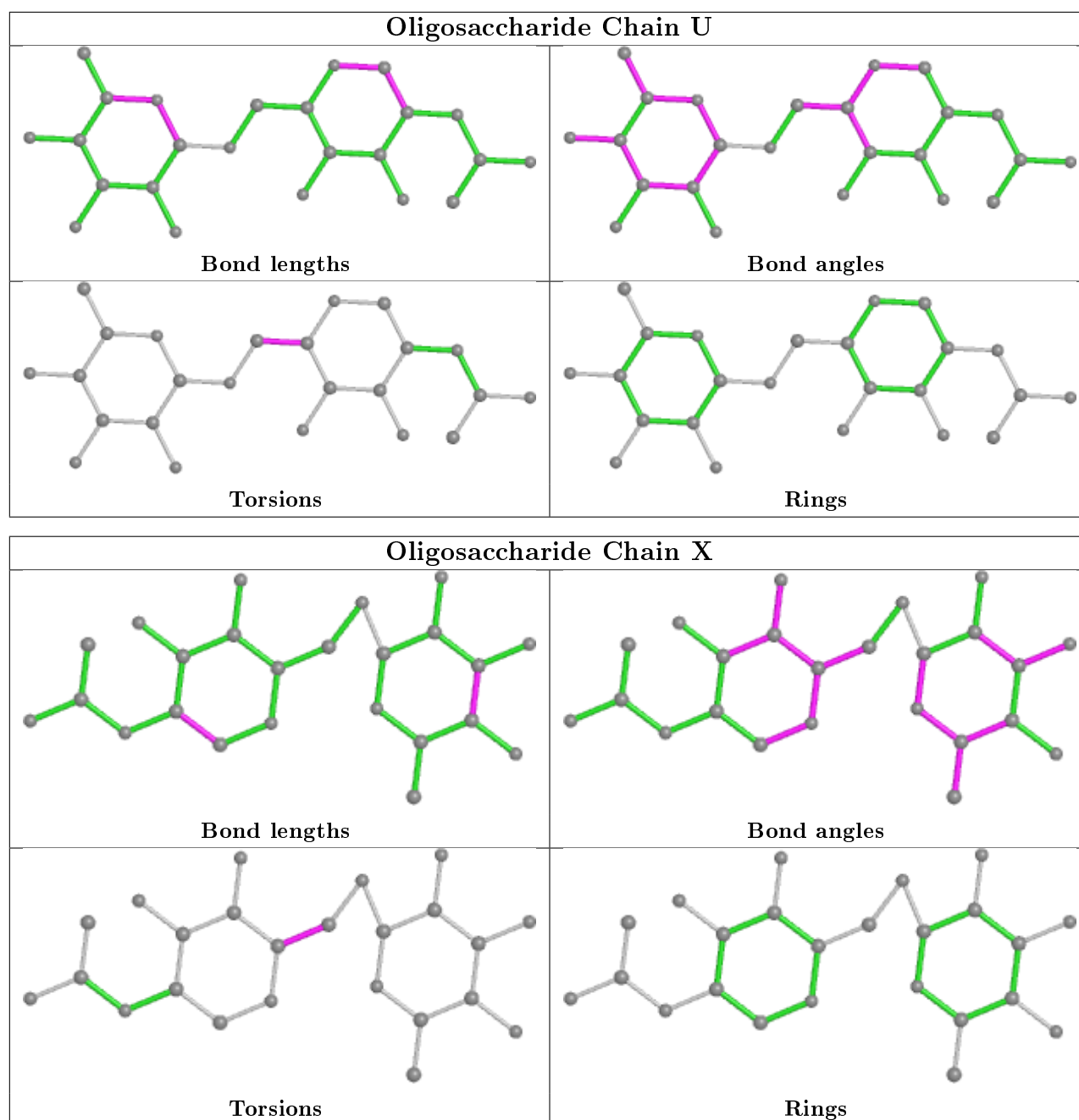


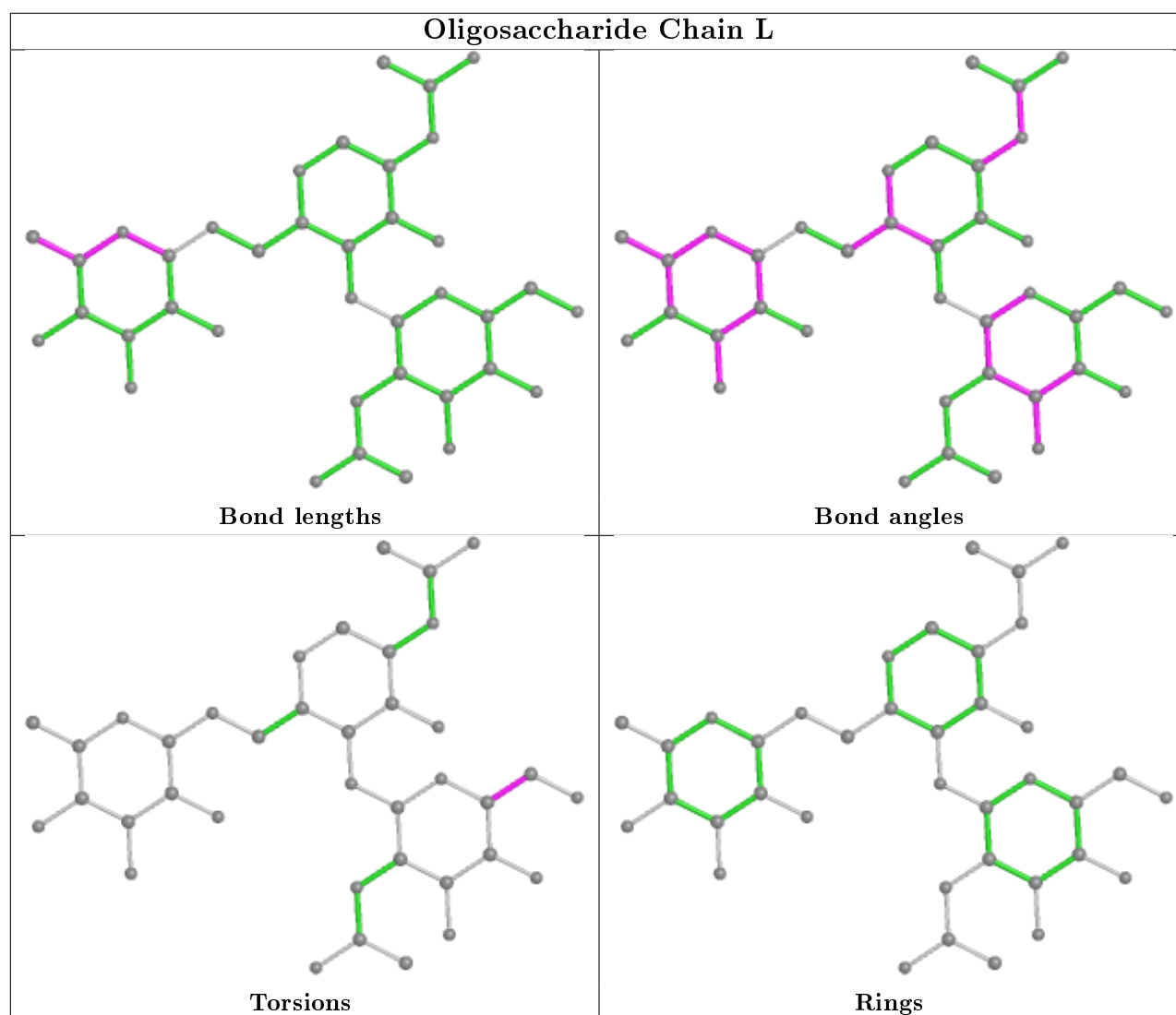












5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 21 are monoatomic - leaving 3 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	$\# Z > 2$
9	GOL	A	764	-	5,5,5	0.51	0	5,5,5	0.44	0
10	NAG	B	1772	1	14,14,15	0.76	0	17,19,21	3.26	10 (58%)
10	NAG	D	1775	1	14,14,15	0.69	0	17,19,21	1.93	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
9	GOL	A	764	-	-	2/4/4/4	-
10	NAG	B	1772	1	-	6/6/23/26	0/1/1/1
10	NAG	D	1775	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1772	NAG	C4-C3-C2	-7.61	99.87	111.02
10	B	1772	NAG	C1-O5-C5	7.42	122.25	112.19
10	B	1772	NAG	C1-C2-N2	5.20	119.37	110.49
10	D	1775	NAG	C2-N2-C7	4.69	129.58	122.90
10	D	1775	NAG	C1-O5-C5	3.97	117.57	112.19

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	1775	NAG	C3-C2-N2-C7
9	A	764	GOL	O1-C1-C2-O2
10	B	1772	NAG	C1-C2-N2-C7
10	B	1772	NAG	C4-C5-C6-O6
10	B	1772	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1772	NAG	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	704/748 (94%)	0.47	1 (0%) 95 96	13, 39, 43, 63	0
1	B	704/748 (94%)	0.35	3 (0%) 92 93	12, 39, 43, 65	0
1	C	708/748 (94%)	0.33	1 (0%) 95 96	16, 39, 45, 73	0
1	D	710/748 (94%)	0.40	4 (0%) 89 89	16, 39, 46, 68	0
1	E	701/748 (93%)	0.29	8 (1%) 80 80	22, 39, 49, 76	0
1	F	700/748 (93%)	0.76	56 (8%) 12 9	26, 39, 47, 69	0
1	G	704/748 (94%)	1.03	109 (15%) 2 1	32, 39, 49, 82	0
All	All	4931/5236 (94%)	0.52	182 (3%) 41 37	12, 39, 46, 82	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	741	CYS	5.0
1	G	352	VAL	4.2
1	F	489	PHE	4.1
1	G	79	LEU	4.1
1	G	121	ALA	3.8

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPQ	G	471	14/15	0.86	0.44	44,60,67,84	0
1	TPQ	F	471	14/15	0.90	0.29	36,40,50,58	0
1	TPQ	C	471	14/15	0.92	0.27	22,47,61,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TPQ	E	471	14/15	0.94	0.26	36,45,58,65	0
1	TPQ	D	471	14/15	0.95	0.23	21,31,48,64	0
1	TPQ	B	471	14/15	0.95	0.25	24,31,57,62	0
1	TPQ	A	471	14/15	0.97	0.20	17,28,56,58	0

6.3 Carbohydrates

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

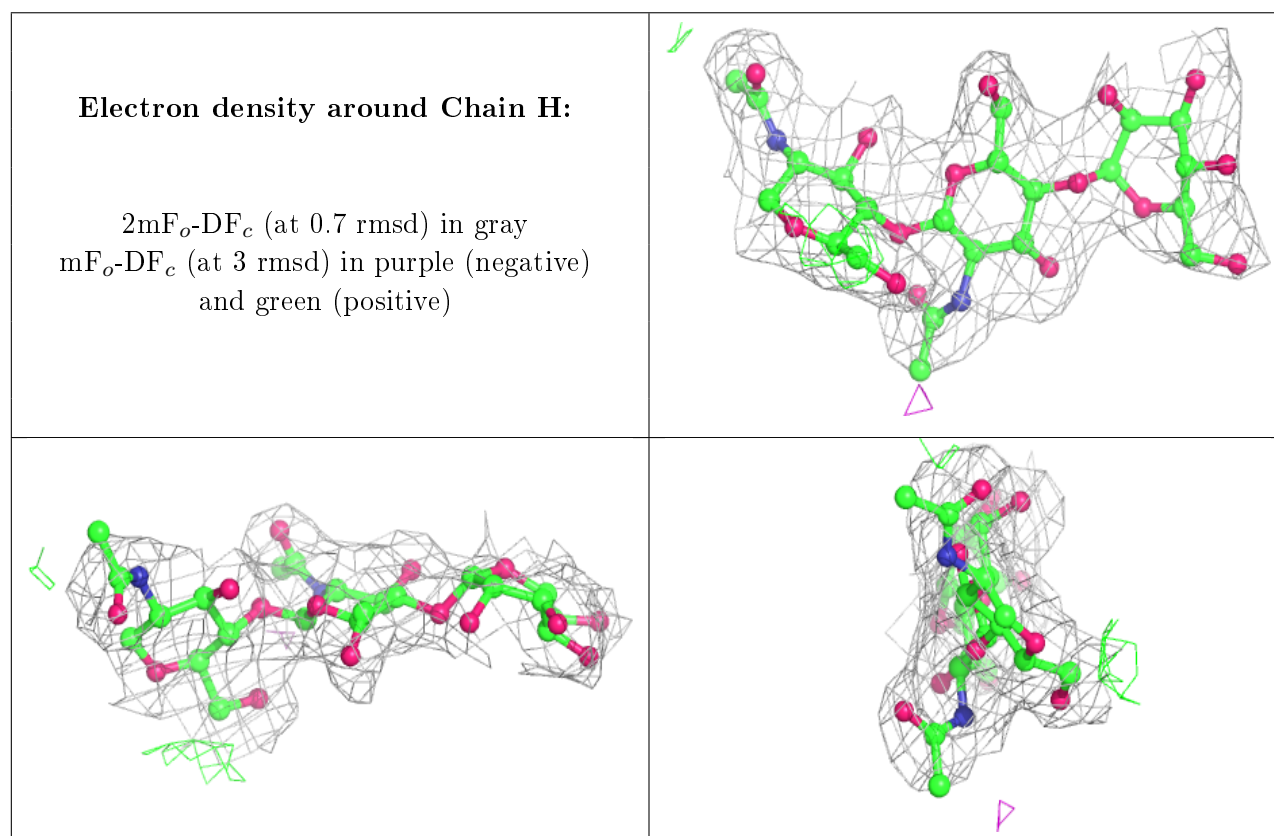
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BMA	V	3	11/12	0.48	0.26	97,102,107,110	0
2	BMA	Y	3	11/12	0.59	0.25	76,88,92,93	0
3	NAG	W	2	14/15	0.70	0.31	73,85,91,91	0
3	NAG	Z	2	14/15	0.71	0.41	83,100,107,111	0
2	BMA	M	3	11/12	0.73	0.23	58,73,74,75	0
2	BMA	H	3	11/12	0.73	0.22	57,73,77,77	0
2	BMA	K	3	11/12	0.74	0.17	53,61,69,71	0
3	NAG	N	2	14/15	0.76	0.31	56,75,81,82	0
2	BMA	P	3	11/12	0.77	0.18	42,68,74,76	0
2	BMA	S	3	11/12	0.78	0.17	58,76,83,87	0
3	NAG	T	2	14/15	0.78	0.22	60,80,85,86	0
6	NAG	a	1	14/15	0.81	0.18	55,76,89,89	0
3	NAG	W	1	14/15	0.81	0.20	48,66,75,79	0
4	NAG	U	1	14/15	0.81	0.24	39,72,84,89	0
3	NAG	Q	2	14/15	0.83	0.25	46,72,77,78	0
3	NAG	T	1	14/15	0.84	0.20	68,77,87,88	0
2	NAG	S	2	14/15	0.84	0.22	74,85,87,88	0
3	NAG	Z	1	14/15	0.85	0.22	70,79,85,92	0
2	NAG	M	2	14/15	0.86	0.21	43,53,66,67	0
4	NAG	R	1	14/15	0.86	0.18	34,68,74,90	0
6	FUC	a	2	10/11	0.86	0.24	39,68,73,76	0
5	NAG	L	2	14/15	0.87	0.22	51,59,71,74	0
2	NAG	P	2	14/15	0.87	0.24	45,68,74,77	0
4	NAG	J	1	14/15	0.87	0.17	21,56,68,72	0
4	NAG	O	1	14/15	0.87	0.19	29,40,47,51	0
2	NAG	K	2	14/15	0.88	0.19	34,55,65,66	0
2	NAG	Y	1	14/15	0.89	0.26	65,73,76,78	0
2	NAG	Y	2	14/15	0.89	0.24	63,80,85,89	0
2	NAG	V	1	14/15	0.90	0.16	32,56,60,67	0

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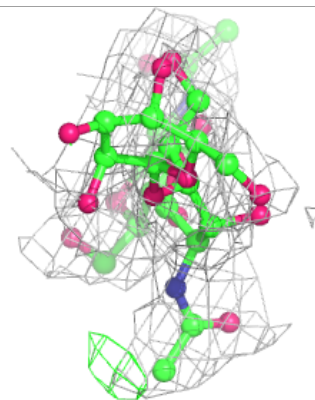
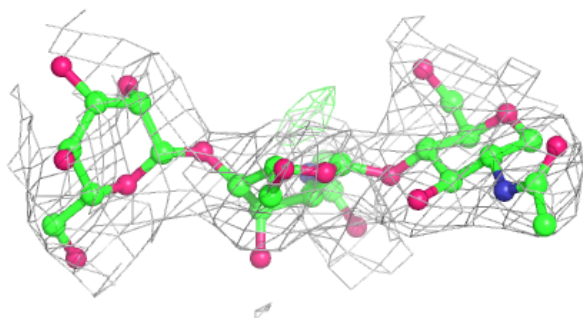
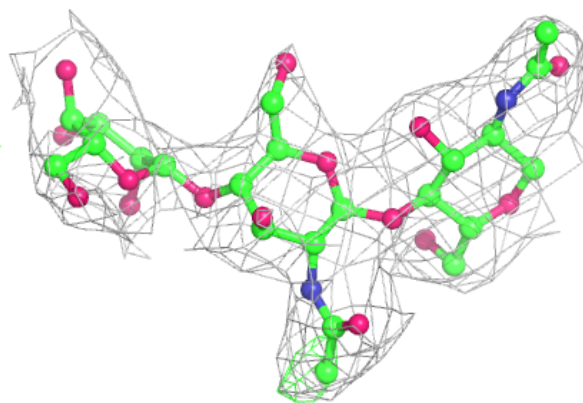
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FUL	R	2	10/11	0.90	0.16	15,51,58,58	0
4	FUL	X	2	10/11	0.90	0.13	33,47,56,57	0
2	NAG	V	2	14/15	0.91	0.18	49,66,83,86	0
3	NAG	I	2	14/15	0.92	0.17	39,54,56,60	0
4	NAG	X	1	14/15	0.92	0.14	33,45,55,59	0
4	FUL	U	2	10/11	0.92	0.16	46,55,58,61	0
2	NAG	H	2	14/15	0.93	0.14	31,46,56,62	0
3	NAG	Q	1	14/15	0.94	0.18	7,32,40,50	0
5	FUL	L	3	10/11	0.94	0.17	21,29,43,47	0
2	NAG	S	1	14/15	0.94	0.14	34,50,64,74	0
5	NAG	L	1	14/15	0.95	0.15	27,39,51,51	0
4	FUL	J	2	10/11	0.95	0.16	14,34,41,44	0
2	NAG	P	1	14/15	0.95	0.15	18,40,55,56	0
3	NAG	I	1	14/15	0.95	0.15	14,37,43,46	0
2	NAG	H	1	14/15	0.96	0.14	20,26,34,41	0
3	NAG	N	1	14/15	0.96	0.20	34,48,72,77	0
2	NAG	K	1	14/15	0.97	0.17	15,23,40,42	0
2	NAG	M	1	14/15	0.97	0.15	15,23,37,49	0
4	FUL	O	2	10/11	0.98	0.13	16,28,30,30	0

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

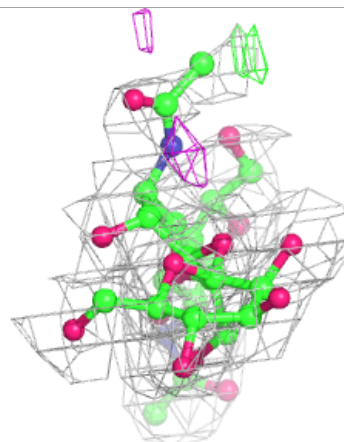
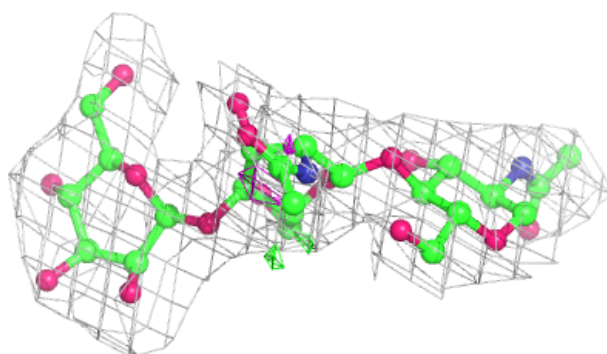
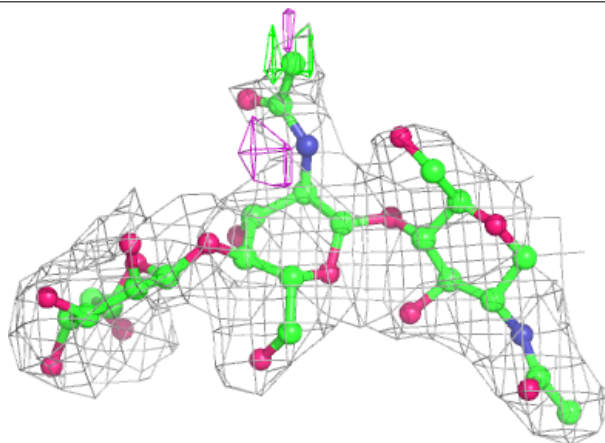


Electron density around Chain K:

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

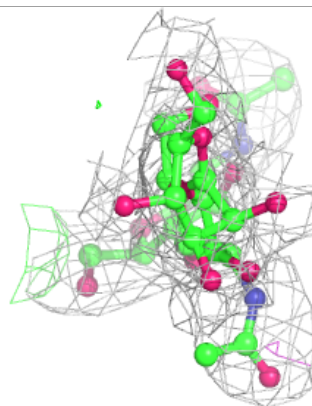
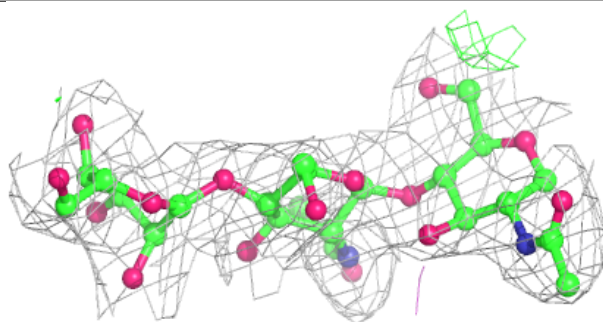
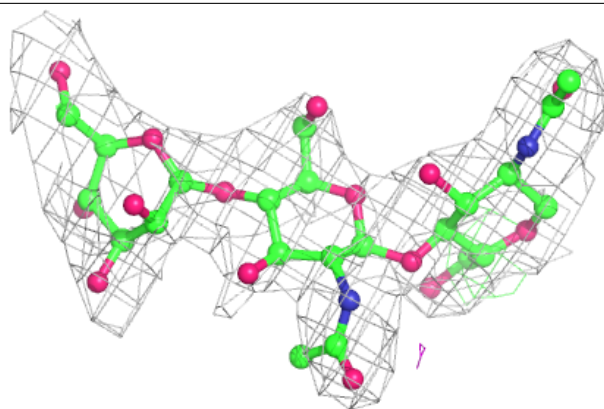
**Electron density around Chain M:**

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

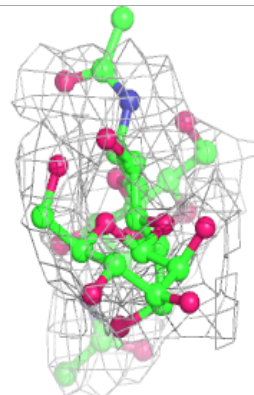
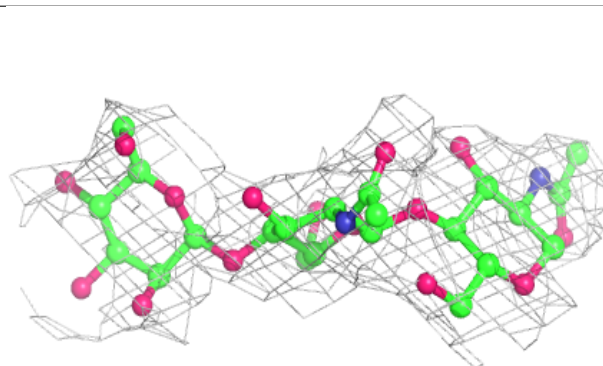
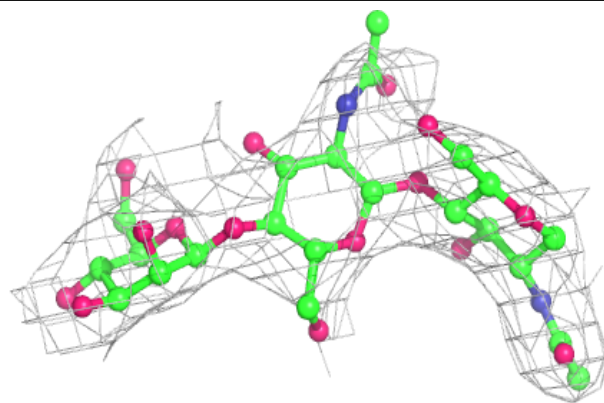


Electron density around Chain P:

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

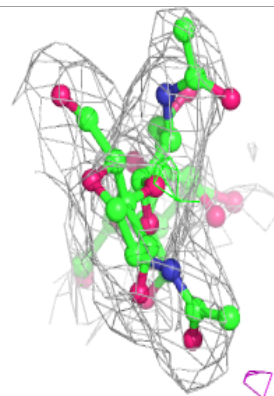
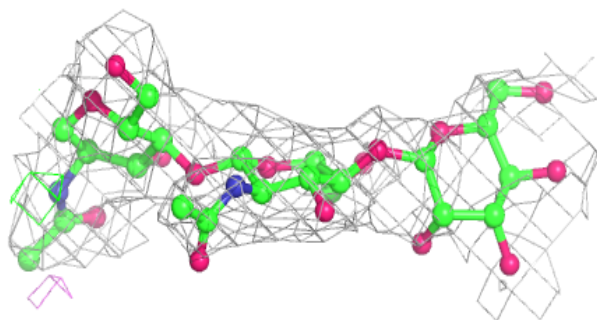
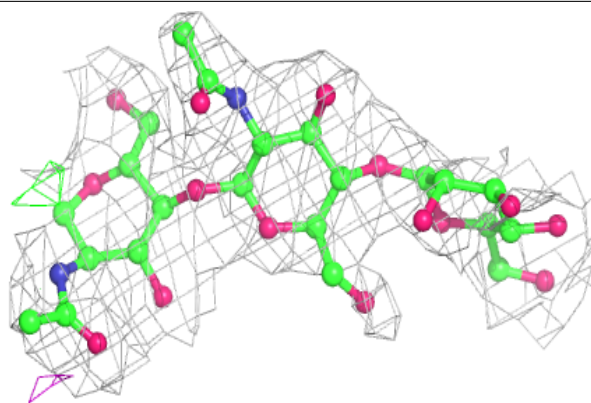
**Electron density around Chain S:**

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

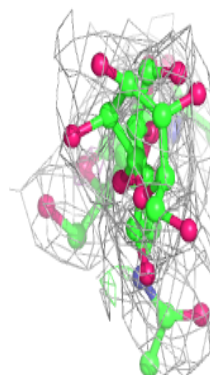
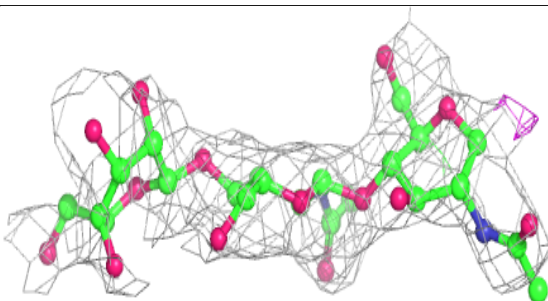
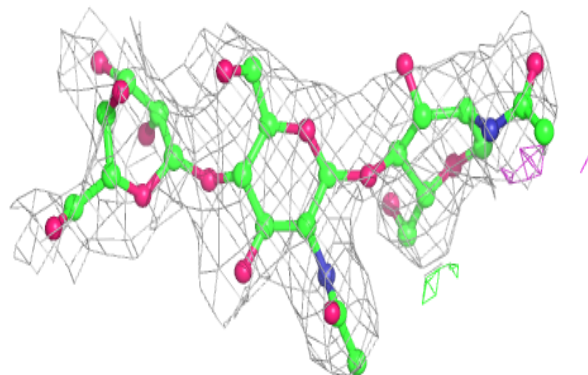


Electron density around Chain V:

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

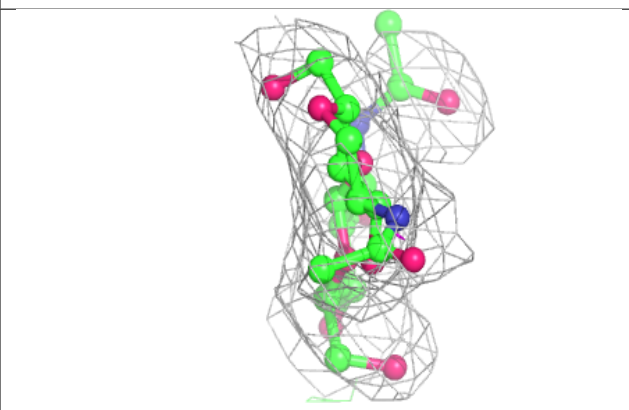
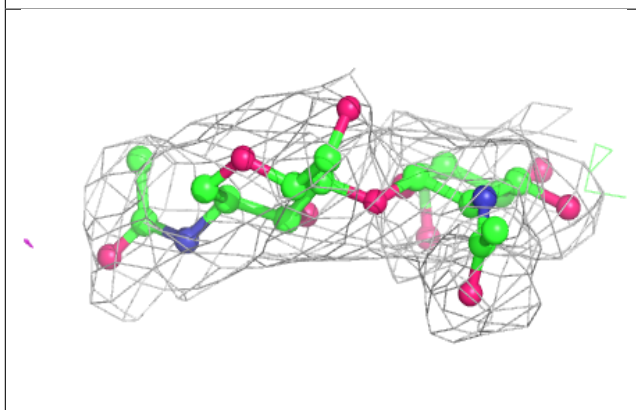
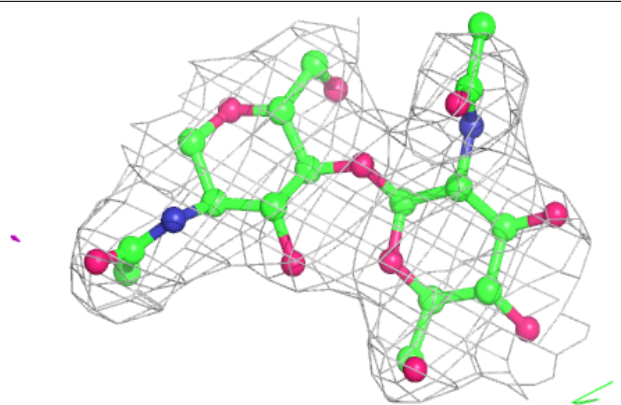
**Electron density around Chain Y:**

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



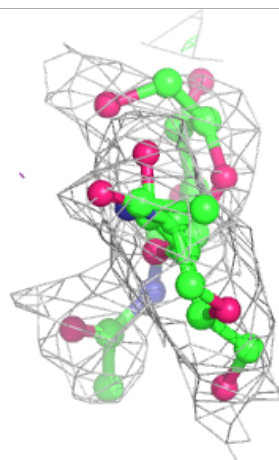
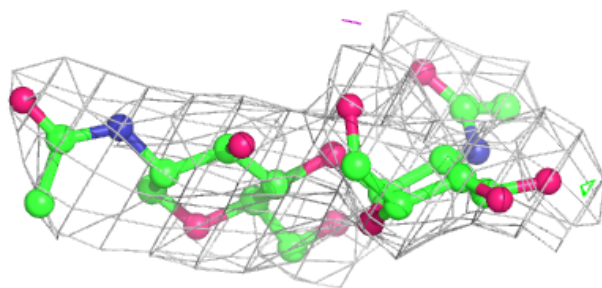
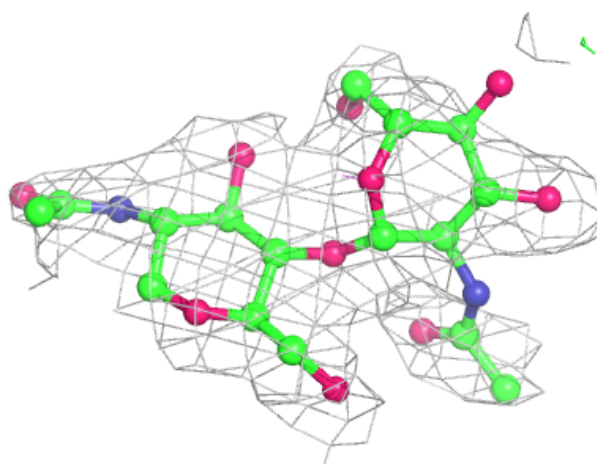
Electron density around Chain I:

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



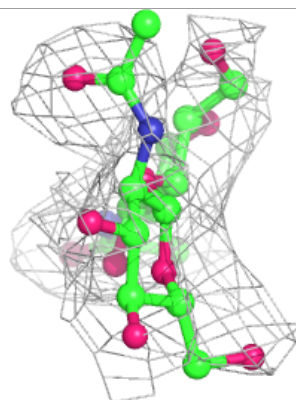
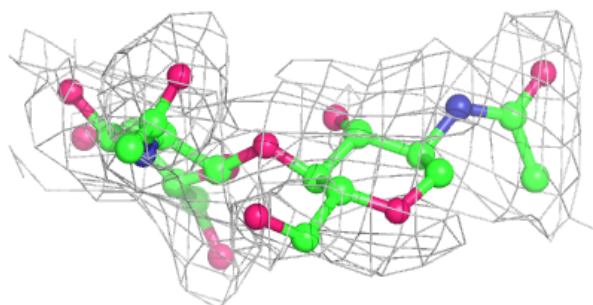
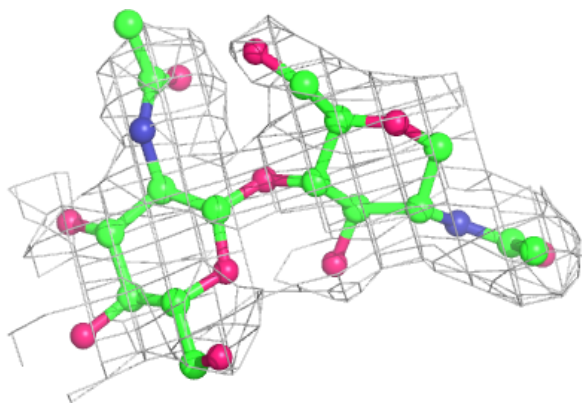
Electron density around Chain N:

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

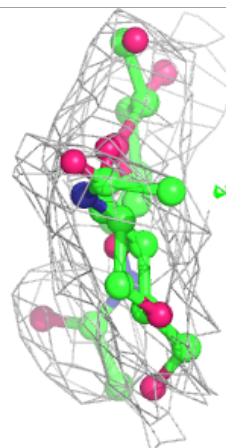
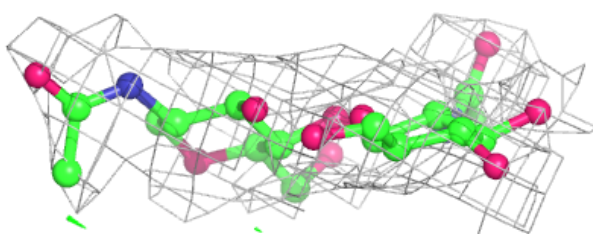
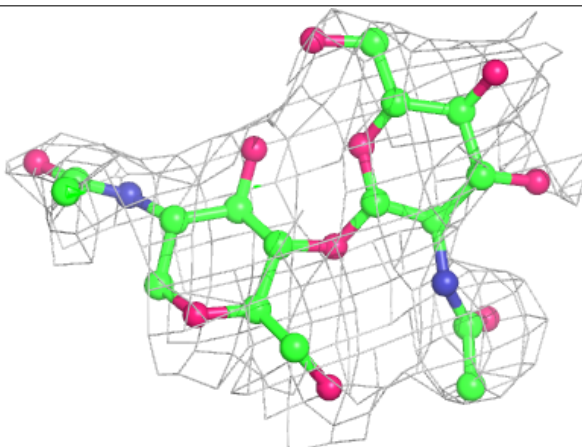


Electron density around Chain Q:

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

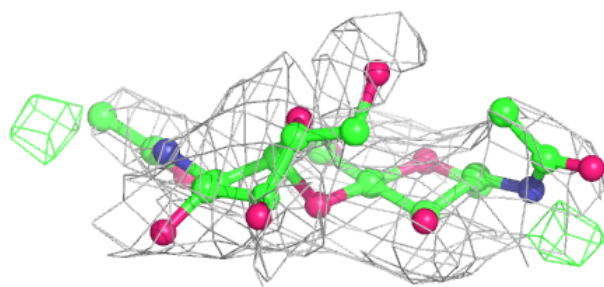
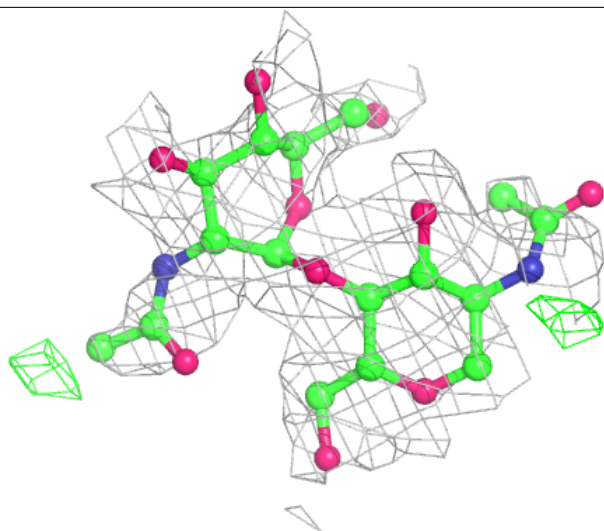
**Electron density around Chain T:**

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



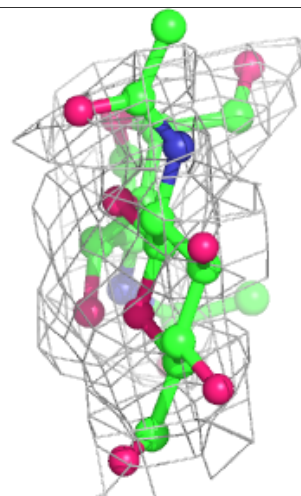
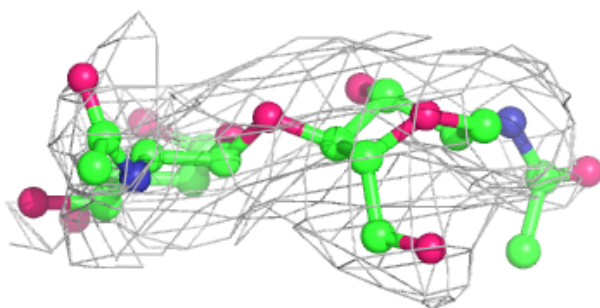
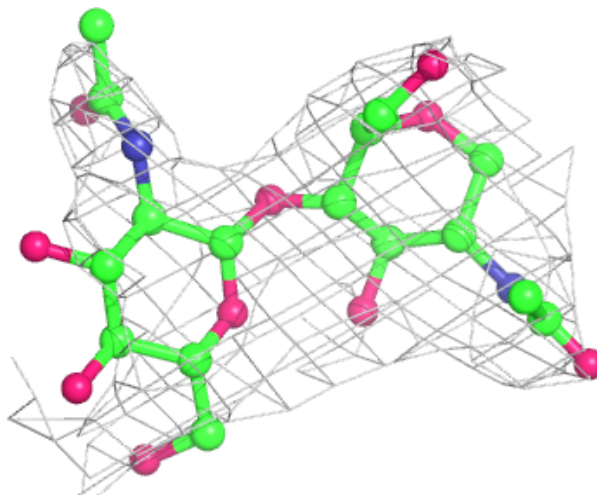
Electron density around Chain W:

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



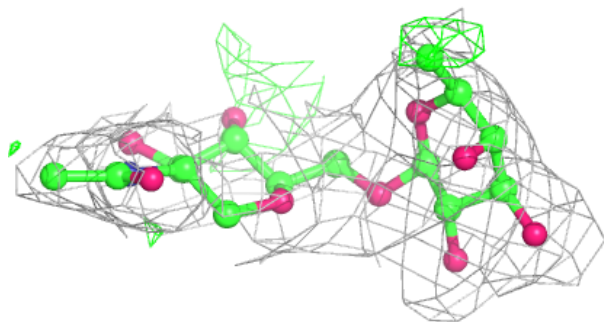
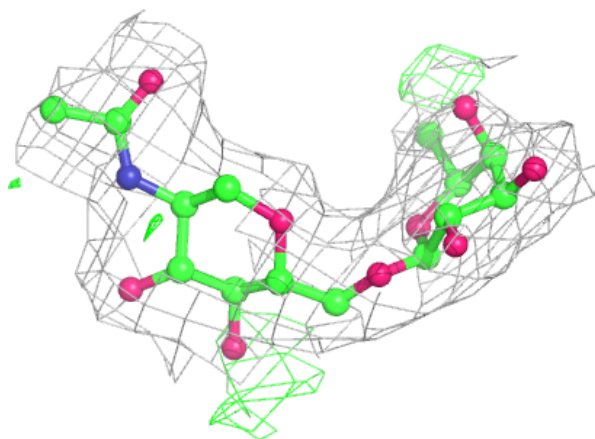
Electron density around Chain Z:

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



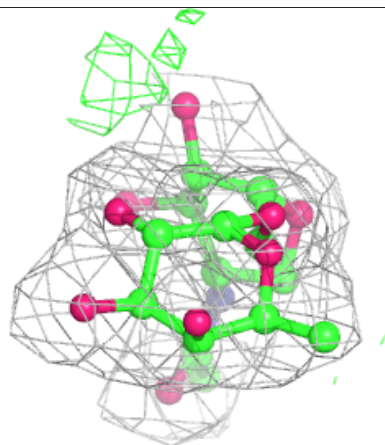
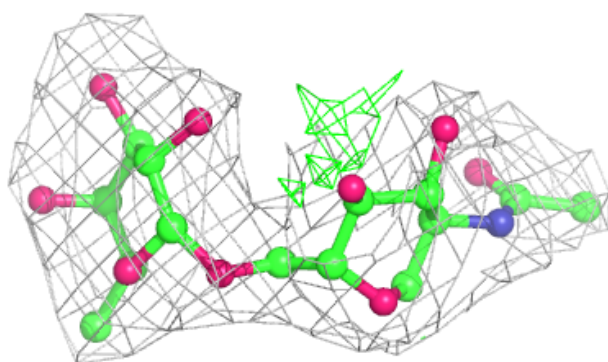
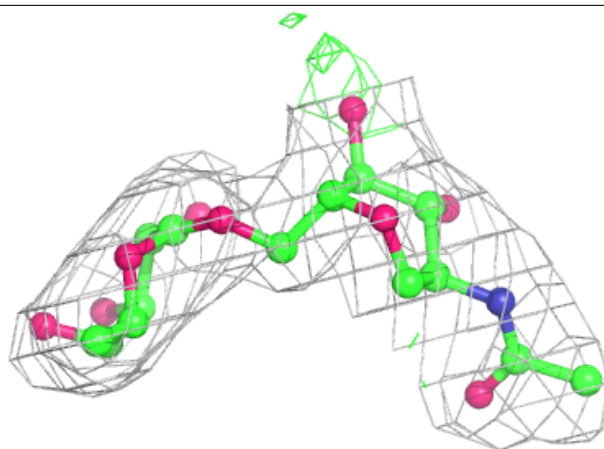
Electron density around Chain J:

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

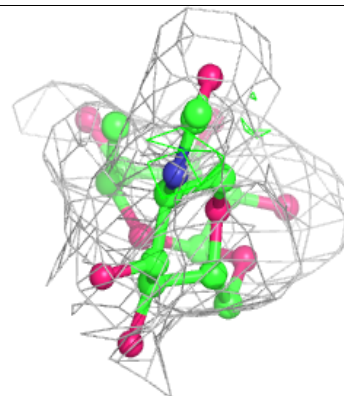
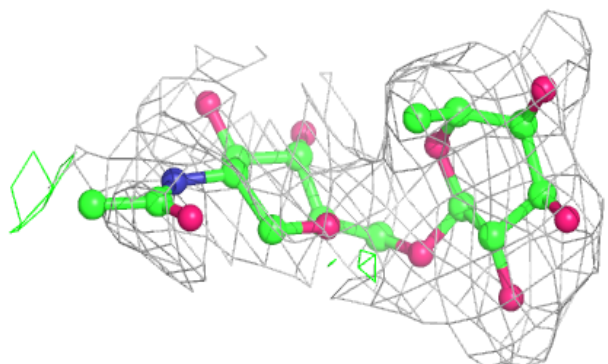
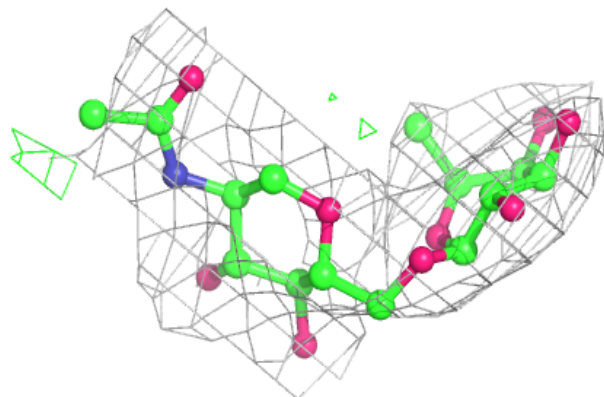


Electron density around Chain O:

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

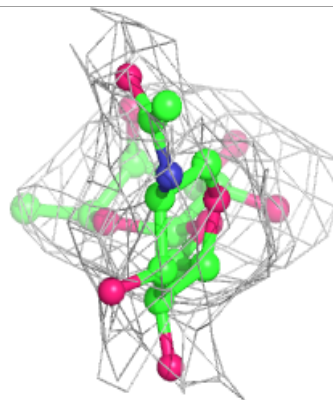
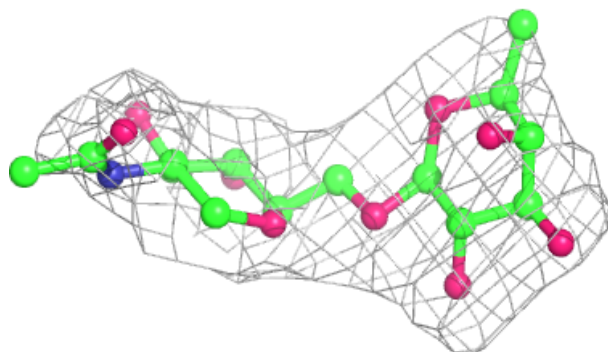
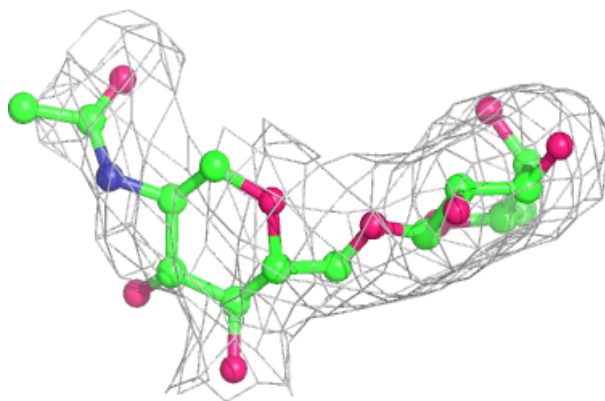
**Electron density around Chain R:**

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

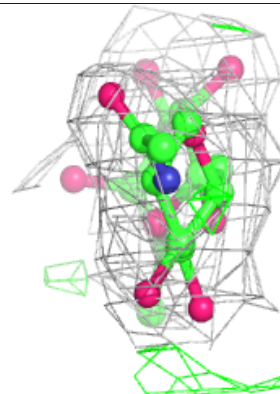
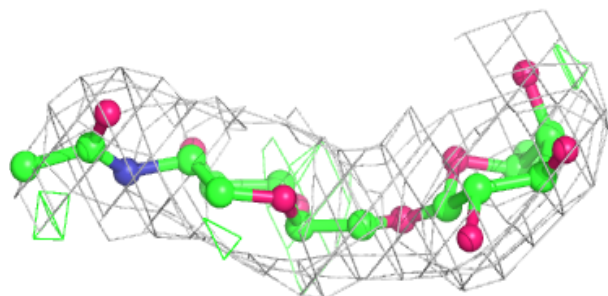
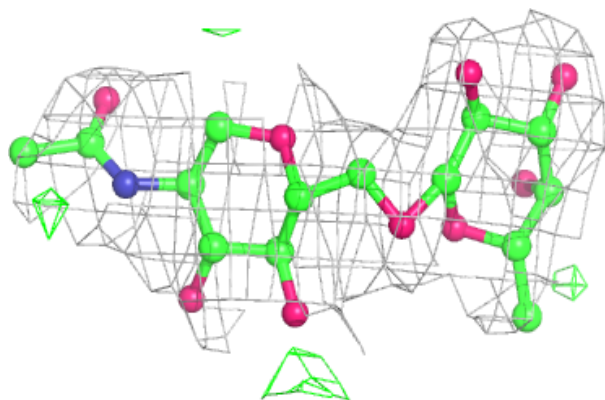


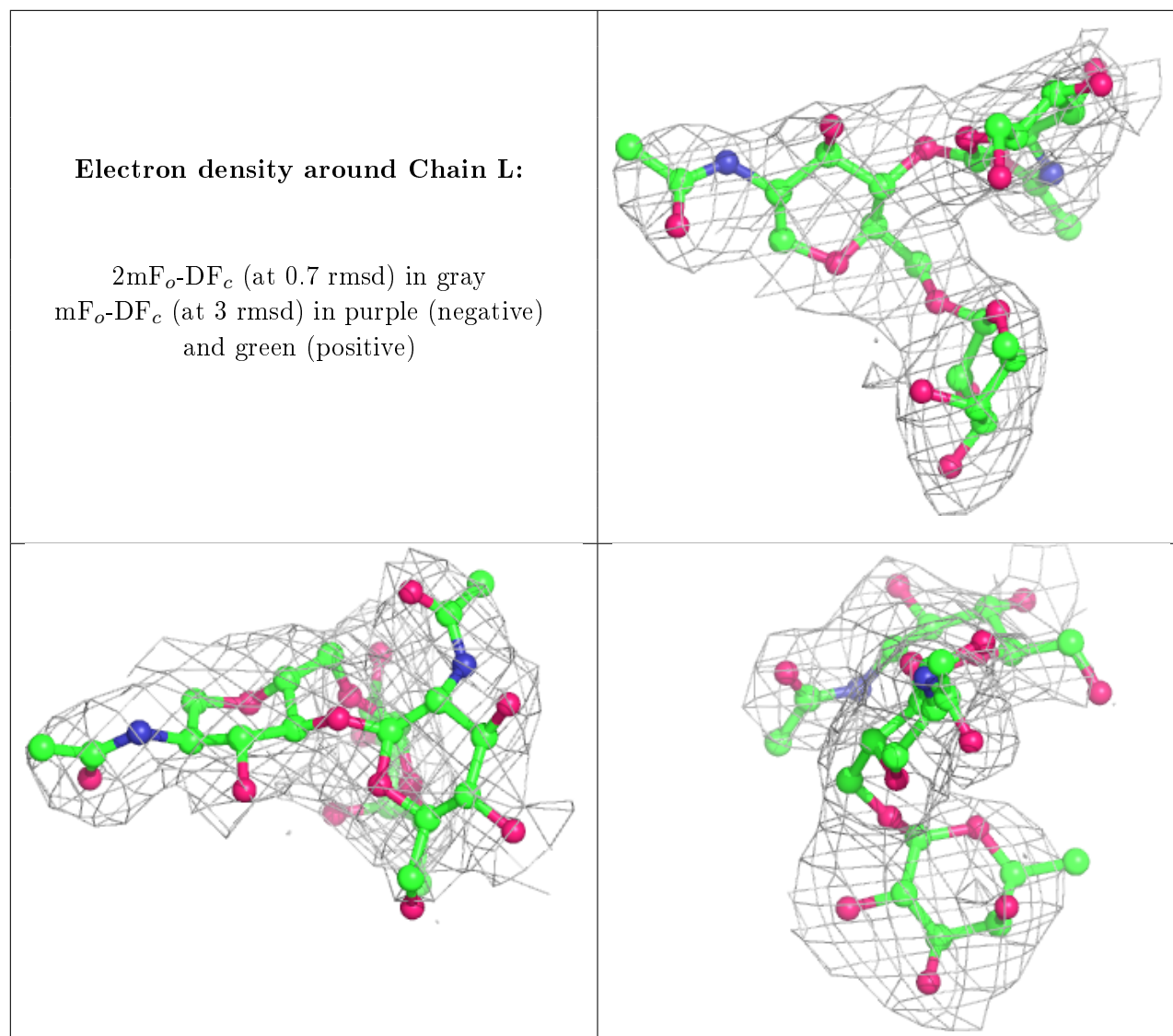
Electron density around Chain U:

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

**Electron density around Chain X:**

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





6.4 Ligands [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
10	NAG	B	1772	14/15	0.81	0.36	50,66,69,72	0
10	NAG	D	1775	14/15	0.82	0.19	74,84,90,90	0
8	CA	G	1763	1/1	0.89	0.09	51,51,51,51	0
9	GOL	A	764	6/6	0.91	0.16	43,43,43,43	0
7	CU	G	1762	1/1	0.92	0.05	69,69,69,69	0
8	CA	G	1764	1/1	0.93	0.17	94,94,94,94	0
8	CA	B	1764	1/1	0.93	0.31	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	CA	F	1763	1/1	0.94	0.10	42,42,42,42	0
8	CA	F	1764	1/1	0.94	0.09	91,91,91,91	0
8	CA	C	1763	1/1	0.95	0.11	34,34,34,34	0
7	CU	C	1762	1/1	0.96	0.06	58,58,58,58	0
8	CA	E	1763	1/1	0.96	0.12	43,43,43,43	0
8	CA	D	1764	1/1	0.96	0.09	65,65,65,65	0
8	CA	B	1763	1/1	0.96	0.14	35,35,35,35	0
7	CU	E	1762	1/1	0.97	0.05	49,49,49,49	0
8	CA	C	1764	1/1	0.97	0.10	53,53,53,53	0
7	CU	A	1762	1/1	0.97	0.08	43,43,43,43	0
7	CU	F	1762	1/1	0.97	0.08	60,60,60,60	0
8	CA	D	1763	1/1	0.97	0.13	39,39,39,39	0
8	CA	A	1764	1/1	0.98	0.12	50,50,50,50	0
8	CA	A	1763	1/1	0.98	0.08	32,32,32,32	0
8	CA	E	1764	1/1	0.98	0.06	46,46,46,46	0
7	CU	B	1762	1/1	0.98	0.07	49,49,49,49	0
7	CU	D	1762	1/1	1.00	0.10	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.