



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:06 PM UTC

PDB ID : 8BRN / pdb_00008brn
Title : Crystal structure of red kidney bean purple acid phosphatase in complex with an alpha-aminonaphthylmethylphosphonic acid inhibitor
Authors : Feder, D.; Hussein, W.M.; Guddat, L.W.; Schenk, G.
Deposited on : 2022-11-23
Resolution : 2.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

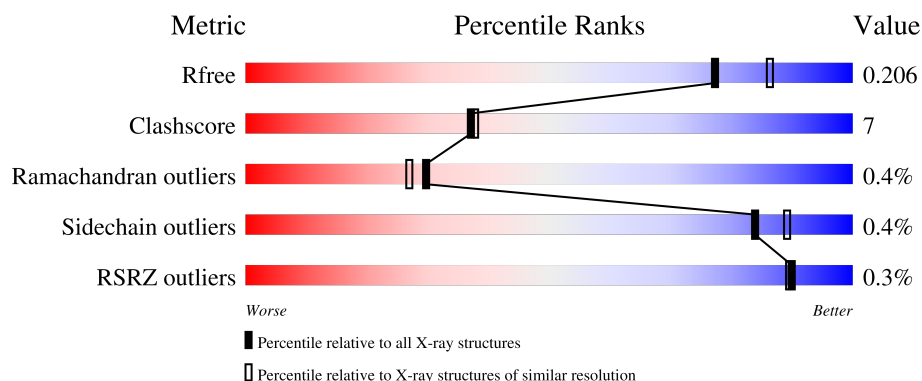
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

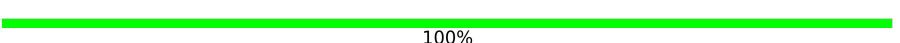
The reported resolution of this entry is 2.00 Å.

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.



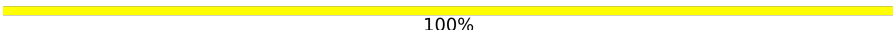
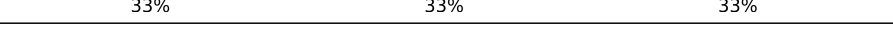
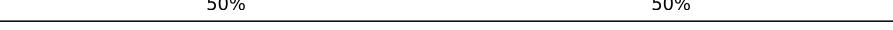
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	428	
1	B	428	
1	C	428	
1	D	428	
2	E	2	

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Mol	Chain	Length	Quality of chain
2	K	2	 100%
2	Q	2	 50% 50%
3	F	6	 50% 33% 17%
4	G	4	 75% 25%
4	I	4	 50% 25% 25%
4	N	4	 75% 25%
4	P	4	 75% 25%
4	S	4	 75% 25%
4	V	4	 75% 25%
5	H	6	 33% 67%
5	J	6	 50% 50%
6	L	5	 40% 60%
7	M	3	 33% 33% 33%
8	O	2	 50% 50%
9	R	4	 50% 50%
10	T	2	 50% 50%

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
13	FLC	A	505	-	X	-	-
13	FLC	A	530	-	X	-	-
13	FLC	B	503	-	X	-	-
13	FLC	B	505	-	-	X	-
13	FLC	C	627	-	X	-	-
14	PGE	D	504	-	-	X	-
16	SO4	A	510	-	-	X	-
16	SO4	A	512	-	-	X	-
16	SO4	C	608	-	-	X	-
16	SO4	C	613	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	GOL	D	522	-	-	X	-
20	R9X	A	532[A]	X	-	-	-
20	R9X	A	532[B]	X	-	-	-
20	R9X	C	633[B]	X	-	-	-
20	R9X	D	535[A]	X	-	-	-
20	R9X	D	535[B]	X	-	-	-
9	BMA	R	3	X	-	-	-

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 18800 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 Fe(3+)-Zn(2+) purple acid phosphatase.

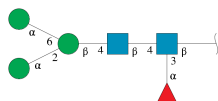
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	4	12	0
			3569	2299	620	640	10			
1	B	428	Total	C	N	O	S	3	5	0
			3558	2284	618	645	11			
1	C	428	Total	C	N	O	S	0	11	0
			3584	2304	619	650	11			
1	D	426	Total	C	N	O	S	5	12	0
			3586	2307	626	642	11			

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



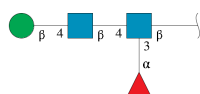
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



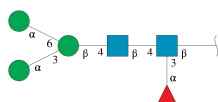
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

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



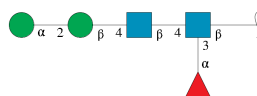
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	I	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	N	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	P	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	S	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	V	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



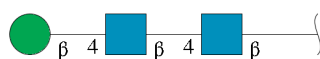
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	6	Total	C	N	O	0	0	0
			71	40	2	29			
5	J	6	Total	C	N	O	0	0	0
			71	40	2	29			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 7 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
7	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(5-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	R	4	Total	C	N	O	0	0	0
			48	27	2	19			

- Molecule 10 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

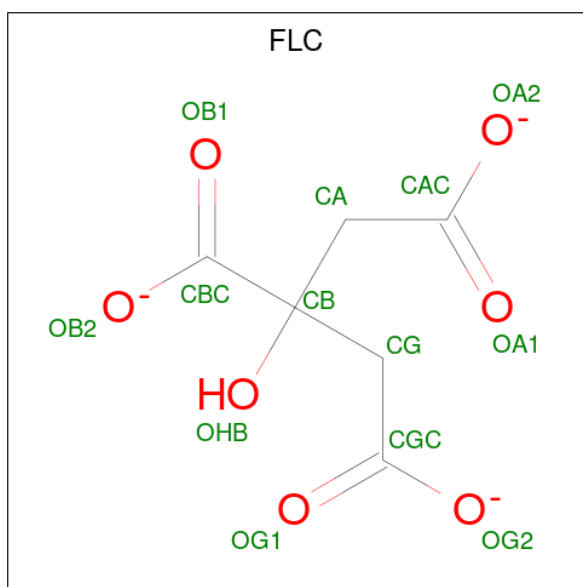
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		
11	C	1	Total	Zn	0	0
			1	1		
11	D	1	Total	Zn	0	0
			1	1		

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

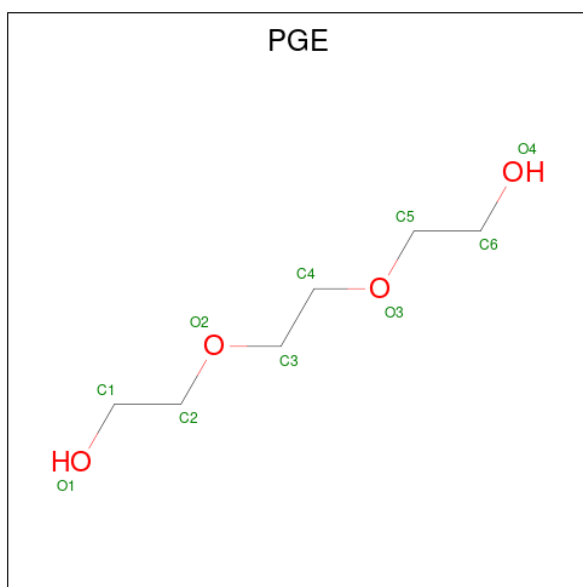
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Fe	0	0
			1	1		
12	B	1	Total	Fe	0	0
			1	1		
12	C	1	Total	Fe	0	0
			1	1		
12	D	1	Total	Fe	0	0
			1	1		

- Molecule 13 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



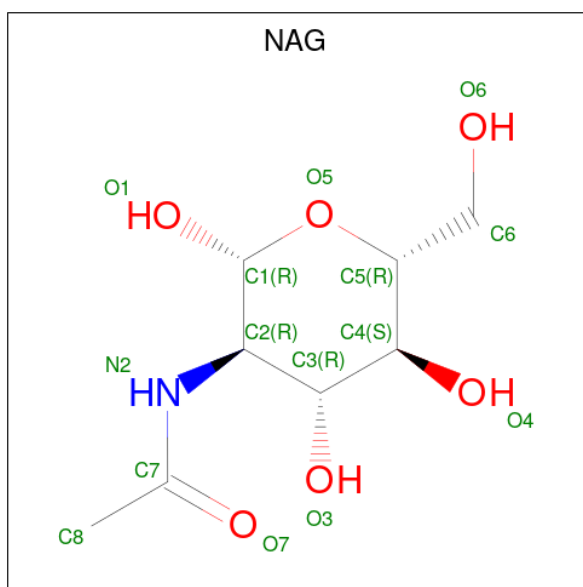
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			13	6	7		
13	A	1	Total	C	O	0	0
			13	6	7		
13	A	1	Total	C	O	0	0
			13	6	7		
13	B	1	Total	C	O	0	0
			13	6	7		
13	B	1	Total	C	O	0	0
			13	6	7		
13	B	1	Total	C	O	0	0
			13	6	7		
13	B	1	Total	C	O	0	0
			13	6	7		
13	C	1	Total	C	O	0	0
			13	6	7		
13	C	1	Total	C	O	0	0
			13	6	7		
13	C	1	Total	C	O	0	0
			13	6	7		
13	C	1	Total	C	O	0	0
			13	6	7		
13	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 14 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



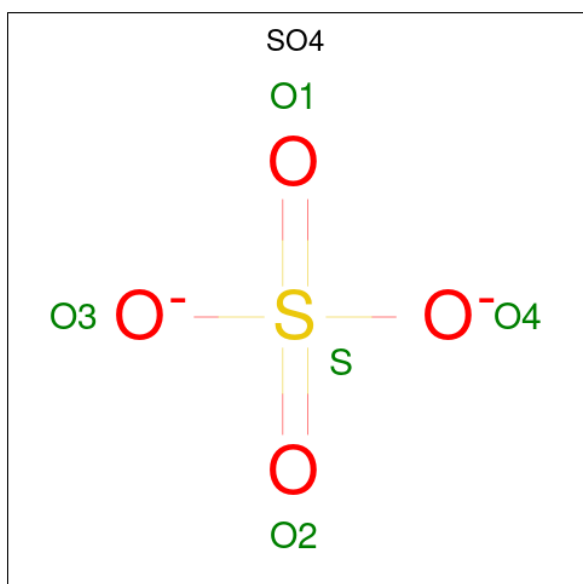
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			10	6	4		
14	A	1	Total	C	O	0	0
			7	4	3		
14	B	1	Total	C	O	0	0
			10	6	4		
14	B	1	Total	C	O	0	0
			10	6	4		
14	C	1	Total	C	O	0	0
			10	6	4		
14	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 16 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



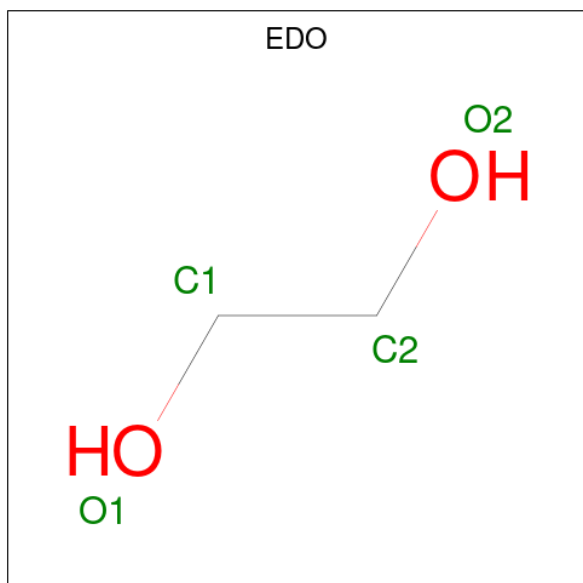
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total	O	S	0	0
			5	4	1		
16	A	1	Total	O	S	0	0
			5	4	1		
16	A	1	Total	O	S	0	0
			5	4	1		
16	A	1	Total	O	S	0	0
			5	4	1		
16	A	1	Total	O	S	0	0
			5	4	1		
16	B	1	Total	O	S	0	0
			5	4	1		
16	B	1	Total	O	S	0	0
			5	4	1		
16	B	1	Total	O	S	0	0
			5	4	1		
16	B	1	Total	O	S	0	0
			5	4	1		
16	B	1	Total	O	S	0	0
			5	4	1		
16	B	1	Total	O	S	0	0
			5	4	1		
16	B	1	Total	O	S	0	0
			5	4	1		
16	B	1	Total	O	S	0	0
			5	4	1		
16	C	1	Total	O	S	0	0
			5	4	1		
16	C	1	Total	O	S	0	0
			5	4	1		
16	C	1	Total	O	S	0	0
			5	4	1		
16	C	1	Total	O	S	0	0
			5	4	1		
16	C	1	Total	O	S	0	0
			5	4	1		
16	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	O	S	0	0
			5	4	1		
16	D	1	Total	O	S	0	0
			5	4	1		
16	D	1	Total	O	S	0	0
			5	4	1		
16	D	1	Total	O	S	0	0
			5	4	1		
16	D	1	Total	O	S	0	0
			5	4	1		
16	D	1	Total	O	S	0	0
			5	4	1		
16	D	1	Total	O	S	0	0
			5	4	1		
16	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 17 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



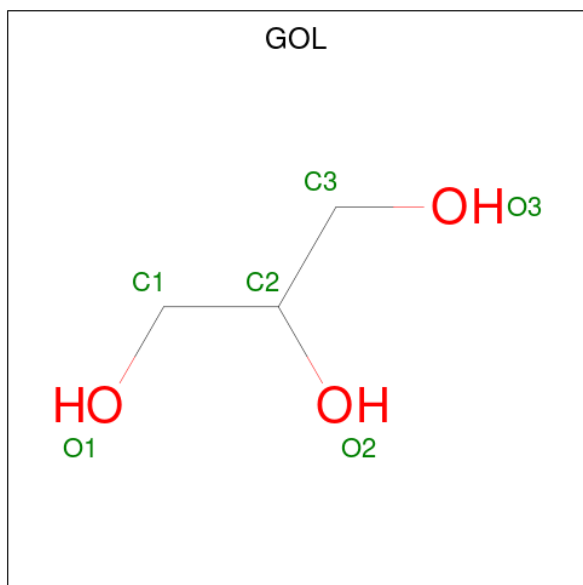
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	B	1	Total	C	O	0	0
			4	2	2		
17	C	1	Total	C	O	0	0
			4	2	2		
17	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 18 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

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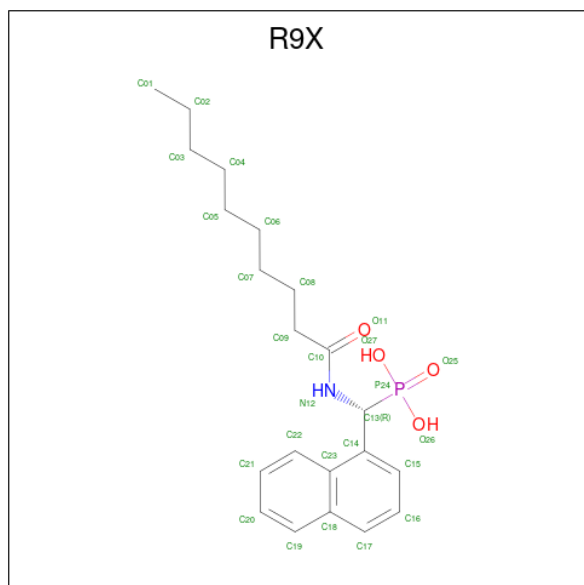
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0

- Molecule 19 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	2	Total	Cl	0	0
			2	2		
19	B	1	Total	Cl	0	0
			1	1		
19	C	1	Total	Cl	0	0
			1	1		
19	D	2	Total	Cl	0	0
			2	2		

- Molecule 20 is [(R)-(decanoylamino)-naphthalen-1-yl-methyl]phosphonic acid (CCD ID: R9X) (formula: C₂₁H₃₀NO₄P) (labeled as "Ligand of Interest" by depositor).

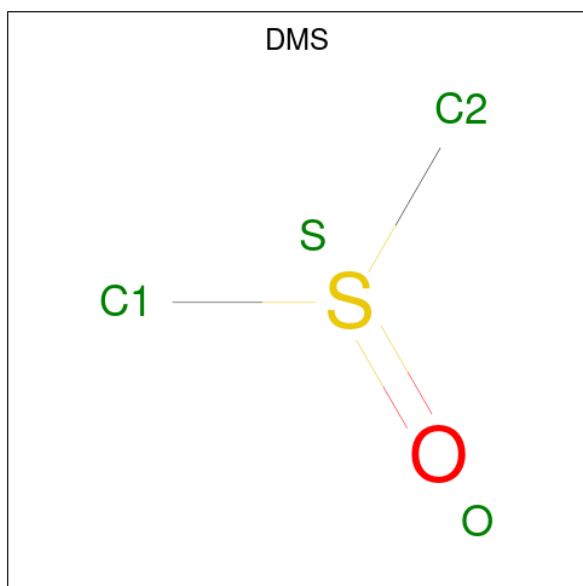


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	N	O	P	0	1
			54	42	2	8	2		
20	B	1	Total	C	N	O	P	0	1
			54	42	2	8	2		
20	C	1	Total	C	N	O	P	0	1
			27	21	1	4	1		
20	C	1	Total	C	N	O	P	0	1
			27	21	1	4	1		
20	D	1	Total	C	N	O	P	0	1
			54	42	2	8	2		

- Molecule 21 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Na	0	0
			1	1		

- Molecule 22 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	D	1	Total	C	O	S	0	0
			4	2	1	1		

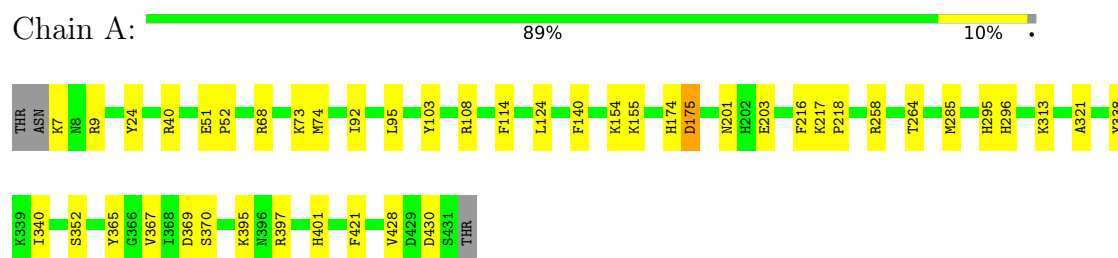
- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	711	Total	O	1	9
			720	720		
23	B	644	Total	O	1	14
			658	658		
23	C	674	Total	O	0	8
			682	682		
23	D	634	Total	O	2	12
			646	646		

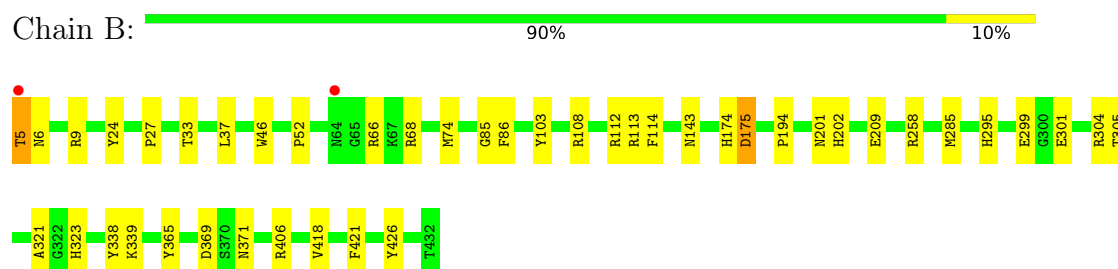
3 Residue-property plots

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.

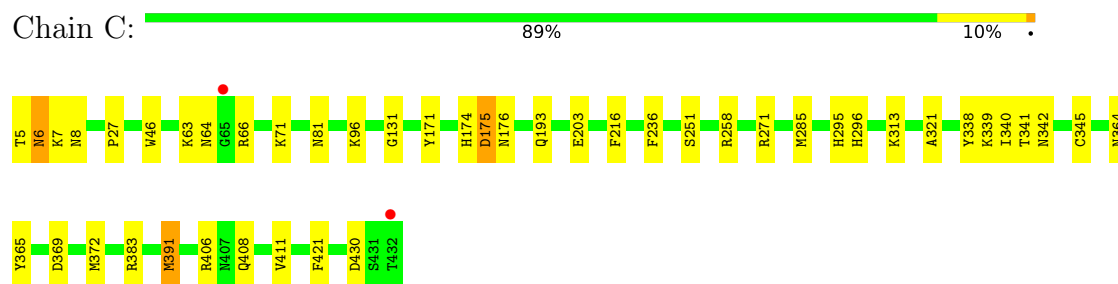
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



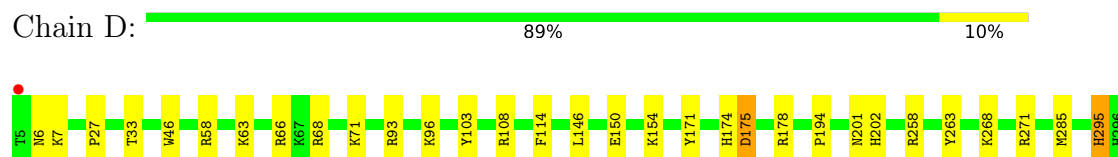
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase





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

Chain E: 100%



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

Chain K: 100%



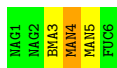
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 50% 50%



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

Chain F: 50% 33% 17%



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

Chain G: 75% 25%



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

Chain I: 50% 25% 25%



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

Chain N:  75% 25%



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

Chain P:  75% 25%



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

Chain S:  75% 25%

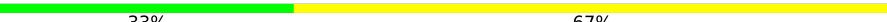


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  75% 25%



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

Chain H:  33% 67%



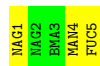
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

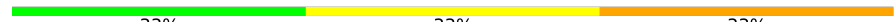


- Molecule 6: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  40% 60%



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 33% 33%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50% 50%



- Molecule 9: beta-D-mannopyranose-(5-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%



- Molecule 10: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.86Å 125.86Å 298.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.96-2.00) 98.5 (19.96-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.157 , 0.206 0.157 , 0.206	Depositor DCC
R_{free} test set	9127 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18800	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, R9X, BMA, GOL, FLC, NAG, DMS, ZN, FUC, SO4, MAN, PGE, NA, EDO, CL

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	0.31	0/3722	0.49	0/5057
1	B	0.30	0/3687	0.49	0/5011
1	C	0.31	0/3734	0.49	0/5076
1	D	0.31	0/3736	0.48	0/5076
All	All	0.31	0/14879	0.49	0/20220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3569	0	3431	45	0
1	B	3558	0	3379	49	0
1	C	3584	0	3423	40	0
1	D	3586	0	3442	40	0
2	E	28	0	25	0	0
2	K	28	0	25	1	0
2	Q	28	0	25	2	0
3	F	71	0	61	1	0
4	G	49	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	49	0	43	2	0
4	N	49	0	43	0	0
4	P	49	0	43	0	0
4	S	49	0	43	0	0
4	V	49	0	43	0	0
5	H	71	0	61	1	0
5	J	71	0	61	0	0
6	L	60	0	52	0	0
7	M	39	0	34	1	0
8	O	28	0	25	0	0
9	R	48	0	41	2	0
10	T	24	0	22	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
13	A	39	0	15	5	0
13	B	52	0	20	9	0
13	C	65	0	25	6	0
13	D	13	0	5	3	0
14	A	17	0	23	6	0
14	B	20	0	28	4	0
14	C	10	0	14	1	0
14	D	10	0	14	8	0
15	A	14	0	13	0	0
15	C	28	0	26	1	0
15	D	28	0	26	3	0
16	A	30	0	0	6	0
16	B	45	0	0	3	0
16	C	40	0	0	6	0
16	D	45	0	0	3	0
17	A	4	0	6	0	0
17	B	4	0	6	0	0
17	C	4	0	6	1	0
17	D	4	0	6	0	0
18	A	84	0	111	12	0
18	B	60	0	80	5	0
18	C	66	0	88	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	D	90	0	120	10	0
19	A	2	0	0	1	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	D	2	0	0	1	0
20	A	54	0	0	12	0
20	B	54	0	0	6	0
20	C	54	0	0	8	0
20	D	54	0	0	8	0
21	B	1	0	0	0	0
22	D	4	0	6	2	0
23	A	720	0	0	12	0
23	B	658	0	0	11	0
23	C	682	0	0	18	0
23	D	646	0	0	12	0
All	All	18800	0	15003	219	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 219 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:397:ARG:HH22	13:A:505:FLC:HG2	1.25	0.98
1:A:68:ARG:NH1	16:A:510:SO4:O4	2.02	0.92
1:C:8:ASN:HD22	17:C:617:EDO:H21	1.37	0.88
1:A:365:TYR:OH	20:A:532[A]:R9X:O11	1.94	0.84
1:D:371:ASN:HB2	13:D:503:FLC:HA2	1.64	0.80

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	435/428 (102%)	417 (96%)	17 (4%)	1 (0%)	43	42
1	B	431/428 (101%)	412 (96%)	18 (4%)	1 (0%)	43	42
1	C	437/428 (102%)	415 (95%)	20 (5%)	2 (0%)	24	21
1	D	436/428 (102%)	414 (95%)	20 (5%)	2 (0%)	24	21
All	All	1739/1712 (102%)	1658 (95%)	75 (4%)	6 (0%)	30	35

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	175	ASP
1	A	175	ASP
1	B	175	ASP
1	C	175	ASP
1	D	63	LYS

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	386/377 (102%)	385 (100%)	1 (0%)	86	91
1	B	382/377 (101%)	381 (100%)	1 (0%)	86	91
1	C	388/377 (103%)	385 (99%)	3 (1%)	73	80
1	D	387/377 (103%)	384 (99%)	3 (1%)	73	80
All	All	1543/1508 (102%)	1535 (100%)	8 (0%)	84	87

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	295[B]	HIS
1	D	295[A]	HIS
1	C	391[B]	MET
1	C	391[A]	MET
1	D	66	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	173	ASN
1	D	193	GLN
1	D	405	ASN
1	A	405	ASN
1	B	138	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

64 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	E	1	1,2	14,14,15	0.56	0	17,19,21	0.56	0
2	NAG	E	2	2	14,14,15	0.49	0	17,19,21	0.50	0
3	NAG	F	1	1,3	14,14,15	0.36	0	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	0.57	0
3	BMA	F	3	3	11,11,12	1.65	3 (27%)	15,15,17	1.31	3 (20%)
3	MAN	F	4	3	11,11,12	1.44	2 (18%)	15,15,17	1.69	4 (26%)
3	MAN	F	5	3	11,11,12	0.99	1 (9%)	15,15,17	1.14	2 (13%)
3	FUC	F	6	3	10,10,11	0.75	0	14,14,16	0.67	0
4	NAG	G	1	1,4	14,14,15	0.51	0	17,19,21	0.65	0
4	NAG	G	2	4	14,14,15	0.47	0	17,19,21	0.76	1 (5%)
4	BMA	G	3	4	11,11,12	0.77	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUC	G	4	4	10,10,11	0.60	0	14,14,16	0.97	0
5	NAG	H	1	1,5	14,14,15	0.48	0	17,19,21	0.70	0
5	NAG	H	2	5	14,14,15	0.28	0	17,19,21	0.51	0
5	BMA	H	3	5	11,11,12	1.13	0	15,15,17	0.94	1 (6%)
5	MAN	H	4	5	11,11,12	0.62	0	15,15,17	1.36	2 (13%)
5	MAN	H	5	5	11,11,12	0.97	1 (9%)	15,15,17	1.14	2 (13%)
5	FUC	H	6	5	10,10,11	0.90	0	14,14,16	0.85	0
4	NAG	I	1	1,4	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
4	NAG	I	2	4	14,14,15	0.38	0	17,19,21	0.55	0
4	BMA	I	3	4	11,11,12	1.59	3 (27%)	15,15,17	1.74	3 (20%)
4	FUC	I	4	4	10,10,11	0.56	0	14,14,16	1.01	0
5	NAG	J	1	1,5	14,14,15	0.53	0	17,19,21	0.57	0
5	NAG	J	2	5	14,14,15	0.44	0	17,19,21	0.54	0
5	BMA	J	3	5	11,11,12	1.15	2 (18%)	15,15,17	1.12	1 (6%)
5	MAN	J	4	5	11,11,12	1.09	1 (9%)	15,15,17	1.20	3 (20%)
5	MAN	J	5	5	11,11,12	0.82	0	15,15,17	1.19	1 (6%)
5	FUC	J	6	5	10,10,11	0.93	0	14,14,16	1.08	0
2	NAG	K	1	1,2	14,14,15	0.48	0	17,19,21	0.60	0
2	NAG	K	2	2	14,14,15	0.17	0	17,19,21	0.90	1 (5%)
6	NAG	L	1	1,6	14,14,15	0.47	0	17,19,21	0.69	1 (5%)
6	NAG	L	2	6	14,14,15	0.31	0	17,19,21	0.56	0
6	BMA	L	3	6	11,11,12	0.97	0	15,15,17	0.78	0
6	MAN	L	4	6	11,11,12	1.16	2 (18%)	15,15,17	1.10	2 (13%)
6	FUC	L	5	6	10,10,11	0.72	0	14,14,16	0.89	1 (7%)
7	NAG	M	1	1,7	14,14,15	0.35	0	17,19,21	0.64	0
7	NAG	M	2	7	14,14,15	0.89	1 (7%)	17,19,21	1.54	1 (5%)
7	BMA	M	3	7	11,11,12	1.69	3 (27%)	15,15,17	1.89	3 (20%)
4	NAG	N	1	1,4	14,14,15	0.55	0	17,19,21	0.67	0
4	NAG	N	2	4	14,14,15	0.40	0	17,19,21	0.70	0
4	BMA	N	3	4	11,11,12	1.58	3 (27%)	15,15,17	1.73	2 (13%)
4	FUC	N	4	4	10,10,11	0.65	0	14,14,16	1.08	0
8	NAG	O	1	1,8	14,14,15	0.76	1 (7%)	17,19,21	1.05	2 (11%)
8	NAG	O	2	8	14,14,15	0.53	0	17,19,21	0.63	0
4	NAG	P	1	1,4	14,14,15	0.48	0	17,19,21	0.67	0
4	NAG	P	2	4	14,14,15	0.59	0	17,19,21	0.68	0
4	BMA	P	3	4	11,11,12	1.33	2 (18%)	15,15,17	1.64	2 (13%)
4	FUC	P	4	4	10,10,11	0.56	0	14,14,16	0.68	0
2	NAG	Q	1	1,2	14,14,15	0.31	0	17,19,21	0.55	0
2	NAG	Q	2	2	14,14,15	0.24	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	R	1	1,9	14,14,15	0.51	0	17,19,21	0.61	0
9	NAG	R	2	9	14,14,15	0.40	0	17,19,21	0.58	0
9	BMA	R	3	9	10,10,12	0.84	0	14,14,17	0.71	0
9	FUC	R	4	9	10,10,11	0.89	0	14,14,16	0.97	0
4	NAG	S	1	1,4	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	S	2	4	14,14,15	0.53	0	17,19,21	0.71	0
4	BMA	S	3	4	11,11,12	1.41	2 (18%)	15,15,17	1.43	1 (6%)
4	FUC	S	4	4	10,10,11	0.79	0	14,14,16	0.79	0
10	NAG	T	1	1,10	14,14,15	0.45	0	17,19,21	0.66	0
10	FUC	T	2	10	10,10,11	1.38	2 (20%)	14,14,16	1.83	3 (21%)
4	NAG	V	1	1,4	14,14,15	0.48	0	17,19,21	0.58	0
4	NAG	V	2	4	14,14,15	0.41	0	17,19,21	0.57	0
4	BMA	V	3	4	11,11,12	0.74	1 (9%)	15,15,17	0.89	0
4	FUC	V	4	4	10,10,11	0.48	0	14,14,16	0.70	0

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	T	1	1,10	-	4/6/23/26	0/1/1/1
10	FUC	T	2	10	-	-	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	BMA	V	3	4	-	2/2/19/22	0/1/1/1
4	FUC	V	4	4	-	-	0/1/1/1

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	3	BMA	C1-C2	3.82	1.61	1.52
7	M	3	BMA	C1-C2	3.62	1.60	1.52
4	I	3	BMA	C1-C2	3.62	1.60	1.52
3	F	4	MAN	C2-C3	3.59	1.58	1.52
3	F	3	BMA	C1-C2	3.48	1.60	1.52

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	3	BMA	C1-O5-C5	5.95	120.16	112.19
7	M	2	NAG	C1-O5-C5	5.88	120.07	112.19
4	P	3	BMA	C1-O5-C5	5.35	119.36	112.19
4	I	3	BMA	C1-O5-C5	5.17	119.12	112.19
4	N	3	BMA	C1-O5-C5	5.14	119.08	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	R	3	BMA	C5

5 of 55 torsion outliers are listed below:

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

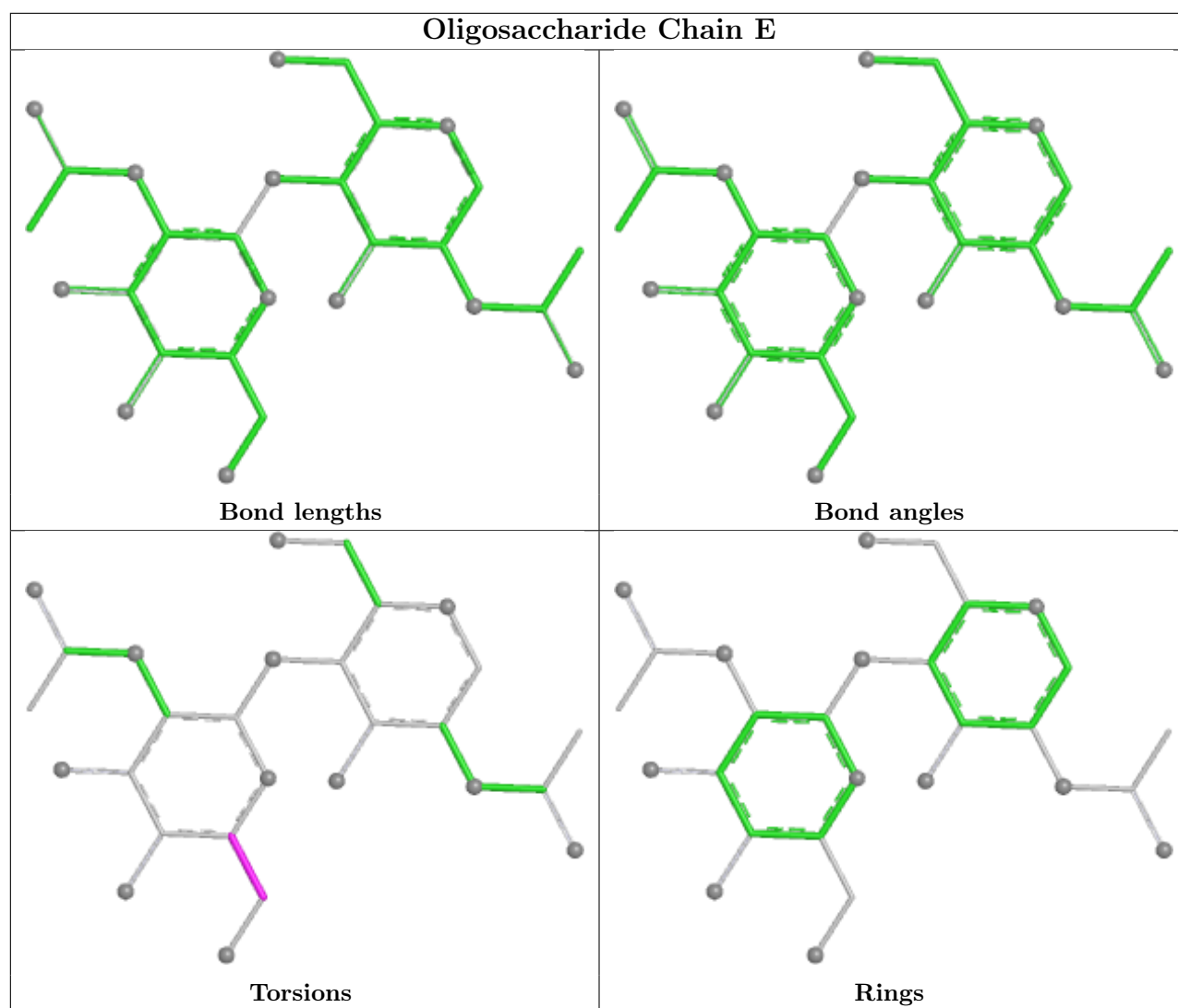
All (4) ring outliers are listed below:

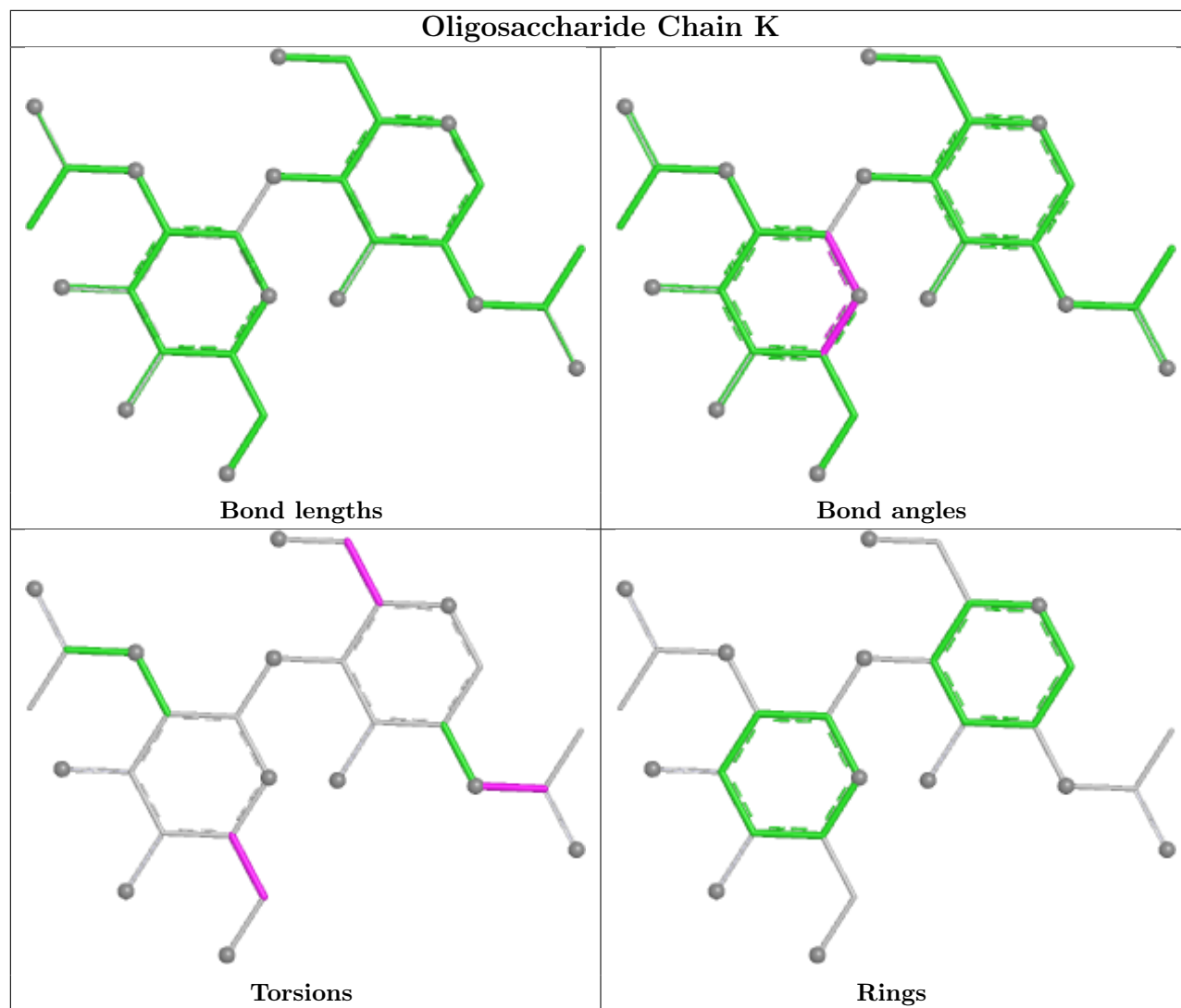
Mol	Chain	Res	Type	Atoms
4	S	3	BMA	C1-C2-C3-C4-C5-O5
6	L	4	MAN	C1-C2-C3-C4-C5-O5
3	F	5	MAN	C1-C2-C3-C4-C5-O5
5	J	4	MAN	C1-C2-C3-C4-C5-O5

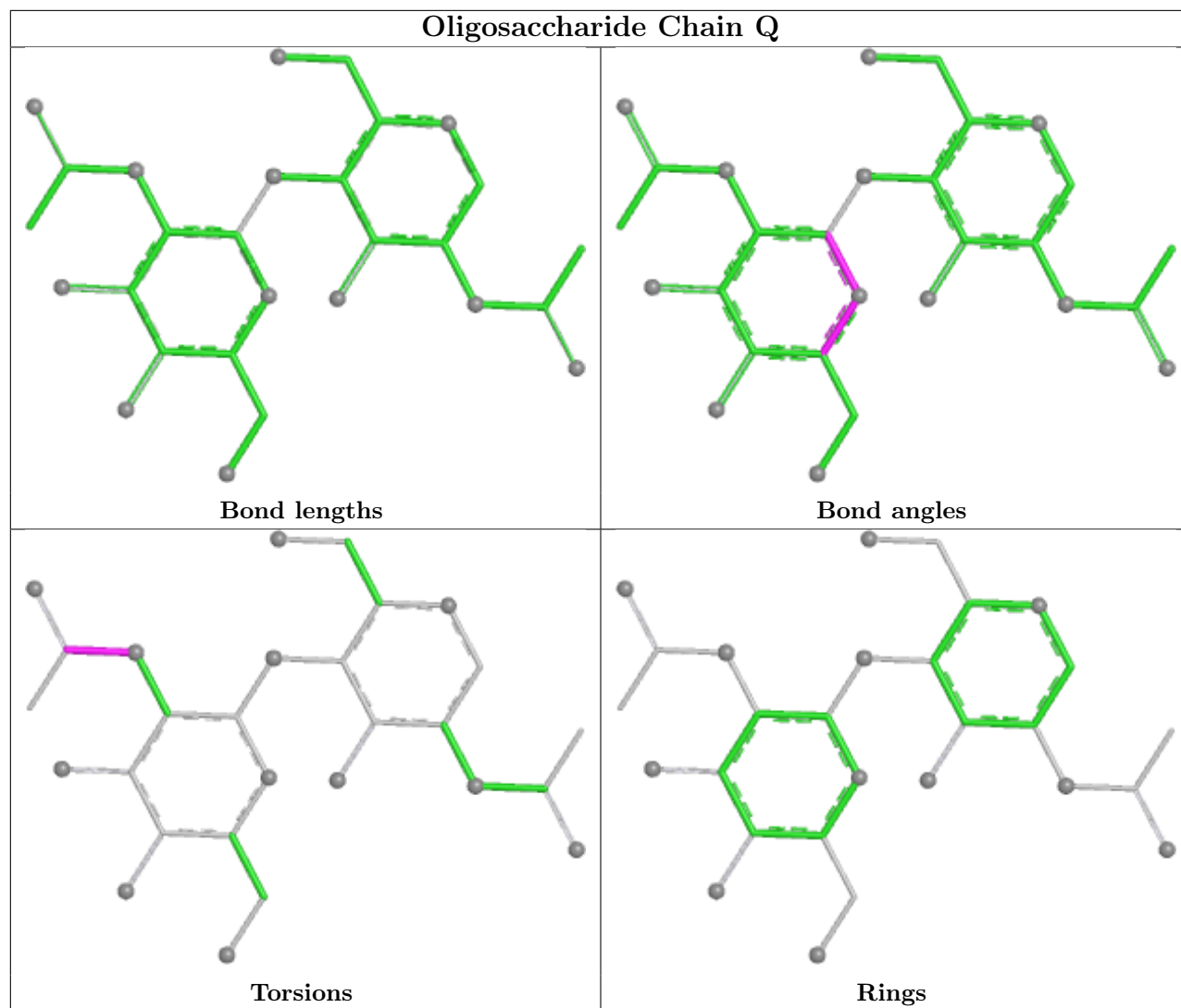
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	2	NAG	1	0
4	I	1	NAG	2	0
2	Q	2	NAG	2	0
2	K	1	NAG	1	0
3	F	4	MAN	1	0
9	R	1	NAG	1	0
7	M	2	NAG	1	0
5	H	2	NAG	1	0

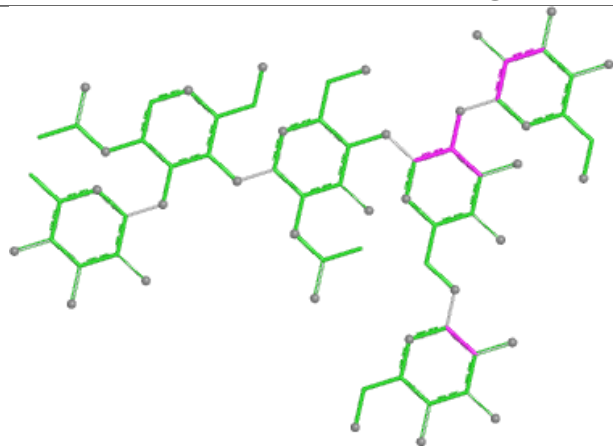
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



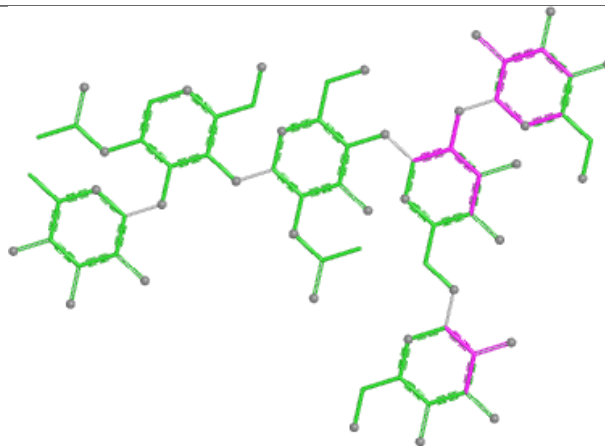




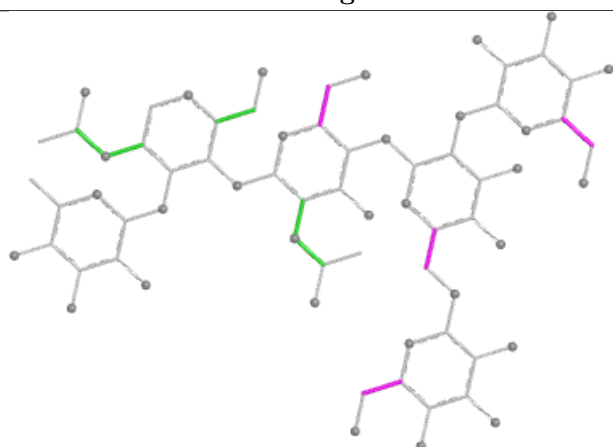
Oligosaccharide Chain F



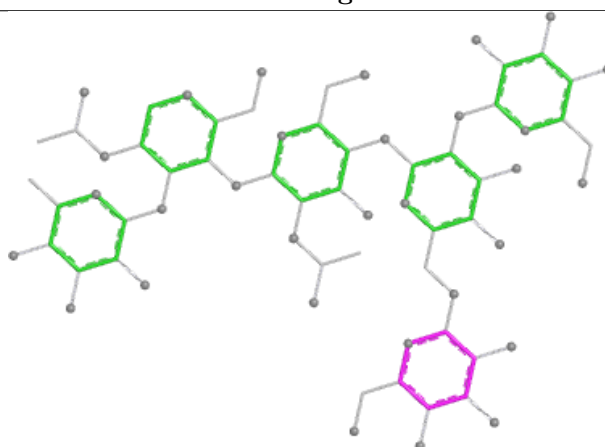
Bond lengths



Bond angles

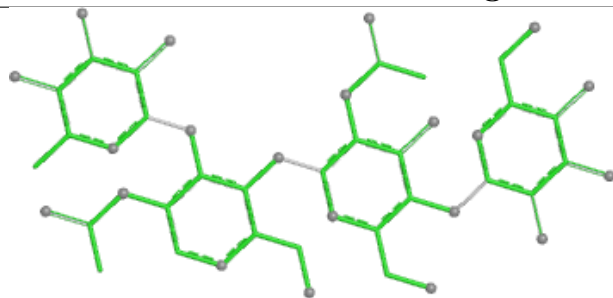


Torsions

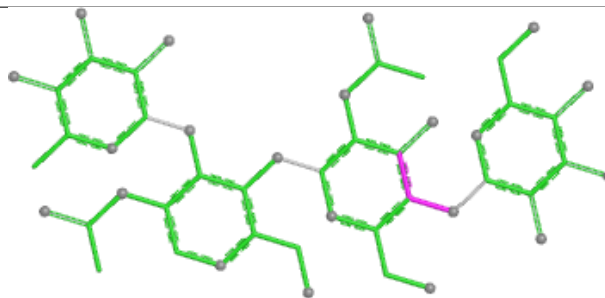


Rings

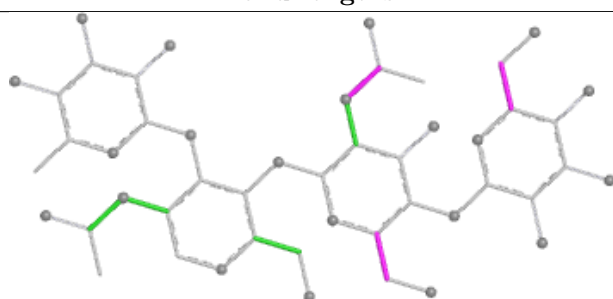
Oligosaccharide Chain G



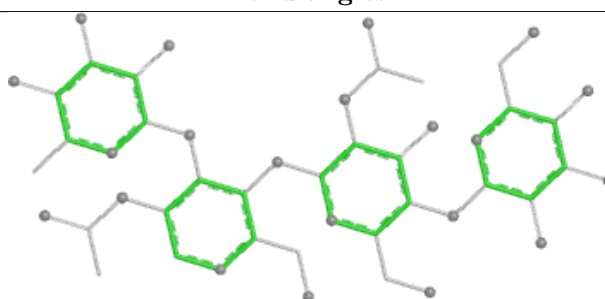
Bond lengths



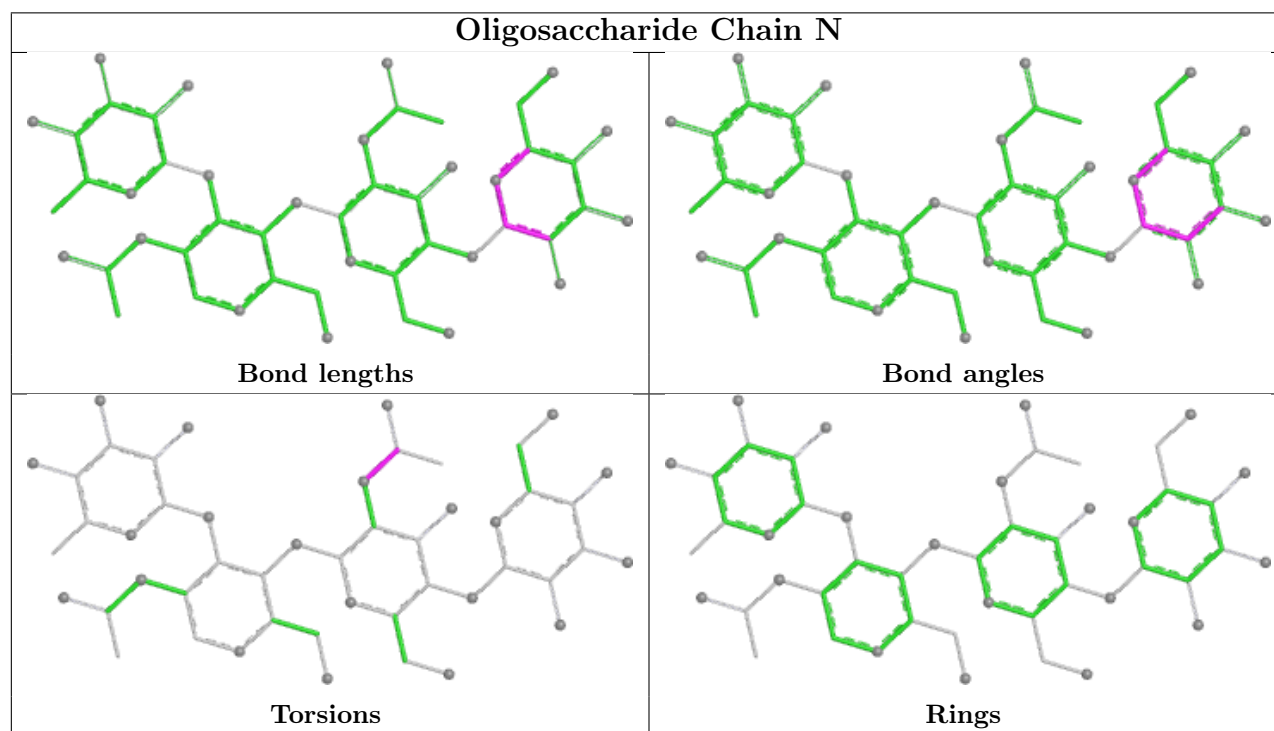
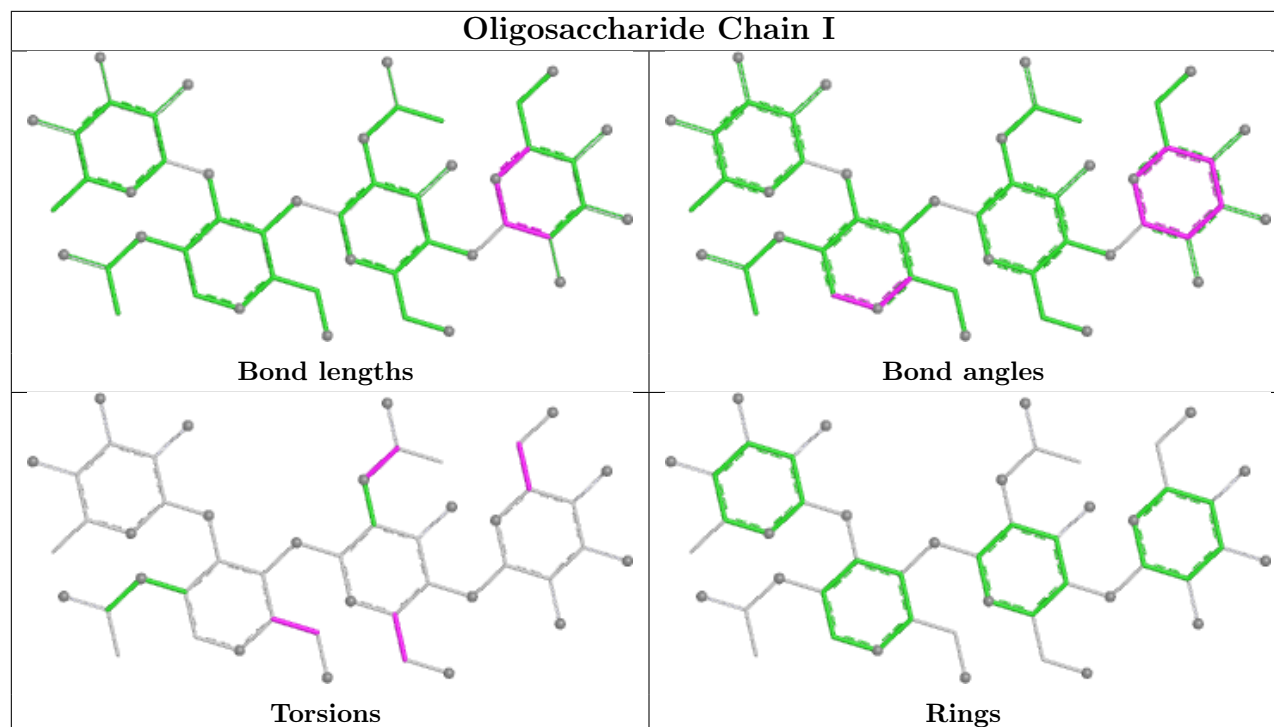
Bond angles



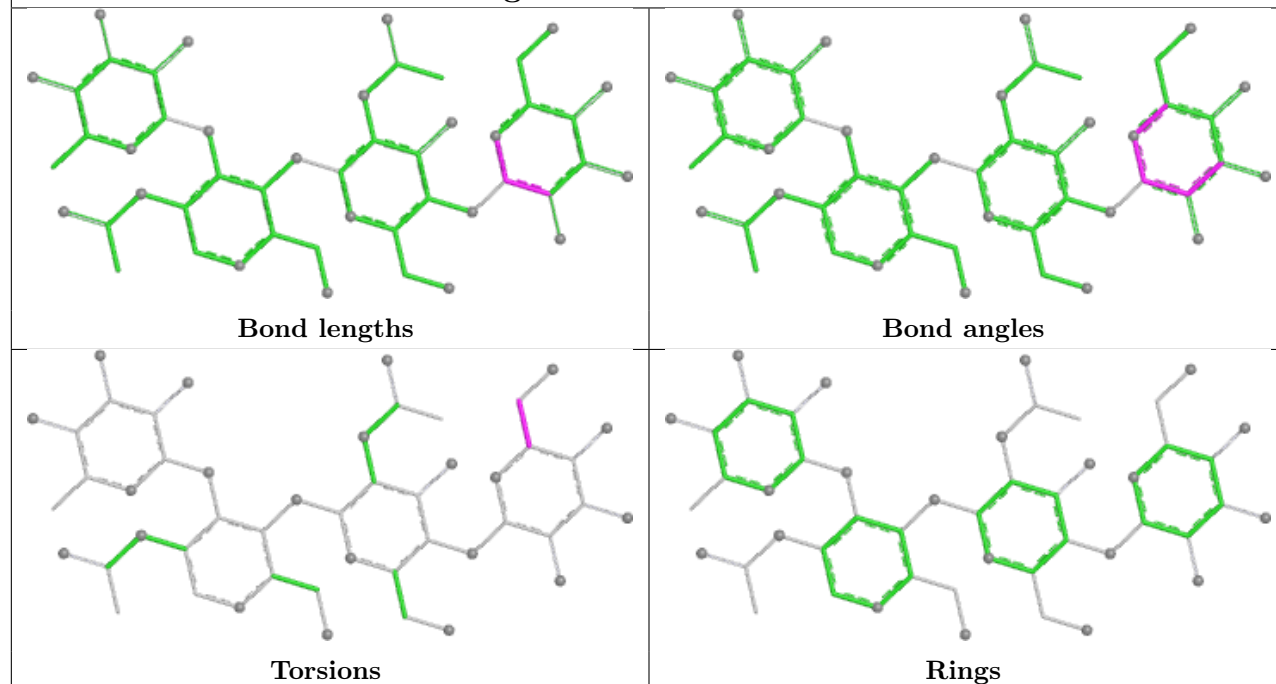
Torsions



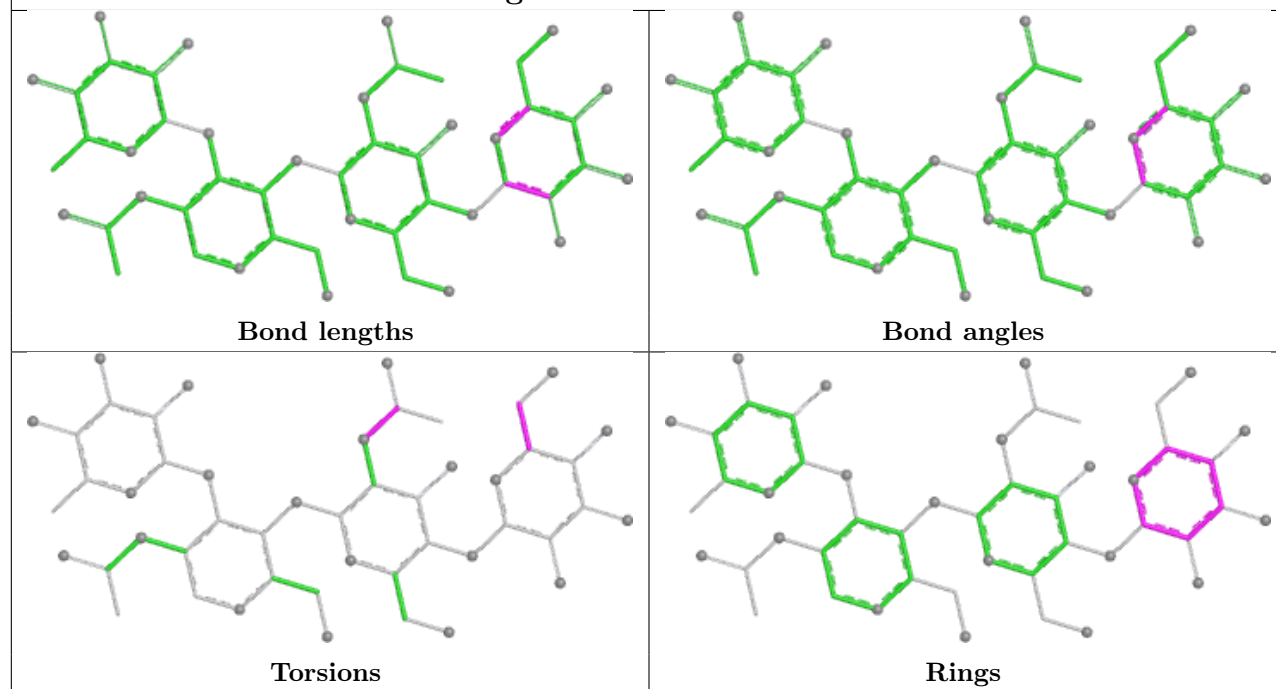
Rings

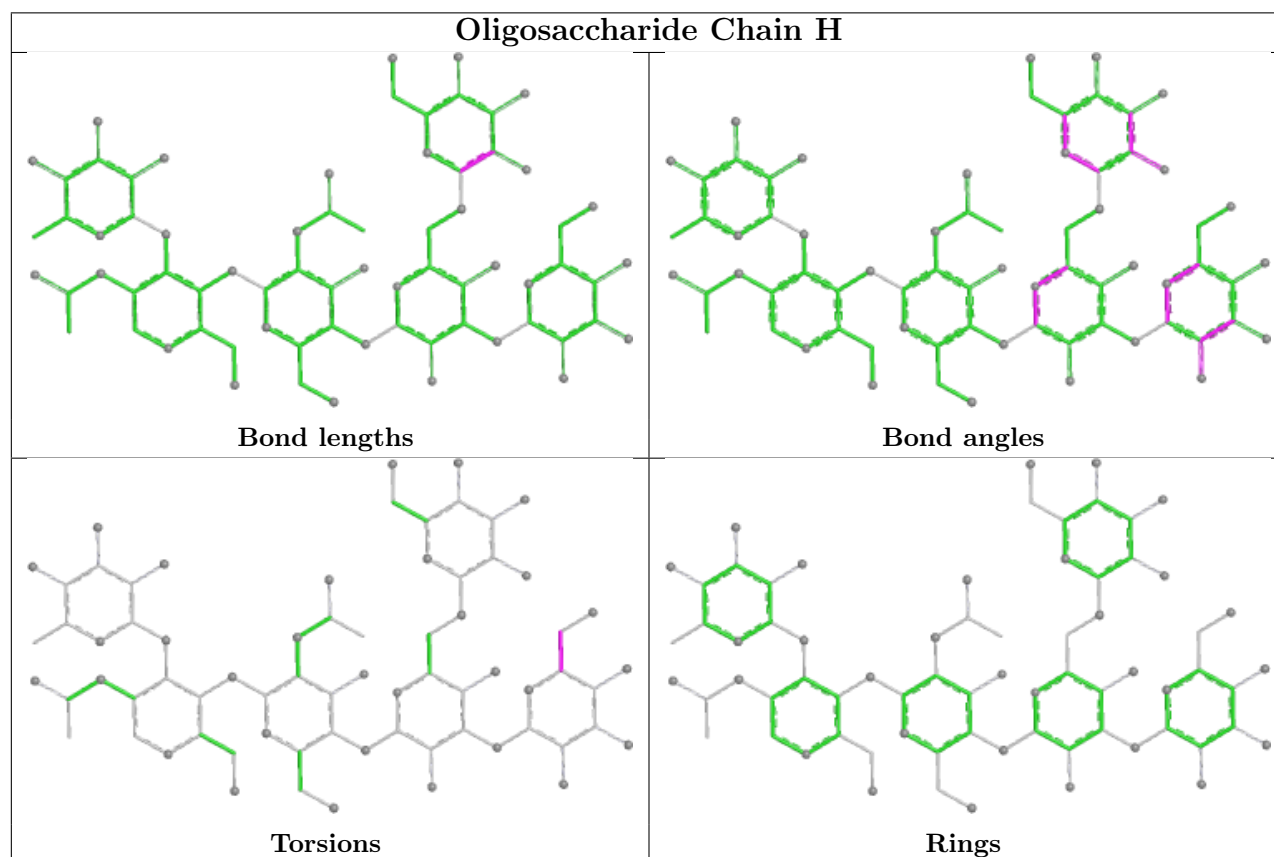
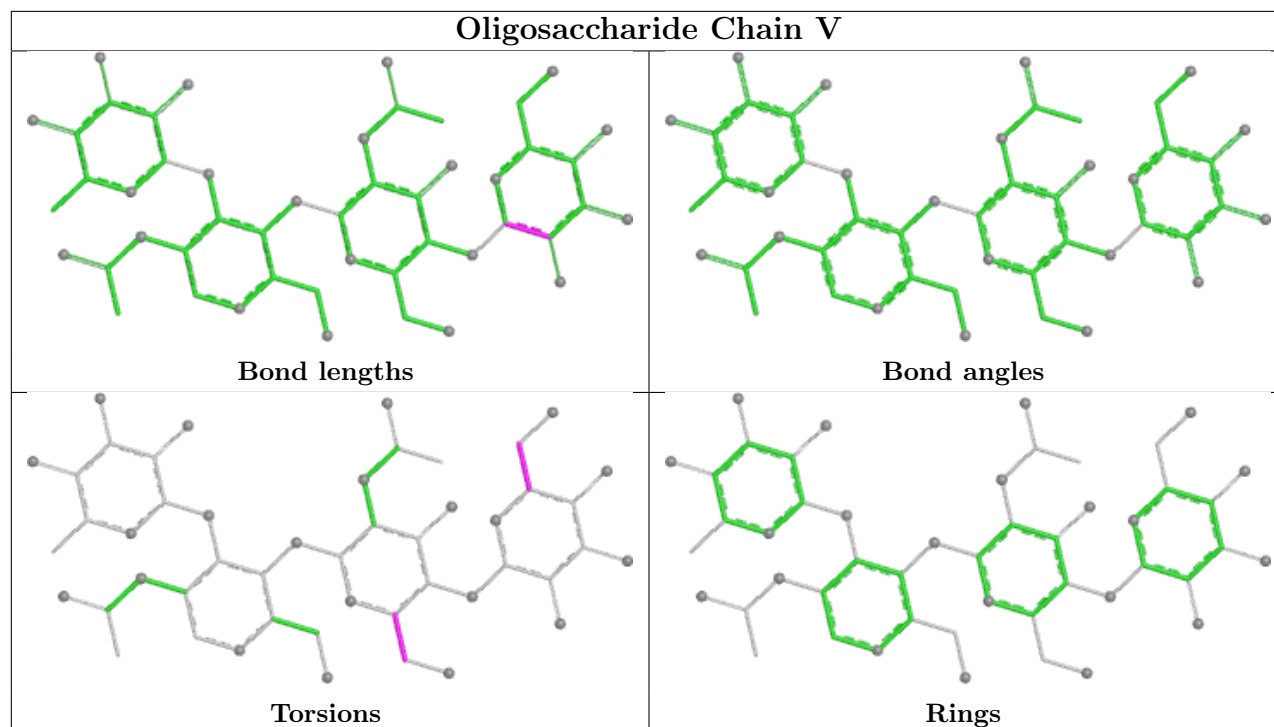


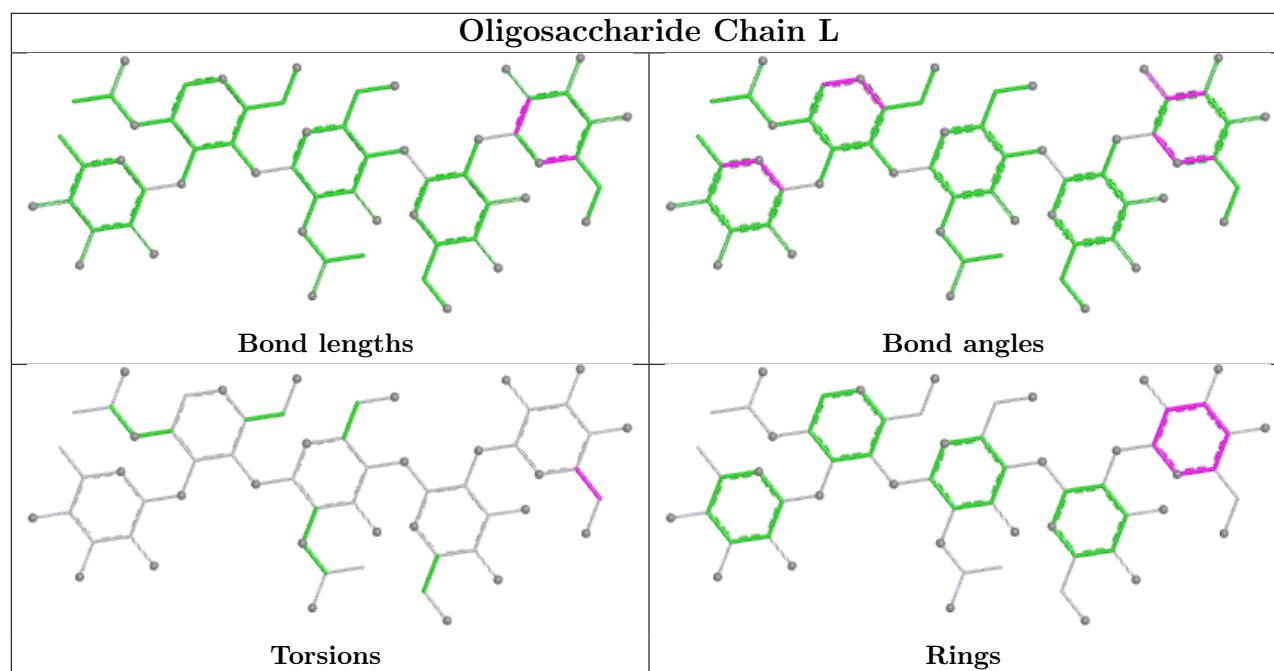
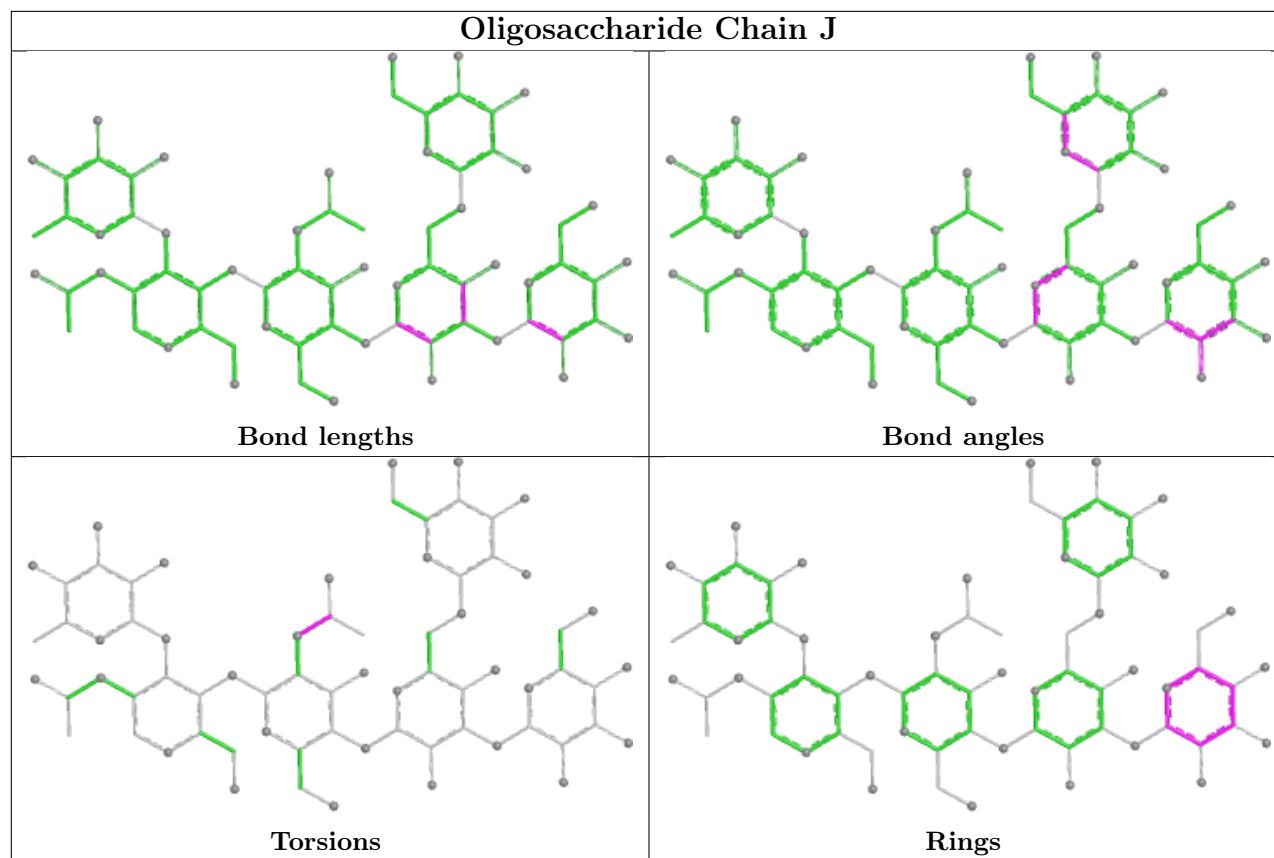
Oligosaccharide Chain P

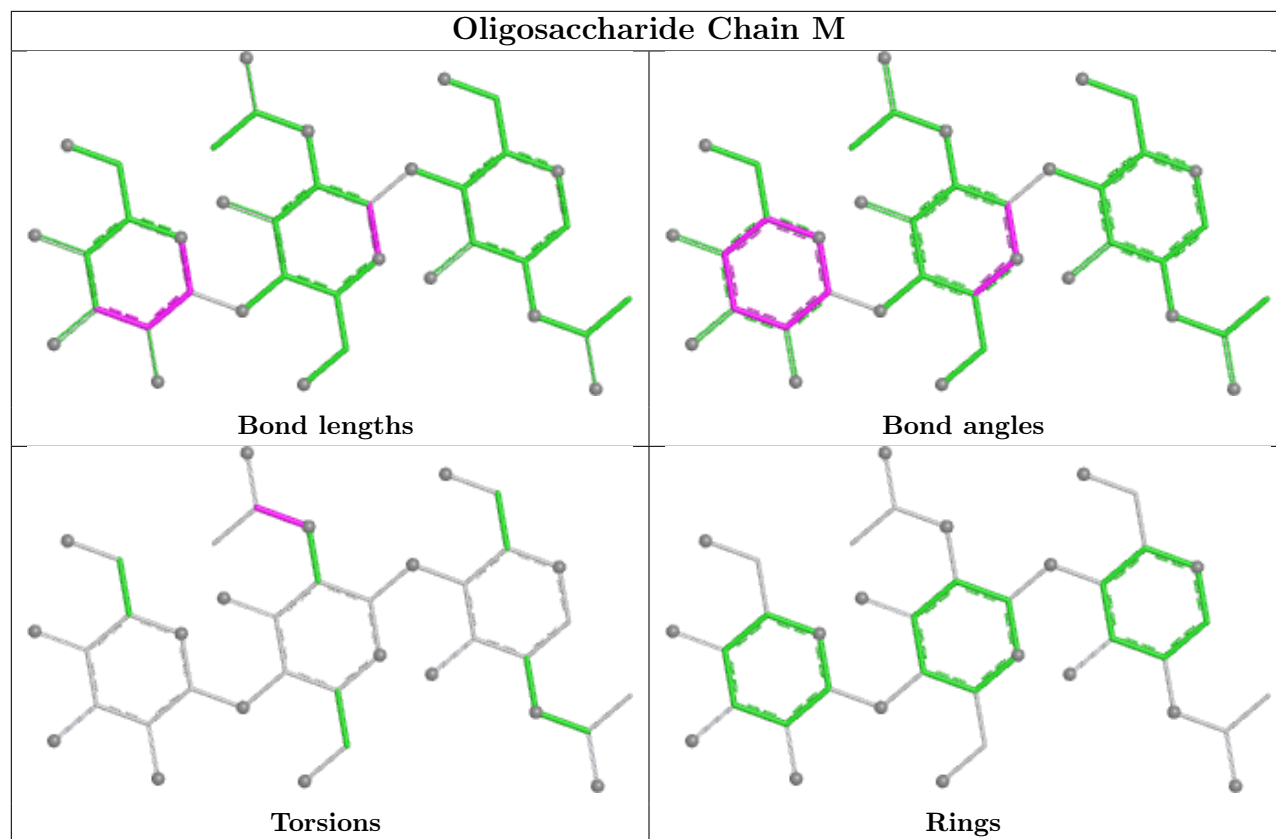


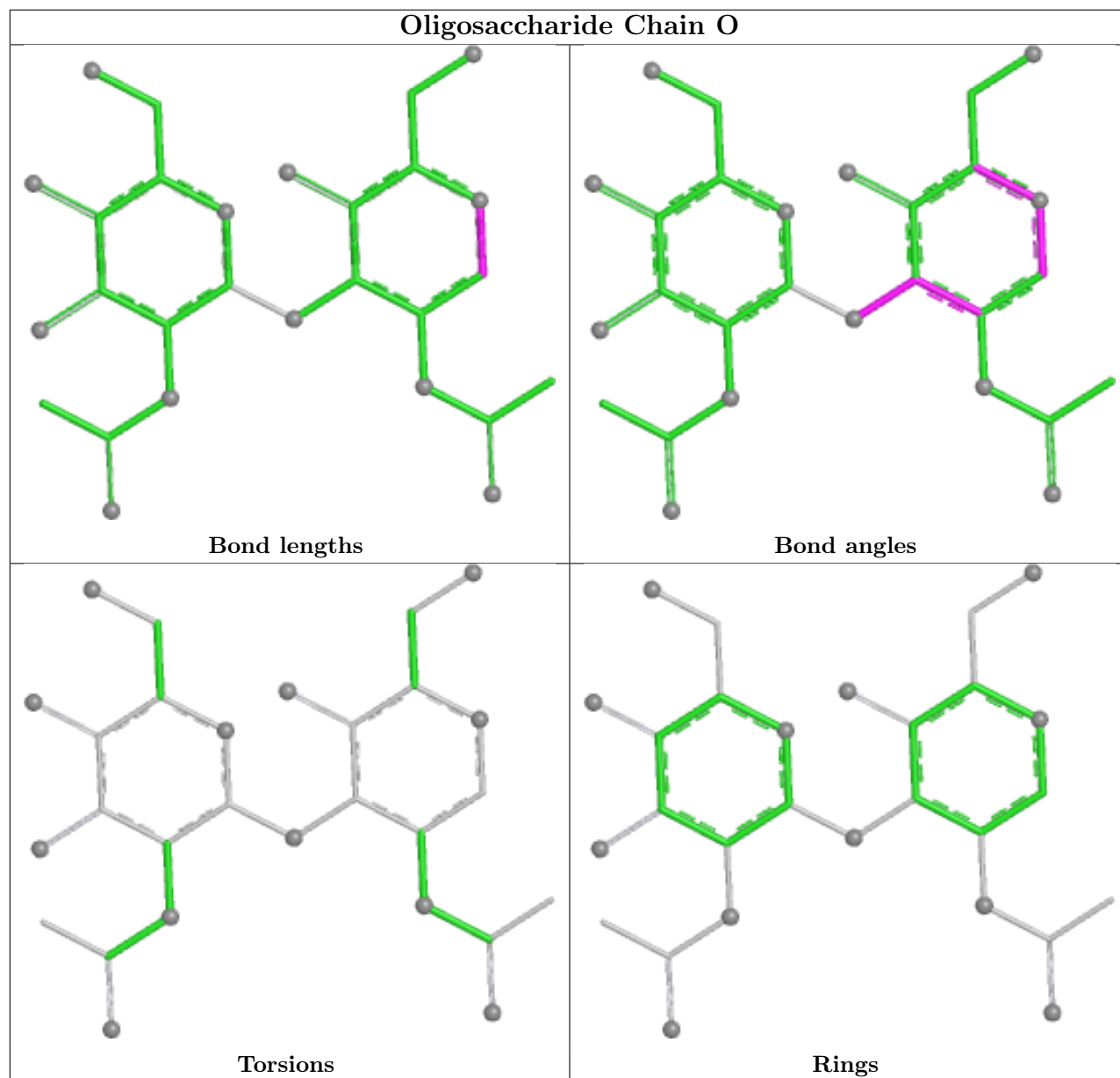
Oligosaccharide Chain S

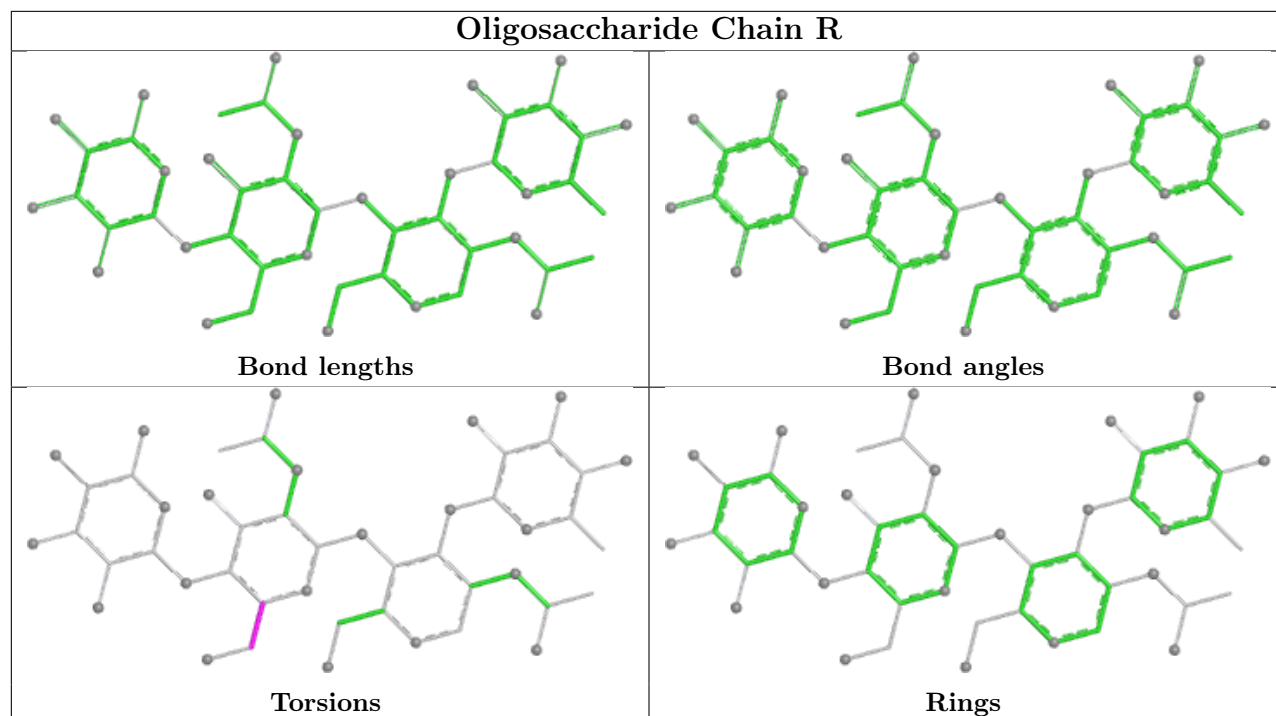


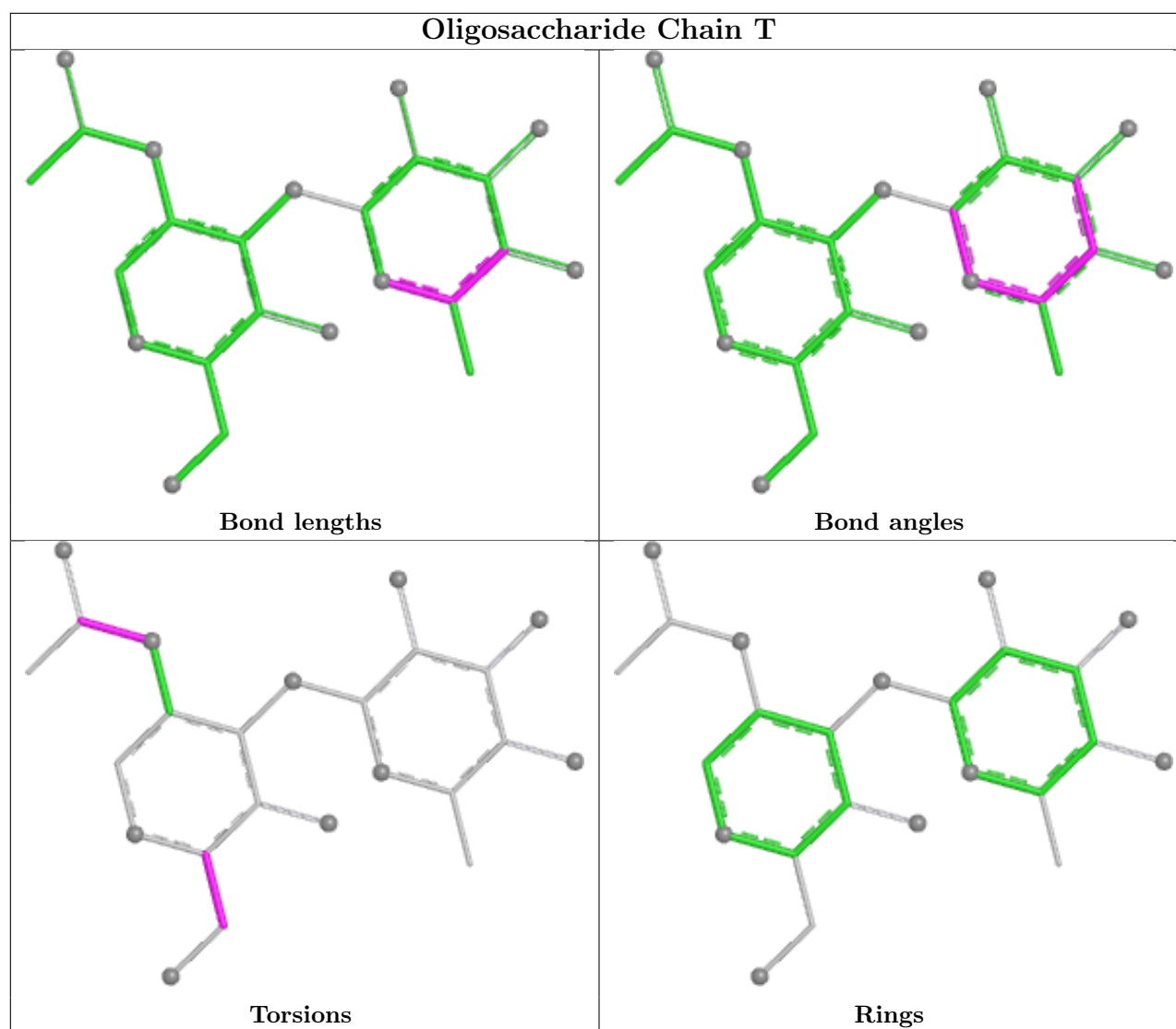












5.6 Ligand geometry [i](#)

Of 134 ligands modelled in this entry, 15 are monoatomic - leaving 119 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	$\# Z > 2$
16	SO4	B	517	-	4,4,4	0.24	0	6,6,6	0.07	0
20	R9X	A	532[A]	-	28,28,28	1.58	5 (17%)	34,37,37	2.22	8 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	SO4	D	510	-	4,4,4	0.19	0	6,6,6	0.18	0
18	GOL	A	523	-	5,5,5	0.84	0	5,5,5	1.24	0
20	R9X	D	535[A]	-	28,28,28	1.42	4 (14%)	34,37,37	2.00	7 (20%)
18	GOL	D	522	-	5,5,5	0.88	0	5,5,5	0.98	0
18	GOL	A	515	-	5,5,5	1.06	0	5,5,5	0.95	0
18	GOL	C	621	-	5,5,5	1.00	0	5,5,5	1.05	0
18	GOL	B	519	-	5,5,5	0.84	0	5,5,5	1.11	0
15	NAG	D	516	1	14,14,15	0.29	0	17,19,21	0.66	1 (5%)
16	SO4	B	512	-	4,4,4	0.26	0	6,6,6	0.15	0
16	SO4	C	608	-	4,4,4	0.27	0	6,6,6	0.43	0
18	GOL	D	523	-	5,5,5	0.88	0	5,5,5	1.12	0
14	PGE	B	508	-	9,9,9	0.29	0	8,8,8	0.45	0
16	SO4	C	610	-	4,4,4	0.24	0	6,6,6	0.11	0
13	FLC	D	503	-	12,12,12	1.55	4 (33%)	17,17,17	2.02	4 (23%)
13	FLC	C	628	-	12,12,12	1.56	4 (33%)	17,17,17	1.94	4 (23%)
18	GOL	D	518	-	5,5,5	0.92	0	5,5,5	1.09	0
18	GOL	B	522	-	5,5,5	0.98	0	5,5,5	1.24	1 (20%)
16	SO4	D	513	-	4,4,4	0.24	0	6,6,6	0.10	0
16	SO4	D	515	-	4,4,4	0.26	0	6,6,6	0.16	0
18	GOL	B	525	-	5,5,5	0.87	0	5,5,5	1.10	0
18	GOL	A	519	-	5,5,5	1.38	1 (20%)	5,5,5	0.89	0
15	NAG	A	506	1	14,14,15	1.07	1 (7%)	17,19,21	1.27	1 (5%)
16	SO4	A	512	-	4,4,4	0.25	0	6,6,6	0.26	0
17	EDO	B	518	-	3,3,3	0.43	0	2,2,2	0.42	0
18	GOL	A	521	-	5,5,5	0.97	0	5,5,5	1.12	0
18	GOL	C	623	-	5,5,5	0.96	0	5,5,5	1.13	0
18	GOL	B	528	-	5,5,5	0.92	0	5,5,5	1.09	0
20	R9X	B	531[A]	-	28,28,28	1.66	6 (21%)	34,37,37	1.52	5 (14%)
13	FLC	A	503	-	12,12,12	0.23	0	17,17,17	0.54	0
18	GOL	D	528	-	5,5,5	0.81	0	5,5,5	1.23	1 (20%)
18	GOL	D	525	-	5,5,5	0.82	0	5,5,5	1.10	0
16	SO4	B	511	-	4,4,4	0.22	0	6,6,6	0.09	0
18	GOL	D	533	-	5,5,5	0.83	0	5,5,5	1.25	1 (20%)
16	SO4	B	514	-	4,4,4	0.24	0	6,6,6	0.11	0
13	FLC	B	503	-	12,12,12	1.54	4 (33%)	17,17,17	1.96	4 (23%)
17	EDO	C	617	-	3,3,3	0.46	0	2,2,2	0.30	0
18	GOL	C	631	-	5,5,5	0.90	0	5,5,5	1.09	0
18	GOL	C	629	-	5,5,5	0.94	0	5,5,5	1.00	0
18	GOL	C	630	-	5,5,5	1.08	0	5,5,5	1.11	0
22	DMS	D	505	-	3,3,3	0.70	0	3,3,3	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	GOL	C	622	-	5,5,5	0.96	0	5,5,5	1.12	0
15	NAG	D	506	1	14,14,15	0.49	0	17,19,21	0.45	0
18	GOL	A	531	-	5,5,5	0.95	0	5,5,5	1.28	1 (20%)
13	FLC	B	506	-	12,12,12	1.17	2 (16%)	17,17,17	1.37	2 (11%)
18	GOL	A	522	-	5,5,5	0.93	0	5,5,5	1.02	0
18	GOL	C	625	-	5,5,5	1.00	0	5,5,5	1.15	1 (20%)
18	GOL	B	523	-	5,5,5	0.75	0	5,5,5	1.21	0
18	GOL	A	517	-	5,5,5	0.88	0	5,5,5	1.06	0
16	SO4	B	515	-	4,4,4	0.24	0	6,6,6	0.08	0
15	NAG	C	605	1	14,14,15	1.05	1 (7%)	17,19,21	1.68	1 (5%)
14	PGE	C	604	-	9,9,9	0.32	0	8,8,8	0.29	0
16	SO4	C	614	-	4,4,4	0.22	0	6,6,6	0.09	0
16	SO4	C	615	-	4,4,4	0.25	0	6,6,6	0.16	0
16	SO4	D	509	-	4,4,4	0.22	0	6,6,6	0.08	0
14	PGE	B	504	-	9,9,9	0.27	0	8,8,8	0.38	0
18	GOL	D	524	-	5,5,5	0.96	0	5,5,5	1.09	0
16	SO4	A	513	-	4,4,4	0.25	0	6,6,6	0.06	0
14	PGE	A	507	-	6,6,9	0.24	0	5,5,8	0.83	0
18	GOL	A	520	-	5,5,5	0.78	0	5,5,5	1.09	1 (20%)
16	SO4	B	513	-	4,4,4	0.23	0	6,6,6	0.08	0
16	SO4	D	511	-	4,4,4	0.21	0	6,6,6	0.19	0
13	FLC	B	507	-	12,12,12	1.61	4 (33%)	17,17,17	2.01	4 (23%)
13	FLC	C	601	-	12,12,12	1.22	2 (16%)	17,17,17	1.04	2 (11%)
18	GOL	B	526	-	5,5,5	0.92	0	5,5,5	1.12	0
18	GOL	D	520	-	5,5,5	1.08	1 (20%)	5,5,5	1.16	0
16	SO4	C	609	-	4,4,4	0.23	0	6,6,6	0.12	0
13	FLC	A	530	-	12,12,12	1.61	4 (33%)	17,17,17	1.39	4 (23%)
18	GOL	D	534	-	5,5,5	0.94	0	5,5,5	1.09	0
13	FLC	A	505	-	12,12,12	1.56	4 (33%)	17,17,17	1.95	4 (23%)
17	EDO	D	517	-	3,3,3	0.47	0	2,2,2	0.31	0
15	NAG	C	616	1	14,14,15	0.28	0	17,19,21	0.52	0
16	SO4	A	508	-	4,4,4	0.27	0	6,6,6	0.22	0
18	GOL	A	525	-	5,5,5	0.91	0	5,5,5	1.06	0
17	EDO	A	514	-	3,3,3	0.34	0	2,2,2	0.47	0
13	FLC	C	602	-	12,12,12	1.08	2 (16%)	17,17,17	1.65	2 (11%)
16	SO4	A	509	-	4,4,4	0.24	0	6,6,6	0.24	0
20	R9X	D	535[B]	-	28,28,28	1.64	4 (14%)	34,37,37	1.06	2 (5%)
18	GOL	C	620	-	5,5,5	1.44	2 (40%)	5,5,5	0.95	0
18	GOL	D	529	-	5,5,5	0.94	0	5,5,5	1.04	0
16	SO4	D	507	-	4,4,4	0.25	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	SO4	D	508	-	4,4,4	0.22	0	6,6,6	0.21	0
18	GOL	C	618	-	5,5,5	1.10	1 (20%)	5,5,5	1.18	1 (20%)
18	GOL	D	519	-	5,5,5	1.13	0	5,5,5	0.92	0
18	GOL	A	516	-	5,5,5	1.07	1 (20%)	5,5,5	0.96	0
18	GOL	D	521	-	5,5,5	0.86	0	5,5,5	1.10	0
16	SO4	D	512	-	4,4,4	0.28	0	6,6,6	0.11	0
16	SO4	B	510	-	4,4,4	0.20	0	6,6,6	0.25	0
16	SO4	C	613	-	4,4,4	0.23	0	6,6,6	0.08	0
16	SO4	B	509	-	4,4,4	0.21	0	6,6,6	0.15	0
18	GOL	C	619	-	5,5,5	0.94	0	5,5,5	0.97	0
18	GOL	D	526	-	5,5,5	0.88	0	5,5,5	1.13	0
18	GOL	A	527	-	5,5,5	0.94	0	5,5,5	0.96	0
18	GOL	B	524	-	5,5,5	0.79	0	5,5,5	1.13	0
18	GOL	D	527	-	5,5,5	1.19	1 (20%)	5,5,5	1.27	1 (20%)
18	GOL	D	532	-	5,5,5	0.87	0	5,5,5	1.08	0
13	FLC	C	627	-	12,12,12	1.94	6 (50%)	17,17,17	2.52	8 (47%)
18	GOL	B	521	-	5,5,5	1.10	1 (20%)	5,5,5	1.08	0
16	SO4	B	516	-	4,4,4	0.24	0	6,6,6	0.13	0
20	R9X	B	531[B]	-	28,28,28	1.50	3 (10%)	34,37,37	1.52	5 (14%)
20	R9X	C	633[B]	-	28,28,28	1.66	3 (10%)	34,37,37	1.38	6 (17%)
16	SO4	A	510	-	4,4,4	0.19	0	6,6,6	0.13	0
18	GOL	A	518	-	5,5,5	0.90	0	5,5,5	1.29	1 (20%)
14	PGE	A	504	-	9,9,9	0.32	0	8,8,8	0.26	0
18	GOL	B	520	-	5,5,5	0.97	0	5,5,5	1.02	0
20	R9X	A	532[B]	-	28,28,28	1.52	5 (17%)	34,37,37	1.07	2 (5%)
18	GOL	A	526	-	5,5,5	0.91	0	5,5,5	1.13	0
16	SO4	D	514	-	4,4,4	0.23	0	6,6,6	0.15	0
18	GOL	A	524	-	5,5,5	0.86	0	5,5,5	1.04	0
14	PGE	D	504	-	9,9,9	0.28	0	8,8,8	0.56	0
16	SO4	C	612	-	4,4,4	0.21	0	6,6,6	0.13	0
18	GOL	B	527	-	5,5,5	1.03	0	5,5,5	0.93	0
13	FLC	B	505	-	12,12,12	0.13	0	17,17,17	0.32	0
13	FLC	C	603	-	12,12,12	1.55	4 (33%)	17,17,17	2.01	4 (23%)
18	GOL	C	624	-	5,5,5	0.89	0	5,5,5	1.13	1 (20%)
16	SO4	A	511	-	4,4,4	0.25	0	6,6,6	0.10	0
16	SO4	C	611	-	4,4,4	0.21	0	6,6,6	0.13	0
20	R9X	C	632[A]	-	28,28,28	1.60	4 (14%)	34,37,37	2.88	6 (17%)

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
20	R9X	A	532[A]	-	1/1/3/4	10/23/23/23	0/2/2/2
18	GOL	A	523	-	-	0/4/4/4	-
20	R9X	D	535[A]	-	1/1/3/4	17/23/23/23	0/2/2/2
18	GOL	D	522	-	-	4/4/4/4	-
18	GOL	A	515	-	-	0/4/4/4	-
18	GOL	C	621	-	-	0/4/4/4	-
18	GOL	B	519	-	-	2/4/4/4	-
15	NAG	D	516	1	-	2/6/23/26	0/1/1/1
18	GOL	D	523	-	-	2/4/4/4	-
14	PGE	B	508	-	-	3/7/7/7	-
13	FLC	D	503	-	-	4/16/16/16	-
13	FLC	C	628	-	-	9/16/16/16	-
18	GOL	D	518	-	-	0/4/4/4	-
18	GOL	B	522	-	-	2/4/4/4	-
18	GOL	B	525	-	-	2/4/4/4	-
18	GOL	A	519	-	-	2/4/4/4	-
15	NAG	A	506	1	-	1/6/23/26	0/1/1/1
17	EDO	B	518	-	-	0/1/1/1	-
18	GOL	A	521	-	-	2/4/4/4	-
18	GOL	C	623	-	-	0/4/4/4	-
18	GOL	B	528	-	-	4/4/4/4	-
20	R9X	B	531[A]	-	-	9/23/23/23	0/2/2/2
13	FLC	A	503	-	-	5/16/16/16	-
18	GOL	D	528	-	-	0/4/4/4	-
18	GOL	D	525	-	-	2/4/4/4	-
18	GOL	D	533	-	-	2/4/4/4	-
13	FLC	B	503	-	-	11/16/16/16	-
17	EDO	C	617	-	-	1/1/1/1	-
18	GOL	C	631	-	-	2/4/4/4	-
18	GOL	C	629	-	-	4/4/4/4	-
18	GOL	C	630	-	-	2/4/4/4	-
18	GOL	C	622	-	-	1/4/4/4	-
15	NAG	D	506	1	-	2/6/23/26	0/1/1/1
18	GOL	A	531	-	-	2/4/4/4	-
13	FLC	B	506	-	-	10/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	GOL	A	522	-	-	2/4/4/4	-
18	GOL	C	625	-	-	3/4/4/4	-
18	GOL	B	523	-	-	0/4/4/4	-
18	GOL	A	517	-	-	3/4/4/4	-
15	NAG	C	605	1	-	4/6/23/26	0/1/1/1
14	PGE	C	604	-	-	6/7/7/7	-
14	PGE	B	504	-	-	6/7/7/7	-
18	GOL	D	524	-	-	2/4/4/4	-
14	PGE	A	507	-	-	3/4/4/7	-
18	GOL	A	520	-	-	2/4/4/4	-
13	FLC	B	507	-	-	9/16/16/16	-
13	FLC	C	601	-	-	2/16/16/16	-
18	GOL	B	526	-	-	1/4/4/4	-
18	GOL	D	520	-	-	0/4/4/4	-
13	FLC	A	530	-	-	10/16/16/16	-
18	GOL	D	534	-	-	2/4/4/4	-
13	FLC	A	505	-	-	14/16/16/16	-
17	EDO	D	517	-	-	1/1/1/1	-
15	NAG	C	616	1	-	4/6/23/26	0/1/1/1
18	GOL	A	525	-	-	2/4/4/4	-
17	EDO	A	514	-	-	0/1/1/1	-
20	R9X	D	535[B]	-	1/1/3/4	14/23/23/23	0/2/2/2
13	FLC	C	602	-	-	3/16/16/16	-
18	GOL	C	620	-	-	2/4/4/4	-
18	GOL	D	529	-	-	1/4/4/4	-
18	GOL	C	618	-	-	0/4/4/4	-
18	GOL	D	519	-	-	0/4/4/4	-
18	GOL	A	516	-	-	1/4/4/4	-
18	GOL	D	521	-	-	2/4/4/4	-
18	GOL	C	619	-	-	1/4/4/4	-
18	GOL	D	526	-	-	0/4/4/4	-
18	GOL	A	527	-	-	1/4/4/4	-
18	GOL	B	524	-	-	4/4/4/4	-
18	GOL	D	527	-	-	2/4/4/4	-
18	GOL	D	532	-	-	0/4/4/4	-
13	FLC	C	627	-	-	9/16/16/16	-
18	GOL	B	521	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	R9X	B	531[B]	-	-	7/23/23/23	0/2/2/2
20	R9X	C	633[B]	-	1/1/3/4	16/23/23/23	0/2/2/2
18	GOL	A	518	-	-	0/4/4/4	-
14	PGE	A	504	-	-	3/7/7/7	-
18	GOL	B	520	-	-	0/4/4/4	-
20	R9X	A	532[B]	-	1/1/3/4	9/23/23/23	0/2/2/2
18	GOL	A	526	-	-	1/4/4/4	-
18	GOL	A	524	-	-	2/4/4/4	-
14	PGE	D	504	-	-	6/7/7/7	-
18	GOL	B	527	-	-	1/4/4/4	-
13	FLC	B	505	-	-	9/16/16/16	-
13	FLC	C	603	-	-	3/16/16/16	-
18	GOL	C	624	-	-	2/4/4/4	-
20	R9X	C	632[A]	-	-	13/23/23/23	0/2/2/2

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	633[B]	R9X	C10-N12	6.47	1.47	1.34
20	C	632[A]	R9X	C10-N12	5.96	1.46	1.34
20	A	532[B]	R9X	C10-N12	5.66	1.46	1.34
20	D	535[B]	R9X	C10-N12	5.58	1.45	1.34
20	B	531[B]	R9X	C10-N12	5.56	1.45	1.34

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	632[A]	R9X	C13-N12-C10	11.49	136.25	121.18
20	C	632[A]	R9X	P24-C13-N12	-8.47	92.58	108.10
20	A	532[A]	R9X	P24-C13-N12	-6.93	95.41	108.10
15	C	605	NAG	C1-O5-C5	6.50	120.89	112.19
20	D	535[A]	R9X	P24-C13-N12	-6.43	96.32	108.10

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	532[A]	R9X	C13
20	A	532[B]	R9X	C13
20	C	633[B]	R9X	C13

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Mol	Chain	Res	Type	Atom
20	D	535[A]	R9X	C13
20	D	535[B]	R9X	C13

5 of 309 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	530	FLC	CAC-CA-CB-CBC
13	A	530	FLC	CAC-CA-CB-CG
13	A	530	FLC	CAC-CA-CB-OHB
13	A	530	FLC	CG-CB-CBC-OB1
13	A	530	FLC	OHB-CB-CBC-OB1

There are no ring outliers.

63 monomers are involved in 137 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	532[A]	R9X	7	0
18	A	523	GOL	2	0
20	D	535[A]	R9X	6	0
18	D	522	GOL	4	0
18	C	621	GOL	2	0
18	B	519	GOL	1	0
16	B	512	SO4	1	0
16	C	608	SO4	2	0
16	C	610	SO4	1	0
13	D	503	FLC	3	0
13	C	628	FLC	2	0
18	B	522	GOL	1	0
16	D	515	SO4	1	0
18	B	525	GOL	1	0
18	A	519	GOL	1	0
16	A	512	SO4	3	0
18	C	623	GOL	1	0
20	B	531[A]	R9X	6	0
13	A	503	FLC	3	0
18	D	533	GOL	1	0
17	C	617	EDO	1	0
22	D	505	DMS	2	0
18	C	622	GOL	1	0
15	D	506	NAG	3	0
18	A	531	GOL	3	0
13	B	506	FLC	3	0

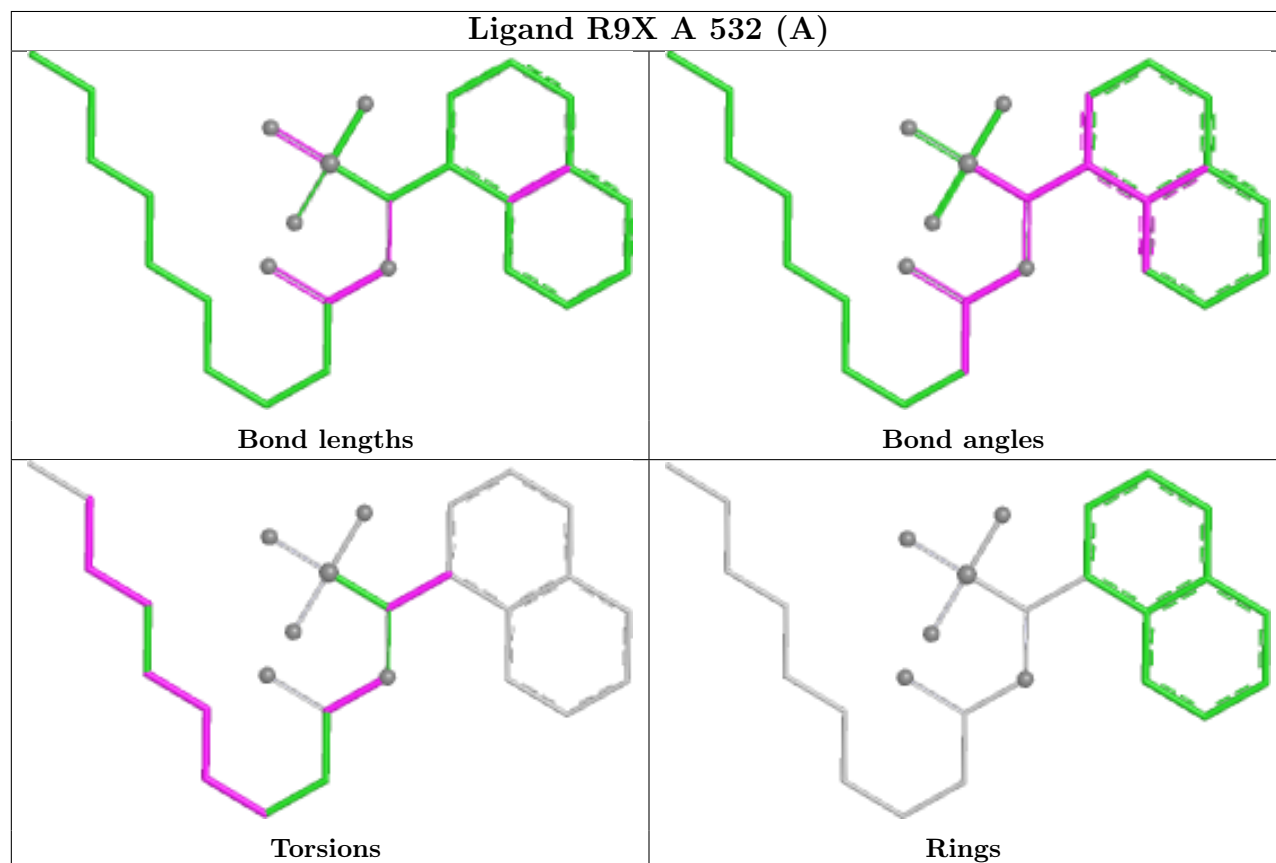
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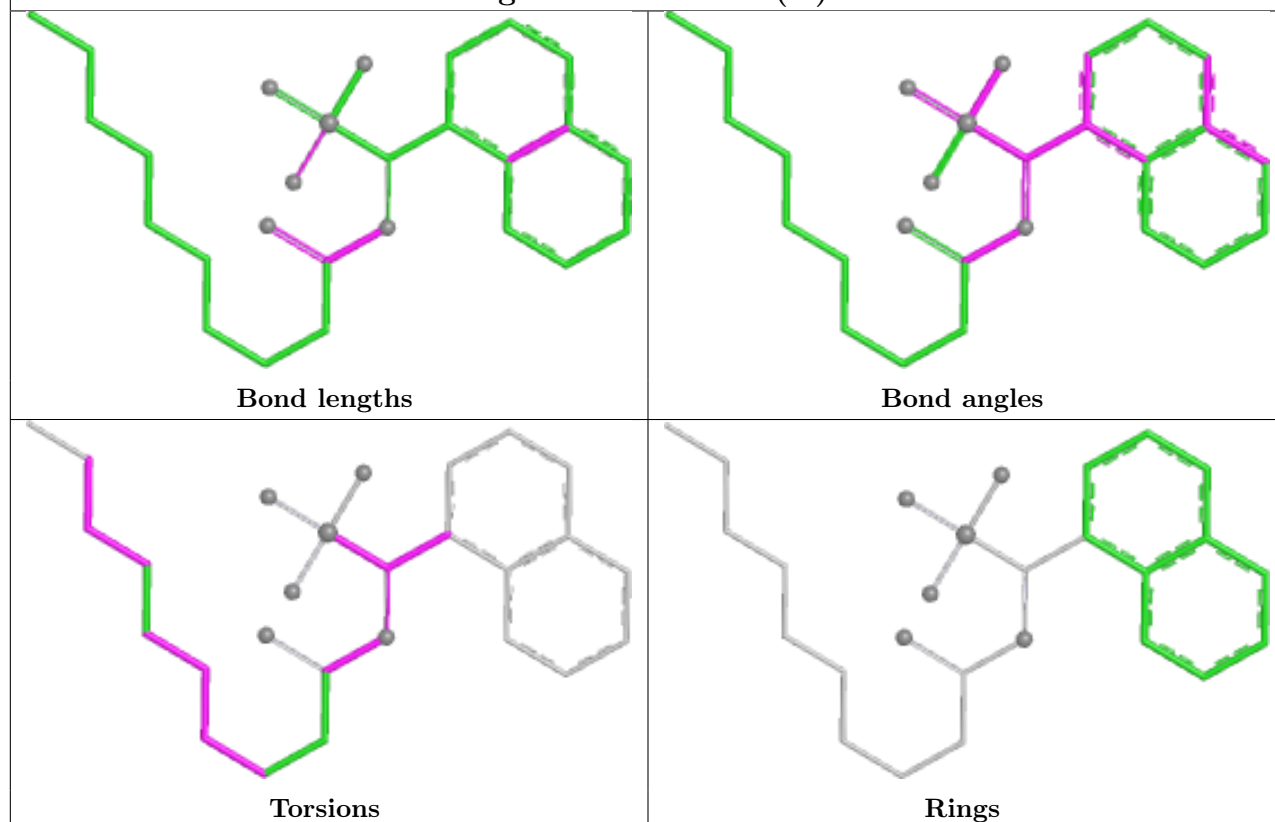
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	625	GOL	1	0
15	C	605	NAG	1	0
14	C	604	PGE	1	0
16	C	615	SO4	1	0
14	B	504	PGE	4	0
18	D	524	GOL	1	0
14	A	507	PGE	4	0
13	B	507	FLC	2	0
13	A	505	FLC	2	0
13	C	602	FLC	1	0
16	A	509	SO4	1	0
20	D	535[B]	R9X	2	0
18	C	620	GOL	3	0
18	D	529	GOL	1	0
16	D	507	SO4	1	0
18	C	618	GOL	1	0
18	A	516	GOL	2	0
16	B	510	SO4	1	0
16	C	613	SO4	2	0
16	B	509	SO4	1	0
18	B	524	GOL	1	0
18	D	527	GOL	3	0
13	C	627	FLC	2	0
18	B	521	GOL	1	0
20	C	633[B]	R9X	6	0
16	A	510	SO4	2	0
18	A	518	GOL	3	0
14	A	504	PGE	2	0
20	A	532[B]	R9X	5	0
18	A	526	GOL	1	0
16	D	514	SO4	1	0
18	A	524	GOL	1	0
14	D	504	PGE	8	0
13	B	505	FLC	4	0
13	C	603	FLC	1	0
18	C	624	GOL	2	0
20	C	632[A]	R9X	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

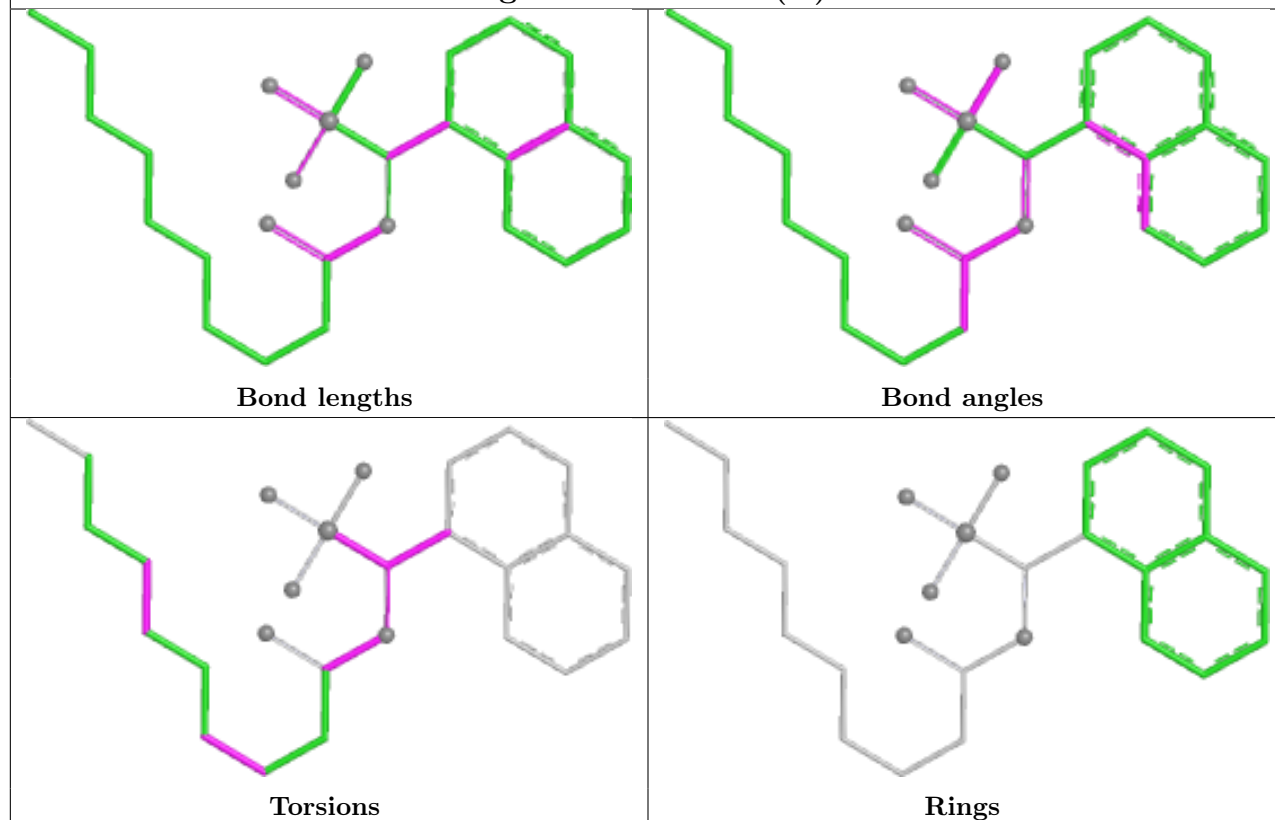
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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



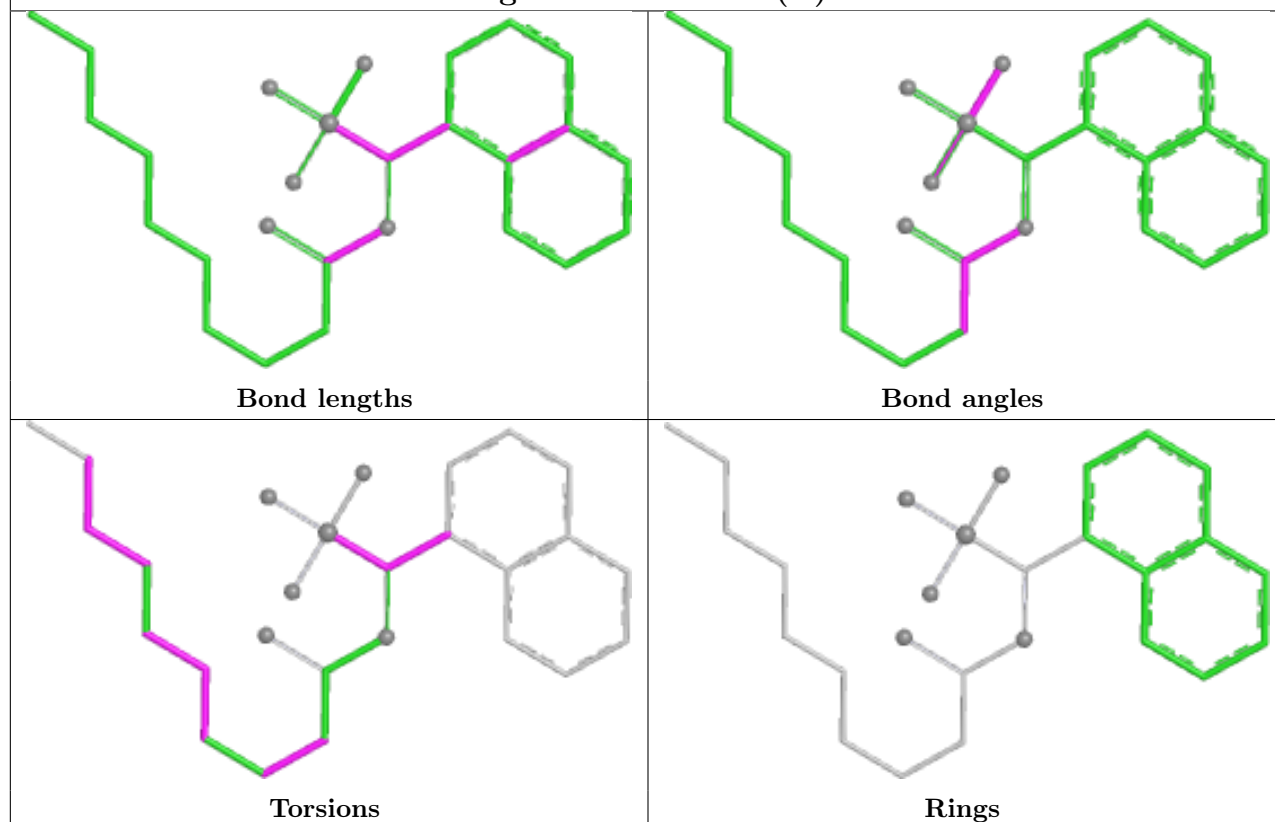
Ligand R9X D 535 (A)



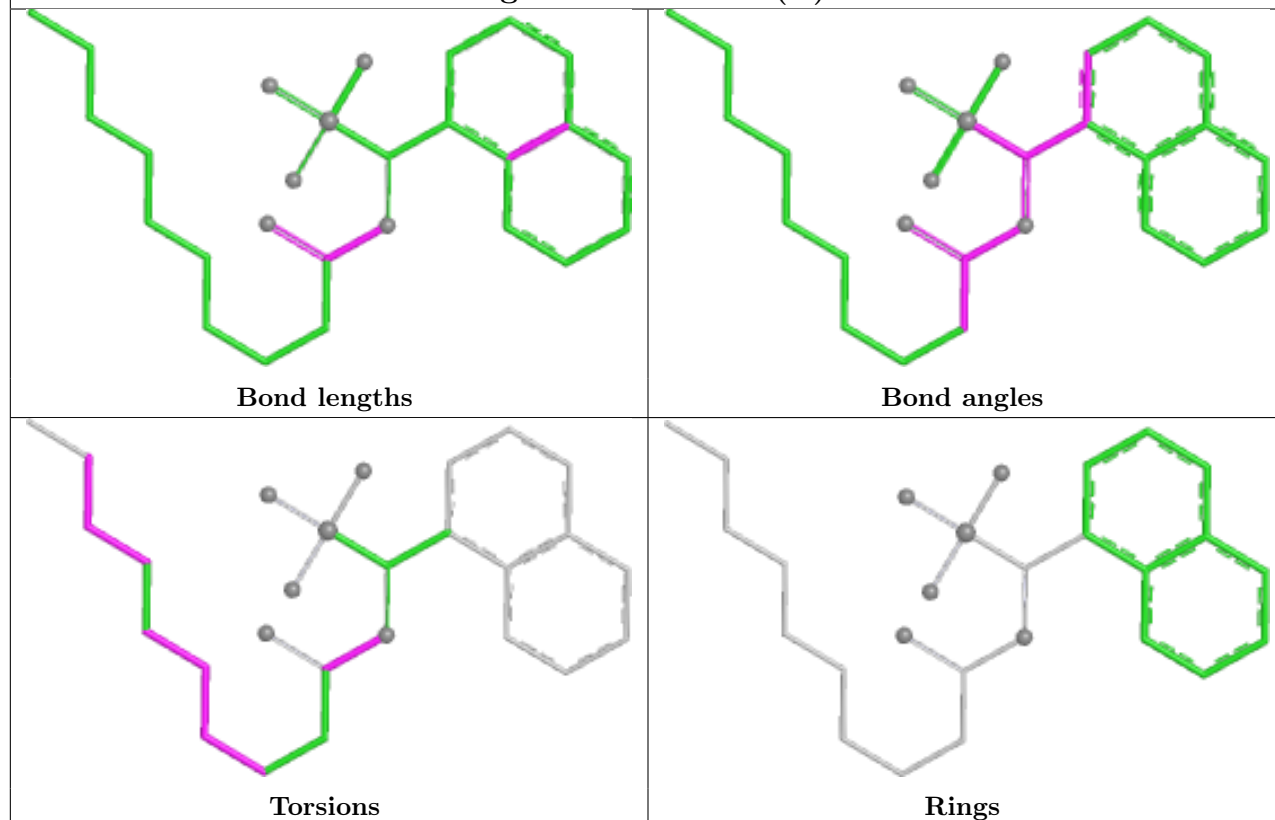
Ligand R9X B 531 (A)



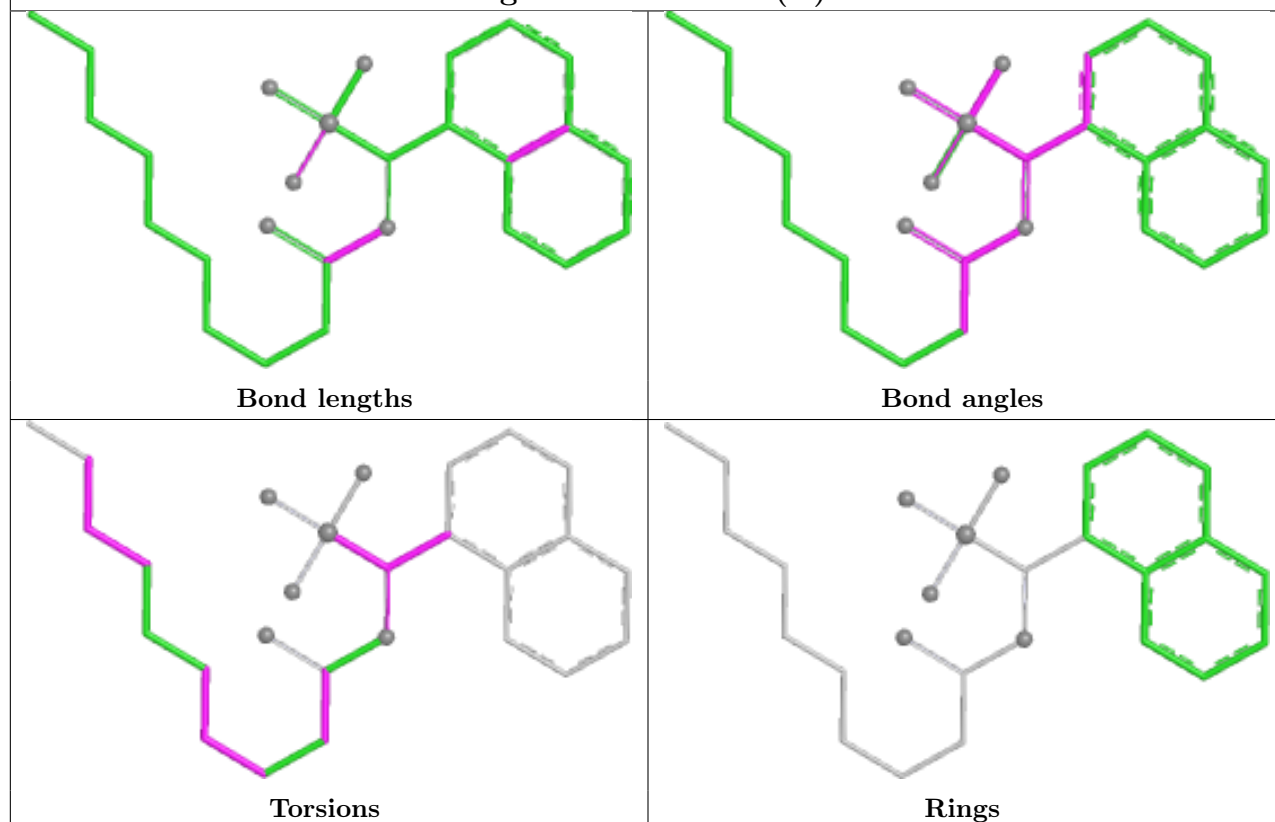
Ligand R9X D 535 (B)



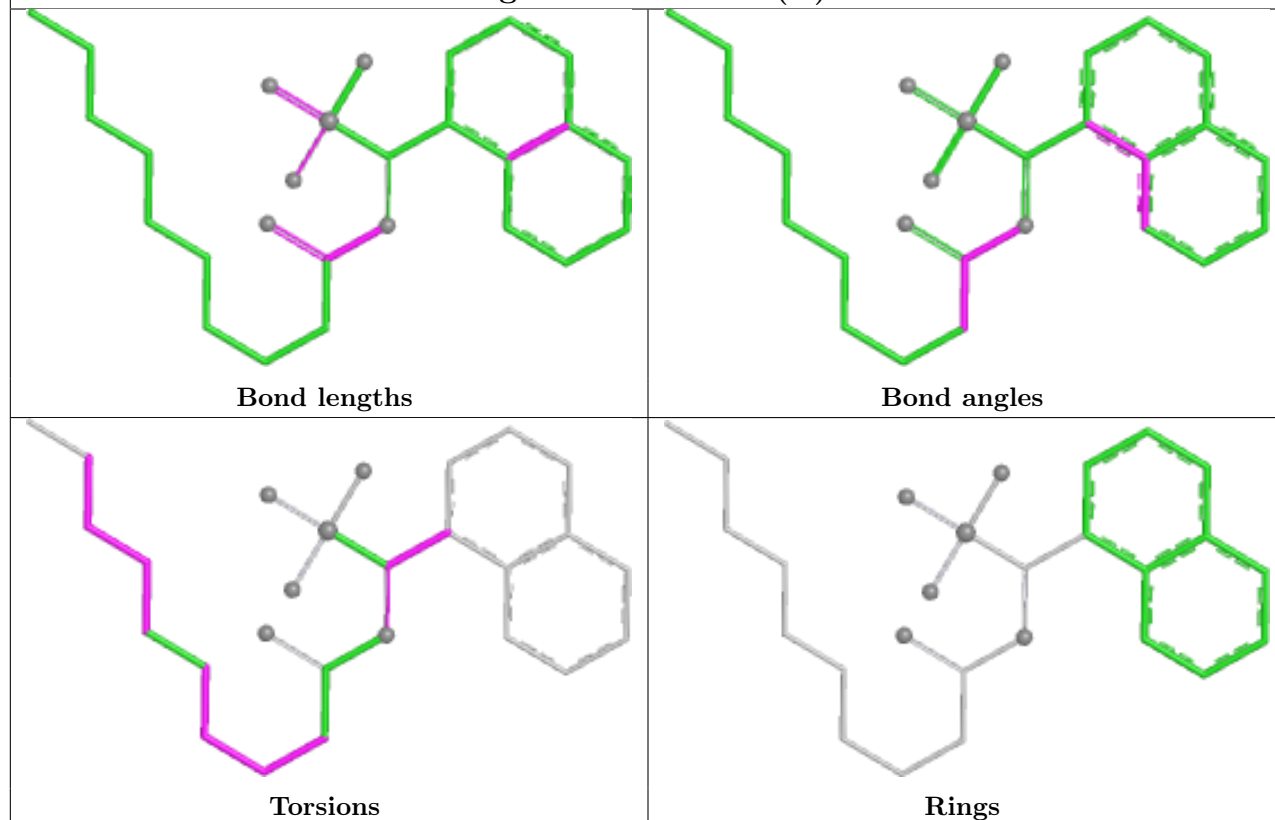
Ligand R9X B 531 (B)

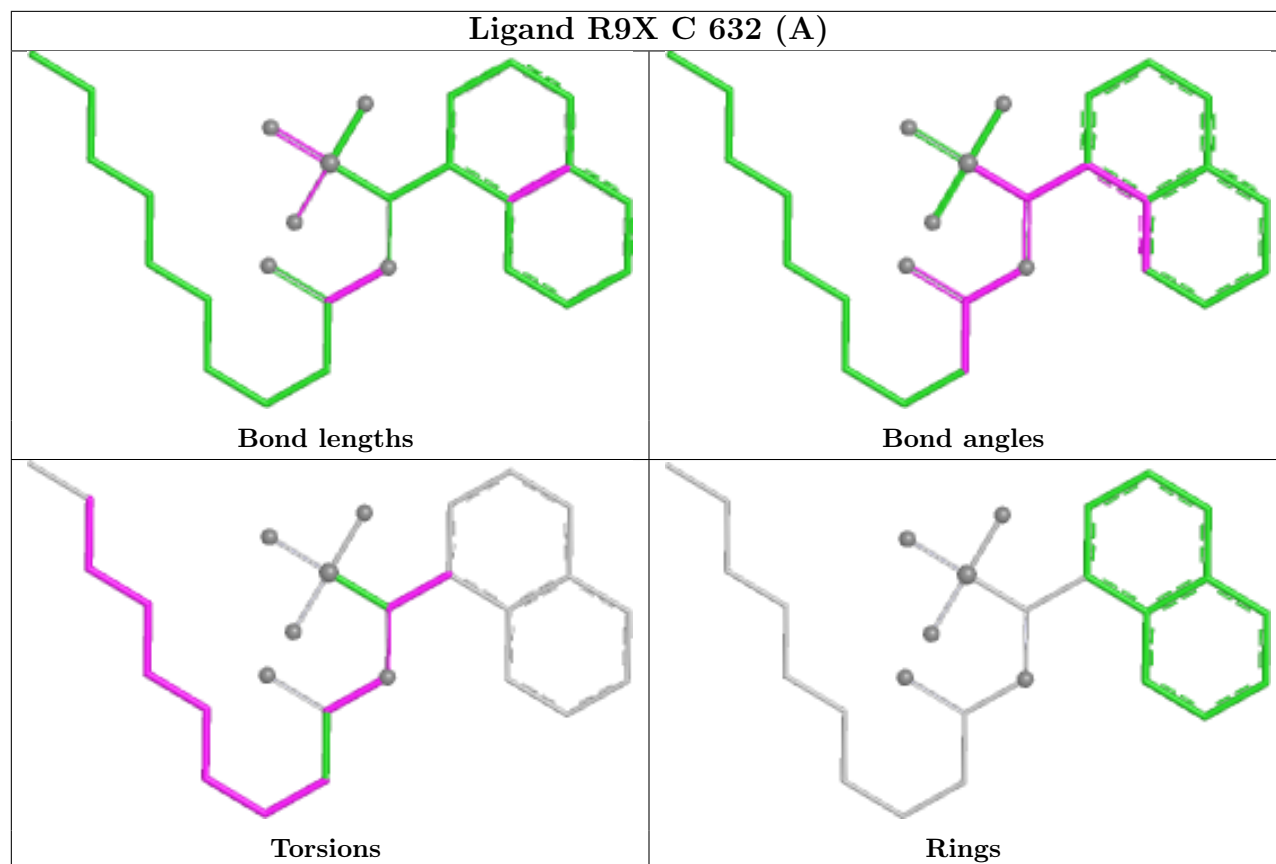


Ligand R9X C 633 (B)



Ligand R9X A 532 (B)





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	425/428 (99%)	-0.92	0 100 100	12, 20, 32, 58	12 (2%)
1	B	428/428 (100%)	-0.83	2 (0%) 87 87	11, 22, 37, 93	5 (1%)
1	C	428/428 (100%)	-0.83	2 (0%) 87 87	10, 21, 36, 79	11 (2%)
1	D	426/428 (99%)	-0.85	1 (0%) 91 90	11, 21, 35, 77	13 (3%)
All	All	1707/1712 (99%)	-0.86	5 (0%) 90 89	10, 21, 35, 93	41 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	ASN	3.0
1	B	5	THR	2.3
1	C	432	THR	2.3
1	D	5	THR	2.2
1	C	65	GLY	2.2

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
7	BMA	M	3	11/12	0.42	0.16	68,72,75,79	11
4	BMA	I	3	11/12	0.45	0.13	83,100,103,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BMA	G	3	11/12	0.54	0.14	68,82,88,88	11
9	FUC	R	4	10/11	0.58	0.15	47,50,56,58	10
4	BMA	N	3	11/12	0.61	0.13	59,62,68,70	11
9	BMA	R	3	10/12	0.61	0.12	64,67,70,71	10
5	MAN	J	4	11/12	0.61	0.18	40,54,64,69	11
3	MAN	F	5	11/12	0.66	0.16	48,51,59,60	11
4	BMA	S	3	11/12	0.66	0.11	59,70,74,75	11
4	NAG	I	2	14/15	0.68	0.14	60,73,82,92	14
4	NAG	S	2	14/15	0.69	0.14	39,52,60,61	14
8	NAG	O	2	14/15	0.69	0.17	41,46,52,58	14
2	NAG	E	2	14/15	0.70	0.13	30,41,48,49	14
4	BMA	P	3	11/12	0.71	0.10	65,75,82,83	0
7	NAG	M	2	14/15	0.72	0.15	40,48,60,65	14
4	NAG	G	2	14/15	0.73	0.12	51,61,74,78	14
4	NAG	N	2	14/15	0.74	0.13	43,49,57,59	14
9	NAG	R	2	14/15	0.75	0.18	38,50,61,63	14
2	NAG	Q	2	14/15	0.75	0.12	27,43,49,50	14
3	MAN	F	4	11/12	0.75	0.15	43,48,51,51	11
3	BMA	F	3	11/12	0.78	0.11	45,49,57,62	11
4	FUC	G	4	10/11	0.78	0.12	44,48,55,59	10
5	MAN	H	5	11/12	0.79	0.12	39,44,49,50	11
10	NAG	T	1	14/15	0.79	0.13	43,48,53,53	14
10	FUC	T	2	10/11	0.79	0.15	46,50,53,55	10
5	MAN	J	5	11/12	0.80	0.11	39,48,52,54	11
5	BMA	J	3	11/12	0.80	0.11	42,44,52,57	11
2	NAG	K	2	14/15	0.80	0.11	38,46,47,48	14
5	NAG	J	2	14/15	0.82	0.12	31,37,42,45	14
4	FUC	I	4	10/11	0.82	0.11	45,60,68,71	0
3	FUC	F	6	10/11	0.83	0.11	39,43,51,53	10
5	FUC	J	6	10/11	0.83	0.11	35,43,47,56	10
4	NAG	V	1	14/15	-	-	19,25,30,30	0
4	NAG	V	2	14/15	-	-	21,38,44,53	14
4	BMA	V	3	11/12	-	-	48,60,68,85	11
4	FUC	V	4	10/11	-	-	34,39,47,48	10
6	MAN	L	4	11/12	0.84	0.12	40,52,67,72	11
8	NAG	O	1	14/15	0.84	0.11	32,35,47,54	14
6	BMA	L	3	11/12	0.85	0.09	39,45,51,57	11
4	FUC	P	4	10/11	0.86	0.10	37,46,51,51	0
4	FUC	N	4	10/11	0.86	0.09	40,44,49,50	10
9	NAG	R	1	14/15	0.88	0.10	34,40,52,53	14
4	NAG	N	1	14/15	0.89	0.09	28,43,49,51	14
4	FUC	S	4	10/11	0.89	0.10	30,43,46,47	10

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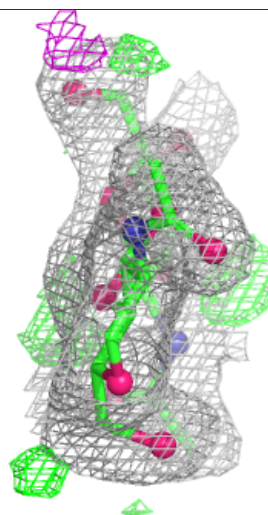
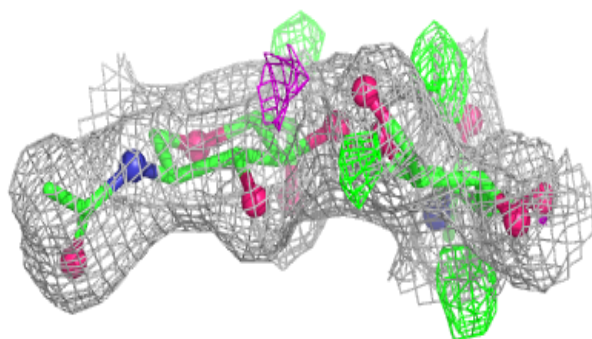
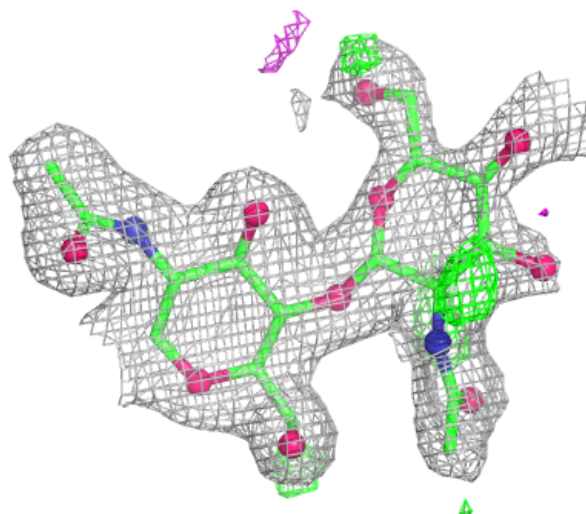
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	I	1	14/15	0.90	0.09	35,44,57,61	0
5	BMA	H	3	11/12	0.90	0.08	25,32,39,42	11
3	NAG	F	2	14/15	0.91	0.08	35,39,44,44	14
4	NAG	S	1	14/15	0.91	0.08	30,39,44,46	14
4	NAG	G	1	14/15	0.91	0.08	30,38,51,55	0
4	NAG	P	2	14/15	0.92	0.08	29,40,52,62	0
3	NAG	F	1	14/15	0.92	0.07	31,34,39,44	0
5	MAN	H	4	11/12	0.92	0.07	27,34,36,40	11
5	NAG	J	1	14/15	0.93	0.07	27,32,36,37	0
5	FUC	H	6	10/11	0.93	0.07	26,30,33,47	0
5	NAG	H	2	14/15	0.95	0.06	22,27,30,31	0
7	NAG	M	1	14/15	0.95	0.06	17,28,38,39	0
2	NAG	Q	1	14/15	0.95	0.06	28,31,39,41	0
2	NAG	K	1	14/15	0.95	0.07	22,31,38,46	0
6	NAG	L	2	14/15	0.95	0.06	22,28,38,39	0
2	NAG	E	1	14/15	0.95	0.06	22,28,34,39	0
6	FUC	L	5	10/11	0.96	0.05	23,29,33,40	0
4	NAG	P	1	14/15	0.96	0.07	25,30,38,42	0
6	NAG	L	1	14/15	0.97	0.05	19,24,30,31	0
5	NAG	H	1	14/15	0.97	0.05	17,22,27,32	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.

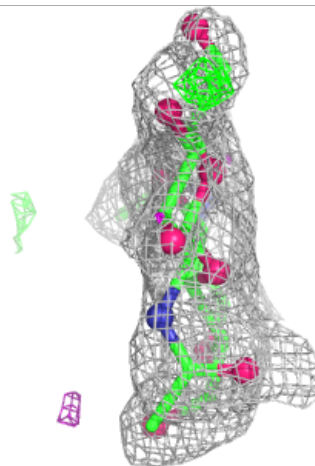
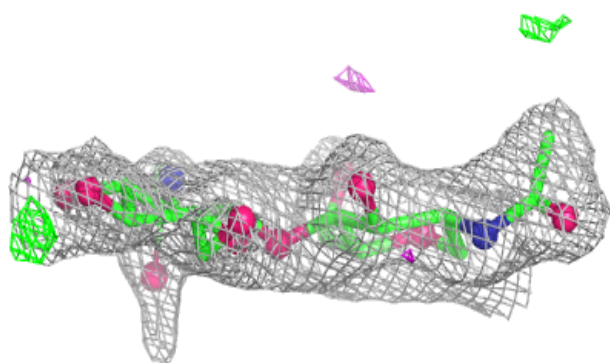
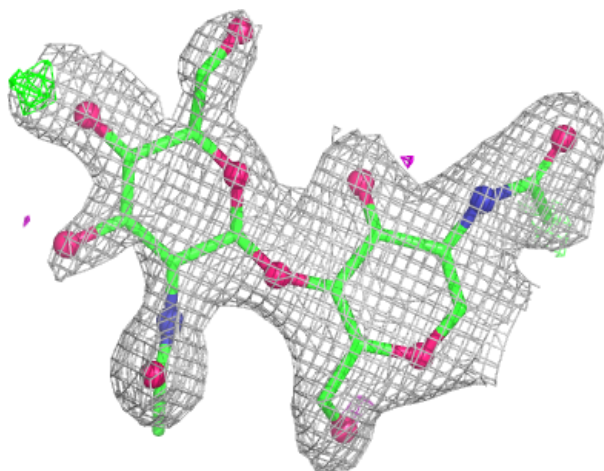
Electron density around Chain E:

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



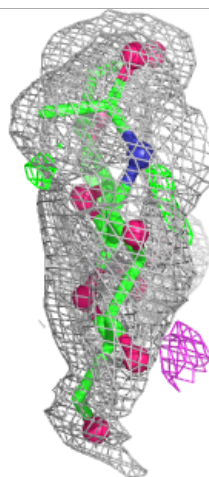
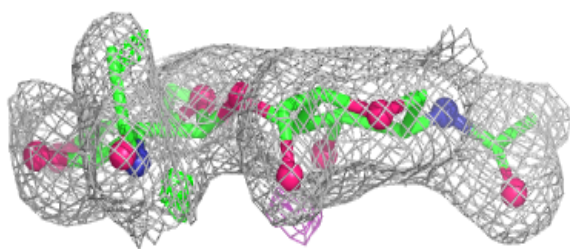
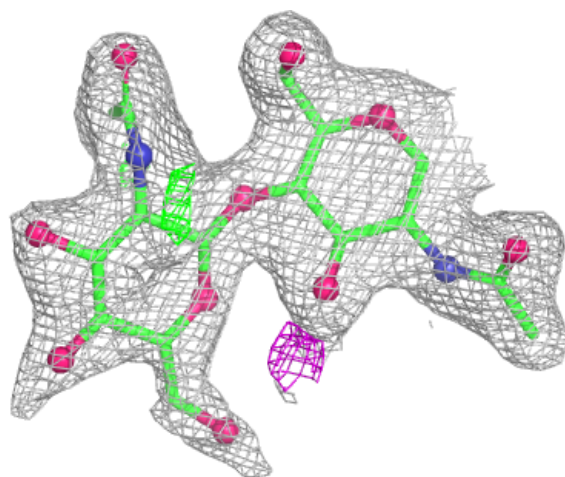
Electron density around Chain K:

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



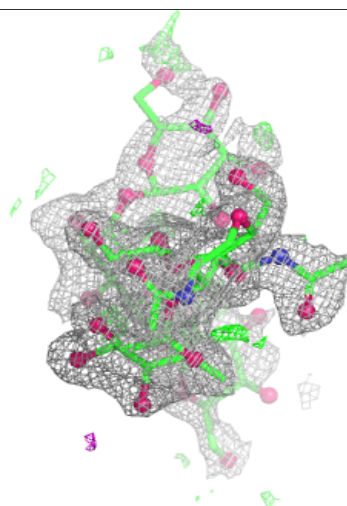
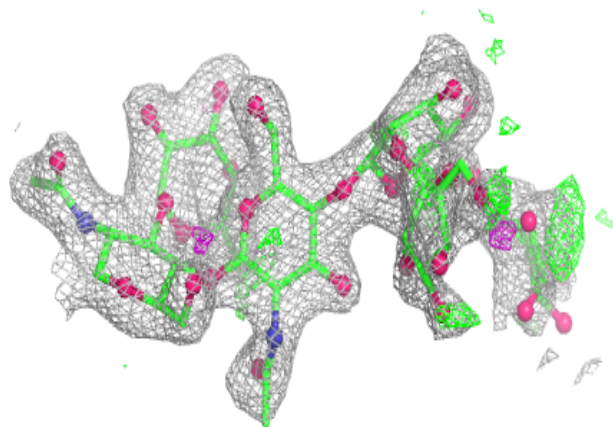
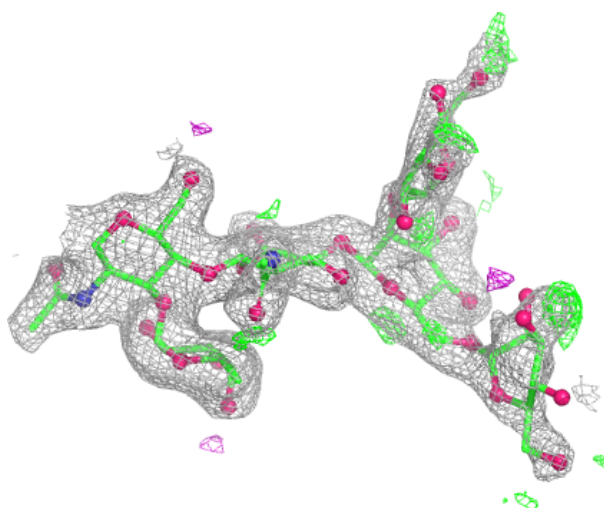
Electron density around Chain Q:

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



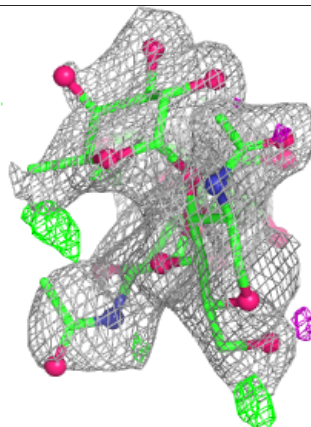
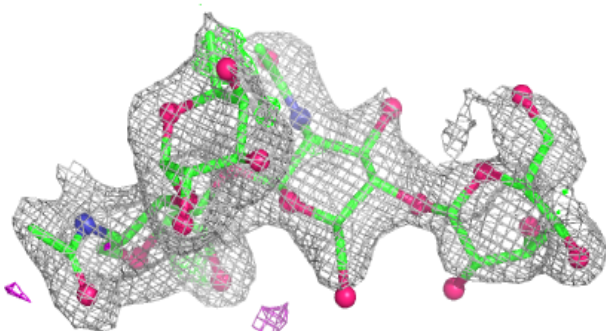
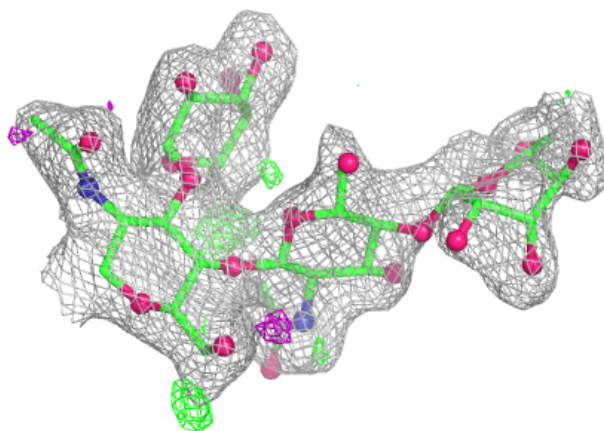
Electron density around Chain F:

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

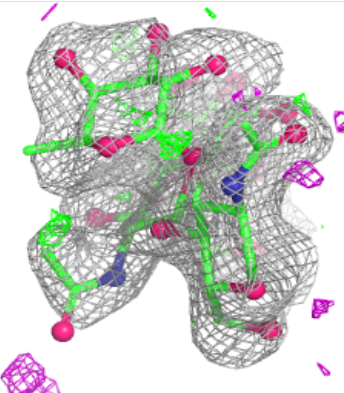
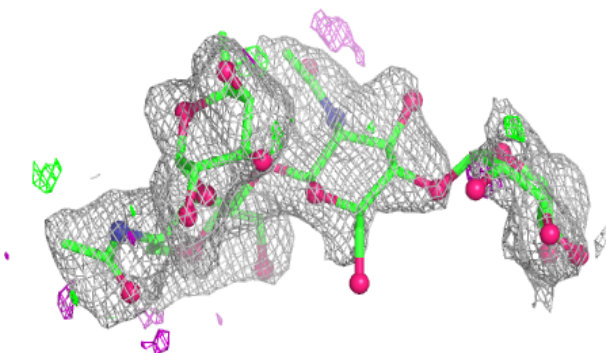
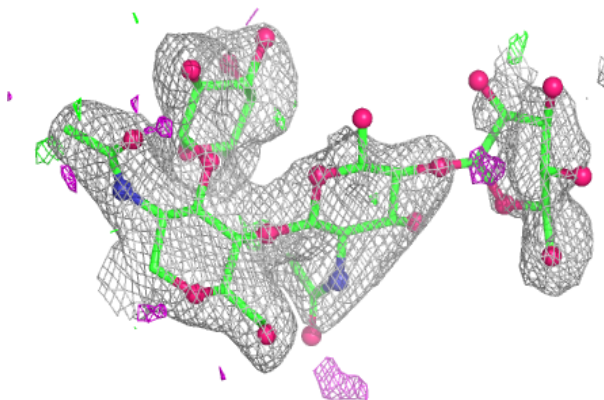


Electron density around Chain G:

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

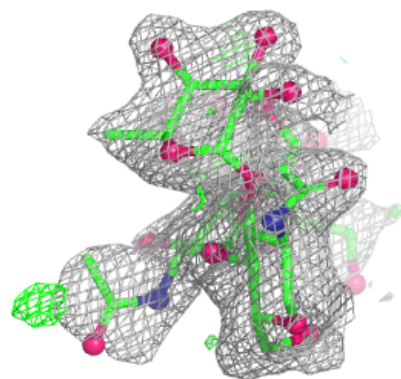
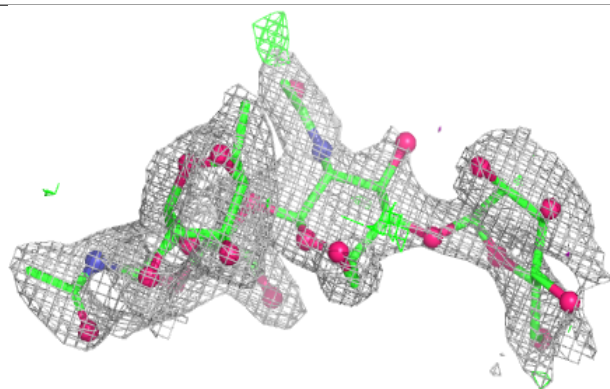
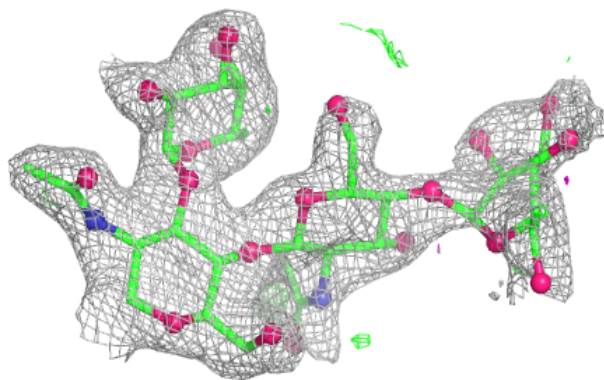
**Electron density around Chain I:**

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and green (positive)

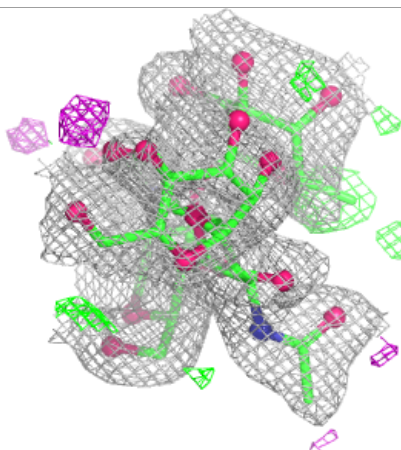
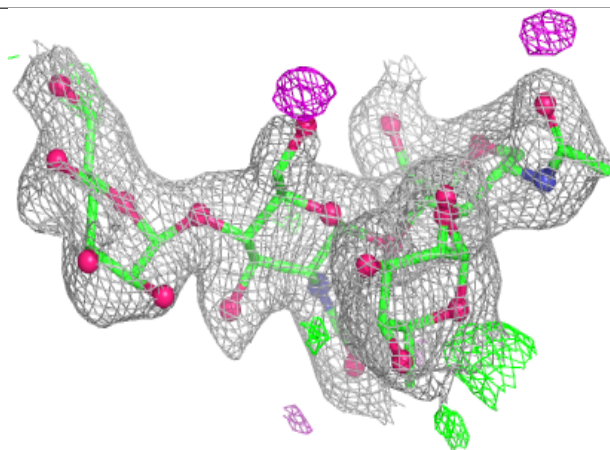
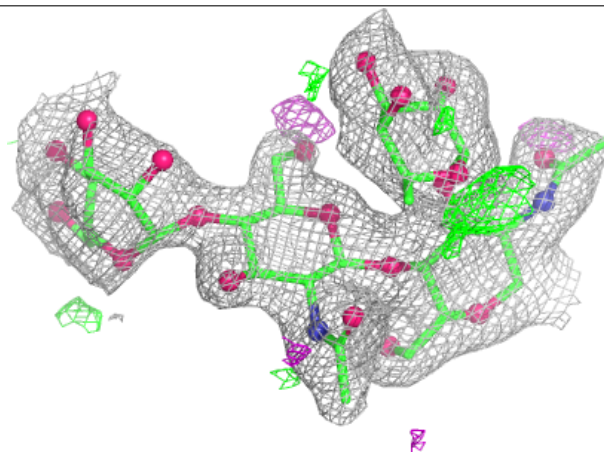


Electron density around Chain N:

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

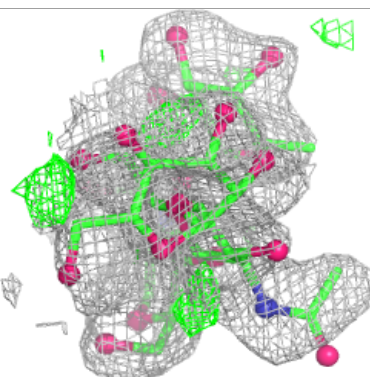
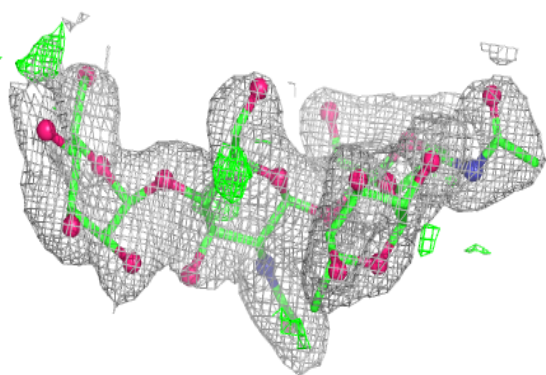
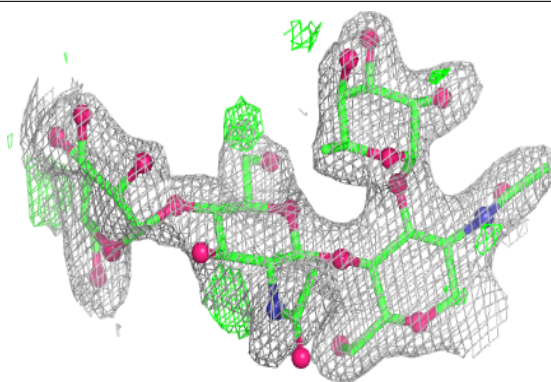
**Electron density around Chain P:**

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

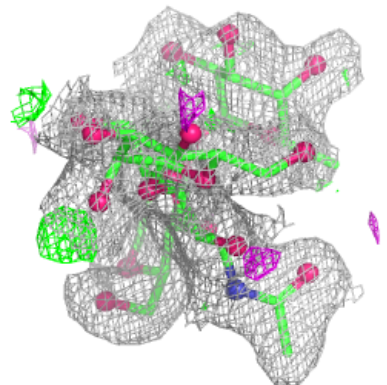
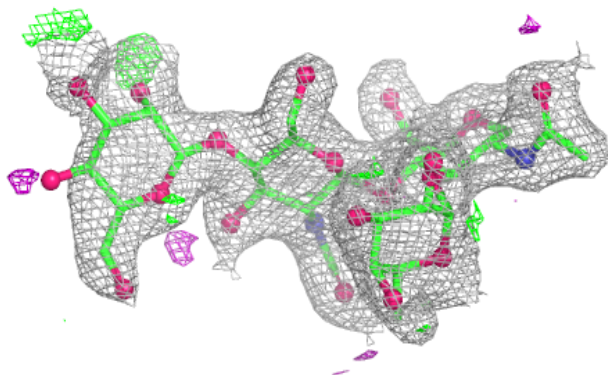
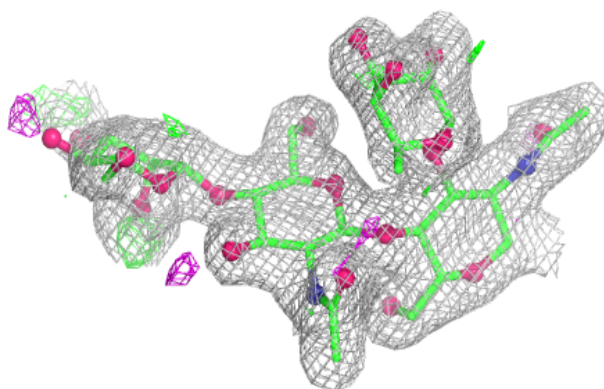


Electron density around Chain S:

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

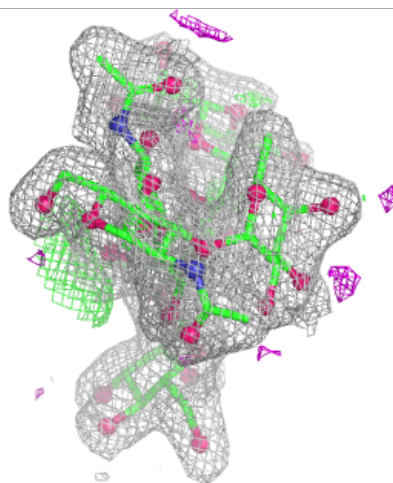
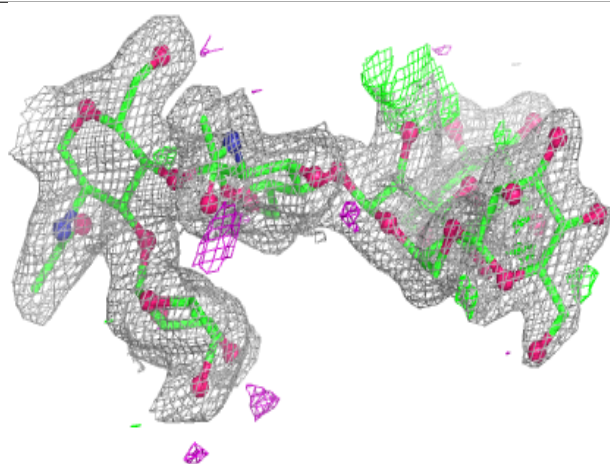
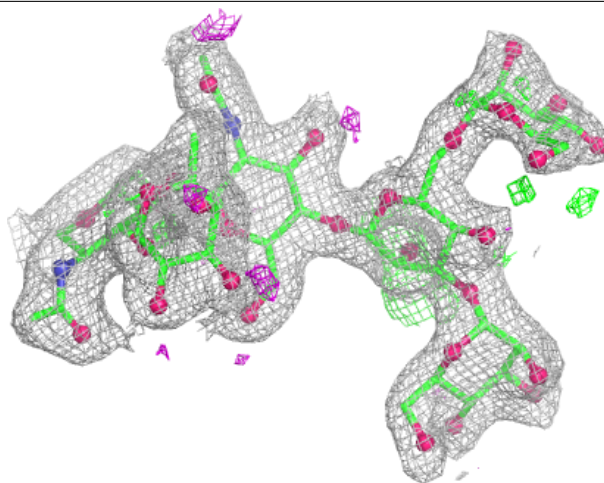
**Electron density around Chain V:**

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



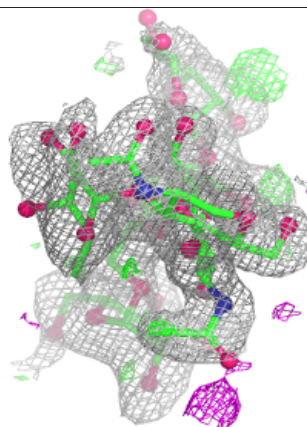
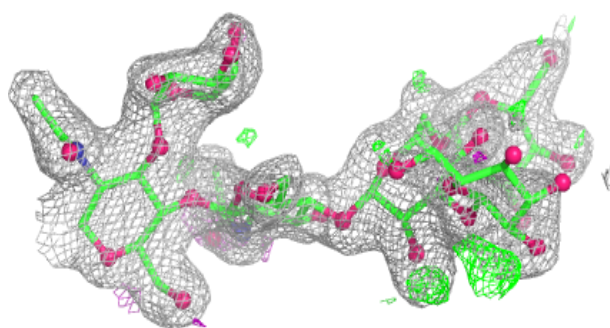
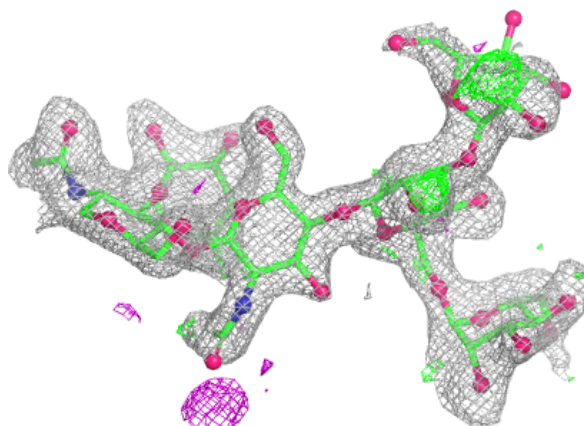
Electron density around Chain H:

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

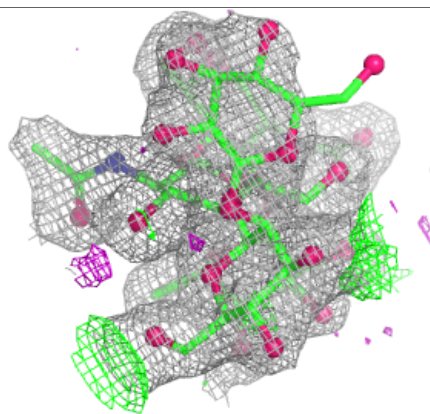
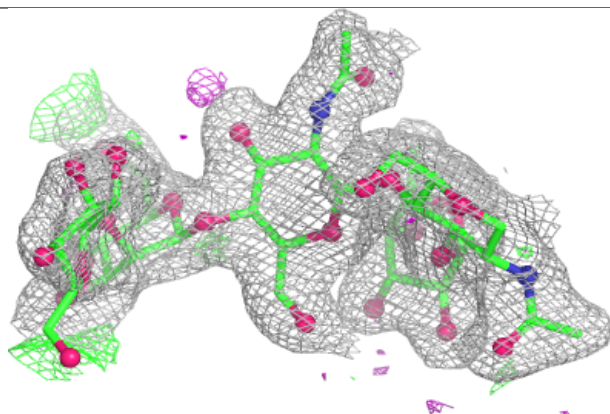
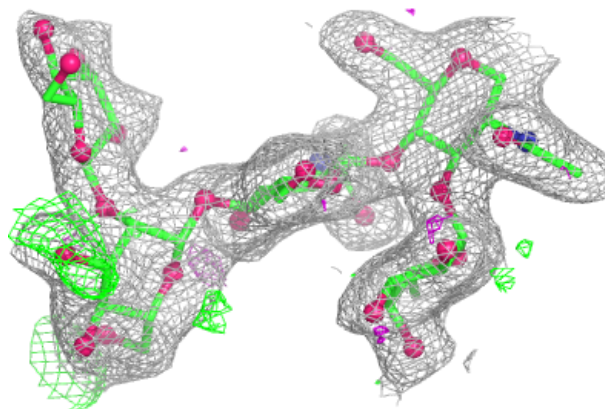


Electron density around Chain J:

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and green (positive)

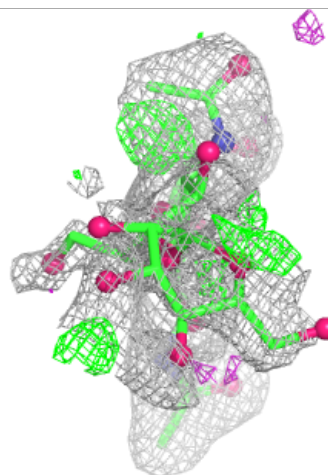
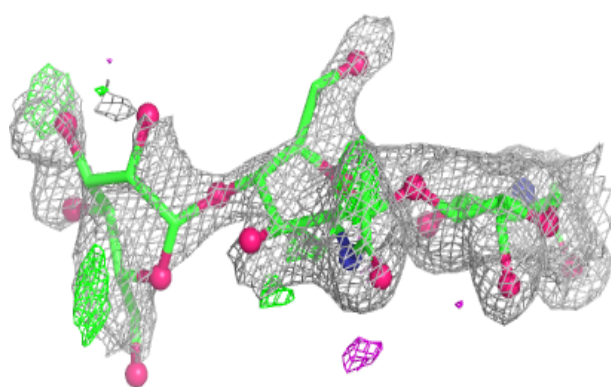
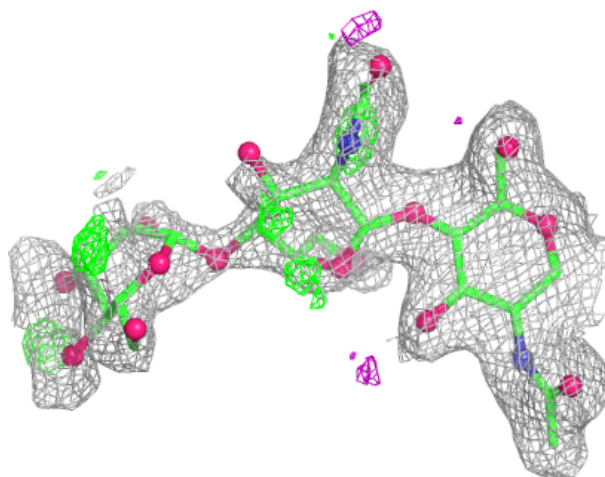
**Electron density around Chain L:**

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



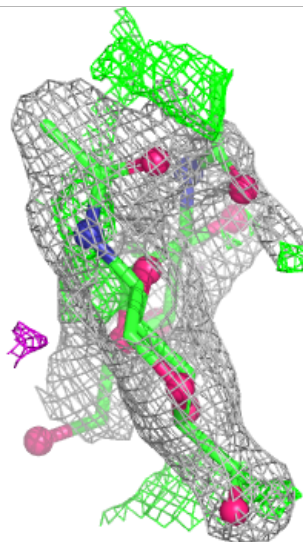
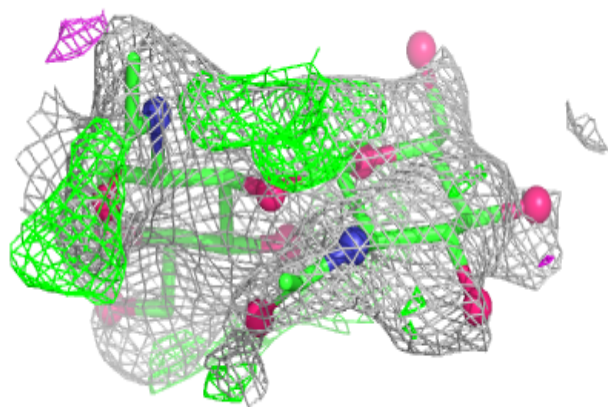
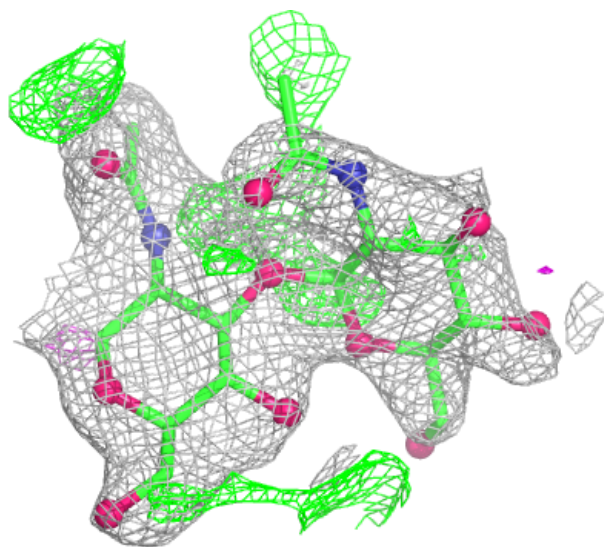
Electron density around Chain M:

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



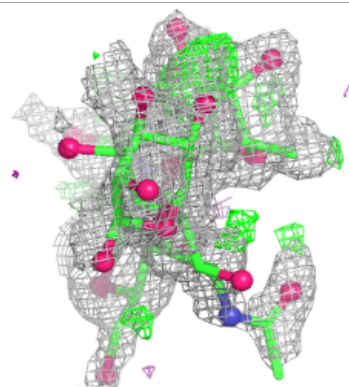
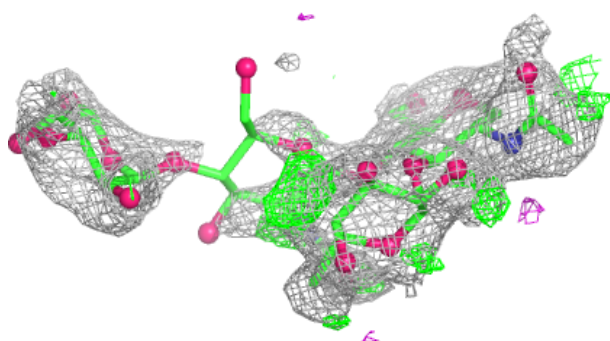
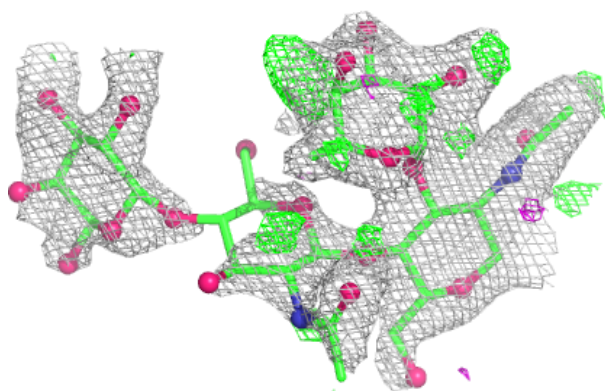
Electron density around Chain O:

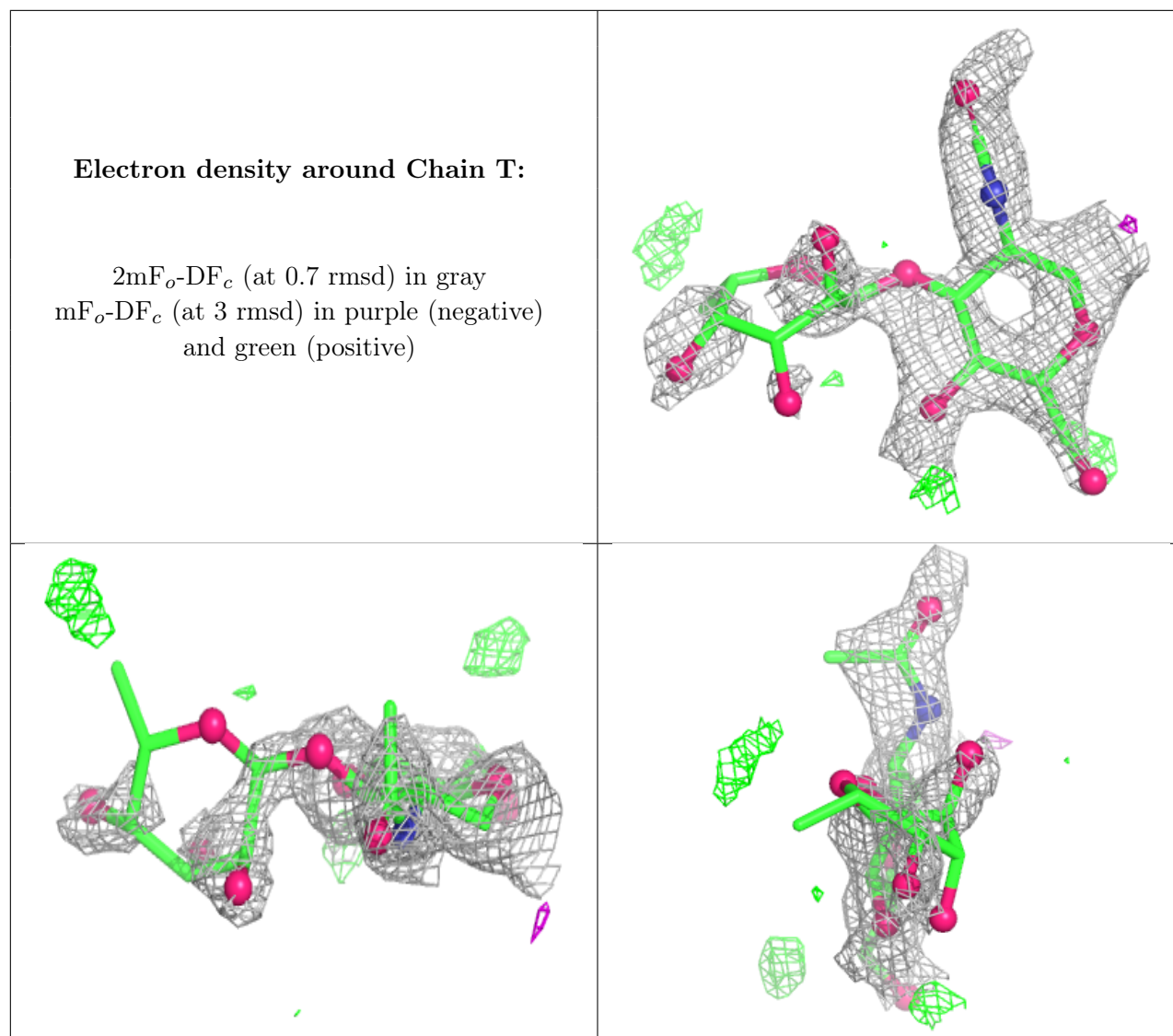
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain R:

$2mF_o-DF_c$ (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
20	R9X	C	632[A]	27/27	0.52	0.25	31,45,48,50	27
18	GOL	A	526	6/6	0.58	0.15	45,50,51,52	6
13	FLC	B	507	13/13	0.61	0.25	17,32,38,38	13
16	SO4	B	517	5/5	0.62	0.20	42,43,49,53	5
20	R9X	A	532[B]	27/27	0.64	0.23	23,44,50,57	27
20	R9X	A	532[A]	27/27	0.64	0.23	29,43,48,49	27
13	FLC	A	505	13/13	0.65	0.17	40,44,49,57	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	R9X	C	633[B]	27/27	0.66	0.21	36,46,50,52	27
15	NAG	A	506	14/15	0.67	0.18	33,44,47,55	14
20	R9X	B	531[A]	27/27	0.68	0.22	25,40,44,46	27
20	R9X	B	531[B]	27/27	0.68	0.22	35,42,46,49	27
14	PGE	B	508	10/10	0.68	0.24	37,43,48,49	10
13	FLC	B	506	13/13	0.68	0.15	47,54,68,68	13
18	GOL	C	631	6/6	0.69	0.15	51,55,59,60	6
20	R9X	D	535[A]	27/27	0.69	0.23	21,37,44,45	27
20	R9X	D	535[B]	27/27	0.69	0.23	36,40,45,51	27
18	GOL	D	529	6/6	0.70	0.18	25,28,34,34	6
18	GOL	A	517	6/6	0.71	0.15	27,32,36,37	6
15	NAG	D	506	14/15	0.71	0.21	53,60,74,80	14
13	FLC	A	530	13/13	0.71	0.16	30,39,45,50	13
13	FLC	A	503	13/13	0.73	0.20	25,32,40,42	13
13	FLC	B	505	13/13	0.73	0.17	33,41,46,50	13
13	FLC	D	503	13/13	0.73	0.21	26,33,38,43	13
18	GOL	A	527	6/6	0.73	0.15	39,44,50,52	6
18	GOL	C	624	6/6	0.73	0.17	31,37,42,43	6
16	SO4	C	615	5/5	0.74	0.14	38,43,46,49	5
18	GOL	D	534	6/6	0.74	0.18	36,37,40,41	6
13	FLC	C	602	13/13	0.74	0.19	25,35,44,49	13
18	GOL	C	629	6/6	0.74	0.12	51,53,56,56	6
15	NAG	C	605	14/15	0.74	0.14	30,43,51,55	14
15	NAG	C	616	14/15	0.75	0.16	42,47,52,61	14
18	GOL	A	531	6/6	0.75	0.15	37,41,43,46	6
18	GOL	B	520	6/6	0.75	0.16	36,39,43,46	6
13	FLC	C	628	13/13	0.75	0.14	43,48,54,54	13
13	FLC	B	503	13/13	0.76	0.16	28,39,48,54	13
13	FLC	C	603	13/13	0.76	0.20	30,35,48,54	13
18	GOL	A	523	6/6	0.76	0.10	56,58,60,60	6
16	SO4	C	611	5/5	0.76	0.11	51,52,67,69	5
13	FLC	C	627	13/13	0.78	0.15	28,33,39,52	13
14	PGE	A	504	10/10	0.78	0.15	31,36,43,44	10
16	SO4	A	513	5/5	0.78	0.09	44,49,51,56	5
18	GOL	D	525	6/6	0.78	0.20	37,47,49,51	6
14	PGE	A	507	7/10	0.78	0.21	25,27,34,38	7
18	GOL	B	523	6/6	0.78	0.15	31,38,41,41	6
18	GOL	C	623	6/6	0.78	0.16	30,39,46,49	6
18	GOL	B	524	6/6	0.79	0.15	33,39,41,50	6
18	GOL	D	520	6/6	0.79	0.14	35,38,44,47	6
18	GOL	D	524	6/6	0.79	0.12	30,32,35,36	6
18	GOL	C	630	6/6	0.79	0.18	33,41,43,45	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	GOL	D	526	6/6	0.79	0.11	32,36,42,43	6
22	DMS	D	505	4/4	0.80	0.13	41,47,53,74	4
18	GOL	C	622	6/6	0.81	0.17	22,28,30,35	6
18	GOL	D	532	6/6	0.81	0.13	40,51,54,57	6
17	EDO	B	518	4/4	0.81	0.14	28,31,32,37	4
18	GOL	B	526	6/6	0.82	0.17	32,36,39,41	6
18	GOL	B	528	6/6	0.82	0.12	43,44,45,46	6
16	SO4	B	515	5/5	0.82	0.10	55,63,69,70	5
18	GOL	B	525	6/6	0.82	0.10	40,52,54,56	0
18	GOL	B	519	6/6	0.83	0.17	27,28,33,35	6
18	GOL	A	522	6/6	0.84	0.14	33,38,41,41	6
16	SO4	D	513	5/5	0.84	0.11	41,44,46,55	5
18	GOL	A	524	6/6	0.84	0.13	24,34,39,41	6
18	GOL	A	520	6/6	0.84	0.14	29,36,43,46	6
18	GOL	D	523	6/6	0.84	0.10	30,36,40,45	6
18	GOL	C	619	6/6	0.85	0.13	24,25,28,34	6
15	NAG	D	516	14/15	0.85	0.10	37,45,47,51	14
16	SO4	B	516	5/5	0.85	0.12	40,41,45,47	5
18	GOL	D	533	6/6	0.85	0.19	26,29,32,33	6
14	PGE	D	504	10/10	0.85	0.14	20,22,26,28	10
18	GOL	C	625	6/6	0.85	0.11	22,36,42,45	6
16	SO4	D	515	5/5	0.85	0.09	47,48,52,62	5
16	SO4	A	511	5/5	0.86	0.09	36,46,63,63	5
18	GOL	D	528	6/6	0.86	0.09	42,44,47,47	0
18	GOL	A	525	6/6	0.86	0.10	36,41,45,47	6
18	GOL	B	527	6/6	0.86	0.12	27,31,37,41	6
14	PGE	B	504	10/10	0.86	0.15	17,25,33,33	10
14	PGE	C	604	10/10	0.87	0.14	25,33,37,42	10
18	GOL	D	522	6/6	0.87	0.10	25,34,38,40	6
18	GOL	D	527	6/6	0.88	0.14	17,26,32,38	6
16	SO4	D	514	5/5	0.88	0.08	55,56,62,63	5
18	GOL	C	618	6/6	0.88	0.11	28,29,36,43	6
17	EDO	D	517	4/4	0.88	0.10	30,30,34,37	4
13	FLC	C	601	13/13	0.88	0.11	21,35,45,48	13
18	GOL	B	521	6/6	0.89	0.13	26,30,35,37	6
18	GOL	C	620	6/6	0.89	0.12	15,27,28,29	6
16	SO4	C	613	5/5	0.89	0.09	56,58,59,63	5
16	SO4	D	510	5/5	0.89	0.14	27,37,39,43	5
17	EDO	C	617	4/4	0.89	0.09	39,41,44,46	4
18	GOL	A	518	6/6	0.90	0.09	19,23,33,34	6
18	GOL	A	519	6/6	0.90	0.12	22,33,39,39	6
16	SO4	D	512	5/5	0.90	0.11	33,36,41,42	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	GOL	A	516	6/6	0.90	0.12	23,26,31,34	6
16	SO4	D	509	5/5	0.90	0.08	38,44,56,56	5
18	GOL	B	522	6/6	0.91	0.14	17,34,36,37	6
18	GOL	D	519	6/6	0.91	0.10	23,26,31,34	6
18	GOL	A	521	6/6	0.91	0.09	15,26,27,31	6
18	GOL	D	521	6/6	0.91	0.09	27,33,40,43	6
16	SO4	C	608	5/5	0.92	0.11	26,28,30,33	5
18	GOL	C	621	6/6	0.92	0.11	20,29,38,48	6
16	SO4	D	508	5/5	0.92	0.10	26,28,32,34	5
16	SO4	C	609	5/5	0.92	0.08	40,43,54,55	5
16	SO4	B	509	5/5	0.93	0.09	36,42,48,52	5
16	SO4	D	511	5/5	0.93	0.08	28,37,39,50	5
16	SO4	B	514	5/5	0.93	0.07	24,28,35,37	5
16	SO4	A	512	5/5	0.94	0.11	26,30,31,34	5
16	SO4	D	507	5/5	0.94	0.07	26,35,40,43	5
16	SO4	C	612	5/5	0.94	0.07	25,34,36,39	5
16	SO4	C	610	5/5	0.94	0.07	22,24,36,42	5
16	SO4	C	614	5/5	0.94	0.10	35,36,45,51	5
17	EDO	A	514	4/4	0.94	0.09	19,22,28,28	4
16	SO4	B	510	5/5	0.95	0.08	18,28,31,32	5
16	SO4	B	513	5/5	0.95	0.07	40,46,50,51	5
16	SO4	A	509	5/5	0.96	0.06	25,30,40,40	5
16	SO4	A	508	5/5	0.97	0.05	22,27,27,28	5
18	GOL	D	518	6/6	0.97	0.05	16,20,22,25	0
16	SO4	B	511	5/5	0.97	0.06	27,29,31,40	5
18	GOL	A	515	6/6	0.97	0.05	17,22,24,24	0
16	SO4	B	512	5/5	0.97	0.07	26,26,32,37	5
19	CL	D	531	1/1	0.98	0.06	30,30,30,30	0
16	SO4	A	510	5/5	0.98	0.05	28,35,36,38	0
19	CL	A	528	1/1	0.99	0.05	24,24,24,24	0
21	NA	B	530	1/1	0.99	0.10	21,21,21,21	0
19	CL	C	626	1/1	0.99	0.03	19,19,19,19	0
11	ZN	A	501	1/1	1.00	0.02	22,22,22,22	0
11	ZN	B	501	1/1	1.00	0.01	24,24,24,24	0
11	ZN	C	606	1/1	1.00	0.02	23,23,23,23	0
11	ZN	D	501	1/1	1.00	0.03	22,22,22,22	0
12	FE	A	502	1/1	1.00	0.05	22,22,22,22	1
12	FE	B	502	1/1	1.00	0.03	27,27,27,27	1
12	FE	C	607	1/1	1.00	0.02	25,25,25,25	1
19	CL	A	529	1/1	1.00	0.03	19,19,19,19	0
19	CL	B	529	1/1	1.00	0.01	19,19,19,19	0
12	FE	D	502	1/1	1.00	0.04	24,24,24,24	1

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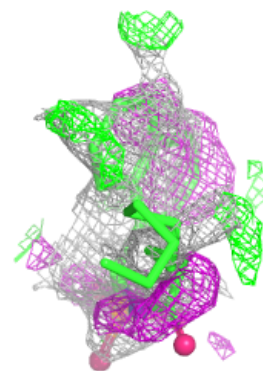
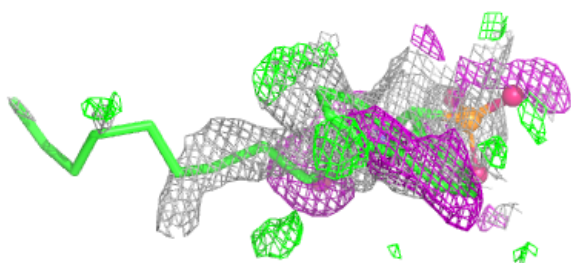
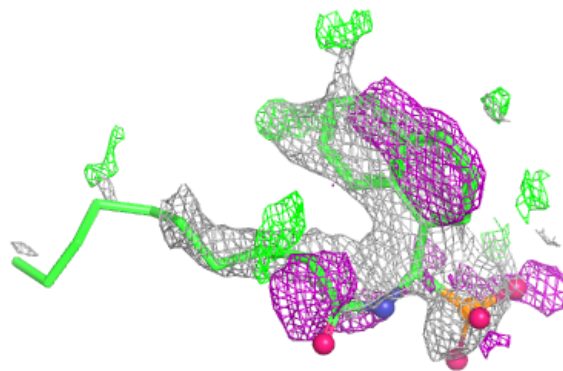
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	CL	D	530	1/1	1.00	0.04	19,19,19,19	0

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

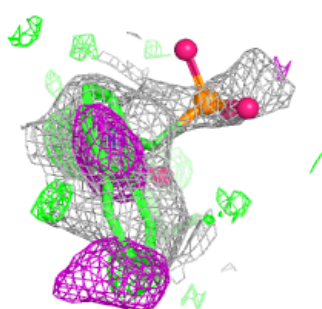
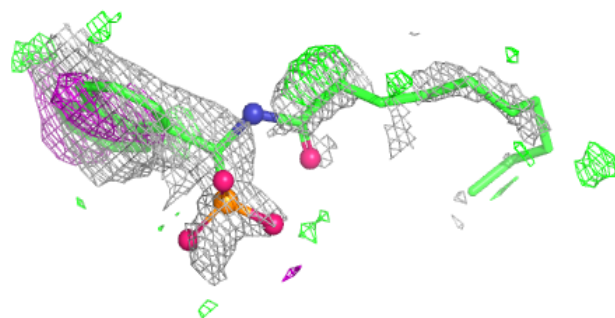
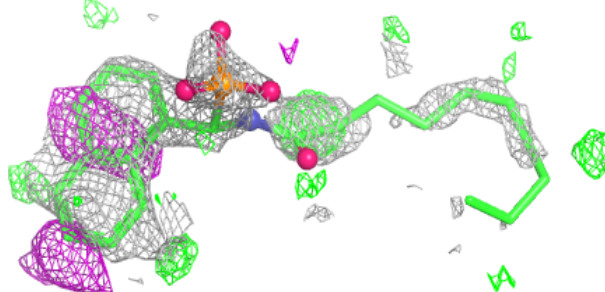
Electron density around R9X C 632 (A):

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

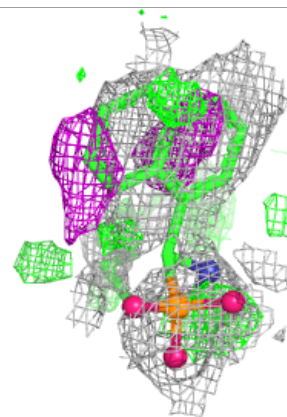
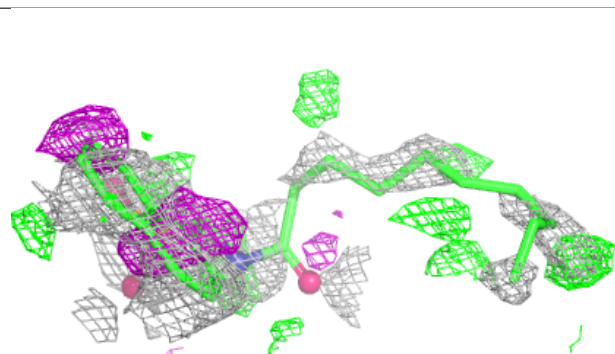
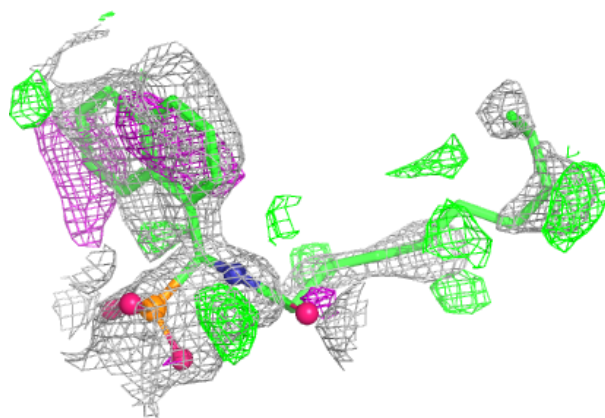


Electron density around R9X A 532 (B):

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

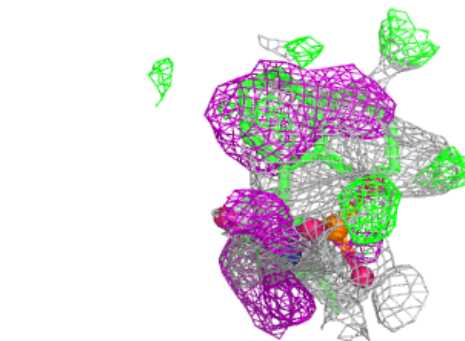
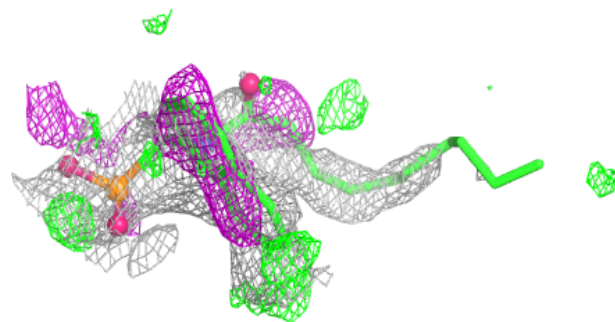
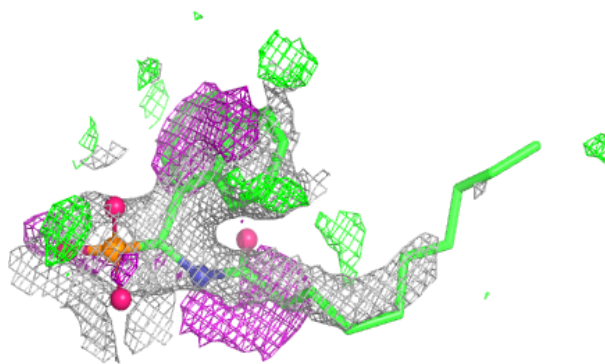
**Electron density around R9X A 532 (A):**

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



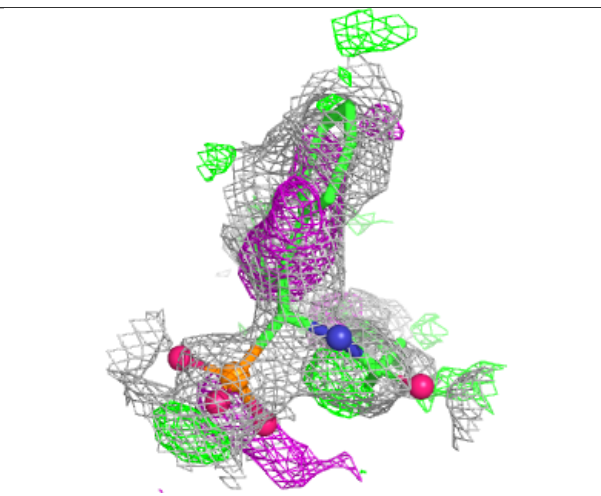
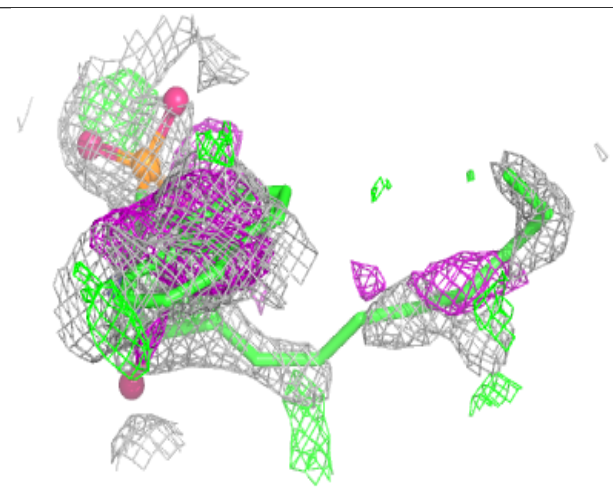
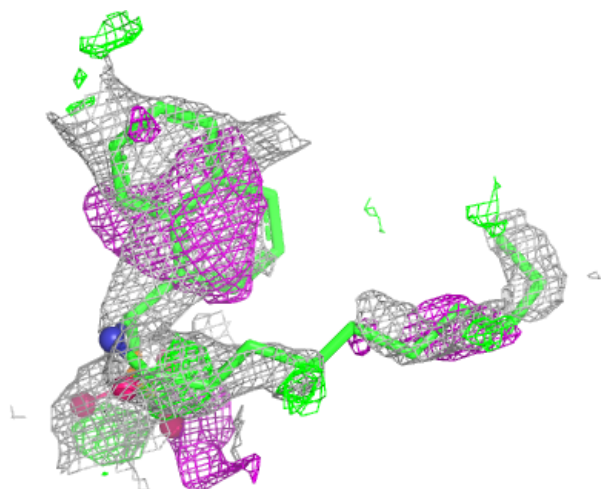
Electron density around R9X C 633 (B):

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



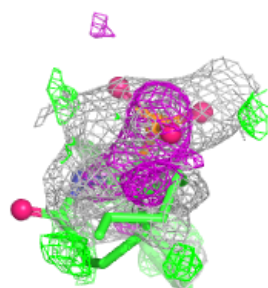
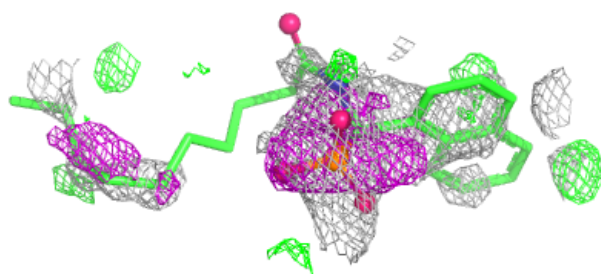
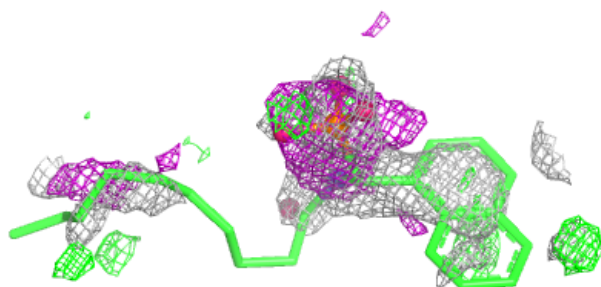
Electron density around R9X B 531 (A):

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



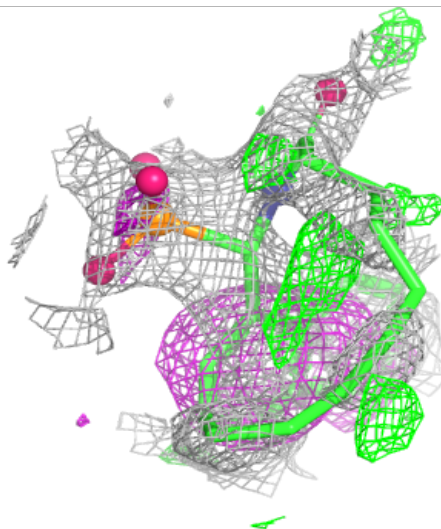
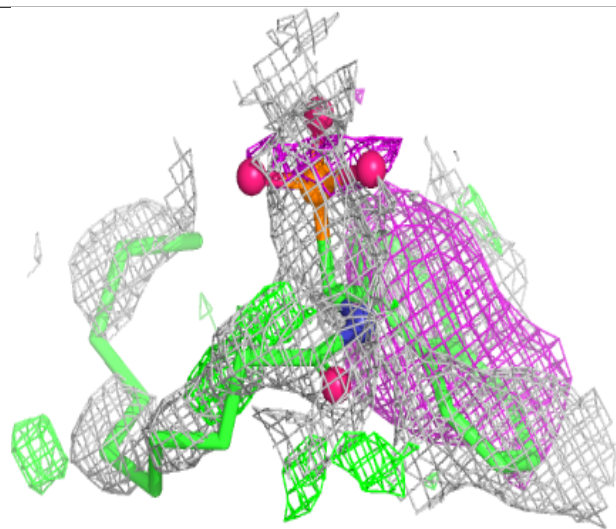
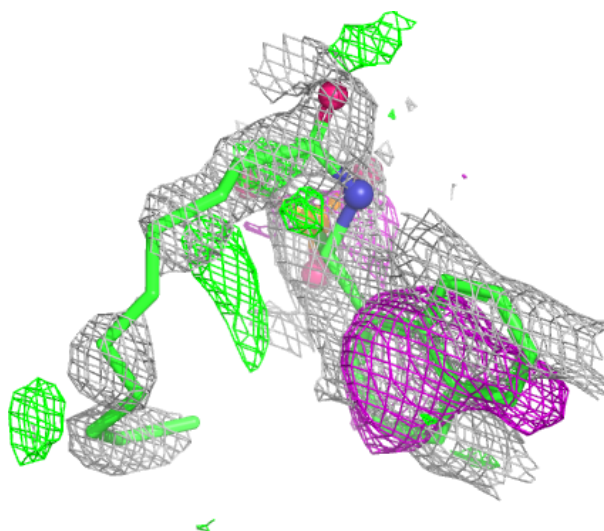
Electron density around R9X B 531 (B):

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



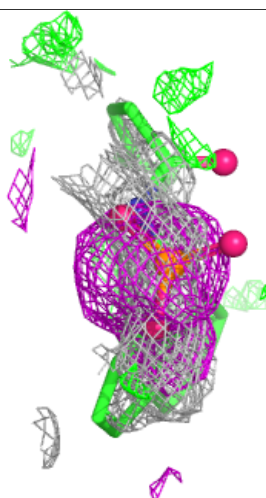
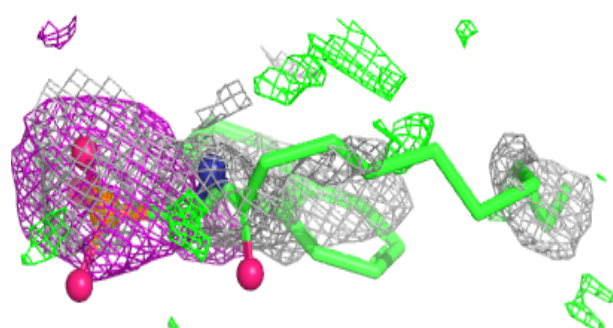
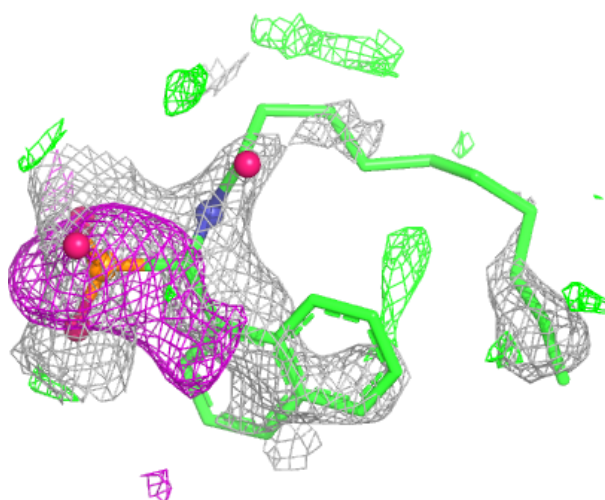
Electron density around R9X D 535 (A):

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



Electron density around R9X D 535 (B):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.