



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:19 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 Full wwPDB X-ray Structure Validation 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

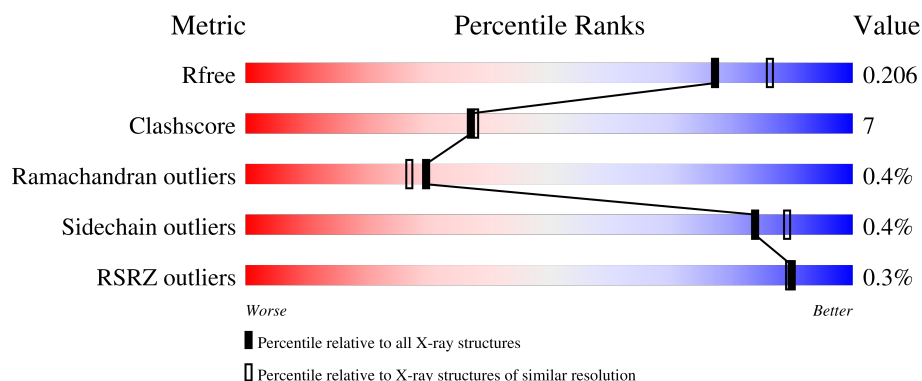
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

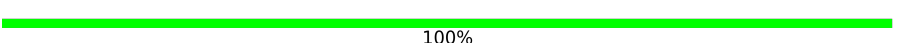
The reported resolution of this entry is 2.00 Å.

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.



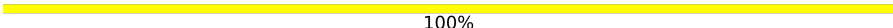
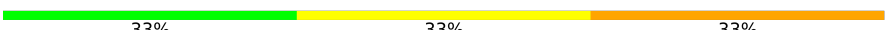
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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.

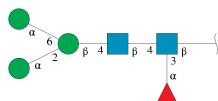
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	4	12	0
			3569	2299	620	640	10			
1	B	428	Total	C	N	O	S	3	5	0
			3558	2284	618	645	11			
1	C	428	Total	C	N	O	S	0	11	0
			3584	2304	619	650	11			
1	D	426	Total	C	N	O	S	5	12	0
			3586	2307	626	642	11			

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



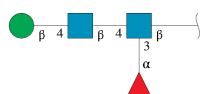
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



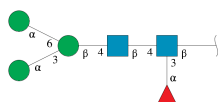
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

- 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.



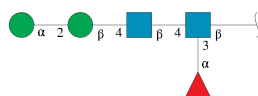
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	I	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	N	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	P	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	S	4	Total	C	N	O	0	0	0
			49	28	2	19			
4	V	4	Total	C	N	O	0	0	0
			49	28	2	19			

- 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.



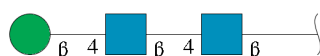
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	6	Total	C	N	O	0	0	0
			71	40	2	29			
5	J	6	Total	C	N	O	0	0	0
			71	40	2	29			

- 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			

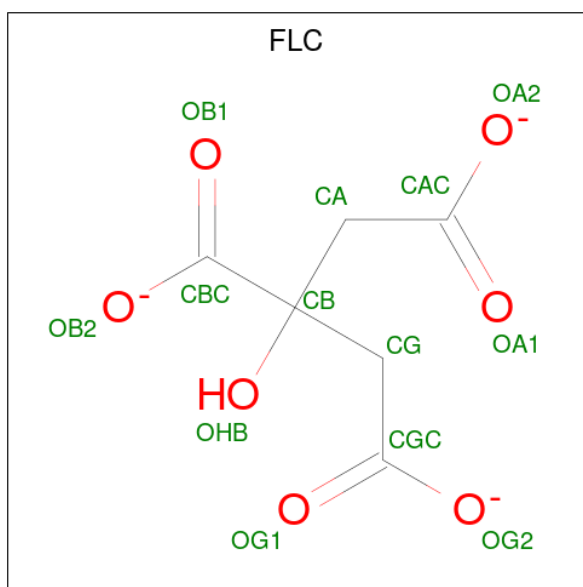
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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).

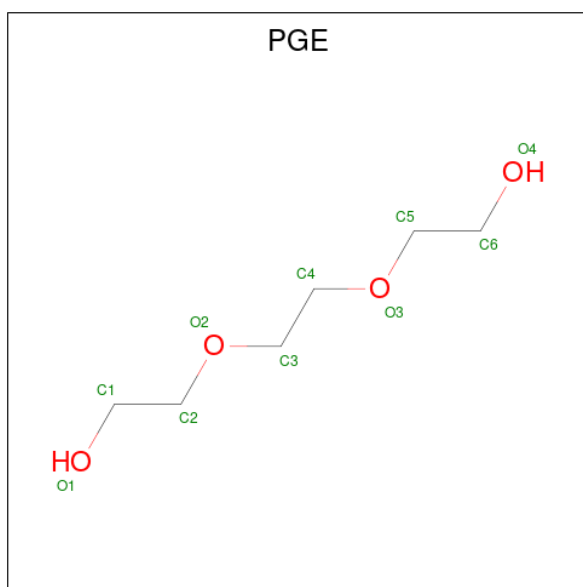
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Fe	0	0
			1	1		
12	B	1	Total	Fe	0	0
			1	1		
12	C	1	Total	Fe	0	0
			1	1		
12	D	1	Total	Fe	0	0
			1	1		

- 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).



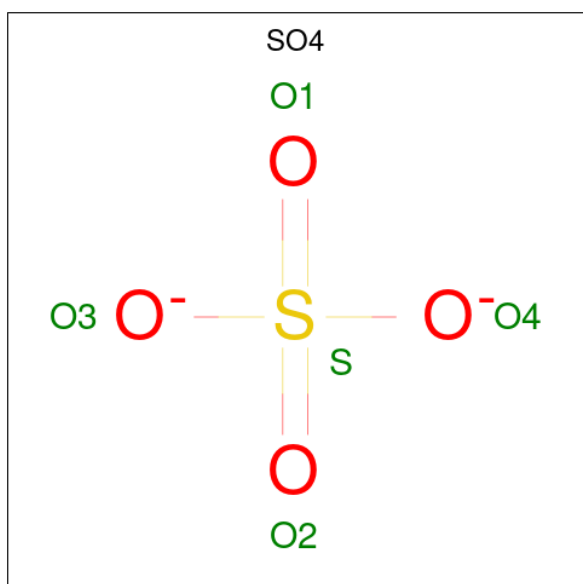
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			10	6	4		
14	A	1	Total	C	O	0	0
			7	4	3		
14	B	1	Total	C	O	0	0
			10	6	4		
14	B	1	Total	C	O	0	0
			10	6	4		
14	C	1	Total	C	O	0	0
			10	6	4		
14	D	1	Total	C	O	0	0
			10	6	4		

- 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).



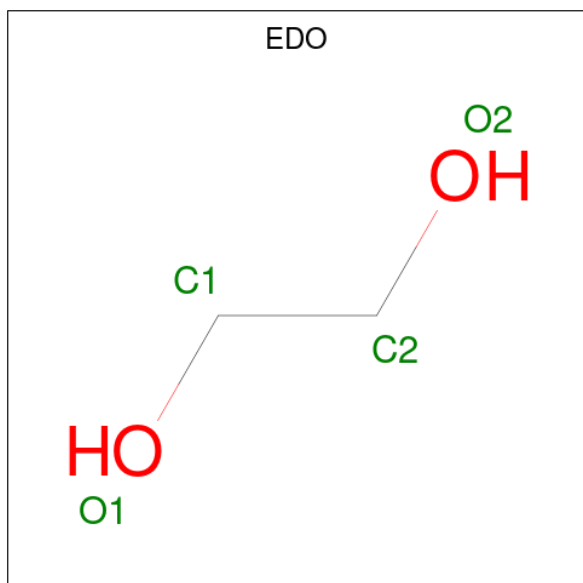
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total O S 5 4 1	0	0
16	A	1	Total O S 5 4 1	0	0
16	A	1	Total O S 5 4 1	0	0
16	A	1	Total O S 5 4 1	0	0
16	A	1	Total O S 5 4 1	0	0
16	A	1	Total O S 5 4 1	0	0
16	B	1	Total O S 5 4 1	0	0
16	B	1	Total O S 5 4 1	0	0
16	B	1	Total O S 5 4 1	0	0
16	B	1	Total O S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

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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).



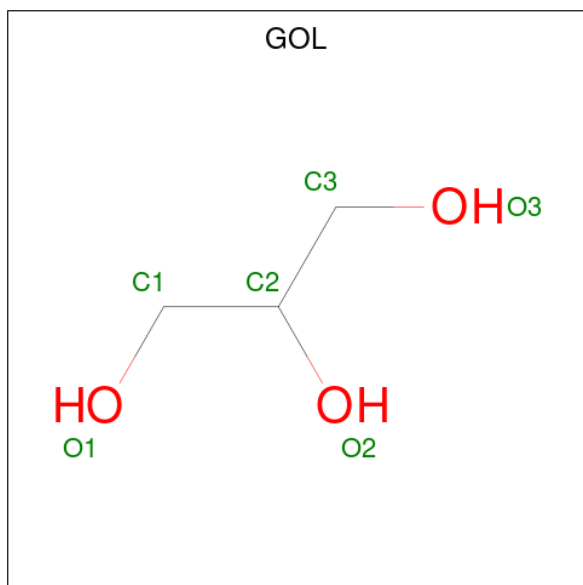
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	A	1	Total	C	O	0	0
			4	2	2		

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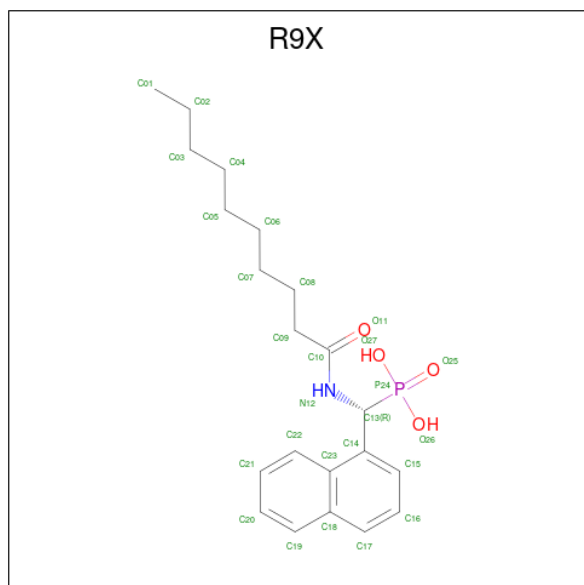
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	C	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C 3	O 3	0	0
18	D	1	Total 6	C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

- 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).

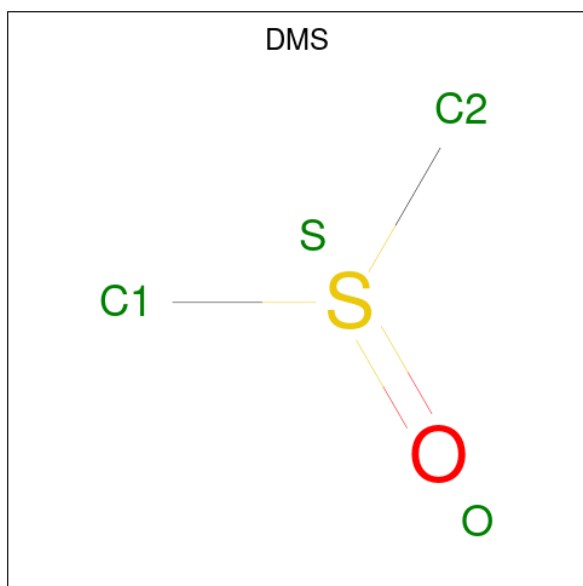


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	N	O	P	0	1
			54	42	2	8	2		
20	B	1	Total	C	N	O	P	0	1
			54	42	2	8	2		
20	C	1	Total	C	N	O	P	0	1
			27	21	1	4	1		
20	C	1	Total	C	N	O	P	0	1
			27	21	1	4	1		
20	D	1	Total	C	N	O	P	0	1
			54	42	2	8	2		

- 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		

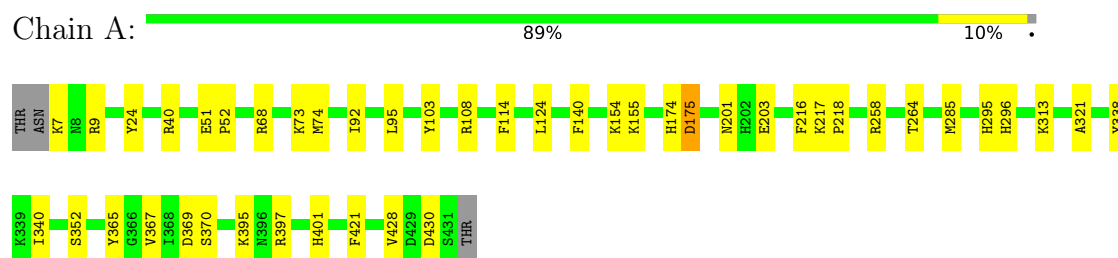
- Molecule 23 is water.

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		

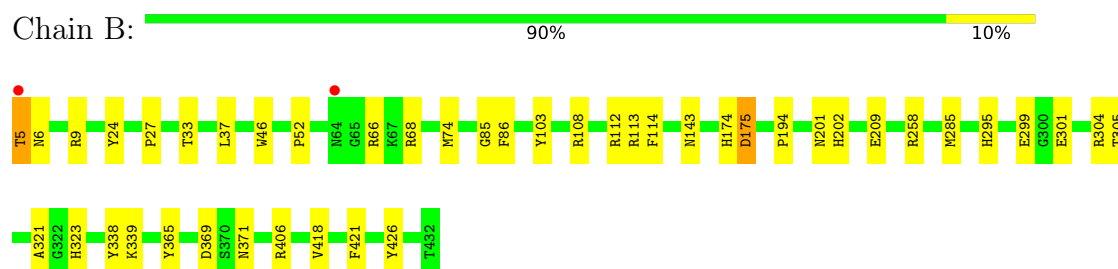
3 Residue-property plots

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.

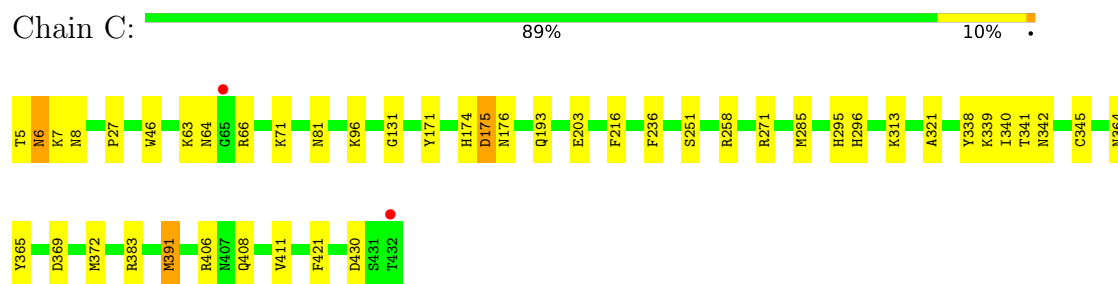
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



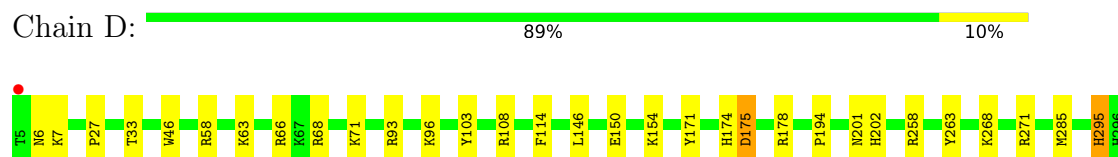
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



- 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%



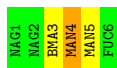
- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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%

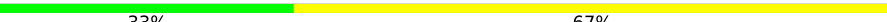


- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

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%



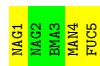
- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

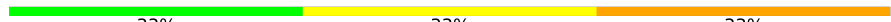


- Molecule 6: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

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.

All (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
1:B:85:GLY:HA2	18:B:519:GOL:H32	1.64	0.79
16:A:509:SO4:O2	23:A:601:HOH:O	1.99	0.79
1:C:296:HIS:NE2	20:C:633[B]:R9X:O26	2.19	0.76
13:C:627:FLC:OA1	13:C:627:FLC:OHB	2.02	0.75
1:A:367[A]:VAL:HG21	18:A:531:GOL:H2	1.71	0.73
16:A:512:SO4:O3	23:A:602:HOH:O	2.05	0.73
16:B:510:SO4:O1	23:B:602:HOH:O	2.05	0.72
14:B:504:PGE:H3	1:D:298:MET:HE2	1.69	0.72
1:A:7:LYS:HE3	18:A:531:GOL:H11	1.73	0.70
1:A:296:HIS:NE2	20:A:532[A]:R9X:O26	2.21	0.70
20:A:532[A]:R9X:O26	23:A:603:HOH:O	2.09	0.69
1:B:143:ASN:HD22	2:K:1:NAG:H83	1.58	0.69
1:A:352:SER:HA	18:A:516:GOL:H32	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ARG:HH22	13:B:506:FLC:HA2	1.59	0.68
1:A:264[A]:THR:HA	14:A:507:PGE:H2	1.75	0.68
1:D:263:TYR:OH	18:D:527:GOL:O2	2.06	0.68
16:B:509:SO4:O3	23:B:604:HOH:O	2.10	0.68
1:B:6:ASN:ND2	23:B:609:HOH:O	2.26	0.68
1:D:68:ARG:HH12	15:D:506:NAG:H3	1.58	0.68
13:B:507:FLC:OA1	13:B:507:FLC:OHB	2.08	0.67
1:C:64:ASN:ND2	16:C:613:SO4:O2	2.28	0.67
1:B:406:ARG:HH12	18:B:525:GOL:H31	1.61	0.66
16:A:512:SO4:S	23:A:602:HOH:O	2.53	0.66
1:B:202:HIS:NE2	20:B:531[A]:R9X:O25	2.27	0.66
1:D:201:ASN:ND2	20:D:535[A]:R9X:O27	2.25	0.66
1:B:338:TYR:HB3	14:B:504:PGE:H52	1.76	0.66
1:D:271[A]:ARG:NH1	23:D:608:HOH:O	2.28	0.66
1:B:66:ARG:HE	1:B:68:ARG:HE	1.44	0.65
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.31	0.65
1:B:112:ARG:HE	13:B:505:FLC:HG1	1.61	0.65
1:A:295:HIS:HB2	13:A:503:FLC:HG2	1.77	0.65
1:C:258:ARG:NH1	23:C:714:HOH:O	2.29	0.65
16:C:610:SO4:O3	23:C:701:HOH:O	2.14	0.65
16:C:608:SO4:O1	23:C:702:HOH:O	2.15	0.64
1:A:295:HIS:HE1	20:A:532[B]:R9X:C15	2.10	0.64
1:B:108:ARG:NH1	23:B:613:HOH:O	2.28	0.64
1:B:112:ARG:HH21	13:B:505:FLC:HG1	1.63	0.63
13:C:602:FLC:OB2	23:C:704:HOH:O	2.15	0.63
20:C:633[B]:R9X:O26	23:C:703:HOH:O	2.15	0.63
1:A:9:ARG:HH22	18:A:523:GOL:H12	1.63	0.63
1:B:258[B]:ARG:NH1	20:D:535[B]:R9X:O25	2.31	0.63
1:C:171:TYR:CD2	13:C:603:FLC:HG2	2.34	0.62
1:A:369:ASP:OD1	13:A:503:FLC:OHB	2.17	0.62
1:D:154:LYS:NZ	23:D:638[B]:HOH:O	2.32	0.62
16:D:507:SO4:O4	23:D:602:HOH:O	2.14	0.62
1:B:201:ASN:ND2	20:B:531[A]:R9X:O27	2.29	0.62
1:C:63:LYS:HE2	1:C:96:LYS:HD2	1.82	0.62
1:B:209:GLU:HB3	18:D:524:GOL:H2	1.82	0.61
18:C:621:GOL:O1	23:C:705:HOH:O	2.16	0.61
1:A:68:ARG:NH1	16:A:510:SO4:S	2.72	0.60
1:B:371:ASN:HB3	13:B:507:FLC:HG2	1.84	0.59
1:C:406:ARG:HH12	13:C:628:FLC:HA2	1.66	0.59
1:C:296:HIS:HE1	20:C:632[A]:R9X:C22	2.15	0.59
1:C:372:MET:H	18:C:621:GOL:H2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:HIS:H	20:A:532[B]:R9X:C09	2.16	0.59
1:C:339:LYS:HB3	18:C:620:GOL:H32	1.84	0.58
18:A:516:GOL:O2	23:A:604:HOH:O	2.16	0.58
1:B:258[A]:ARG:NH1	23:B:624:HOH:O	2.37	0.57
1:C:131:GLY:HA2	1:C:391[B]:MET:HE3	1.86	0.57
1:A:401[B]:HIS:CE1	18:A:524:GOL:H2	2.39	0.57
1:D:96:LYS:HG3	15:D:506:NAG:H61	1.85	0.57
1:C:7:LYS:NZ	23:C:726:HOH:O	2.36	0.57
20:C:633[B]:R9X:O25	23:C:706:HOH:O	2.17	0.57
1:B:66:ARG:NE	1:B:68:ARG:HE	2.02	0.57
1:C:383:ARG:HH21	18:C:618:GOL:H11	1.69	0.57
18:C:624:GOL:H12	23:C:928:HOH:O	2.05	0.57
18:A:518:GOL:O3	23:A:605:HOH:O	2.17	0.56
1:D:6:ASN:ND2	16:D:514:SO4:O1	2.28	0.56
1:A:73:LYS:NZ	23:A:623:HOH:O	2.39	0.56
18:A:523:GOL:O2	18:A:531:GOL:O1	2.19	0.55
1:D:202:HIS:NE2	20:D:535[A]:R9X:O26	2.38	0.55
1:B:304:ARG:HH22	14:D:504:PGE:H2	1.72	0.55
1:D:295[A]:HIS:HE1	20:D:535[A]:R9X:C21	2.19	0.55
20:B:531[A]:R9X:C19	1:D:258[A]:ARG:HH22	2.19	0.55
1:D:371:ASN:N	13:D:503:FLC:OG1	2.33	0.55
16:C:615:SO4:O1	18:C:625:GOL:O3	2.25	0.54
1:A:295:HIS:HE1	20:A:532[A]:R9X:C16	2.19	0.54
1:B:338:TYR:CD2	14:D:504:PGE:H12	2.41	0.54
1:B:365:TYR:OH	20:B:531[A]:R9X:O11	2.09	0.54
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.42	0.54
1:D:96:LYS:HE2	15:D:506:NAG:H4	1.90	0.53
1:B:421[B]:PHE:HD2	1:B:426:TYR:CD1	2.26	0.53
1:C:411:VAL:H	18:C:623:GOL:H32	1.73	0.53
1:D:27:PRO:HB3	1:D:46:TRP:CD1	2.43	0.53
1:D:171:TYR:HE2	18:D:522:GOL:H31	1.74	0.53
1:D:33:THR:HA	1:D:194:PRO:HB3	1.90	0.53
1:D:178:ARG:HE	18:D:522:GOL:C1	2.22	0.53
22:D:505:DMS:O	2:Q:2:NAG:N2	2.35	0.53
1:A:395[B]:LYS:NZ	23:A:605:HOH:O	2.40	0.53
1:C:271:ARG:NH2	23:C:713:HOH:O	2.27	0.52
1:B:299:GLU:HG2	18:D:527:GOL:H32	1.90	0.52
1:A:352:SER:O	23:A:606:HOH:O	2.18	0.52
1:D:178:ARG:HE	18:D:522:GOL:H12	1.74	0.52
18:D:529:GOL:H12	23:D:882:HOH:O	2.09	0.51
13:C:627:FLC:OHB	13:C:627:FLC:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:CYS:HA	14:D:504:PGE:O4	2.10	0.51
1:C:338:TYR:CZ	1:C:340:ILE:HA	2.46	0.51
1:D:295[B]:HIS:HB2	13:D:503:FLC:HG2	1.93	0.50
1:D:297:PHE:HB3	18:D:533:GOL:H2	1.93	0.50
1:A:258:ARG:HE	20:C:633[B]:R9X:C21	2.24	0.50
20:A:532[B]:R9X:C21	1:C:258:ARG:HE	2.24	0.50
22:D:505:DMS:H22	2:Q:2:NAG:H3	1.93	0.50
1:D:174:HIS:O	1:D:175:ASP:C	2.55	0.49
14:A:507:PGE:H32	23:A:940:HOH:O	2.13	0.49
1:A:421:PHE:CD2	1:A:430:ASP:HB3	2.47	0.49
20:A:532[B]:R9X:C22	1:C:258:ARG:HE	2.25	0.49
1:B:6:ASN:HB3	1:B:9:ARG:HH12	1.78	0.49
1:C:174:HIS:O	1:C:175:ASP:C	2.55	0.49
1:C:341:THR:OG1	18:C:620:GOL:H12	2.12	0.49
1:A:174:HIS:O	1:A:175:ASP:C	2.56	0.49
20:A:532[A]:R9X:C20	1:C:258:ARG:HE	2.25	0.49
20:C:633[B]:R9X:C22	20:C:633[B]:R9X:N12	2.76	0.49
1:A:155:LYS:HD2	23:A:716:HOH:O	2.13	0.48
1:D:304:ARG:HH12	14:D:504:PGE:H52	1.78	0.48
1:D:103:TYR:CE1	1:D:114:PHE:HB2	2.48	0.48
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.96	0.48
20:A:532[A]:R9X:C19	1:C:258:ARG:HH21	2.27	0.48
1:D:103:TYR:CZ	1:D:114:PHE:HB2	2.48	0.48
1:B:113:ARG:NH1	13:B:506:FLC:HG2	2.28	0.48
16:C:613:SO4:O2	23:C:708:HOH:O	2.20	0.48
1:C:71:LYS:HD2	23:C:1165:HOH:O	2.14	0.47
1:B:258[A]:ARG:HH21	20:D:535[A]:R9X:C19	2.27	0.47
1:B:295:HIS:HD2	1:B:369:ASP:OD2	1.96	0.47
23:D:1228:HOH:O	3:F:4:MAN:H3	2.13	0.47
1:B:112:ARG:HE	13:B:505:FLC:CG	2.28	0.47
1:B:174:HIS:O	1:B:175:ASP:C	2.57	0.47
1:B:295:HIS:HE1	20:B:531[A]:R9X:C22	2.27	0.47
1:C:27:PRO:HB3	1:C:46:TRP:CD1	2.50	0.46
1:A:40:ARG:NH1	16:A:512:SO4:O1	2.48	0.46
1:A:295:HIS:HD2	1:A:369:ASP:OD2	1.98	0.46
20:D:535[B]:R9X:O25	20:D:535[B]:R9X:C15	2.63	0.46
1:B:24:TYR:CD2	4:I:1:NAG:H82	2.51	0.46
1:A:201:ASN:ND2	20:A:532[A]:R9X:O25	2.33	0.46
1:B:103:TYR:CZ	1:B:114:PHE:HB2	2.51	0.46
1:A:285:MET:O	1:A:321:ALA:HA	2.15	0.46
1:B:295:HIS:CE1	20:B:531[A]:R9X:C22	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:522:GOL:H32	23:B:1068:HOH:O	2.16	0.45
18:C:622:GOL:H11	23:C:1193:HOH:O	2.16	0.45
1:A:258:ARG:HG2	14:A:507:PGE:O3	2.16	0.45
1:B:33:THR:HA	1:B:194:PRO:HB3	1.98	0.45
14:B:504:PGE:H6	23:B:947[B]:HOH:O	2.16	0.45
1:A:108[B]:ARG:HB2	19:A:528:CL:CL	2.53	0.45
1:B:103:TYR:CE1	1:B:114:PHE:HB2	2.51	0.45
18:A:519:GOL:O2	5:H:2:NAG:N2	2.40	0.45
1:B:24:TYR:CE2	4:I:1:NAG:H82	2.52	0.45
14:D:504:PGE:H32	23:D:647:HOH:O	2.17	0.45
16:C:608:SO4:O2	23:C:707:HOH:O	2.20	0.45
1:D:391[A]:MET:HG2	23:D:801:HOH:O	2.16	0.45
23:C:1145:HOH:O	7:M:2:NAG:H5	2.17	0.44
13:A:505:FLC:OA2	13:A:505:FLC:OHB	2.20	0.44
1:B:339:LYS:HD2	18:B:521:GOL:H2	1.99	0.44
1:A:421:PHE:CD2	1:A:428:VAL:HG13	2.53	0.44
1:B:113:ARG:HH12	13:B:506:FLC:HG2	1.83	0.44
1:A:154:LYS:HA	18:A:518:GOL:H31	1.99	0.44
18:D:527:GOL:H2	23:D:634:HOH:O	2.18	0.44
1:D:146:LEU:O	1:D:150:GLU:HG3	2.17	0.44
1:A:338:TYR:CE1	1:C:345:CYS:HB2	2.53	0.44
1:B:301:GLU:O	1:B:305:THR:HG23	2.16	0.44
15:C:605:NAG:H83	23:C:712:HOH:O	2.17	0.44
1:D:285:MET:O	1:D:321:ALA:HA	2.17	0.44
14:A:507:PGE:H4	20:C:633[B]:R9X:C19	2.47	0.44
1:D:108:ARG:HB2	19:D:531:CL:CL	2.54	0.44
1:D:364:ASN:OD1	1:D:365:TYR:N	2.51	0.44
1:B:285:MET:O	1:B:321:ALA:HA	2.18	0.43
1:A:258:ARG:HE	20:C:632[A]:R9X:C21	2.31	0.43
1:D:71:LYS:NZ	23:D:615:HOH:O	2.51	0.43
1:B:27:PRO:HB3	1:B:46:TRP:CD1	2.54	0.43
1:B:37:LEU:HD22	18:B:524:GOL:H2	2.00	0.43
1:C:295:HIS:HD1	1:C:369:ASP:CG	2.26	0.43
1:A:313:LYS:NZ	18:A:526:GOL:H2	2.33	0.43
1:A:203:GLU:O	1:A:216:PHE:HA	2.19	0.43
1:C:203:GLU:O	1:C:216:PHE:HA	2.19	0.43
1:A:103:TYR:CE1	1:A:114:PHE:HB2	2.54	0.43
1:A:395[A]:LYS:HA	1:A:395[A]:LYS:HD3	1.83	0.43
14:B:504:PGE:H6	14:B:504:PGE:H42	1.35	0.43
23:B:1003:HOH:O	9:R:2:NAG:O6	2.21	0.43
18:D:522:GOL:H32	23:D:1113:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:TYR:OH	1:A:51:GLU:OE1	2.34	0.43
1:D:304:ARG:HH22	14:D:504:PGE:C5	2.32	0.43
14:D:504:PGE:H62	14:D:504:PGE:H42	1.32	0.43
20:D:535[A]:R9X:N12	20:D:535[A]:R9X:C22	2.82	0.42
1:D:414:GLU:HG2	23:D:638[A]:HOH:O	2.20	0.42
1:B:52:PRO:HB3	1:B:74:MET:HE2	2.02	0.42
1:B:112:ARG:NH2	13:B:505:FLC:HG1	2.33	0.42
20:A:532[B]:R9X:C22	1:C:258:ARG:HH21	2.33	0.42
1:D:58:ARG:O	1:D:103:TYR:HA	2.19	0.42
1:C:408:GLN:HE21	13:C:628:FLC:CGC	2.33	0.42
1:B:24:TYR:OH	9:R:1:NAG:H61	2.19	0.41
1:C:193:GLN:HB3	14:C:604:PGE:H5	2.01	0.41
1:A:52:PRO:HB3	1:A:74:MET:HE2	2.02	0.41
1:C:342:ASN:N	18:C:620:GOL:H11	2.35	0.41
1:D:93:ARG:NH2	23:D:643:HOH:O	2.51	0.41
1:A:9:ARG:HD3	14:A:504:PGE:H5	2.02	0.41
18:A:518:GOL:H32	23:A:1081:HOH:O	2.20	0.41
1:B:5:THR:HB	1:B:6:ASN:H	1.52	0.41
1:B:86:PHE:HZ	1:C:81:ASN:HA	1.86	0.41
1:A:92[A]:ILE:CG2	1:A:95:LEU:HD21	2.51	0.41
16:B:512:SO4:O4	23:B:605:HOH:O	2.21	0.41
1:C:66:ARG:NH1	23:C:761:HOH:O	2.53	0.41
1:C:313:LYS:HZ1	18:C:624:GOL:H11	1.86	0.41
1:D:7:LYS:NZ	16:D:515:SO4:S	2.92	0.41
1:B:418:VAL:HG21	23:B:1121:HOH:O	2.21	0.41
1:A:140:PHE:CG	14:A:504:PGE:H22	2.56	0.40
1:B:323:HIS:HA	23:B:601:HOH:O	2.22	0.40
1:C:285:MET:O	1:C:321:ALA:HA	2.21	0.40
1:C:364:ASN:OD1	1:C:365:TYR:N	2.53	0.40
1:B:258[A]:ARG:HE	20:D:535[A]:R9X:C17	2.34	0.40
1:A:370:SER:N	13:A:503:FLC:OA1	2.54	0.40
1:D:268[B]:LYS:HB3	1:D:268[B]:LYS:HE3	1.97	0.40
1:A:338:TYR:CZ	1:A:340:ILE:HA	2.56	0.40
1:C:5:THR:O	1:C:6:ASN:HB2	2.22	0.40
1:C:5:THR:HG23	23:C:950:HOH:O	2.21	0.40
1:C:236:PHE:O	1:C:251:SER:HB2	2.21	0.40
1:D:338:TYR:CE2	14:D:504:PGE:H22	2.57	0.40

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

All (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
1	C	6	ASN

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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1543/1508 (102%)	1535 (100%)	8 (0%)	84 87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
1	B	5	THR
1	C	176	ASN
1	C	391[A]	MET
1	C	391[B]	MET
1	D	66	ARG
1	D	295[A]	HIS
1	D	295[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	193	GLN
1	A	295	HIS
1	A	405	ASN
1	B	138	GLN
1	B	295	HIS
1	C	193	GLN
1	D	173	ASN
1	D	193	GLN
1	D	405	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
4	P	3	BMA	C1-C2	3.17	1.59	1.52
7	M	2	NAG	O5-C1	3.11	1.48	1.43
7	M	3	BMA	O5-C1	3.06	1.48	1.43
10	T	2	FUC	C4-C5	2.96	1.59	1.52
4	S	3	BMA	C1-C2	2.85	1.59	1.52
4	I	3	BMA	O5-C1	2.76	1.48	1.43
8	O	1	NAG	O5-C1	2.70	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	C2-C3	2.70	1.56	1.52
3	F	3	BMA	O2-C2	2.56	1.48	1.43
4	P	3	BMA	O5-C1	2.44	1.47	1.43
3	F	4	MAN	C1-C2	2.39	1.57	1.52
4	N	3	BMA	O5-C1	2.38	1.47	1.43
5	H	5	MAN	C1-C2	2.37	1.57	1.52
6	L	4	MAN	C1-C2	2.36	1.57	1.52
10	T	2	FUC	O5-C5	2.32	1.48	1.43
6	L	4	MAN	O5-C5	2.27	1.47	1.43
5	J	4	MAN	C1-C2	2.23	1.57	1.52
7	M	3	BMA	C2-C3	2.14	1.55	1.52
4	N	3	BMA	O5-C5	2.11	1.47	1.43
3	F	5	MAN	C1-C2	2.10	1.57	1.52
4	S	3	BMA	O5-C5	2.08	1.47	1.43
4	V	3	BMA	C1-C2	2.08	1.57	1.52
5	J	3	BMA	C1-C2	2.08	1.57	1.52
5	J	3	BMA	C4-C3	2.04	1.57	1.52
4	I	3	BMA	O5-C5	2.00	1.47	1.43

All (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
10	T	2	FUC	O5-C5-C4	4.64	117.91	109.55
4	S	3	BMA	C1-O5-C5	4.63	118.39	112.19
5	H	4	MAN	C1-O5-C5	4.41	118.10	112.19
3	F	4	MAN	C1-C2-C3	4.14	115.67	109.64
5	J	5	MAN	C1-O5-C5	3.65	117.07	112.19
10	T	2	FUC	C3-C4-C5	3.63	115.33	109.81
2	K	2	NAG	C1-O5-C5	3.37	116.71	112.19
8	O	1	NAG	O3-C3-C2	-2.93	103.31	109.40
5	J	3	BMA	C1-O5-C5	2.82	115.96	112.19
3	F	3	BMA	C1-C2-C3	2.77	113.68	109.64
3	F	3	BMA	O2-C2-C1	2.74	115.49	109.22
3	F	4	MAN	C2-C3-C4	2.58	115.40	110.86
5	H	5	MAN	C1-O5-C5	2.57	115.63	112.19
10	T	2	FUC	C1-O5-C5	2.57	119.02	112.97
4	I	3	BMA	C1-C2-C3	2.48	113.26	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	4	MAN	C1-C2-C3	-2.44	106.09	109.64
5	H	4	MAN	O2-C2-C3	-2.44	105.10	110.15
4	N	3	BMA	C1-C2-C3	2.35	113.06	109.64
3	F	4	MAN	C1-O5-C5	2.32	115.30	112.19
6	L	4	MAN	C1-O5-C5	2.31	115.28	112.19
8	O	1	NAG	C1-O5-C5	2.29	115.26	112.19
4	I	1	NAG	C1-O5-C5	2.26	115.21	112.19
6	L	4	MAN	O2-C2-C3	-2.24	105.52	110.15
3	F	4	MAN	O2-C2-C3	-2.23	105.52	110.15
3	F	5	MAN	C1-C2-C3	-2.23	106.40	109.64
5	H	3	BMA	C1-O5-C5	2.21	115.15	112.19
7	M	3	BMA	C3-C4-C5	-2.21	106.22	110.23
5	J	4	MAN	O2-C2-C3	-2.19	105.61	110.15
7	M	3	BMA	C1-C2-C3	2.17	112.80	109.64
4	G	2	NAG	O4-C4-C3	-2.15	105.32	110.38
6	L	5	FUC	C1-O5-C5	2.13	117.99	112.97
3	F	3	BMA	C2-C3-C4	2.11	114.58	110.86
5	J	4	MAN	O2-C2-C1	2.11	114.05	109.22
2	Q	2	NAG	C1-O5-C5	2.10	115.00	112.19
3	F	5	MAN	O2-C2-C1	2.09	114.01	109.22
5	H	5	MAN	O2-C2-C3	-2.09	105.82	110.15
6	L	1	NAG	C1-O5-C5	2.08	114.97	112.19
4	P	3	BMA	C1-C2-C3	2.07	112.65	109.64
4	I	3	BMA	C3-C4-C5	-2.07	106.49	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	R	3	BMA	C5

All (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
4	G	2	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	3	BMA	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
6	L	4	MAN	C4-C5-C6-O6
10	T	1	NAG	C4-C5-C6-O6
9	R	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
10	T	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
5	J	2	NAG	C8-C7-N2-C2
5	J	2	NAG	O7-C7-N2-C2
7	M	2	NAG	C8-C7-N2-C2
7	M	2	NAG	O7-C7-N2-C2
10	T	1	NAG	C8-C7-N2-C2
10	T	1	NAG	O7-C7-N2-C2
2	K	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
3	F	5	MAN	O5-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
4	P	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	V	3	BMA	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
4	V	3	BMA	O5-C5-C6-O6
4	S	3	BMA	O5-C5-C6-O6

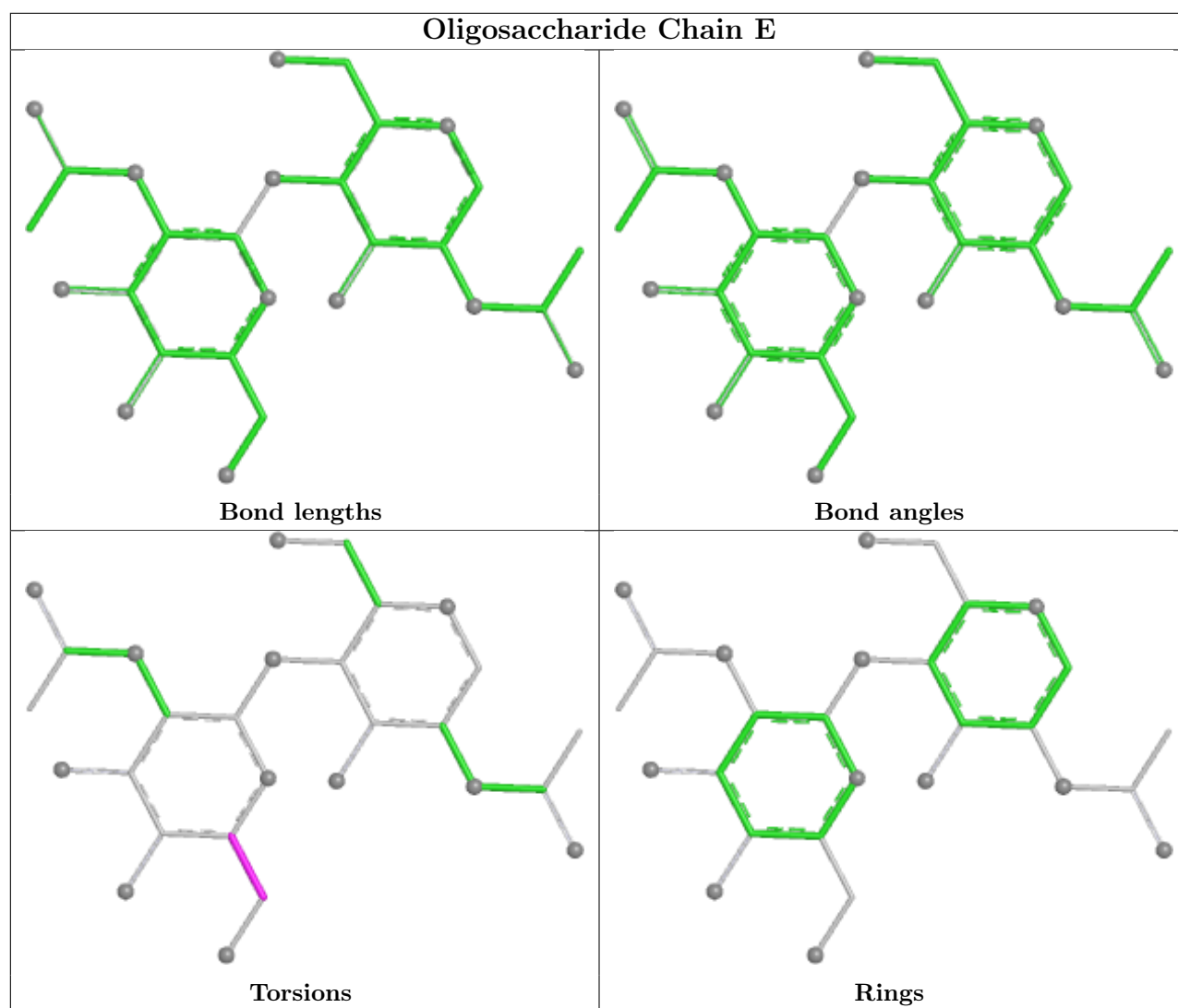
All (4) ring outliers are listed below:

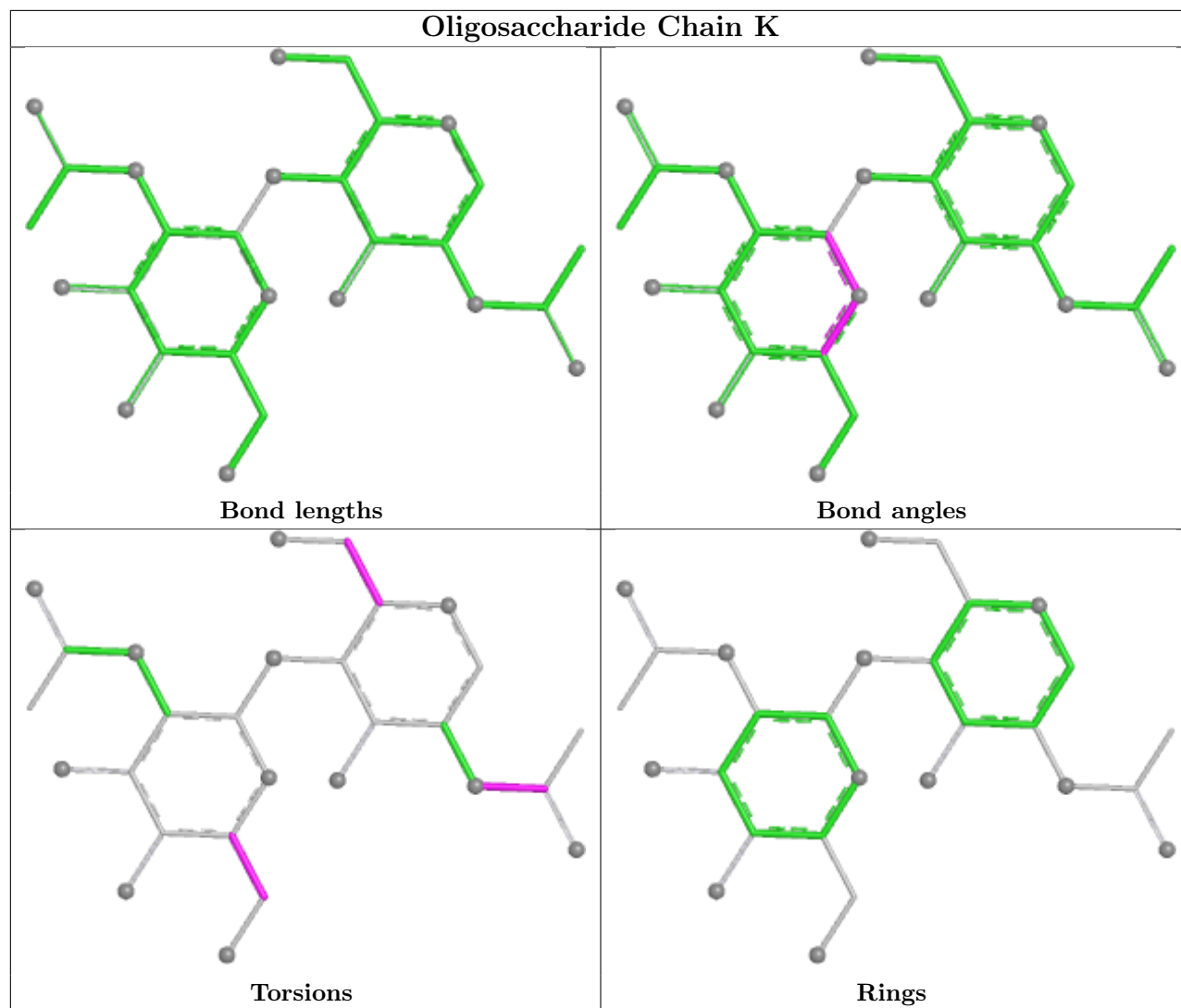
Mol	Chain	Res	Type	Atoms
4	S	3	BMA	C1-C2-C3-C4-C5-O5
6	L	4	MAN	C1-C2-C3-C4-C5-O5
3	F	5	MAN	C1-C2-C3-C4-C5-O5
5	J	4	MAN	C1-C2-C3-C4-C5-O5

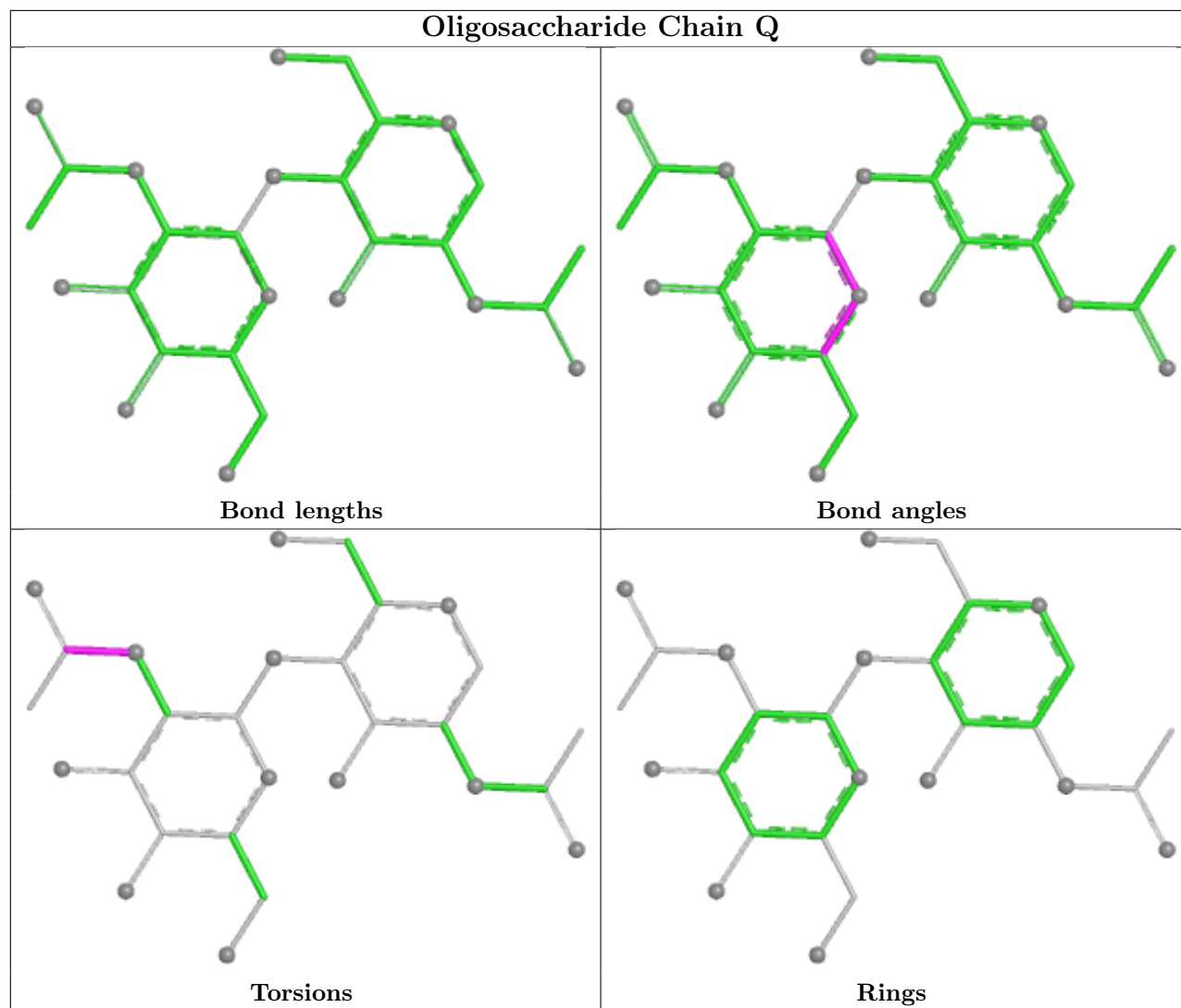
8 monomers are involved in 10 short contacts:

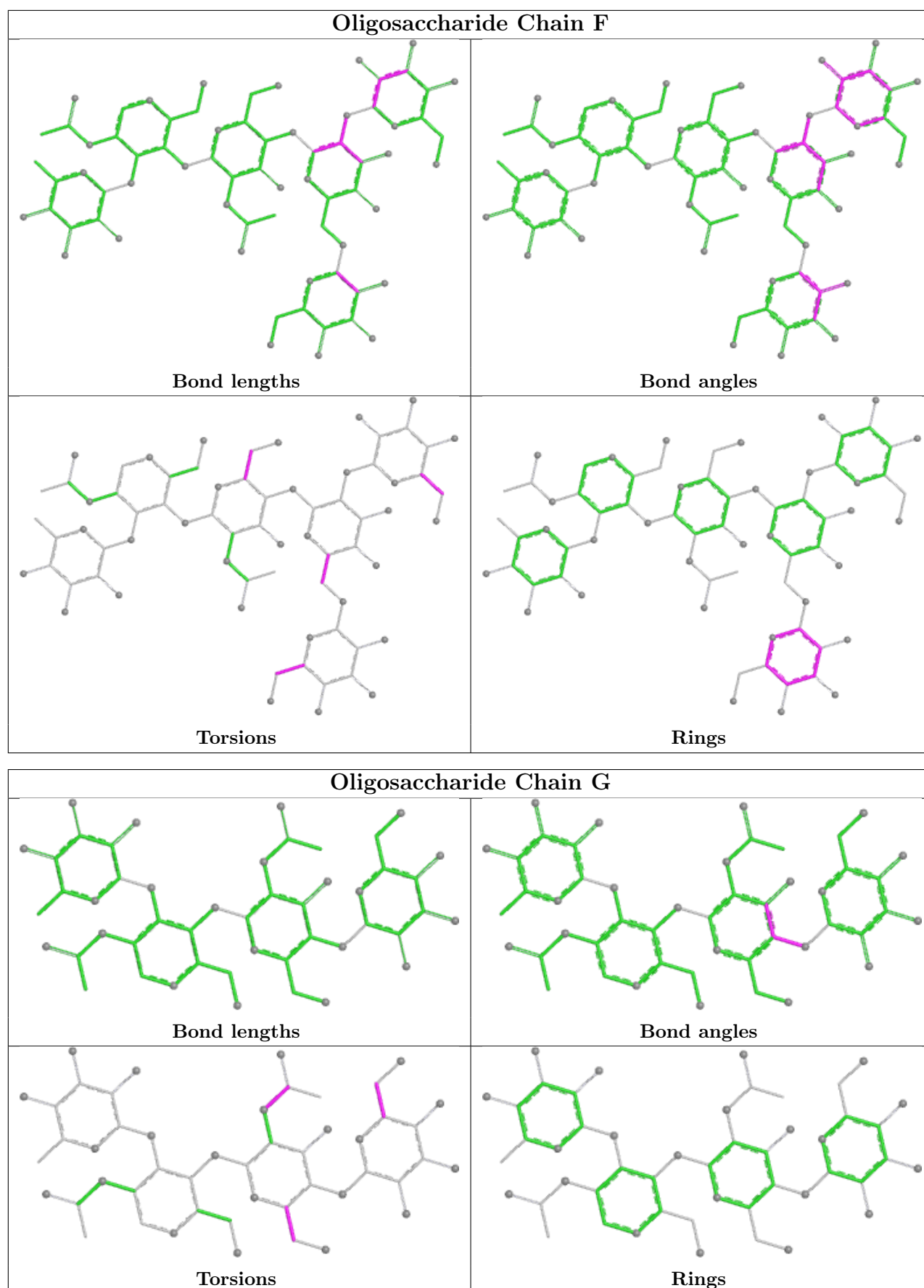
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	R	2	NAG	1	0
4	I	1	NAG	2	0
2	Q	2	NAG	2	0
2	K	1	NAG	1	0
3	F	4	MAN	1	0
9	R	1	NAG	1	0
7	M	2	NAG	1	0
5	H	2	NAG	1	0

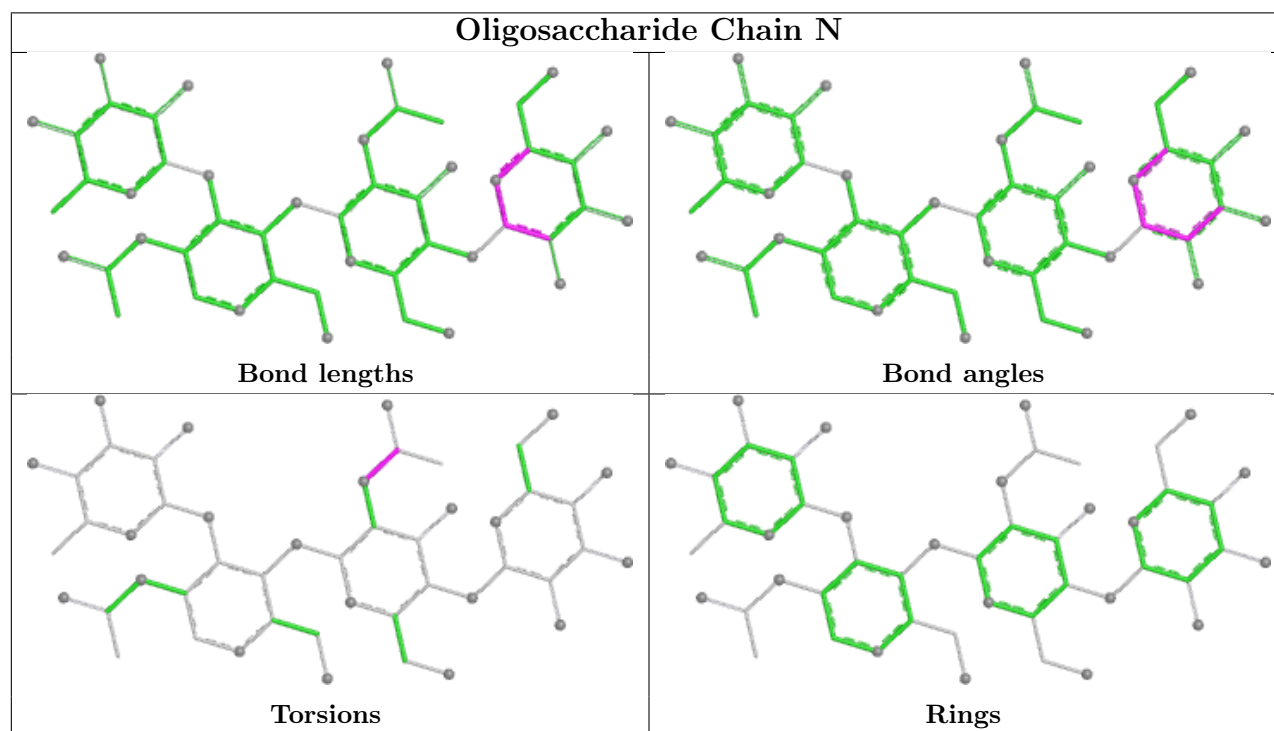
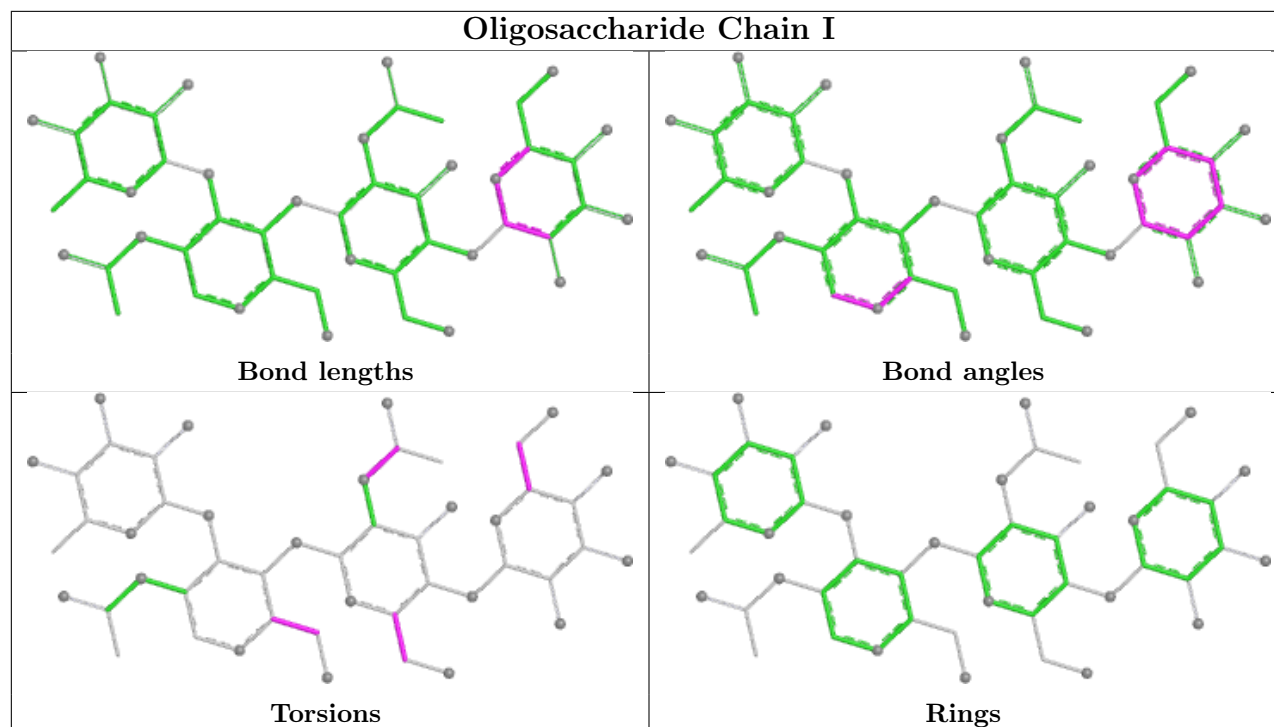
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

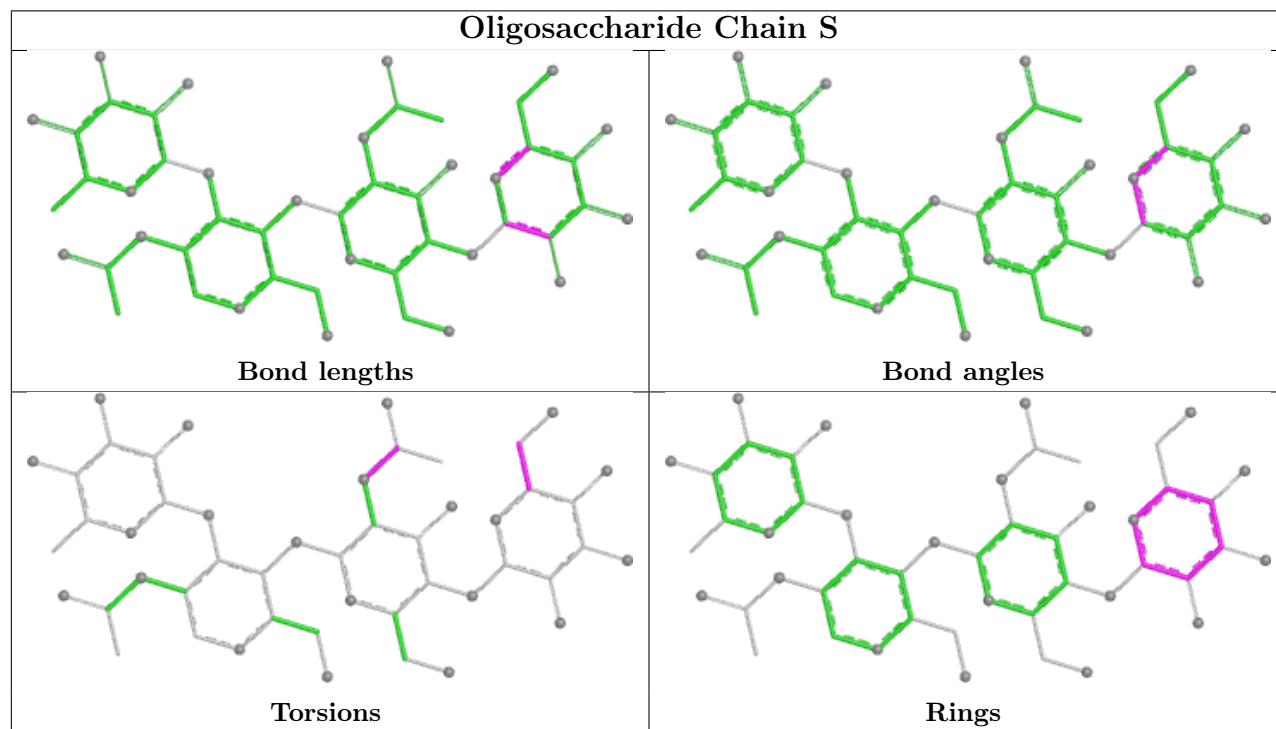
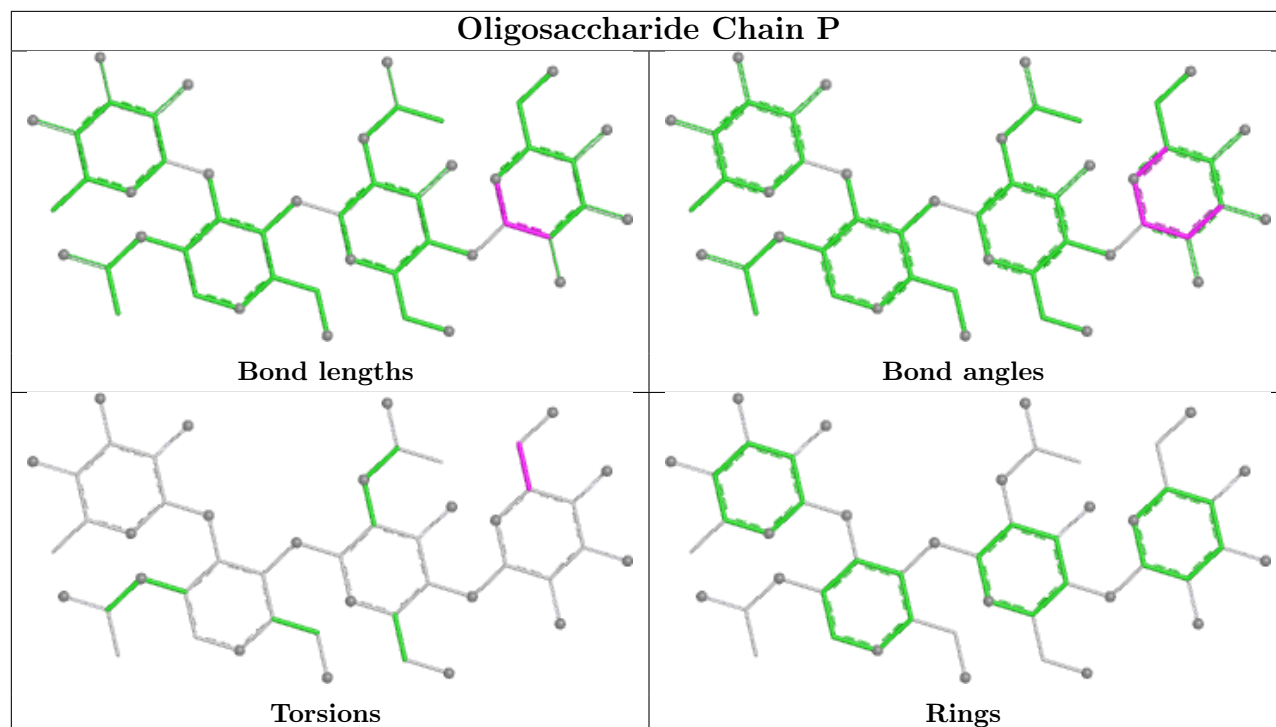


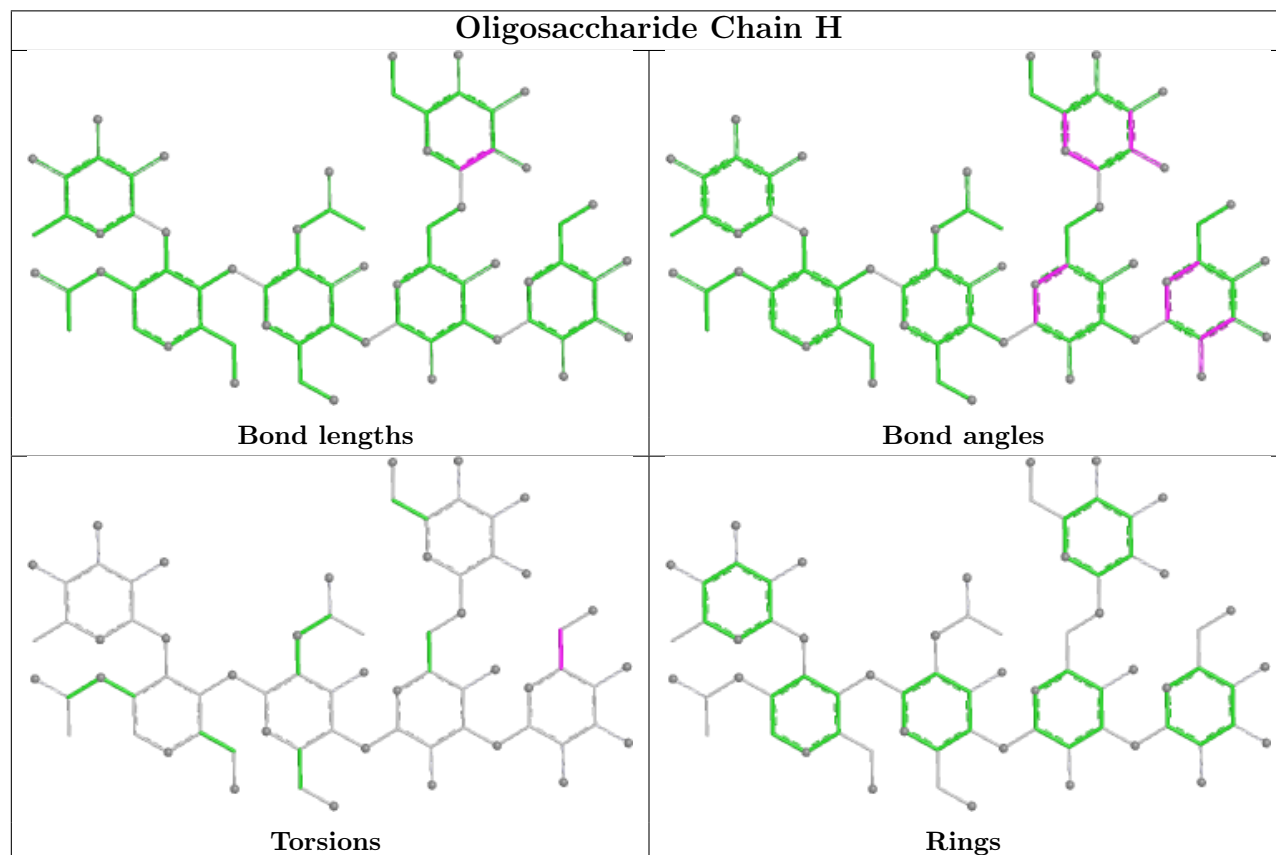
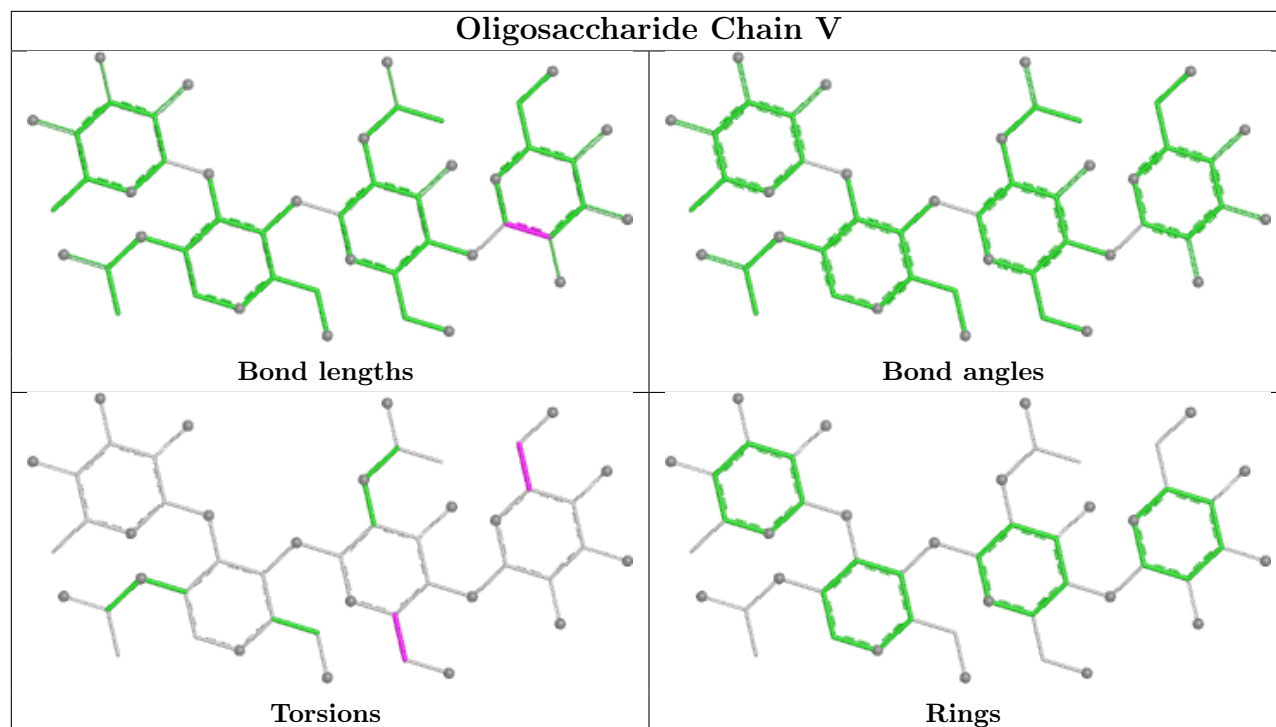


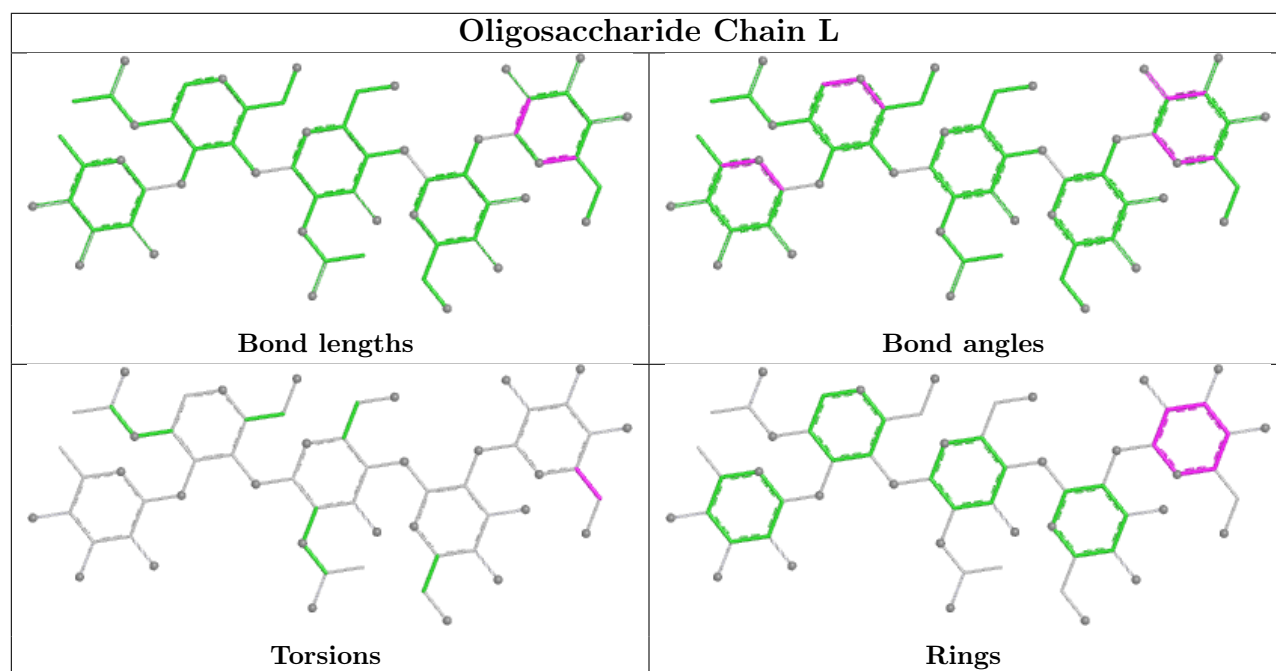
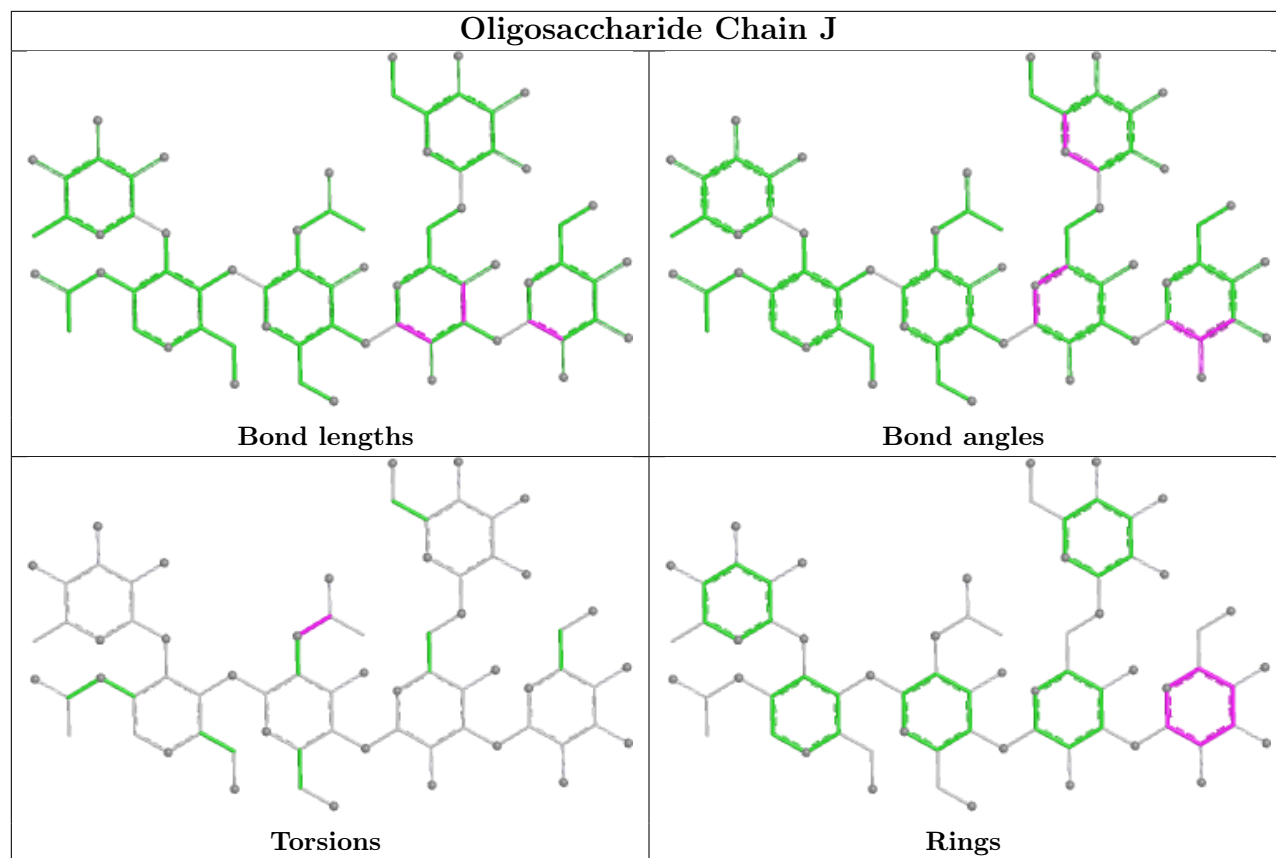


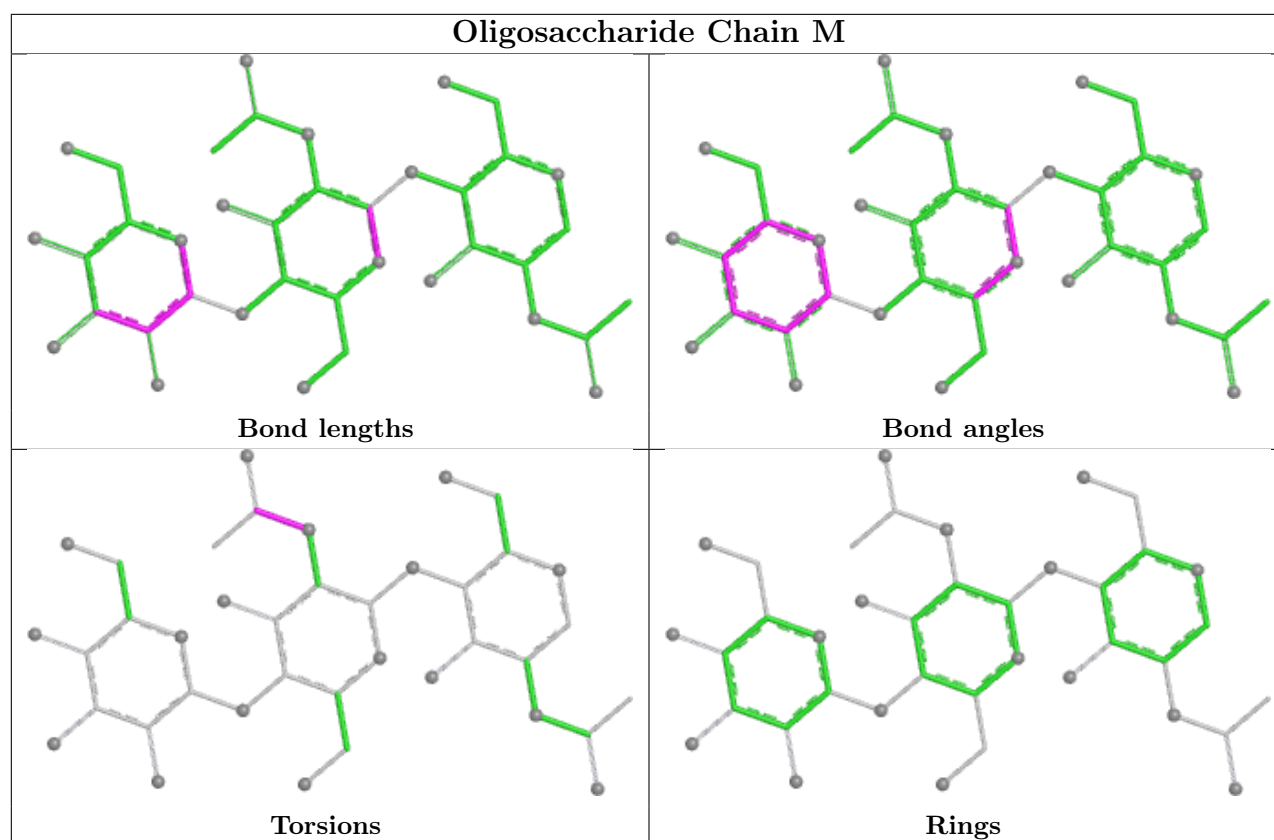


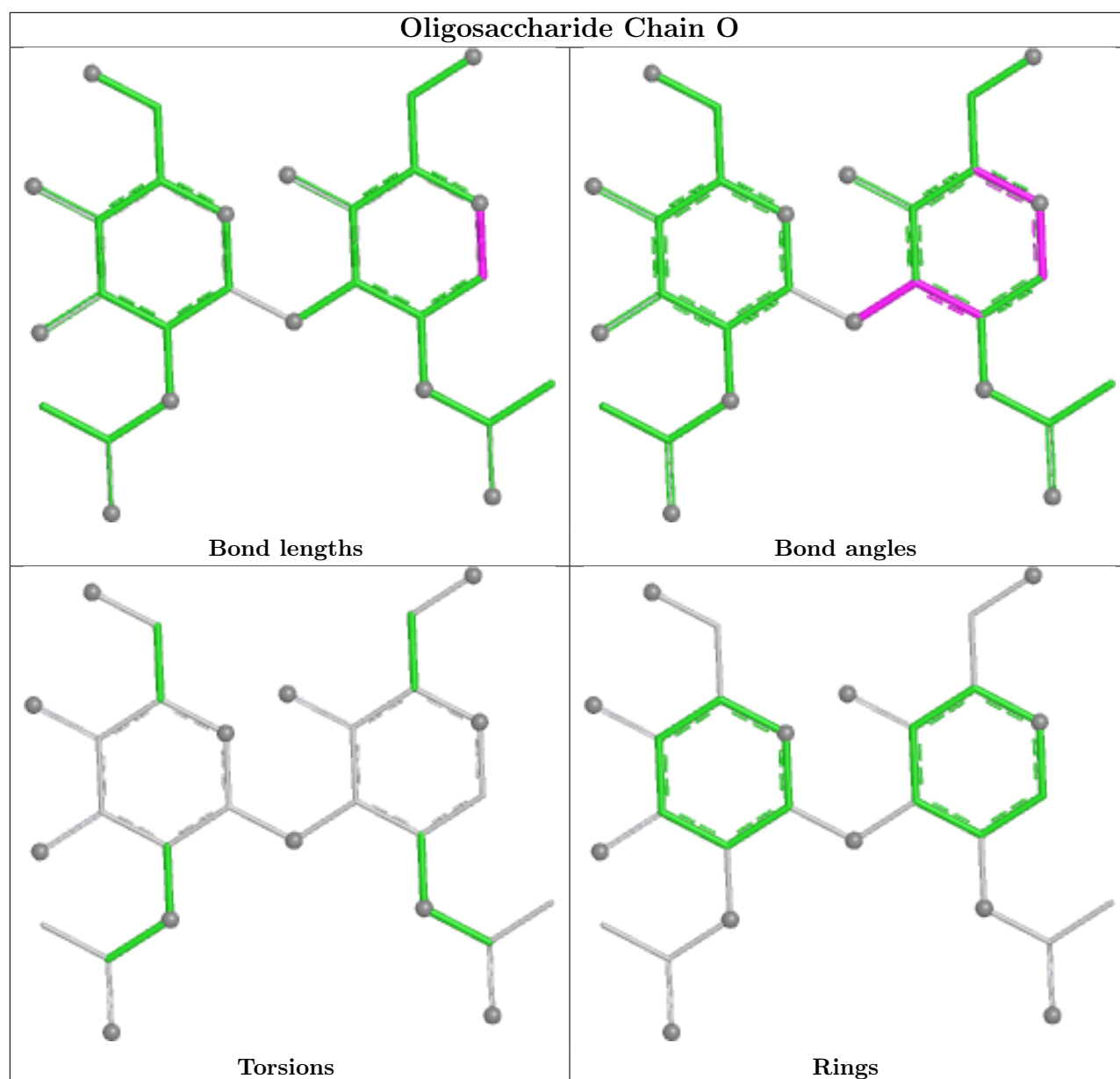


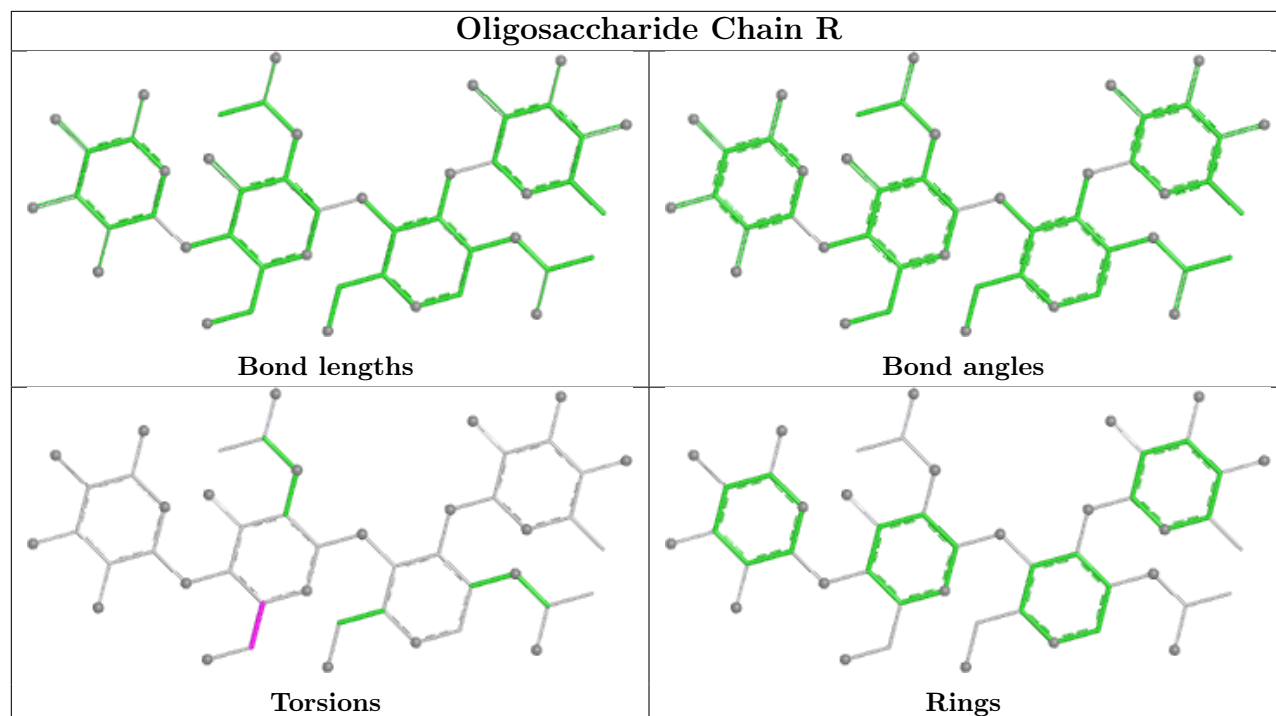


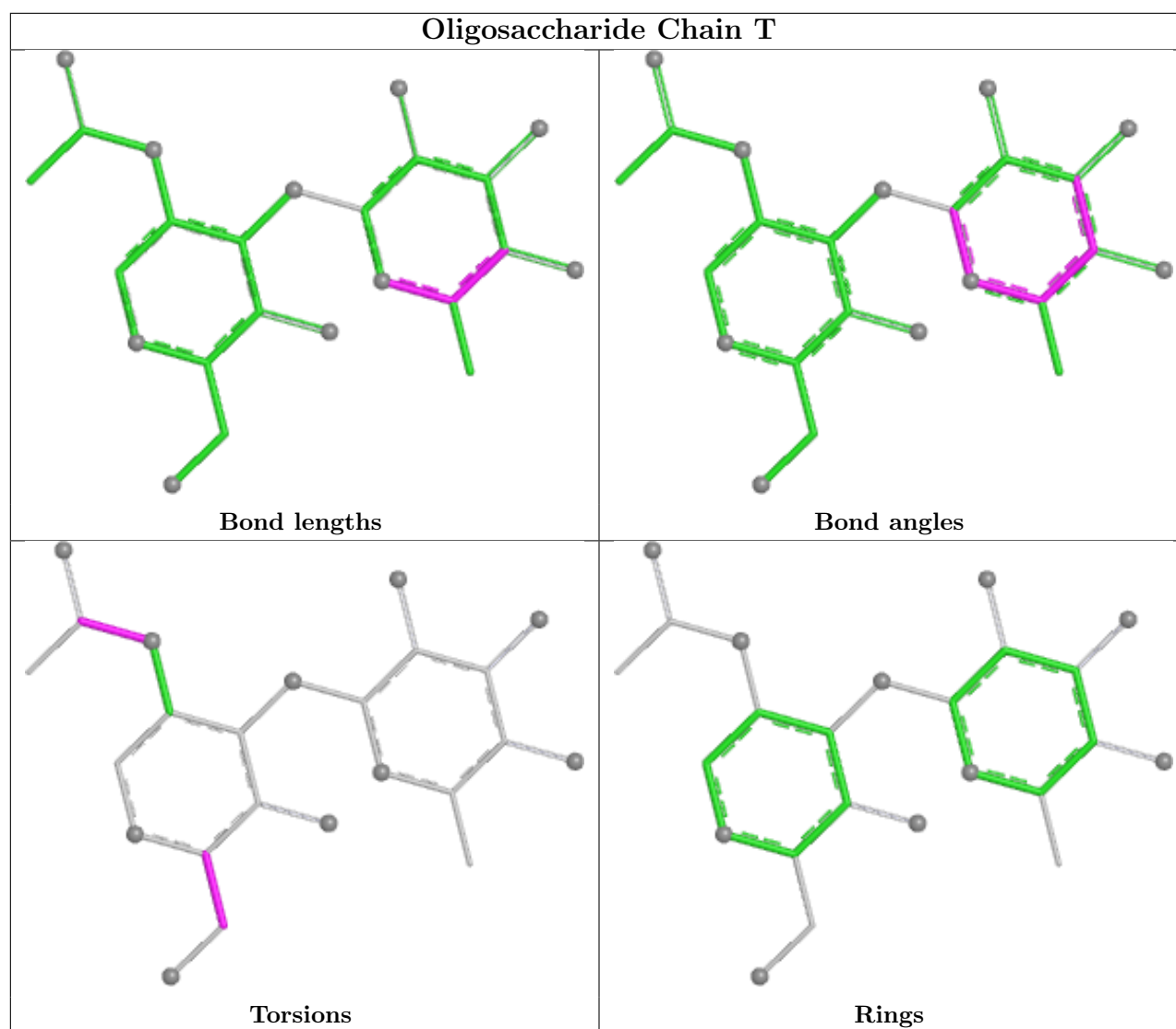












5.6 Ligand geometry [i](#)

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

All (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
20	B	531[A]	R9X	C10-N12	5.41	1.45	1.34
20	D	535[A]	R9X	C10-N12	4.99	1.44	1.34
20	A	532[A]	R9X	C10-N12	4.12	1.42	1.34
20	A	532[A]	R9X	C13-N12	-3.99	1.42	1.46
15	C	605	NAG	O5-C1	3.78	1.50	1.43
15	A	506	NAG	O5-C1	3.74	1.50	1.43
20	B	531[A]	R9X	C14-C13	3.40	1.55	1.52
20	D	535[B]	R9X	P24-C13	3.19	1.88	1.84
13	C	601	FLC	OG2-CGC	-3.17	1.20	1.30
13	C	628	FLC	OG1-CGC	2.94	1.31	1.22
13	B	507	FLC	OB1-CBC	2.93	1.31	1.22
13	A	530	FLC	OA1-CAC	2.92	1.31	1.22
13	C	628	FLC	OB1-CBC	2.92	1.31	1.22
13	A	505	FLC	OB1-CBC	2.92	1.31	1.22
13	C	603	FLC	OB1-CBC	2.90	1.31	1.22
13	C	627	FLC	OB1-CBC	2.88	1.31	1.22
13	A	530	FLC	OG1-CGC	2.87	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	503	FLC	OB1-CBC	2.86	1.31	1.22
13	C	627	FLC	OA2-CAC	-2.86	1.21	1.30
13	B	503	FLC	OB1-CBC	2.85	1.31	1.22
13	B	507	FLC	OA1-CAC	2.84	1.31	1.22
13	C	603	FLC	OG1-CGC	2.84	1.31	1.22
18	A	519	GOL	O2-C2	-2.83	1.35	1.43
13	C	602	FLC	OB1-CBC	2.82	1.30	1.22
13	A	505	FLC	OG1-CGC	2.81	1.31	1.22
13	B	506	FLC	OA1-CAC	2.81	1.31	1.22
20	D	535[B]	R9X	C23-C18	-2.80	1.37	1.43
13	C	627	FLC	OA1-CAC	2.80	1.31	1.22
13	B	503	FLC	OG1-CGC	2.80	1.31	1.22
13	B	507	FLC	OA2-CAC	-2.79	1.21	1.30
20	C	633[B]	R9X	C23-C18	-2.79	1.37	1.43
20	C	632[A]	R9X	C23-C18	-2.79	1.37	1.43
13	C	627	FLC	OG1-CGC	2.78	1.31	1.22
13	B	506	FLC	OA2-CAC	-2.78	1.21	1.30
13	A	505	FLC	OG2-CGC	-2.75	1.21	1.30
20	B	531[B]	R9X	C23-C18	-2.69	1.38	1.43
20	A	532[A]	R9X	O11-C10	-2.69	1.17	1.23
13	C	603	FLC	OG2-CGC	-2.68	1.22	1.30
13	C	601	FLC	OG1-CGC	2.68	1.30	1.22
13	A	530	FLC	OG2-CGC	-2.67	1.22	1.30
13	A	530	FLC	OA2-CAC	-2.64	1.22	1.30
13	C	628	FLC	OG2-CGC	-2.62	1.22	1.30
13	D	503	FLC	OG1-CGC	2.62	1.30	1.22
20	A	532[B]	R9X	C23-C18	-2.56	1.38	1.43
20	B	531[A]	R9X	P24-O27	-2.55	1.50	1.54
13	C	627	FLC	OG2-CGC	-2.53	1.22	1.30
13	D	503	FLC	OG2-CGC	-2.52	1.22	1.30
13	B	503	FLC	OG2-CGC	-2.52	1.22	1.30
20	A	532[A]	R9X	P24-O26	-2.51	1.50	1.54
20	C	632[A]	R9X	P24-O27	-2.48	1.50	1.54
20	B	531[A]	R9X	C23-C18	-2.48	1.38	1.43
13	C	627	FLC	OB2-CBC	-2.46	1.21	1.30
20	A	532[A]	R9X	C23-C18	-2.41	1.38	1.43
20	D	535[A]	R9X	P24-O27	-2.40	1.51	1.54
20	C	633[B]	R9X	P24-O27	-2.38	1.51	1.54
13	B	503	FLC	OB2-CBC	-2.37	1.21	1.30
13	C	602	FLC	OB2-CBC	-2.35	1.22	1.30
13	D	503	FLC	OB2-CBC	-2.34	1.22	1.30
13	B	507	FLC	OB2-CBC	-2.31	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	531[A]	R9X	O11-C10	-2.29	1.18	1.23
13	A	505	FLC	OB2-CBC	-2.29	1.22	1.30
20	D	535[B]	R9X	C14-C13	2.26	1.54	1.52
13	C	628	FLC	OB2-CBC	-2.24	1.22	1.30
20	C	632[A]	R9X	P24-O26	-2.22	1.51	1.54
18	C	620	GOL	C3-C2	2.20	1.60	1.51
13	C	603	FLC	OB2-CBC	-2.19	1.22	1.30
18	C	620	GOL	O2-C2	-2.19	1.37	1.43
20	A	532[B]	R9X	P24-O26	-2.17	1.51	1.54
20	B	531[B]	R9X	O11-C10	-2.13	1.19	1.23
20	D	535[A]	R9X	O11-C10	-2.09	1.19	1.23
20	B	531[A]	R9X	P24-O26	-2.08	1.51	1.54
20	D	535[A]	R9X	C23-C18	-2.07	1.39	1.43
18	B	521	GOL	O2-C2	-2.07	1.37	1.43
18	D	520	GOL	O2-C2	-2.07	1.37	1.43
18	A	516	GOL	O2-C2	-2.07	1.37	1.43
20	A	532[B]	R9X	O11-C10	-2.06	1.19	1.23
18	D	527	GOL	O2-C2	-2.03	1.37	1.43
20	A	532[B]	R9X	P24-O27	-2.03	1.51	1.54
18	C	618	GOL	O2-C2	-2.02	1.37	1.43

All (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
20	A	532[A]	R9X	P24-C13-C14	6.15	121.28	111.31
20	C	632[A]	R9X	C09-C10-N12	5.50	125.55	115.86
13	B	507	FLC	OB2-CBC-CB	5.20	123.12	113.14
13	C	603	FLC	OB2-CBC-CB	5.02	122.77	113.14
13	A	505	FLC	OB2-CBC-CB	5.01	122.75	113.14
13	C	628	FLC	OB2-CBC-CB	4.98	122.69	113.14
13	C	602	FLC	OB2-CBC-CB	4.92	122.57	113.14
13	B	503	FLC	OB2-CBC-CB	4.89	122.53	113.14
15	A	506	NAG	C1-O5-C5	4.86	118.70	112.19
13	D	503	FLC	OB2-CBC-CB	4.84	122.42	113.14
20	D	535[A]	R9X	C13-N12-C10	-4.81	114.88	121.18
13	C	627	FLC	OB2-CBC-CB	4.80	122.34	113.14
13	B	503	FLC	OB1-CBC-CB	-4.79	112.81	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	505	FLC	OB1-CBC-CB	-4.68	113.03	122.09
13	C	603	FLC	OB1-CBC-CB	-4.65	113.09	122.09
13	D	503	FLC	OB1-CBC-CB	-4.63	113.13	122.09
13	C	602	FLC	OB1-CBC-CB	-4.59	113.20	122.09
13	C	628	FLC	OB1-CBC-CB	-4.50	113.37	122.09
13	B	507	FLC	OB1-CBC-CB	-4.46	113.46	122.09
20	A	532[A]	R9X	O11-C10-N12	-4.45	115.42	122.95
20	B	531[A]	R9X	C09-C10-N12	4.27	123.38	115.86
13	C	627	FLC	OB1-CBC-CB	-4.25	113.85	122.09
20	C	632[A]	R9X	O11-C10-N12	-4.16	115.90	122.95
20	B	531[A]	R9X	C13-N12-C10	4.09	126.55	121.18
20	D	535[A]	R9X	C15-C14-C13	-3.76	116.48	121.11
13	C	627	FLC	OG1-CGC-CG	-3.73	112.39	122.95
13	D	503	FLC	OG1-CGC-CG	-3.66	112.58	122.95
13	B	506	FLC	OA1-CAC-CA	-3.55	112.90	122.95
20	B	531[B]	R9X	P24-C13-N12	-3.54	101.61	108.10
20	D	535[A]	R9X	O25-P24-C13	-3.52	105.21	110.89
20	D	535[A]	R9X	C13-C14-C23	3.51	125.49	120.43
13	C	627	FLC	OA1-CAC-CA	-3.48	113.08	122.95
20	B	531[B]	R9X	C15-C14-C13	-3.45	116.86	121.11
20	B	531[A]	R9X	O11-C10-N12	-3.43	117.14	122.95
13	C	628	FLC	OG1-CGC-CG	-3.27	113.69	122.95
13	A	505	FLC	OG1-CGC-CG	-3.24	113.77	122.95
20	C	633[B]	R9X	P24-C13-N12	3.22	114.00	108.10
13	B	507	FLC	OA1-CAC-CA	-3.19	113.91	122.95
20	A	532[A]	R9X	C22-C23-C14	-3.17	119.52	123.37
13	C	603	FLC	OG1-CGC-CG	-3.16	114.00	122.95
20	B	531[B]	R9X	C09-C10-N12	3.16	121.43	115.86
13	C	627	FLC	OA2-CAC-CA	3.14	124.30	114.35
20	B	531[A]	R9X	O26-P24-O25	-3.12	105.64	113.45
13	D	503	FLC	OG2-CGC-CG	3.12	124.22	114.35
13	B	506	FLC	OA2-CAC-CA	3.10	124.17	114.35
13	A	530	FLC	OA1-CAC-CA	-3.07	114.27	122.95
20	D	535[A]	R9X	O26-P24-O25	-3.05	105.80	113.45
13	B	503	FLC	OG1-CGC-CG	-3.04	114.33	122.95
13	A	530	FLC	OG1-CGC-CG	-3.02	114.41	122.95
20	C	633[B]	R9X	O27-P24-O25	-2.99	105.95	113.45
20	B	531[B]	R9X	C13-N12-C10	2.95	125.06	121.18
13	C	627	FLC	CA-CB-CBC	2.95	116.55	110.03
13	C	627	FLC	OG2-CGC-CG	2.92	123.60	114.35
20	A	532[A]	R9X	C13-N12-C10	-2.85	117.45	121.18
20	C	633[B]	R9X	C15-C14-C13	-2.83	117.62	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	601	FLC	OG1-CGC-CG	-2.81	114.99	122.95
20	A	532[A]	R9X	C09-C10-N12	2.81	120.82	115.86
20	C	632[A]	R9X	C22-C23-C14	-2.78	119.99	123.37
20	C	633[B]	R9X	O26-P24-O25	-2.71	106.67	113.45
13	B	507	FLC	OA2-CAC-CA	2.69	122.88	114.35
13	C	628	FLC	OG2-CGC-CG	2.69	122.87	114.35
13	C	603	FLC	OG2-CGC-CG	2.68	122.85	114.35
20	A	532[B]	R9X	C22-C23-C14	-2.68	120.11	123.37
20	C	633[B]	R9X	C09-C10-N12	2.66	120.55	115.86
20	B	531[B]	R9X	O11-C10-N12	-2.64	118.48	122.95
13	A	505	FLC	OG2-CGC-CG	2.62	122.66	114.35
13	A	530	FLC	OG2-CGC-CG	2.58	122.52	114.35
18	A	518	GOL	C3-C2-C1	-2.53	102.51	111.80
13	B	503	FLC	OG2-CGC-CG	2.53	122.36	114.35
13	C	627	FLC	CB-CA-CAC	-2.51	107.05	113.92
13	A	530	FLC	OA2-CAC-CA	2.51	122.30	114.35
20	A	532[A]	R9X	C15-C14-C13	-2.51	118.02	121.11
20	A	532[B]	R9X	C09-C10-N12	2.50	120.27	115.86
13	C	601	FLC	OG2-CGC-CG	2.45	122.11	114.35
18	B	522	GOL	C3-C2-C1	-2.32	103.27	111.80
20	C	633[B]	R9X	O11-C10-C09	-2.30	117.85	122.02
20	B	531[A]	R9X	C22-C23-C14	-2.30	120.58	123.37
15	D	516	NAG	C1-O5-C5	2.18	115.11	112.19
18	C	625	GOL	C3-C2-C1	-2.18	103.81	111.80
20	C	632[A]	R9X	P24-C13-C14	-2.18	107.78	111.31
18	D	527	GOL	C3-C2-C1	-2.16	103.86	111.80
18	C	618	GOL	C3-C2-C1	-2.15	103.90	111.80
20	D	535[A]	R9X	C19-C18-C17	-2.12	118.18	123.01
18	D	528	GOL	C3-C2-C1	-2.12	104.04	111.80
20	A	532[A]	R9X	C22-C23-C18	2.11	120.64	117.92
18	D	533	GOL	C3-C2-C1	-2.08	104.17	111.80
18	A	531	GOL	C3-C2-C1	-2.06	104.23	111.80
20	D	535[B]	R9X	O27-P24-O25	-2.05	108.32	113.45
18	A	520	GOL	C3-C2-C1	-2.03	104.36	111.80
20	D	535[B]	R9X	C09-C10-N12	2.03	119.43	115.86
18	C	624	GOL	C3-C2-C1	-2.01	104.41	111.80

All (5) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
20	C	633[B]	R9X	C13
20	D	535[A]	R9X	C13
20	D	535[B]	R9X	C13

All (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
13	A	530	FLC	OHB-CB-CBC-OB2
13	B	503	FLC	CG-CB-CBC-OB1
13	B	503	FLC	CG-CB-CBC-OB2
13	B	503	FLC	OHB-CB-CBC-OB1
13	B	503	FLC	OHB-CB-CBC-OB2
13	B	503	FLC	CA-CB-CG-CGC
13	B	503	FLC	OHB-CB-CG-CGC
13	B	505	FLC	CAC-CA-CB-CBC
13	B	505	FLC	CAC-CA-CB-OHB
13	B	505	FLC	CA-CB-CBC-OB1
13	B	505	FLC	CA-CB-CBC-OB2
13	B	505	FLC	OHB-CB-CBC-OB1
13	B	505	FLC	OHB-CB-CBC-OB2
13	B	506	FLC	OHB-CB-CG-CGC
13	B	507	FLC	CAC-CA-CB-CBC
13	B	507	FLC	CAC-CA-CB-OHB
13	B	507	FLC	CG-CB-CBC-OB1
13	B	507	FLC	CG-CB-CBC-OB2
13	B	507	FLC	OHB-CB-CBC-OB1
13	B	507	FLC	OHB-CB-CBC-OB2
13	C	627	FLC	CG-CB-CBC-OB1
13	C	627	FLC	CG-CB-CBC-OB2
13	C	627	FLC	OHB-CB-CBC-OB1
13	C	627	FLC	OHB-CB-CBC-OB2
13	C	627	FLC	CA-CB-CG-CGC
13	C	627	FLC	CBC-CB-CG-CGC
13	C	627	FLC	OHB-CB-CG-CGC
13	C	628	FLC	OHB-CB-CBC-OB1
13	C	628	FLC	CBC-CB-CG-CGC
13	C	628	FLC	OHB-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
13	D	503	FLC	CA-CB-CBC-OB1
13	D	503	FLC	CA-CB-CBC-OB2
13	D	503	FLC	OHB-CB-CBC-OB1
13	D	503	FLC	OHB-CB-CBC-OB2
18	A	517	GOL	C1-C2-C3-O3
18	A	521	GOL	O1-C1-C2-C3
18	A	522	GOL	C1-C2-C3-O3
18	A	524	GOL	C1-C2-C3-O3
18	A	531	GOL	O1-C1-C2-O2
18	A	531	GOL	O1-C1-C2-C3
18	B	519	GOL	O1-C1-C2-C3
18	B	521	GOL	C1-C2-C3-O3
18	B	522	GOL	O1-C1-C2-C3
18	B	524	GOL	O1-C1-C2-C3
18	B	524	GOL	C1-C2-C3-O3
18	B	525	GOL	C1-C2-C3-O3
18	B	528	GOL	O1-C1-C2-C3
18	B	528	GOL	C1-C2-C3-O3
18	C	620	GOL	C1-C2-C3-O3
18	C	629	GOL	C1-C2-C3-O3
18	D	522	GOL	C1-C2-C3-O3
18	D	523	GOL	O1-C1-C2-C3
18	D	524	GOL	C1-C2-C3-O3
18	D	525	GOL	C1-C2-C3-O3
20	A	532[A]	R9X	N12-C13-C14-C15
20	A	532[A]	R9X	P24-C13-C14-C23
20	A	532[A]	R9X	P24-C13-C14-C15
20	A	532[B]	R9X	N12-C13-C14-C23
20	A	532[B]	R9X	C14-C13-N12-C10
20	A	532[B]	R9X	P24-C13-N12-C10
20	B	531[A]	R9X	N12-C13-C14-C15
20	B	531[A]	R9X	P24-C13-C14-C23
20	B	531[A]	R9X	P24-C13-C14-C15
20	B	531[A]	R9X	P24-C13-N12-C10
20	C	632[A]	R9X	P24-C13-C14-C23
20	C	632[A]	R9X	P24-C13-C14-C15
20	C	632[A]	R9X	C14-C13-N12-C10
20	C	633[B]	R9X	N12-C13-C14-C23
20	C	633[B]	R9X	N12-C13-C14-C15
20	C	633[B]	R9X	C14-C13-N12-C10
20	C	633[B]	R9X	C14-C13-P24-O27
20	C	633[B]	R9X	N12-C13-P24-O25

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Mol	Chain	Res	Type	Atoms
20	C	633[B]	R9X	N12-C13-P24-O26
20	C	633[B]	R9X	N12-C13-P24-O27
20	D	535[A]	R9X	N12-C13-C14-C23
20	D	535[A]	R9X	N12-C13-C14-C15
20	D	535[A]	R9X	C14-C13-N12-C10
20	D	535[A]	R9X	P24-C13-N12-C10
20	D	535[A]	R9X	C14-C13-P24-O26
20	D	535[B]	R9X	N12-C13-C14-C15
20	D	535[B]	R9X	P24-C13-C14-C23
20	D	535[B]	R9X	P24-C13-C14-C15
20	D	535[B]	R9X	C14-C13-P24-O25
20	D	535[B]	R9X	C14-C13-P24-O26
20	D	535[B]	R9X	C14-C13-P24-O27
20	D	535[B]	R9X	N12-C13-P24-O25
20	D	535[B]	R9X	N12-C13-P24-O26
20	D	535[B]	R9X	N12-C13-P24-O27
14	B	504	PGE	C6-C5-O3-C4
15	C	616	NAG	C4-C5-C6-O6
20	A	532[A]	R9X	C09-C10-N12-C13
20	B	531[A]	R9X	C09-C10-N12-C13
20	B	531[B]	R9X	C09-C10-N12-C13
20	C	632[A]	R9X	C09-C10-N12-C13
20	D	535[A]	R9X	C09-C10-N12-C13
20	A	532[B]	R9X	C07-C08-C09-C10
20	D	535[B]	R9X	C07-C08-C09-C10
15	D	506	NAG	O5-C5-C6-O6
20	A	532[A]	R9X	O11-C10-N12-C13
20	B	531[A]	R9X	O11-C10-N12-C13
20	B	531[B]	R9X	O11-C10-N12-C13
20	C	632[A]	R9X	O11-C10-N12-C13
20	D	535[A]	R9X	O11-C10-N12-C13
14	D	504	PGE	O2-C3-C4-O3
15	C	616	NAG	O5-C5-C6-O6
14	B	504	PGE	O2-C3-C4-O3
15	C	605	NAG	O5-C5-C6-O6
20	A	532[A]	R9X	C02-C03-C04-C05
20	C	633[B]	R9X	C05-C06-C07-C08
13	B	505	FLC	CAC-CA-CB-CG
13	B	506	FLC	CA-CB-CG-CGC
13	B	506	FLC	CBC-CB-CG-CGC
13	B	507	FLC	CAC-CA-CB-CG
13	C	602	FLC	CA-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
13	C	602	FLC	CBC-CB-CG-CGC
13	C	602	FLC	OHB-CB-CG-CGC
13	C	628	FLC	CA-CB-CG-CGC
14	D	504	PGE	C6-C5-O3-C4
15	D	506	NAG	C4-C5-C6-O6
15	C	605	NAG	C8-C7-N2-C2
15	C	605	NAG	O7-C7-N2-C2
15	C	616	NAG	C8-C7-N2-C2
15	C	616	NAG	O7-C7-N2-C2
15	D	516	NAG	C8-C7-N2-C2
15	D	516	NAG	O7-C7-N2-C2
18	A	517	GOL	O2-C2-C3-O3
18	B	521	GOL	O2-C2-C3-O3
18	B	528	GOL	O2-C2-C3-O3
18	D	525	GOL	O2-C2-C3-O3
14	A	507	PGE	O2-C3-C4-O3
15	C	605	NAG	C4-C5-C6-O6
14	A	504	PGE	O1-C1-C2-O2
14	B	504	PGE	O1-C1-C2-O2
14	D	504	PGE	O1-C1-C2-O2
18	A	519	GOL	O1-C1-C2-C3
18	A	520	GOL	O1-C1-C2-C3
18	A	525	GOL	O1-C1-C2-C3
18	C	624	GOL	C1-C2-C3-O3
18	C	629	GOL	O1-C1-C2-C3
18	C	630	GOL	C1-C2-C3-O3
18	D	521	GOL	C1-C2-C3-O3
18	D	522	GOL	O1-C1-C2-C3
18	D	527	GOL	C1-C2-C3-O3
18	D	529	GOL	O1-C1-C2-C3
18	D	533	GOL	C1-C2-C3-O3
18	D	534	GOL	O1-C1-C2-C3
14	B	508	PGE	O1-C1-C2-O2
20	B	531[A]	R9X	C06-C07-C08-C09
13	A	530	FLC	CG-CB-CBC-OB2
13	C	628	FLC	CA-CB-CBC-OB1
20	D	535[B]	R9X	C02-C03-C04-C05
18	A	521	GOL	O1-C1-C2-O2
18	A	522	GOL	O2-C2-C3-O3
18	A	524	GOL	O2-C2-C3-O3
18	B	519	GOL	O1-C1-C2-O2
18	B	524	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
18	B	524	GOL	O2-C2-C3-O3
18	B	525	GOL	O2-C2-C3-O3
18	C	620	GOL	O2-C2-C3-O3
18	C	624	GOL	O2-C2-C3-O3
18	C	629	GOL	O2-C2-C3-O3
18	D	523	GOL	O1-C1-C2-O2
18	D	524	GOL	O2-C2-C3-O3
18	D	527	GOL	O2-C2-C3-O3
20	C	633[B]	R9X	C14-C13-P24-O25
20	C	632[A]	R9X	C07-C08-C09-C10
14	B	504	PGE	O3-C5-C6-O4
14	C	604	PGE	O3-C5-C6-O4
20	C	632[A]	R9X	C06-C07-C08-C09
13	A	503	FLC	CAC-CA-CB-CBC
13	A	505	FLC	CBC-CB-CG-CGC
13	A	505	FLC	OHB-CB-CG-CGC
13	B	503	FLC	CBC-CB-CG-CGC
20	C	632[A]	R9X	C02-C03-C04-C05
20	A	532[B]	R9X	C02-C03-C04-C05
20	B	531[B]	R9X	C02-C03-C04-C05
20	C	633[B]	R9X	C06-C07-C08-C09
20	D	535[A]	R9X	C01-C02-C03-C04
20	D	535[A]	R9X	C04-C05-C06-C07
20	D	535[A]	R9X	N12-C13-P24-O25
20	A	532[A]	R9X	C04-C05-C06-C07
20	B	531[B]	R9X	C06-C07-C08-C09
14	D	504	PGE	O3-C5-C6-O4
20	C	632[A]	R9X	C03-C04-C05-C06
13	A	505	FLC	CA-CB-CG-CGC
20	A	532[B]	R9X	C05-C06-C07-C08
18	B	522	GOL	O1-C1-C2-O2
18	B	528	GOL	O1-C1-C2-O2
18	D	522	GOL	O2-C2-C3-O3
20	C	632[A]	R9X	C01-C02-C03-C04
20	C	632[A]	R9X	C04-C05-C06-C07
20	C	633[B]	R9X	C02-C03-C04-C05
17	C	617	EDO	O1-C1-C2-O2
20	D	535[A]	R9X	C02-C03-C04-C05
20	A	532[B]	R9X	C03-C04-C05-C06
18	A	517	GOL	O1-C1-C2-C3
20	D	535[B]	R9X	C05-C06-C07-C08
15	A	506	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
20	A	532[A]	R9X	C01-C02-C03-C04
13	A	505	FLC	OHB-CB-CBC-OB1
13	C	628	FLC	OHB-CB-CBC-OB2
13	A	505	FLC	CG-CB-CBC-OB2
13	C	628	FLC	CA-CB-CBC-OB2
20	C	633[B]	R9X	C01-C02-C03-C04
18	A	520	GOL	O1-C1-C2-O2
20	C	632[A]	R9X	N12-C13-C14-C15
13	B	506	FLC	CAC-CA-CB-OHB
13	C	603	FLC	OHB-CB-CG-CGC
20	B	531[B]	R9X	C04-C05-C06-C07
20	A	532[B]	R9X	C06-C07-C08-C09
20	D	535[A]	R9X	C06-C07-C08-C09
20	D	535[B]	R9X	C04-C05-C06-C07
18	B	526	GOL	O2-C2-C3-O3
18	C	622	GOL	O1-C1-C2-O2
18	C	625	GOL	O1-C1-C2-O2
18	C	625	GOL	O2-C2-C3-O3
18	C	630	GOL	O2-C2-C3-O3
18	D	533	GOL	O2-C2-C3-O3
14	B	508	PGE	C4-C3-O2-C2
14	C	604	PGE	C1-C2-O2-C3
20	A	532[A]	R9X	C06-C07-C08-C09
14	B	504	PGE	C4-C3-O2-C2
20	D	535[A]	R9X	N12-C13-P24-O26
20	D	535[A]	R9X	N12-C13-P24-O27
14	A	504	PGE	C3-C4-O3-C5
20	A	532[B]	R9X	C01-C02-C03-C04
18	B	527	GOL	O1-C1-C2-C3
18	C	625	GOL	C1-C2-C3-O3
18	C	631	GOL	C1-C2-C3-O3
14	D	504	PGE	C1-C2-O2-C3
14	A	504	PGE	C6-C5-O3-C4
14	A	507	PGE	O1-C1-C2-O2
13	B	503	FLC	CB-CA-CAC-OA1
13	B	503	FLC	CB-CA-CAC-OA2
14	C	604	PGE	C3-C4-O3-C5
20	B	531[B]	R9X	C01-C02-C03-C04
20	A	532[A]	R9X	C05-C06-C07-C08
20	B	531[A]	R9X	C14-C13-P24-O26
20	C	633[B]	R9X	C14-C13-P24-O26
20	D	535[A]	R9X	C14-C13-P24-O27

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Mol	Chain	Res	Type	Atoms
13	A	505	FLC	CA-CB-CBC-OB1
13	A	505	FLC	CA-CB-CBC-OB2
13	A	530	FLC	CA-CB-CBC-OB2
13	B	507	FLC	CA-CB-CBC-OB1
13	B	507	FLC	CA-CB-CBC-OB2
13	C	628	FLC	CG-CB-CBC-OB2
18	C	629	GOL	O1-C1-C2-O2
20	B	531[A]	R9X	C03-C04-C05-C06
13	A	503	FLC	OHB-CB-CG-CGC
13	A	505	FLC	CAC-CA-CB-CBC
14	D	504	PGE	C4-C3-O2-C2
20	D	535[A]	R9X	C05-C06-C07-C08
20	C	632[A]	R9X	C05-C06-C07-C08
13	B	506	FLC	CB-CA-CAC-OA2
13	A	503	FLC	CAC-CA-CB-CG
20	B	531[B]	R9X	C05-C06-C07-C08
13	C	601	FLC	CB-CA-CAC-OA2
14	B	508	PGE	C6-C5-O3-C4
13	A	505	FLC	OHB-CB-CBC-OB2
13	A	505	FLC	CG-CB-CBC-OB1
13	B	506	FLC	CG-CB-CBC-OB1
13	B	506	FLC	CG-CB-CBC-OB2
13	C	603	FLC	CG-CB-CBC-OB1
13	C	627	FLC	CA-CB-CBC-OB2
13	C	628	FLC	CG-CB-CBC-OB1
20	D	535[B]	R9X	C01-C02-C03-C04
13	B	503	FLC	CAC-CA-CB-CBC
13	B	506	FLC	CB-CA-CAC-OA1
18	A	516	GOL	O1-C1-C2-C3
18	A	527	GOL	C1-C2-C3-O3
13	A	503	FLC	CA-CB-CG-CGC
13	A	505	FLC	CAC-CA-CB-OHB
13	B	503	FLC	CAC-CA-CB-CG
18	A	519	GOL	O1-C1-C2-O2
18	A	525	GOL	O1-C1-C2-O2
18	D	521	GOL	O2-C2-C3-O3
18	D	522	GOL	O1-C1-C2-O2
14	A	507	PGE	C4-C3-O2-C2
13	C	601	FLC	CB-CA-CAC-OA1
14	B	504	PGE	C3-C4-O3-C5
13	B	506	FLC	CA-CB-CBC-OB1
13	C	603	FLC	CG-CB-CBC-OB2

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Mol	Chain	Res	Type	Atoms
13	C	627	FLC	CA-CB-CBC-OB1
14	C	604	PGE	O1-C1-C2-O2
13	B	505	FLC	CB-CG-CGC-OG2
14	C	604	PGE	O2-C3-C4-O3
18	C	619	GOL	O1-C1-C2-O2
18	C	631	GOL	O2-C2-C3-O3
18	D	534	GOL	O1-C1-C2-O2
20	C	633[B]	R9X	C08-C09-C10-O11
18	A	526	GOL	O1-C1-C2-C3
20	D	535[A]	R9X	C14-C13-P24-O25
17	D	517	EDO	O1-C1-C2-O2
20	C	633[B]	R9X	C08-C09-C10-N12
13	A	505	FLC	CB-CA-CAC-OA1
13	A	505	FLC	CB-CA-CAC-OA2
13	B	505	FLC	CB-CG-CGC-OG1
13	B	506	FLC	CA-CB-CBC-OB2
13	A	530	FLC	OHB-CB-CG-CGC
13	A	530	FLC	CBC-CB-CG-CGC
20	C	633[B]	R9X	P24-C13-N12-C10
14	C	604	PGE	C6-C5-O3-C4
13	A	503	FLC	CAC-CA-CB-OHB
13	A	505	FLC	CAC-CA-CB-CG

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

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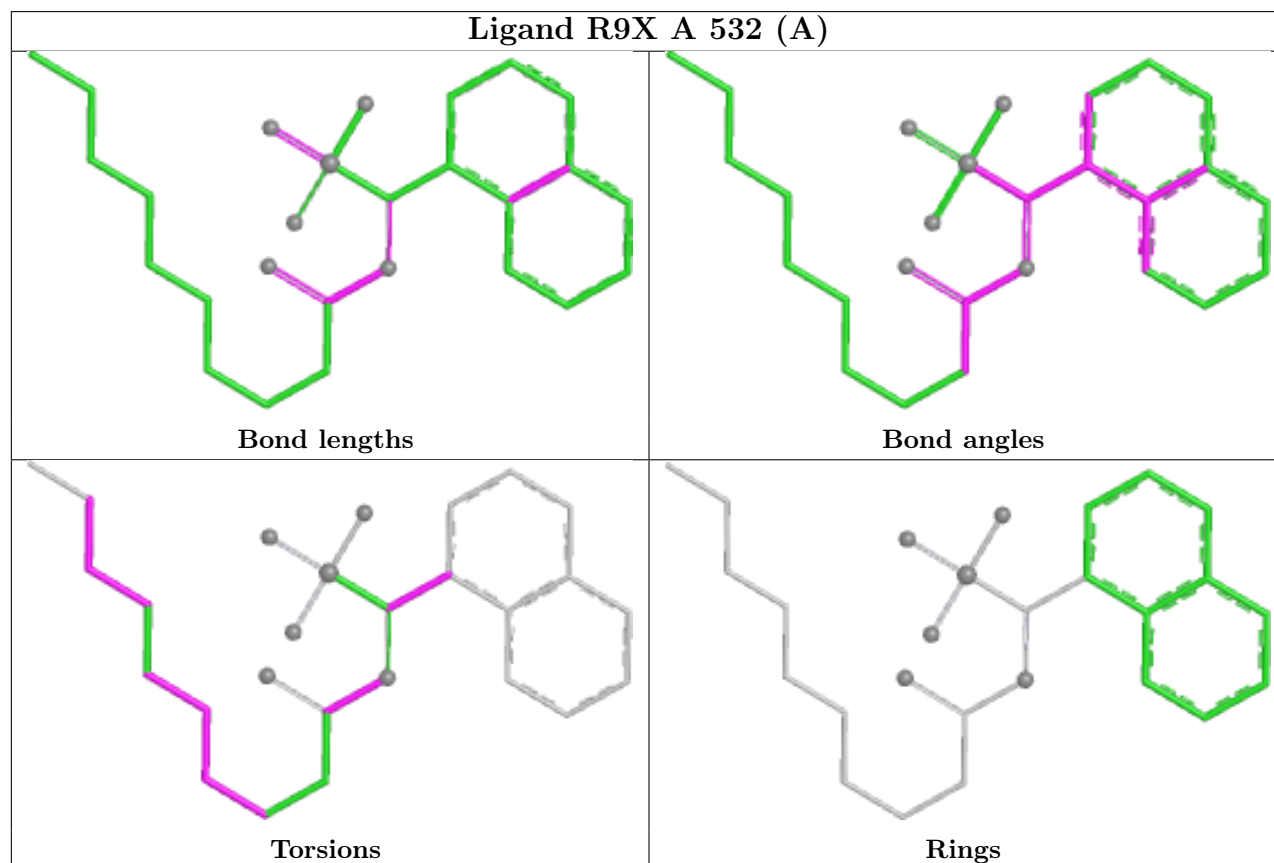
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	512	SO4	3	0
18	C	623	GOL	1	0
20	B	531[A]	R9X	6	0
13	A	503	FLC	3	0
18	D	533	GOL	1	0
17	C	617	EDO	1	0
22	D	505	DMS	2	0
18	C	622	GOL	1	0
15	D	506	NAG	3	0
18	A	531	GOL	3	0
13	B	506	FLC	3	0
18	C	625	GOL	1	0
15	C	605	NAG	1	0
14	C	604	PGE	1	0
16	C	615	SO4	1	0
14	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

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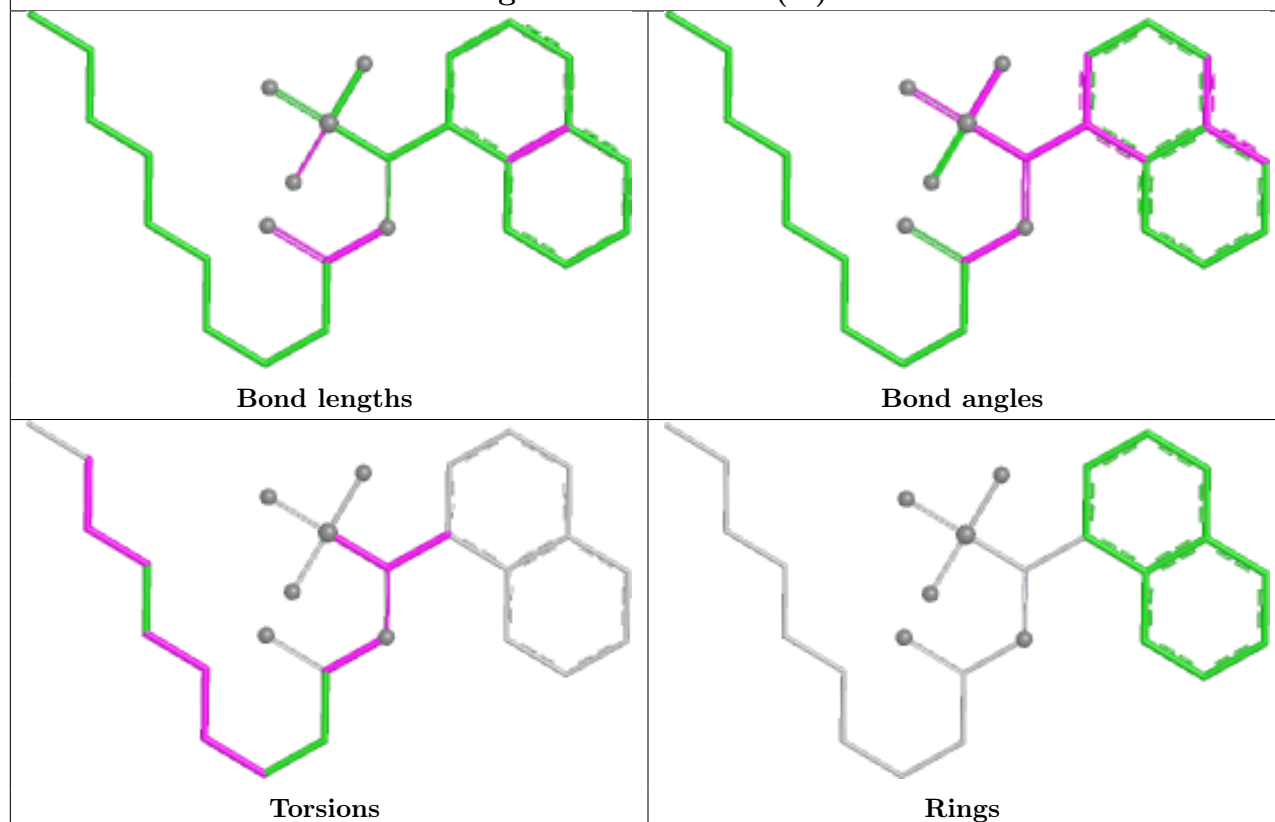
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	524	GOL	1	0
14	D	504	PGE	8	0
13	B	505	FLC	4	0
13	C	603	FLC	1	0
18	C	624	GOL	2	0
20	C	632[A]	R9X	2	0

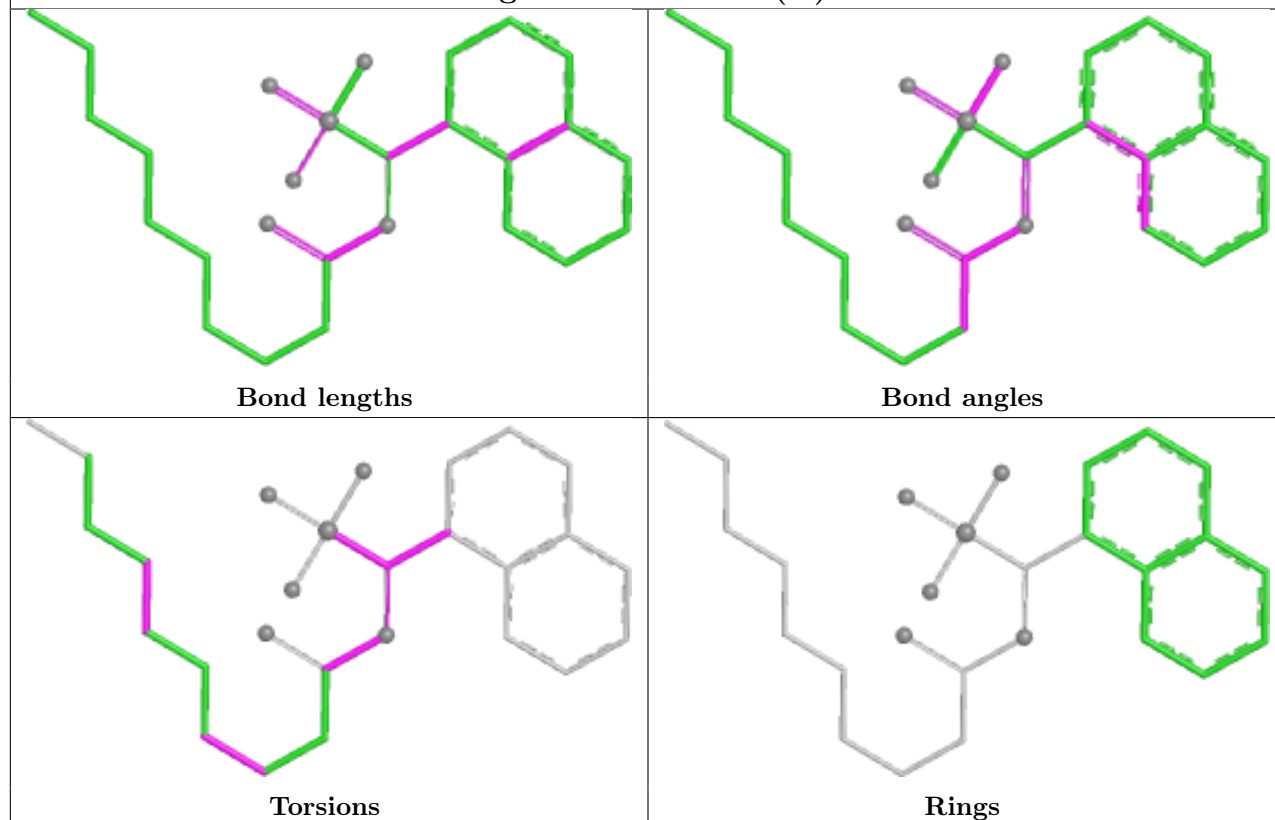
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



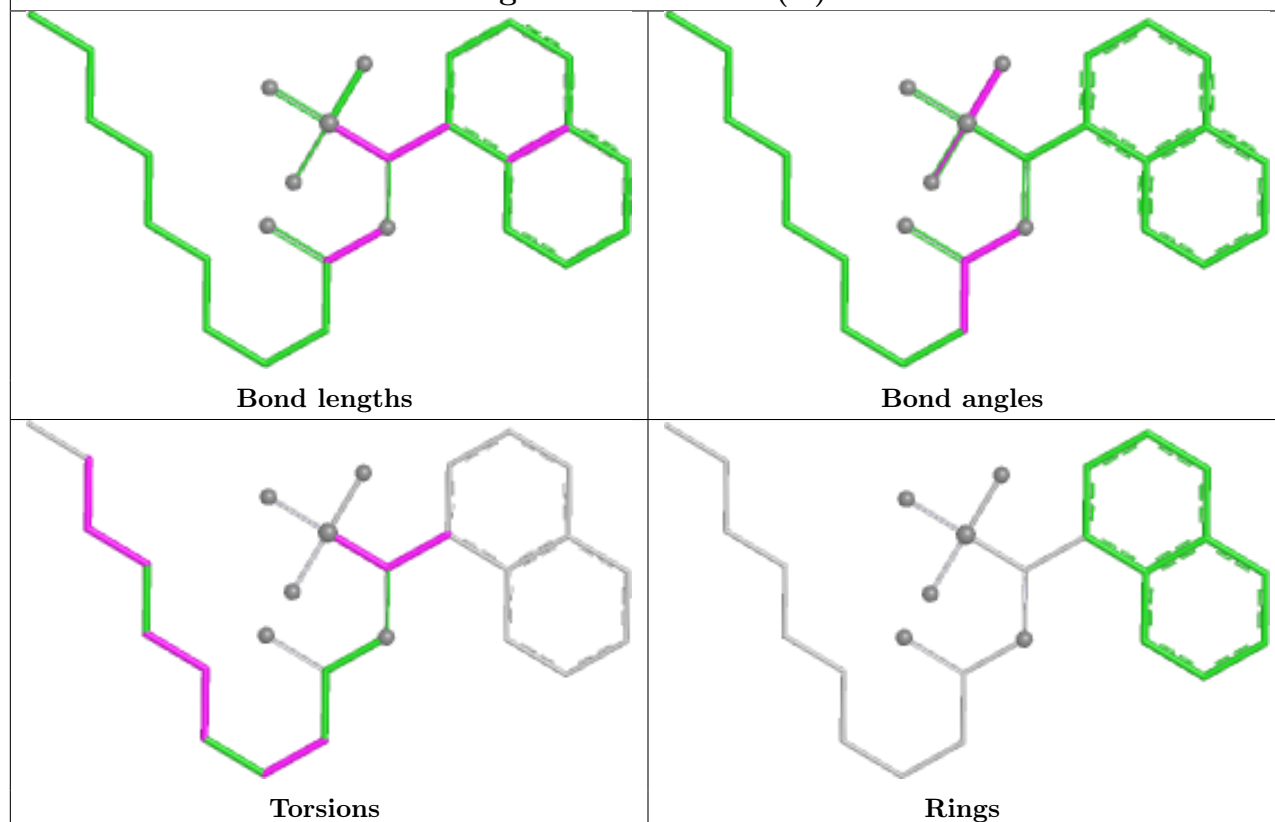
Ligand R9X D 535 (A)



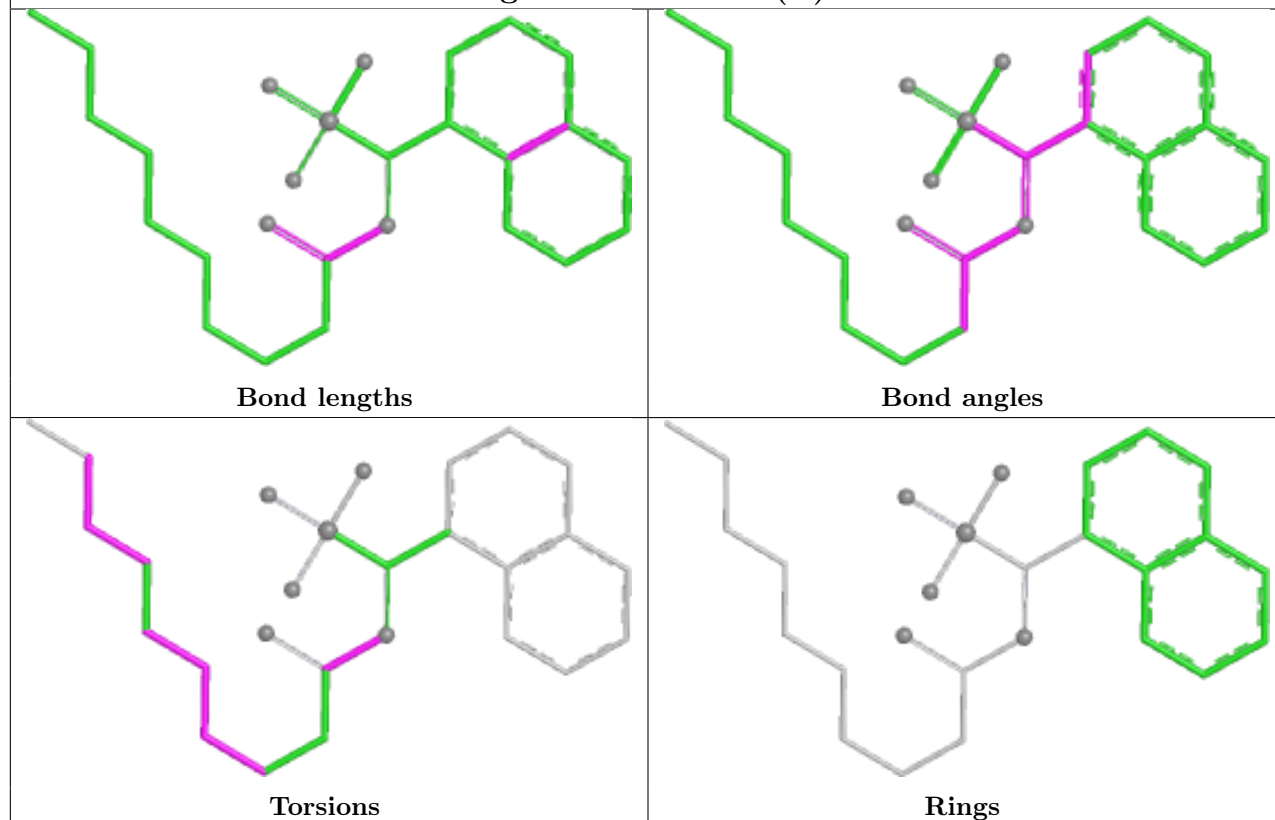
Ligand R9X B 531 (A)



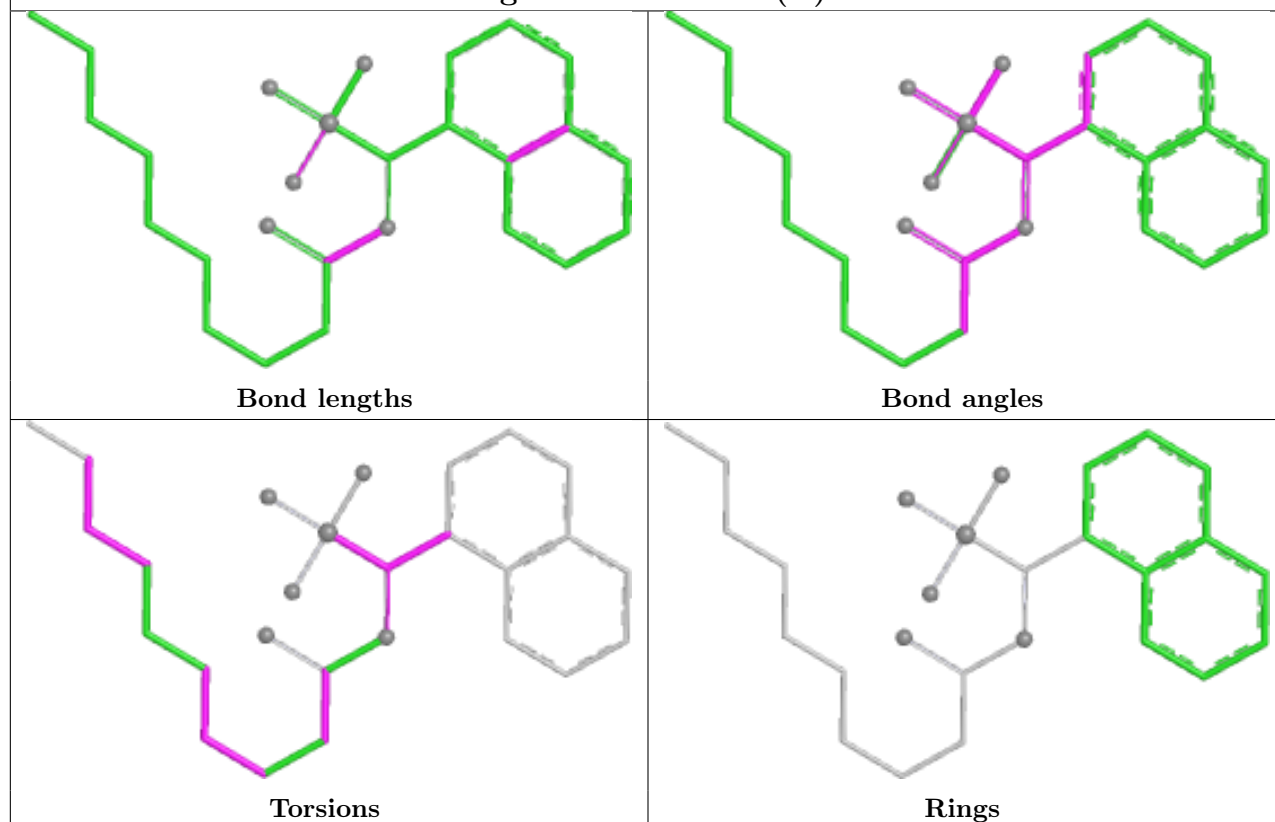
Ligand R9X D 535 (B)



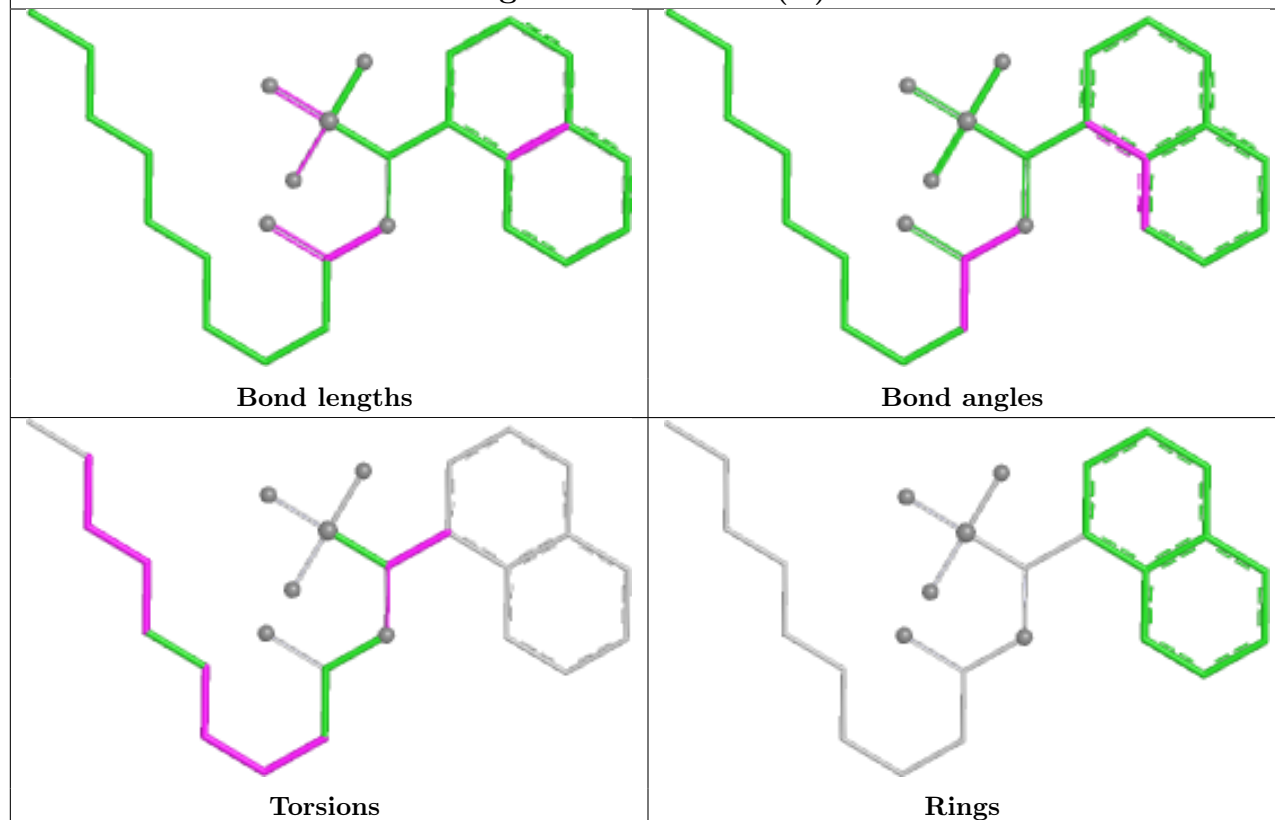
Ligand R9X B 531 (B)

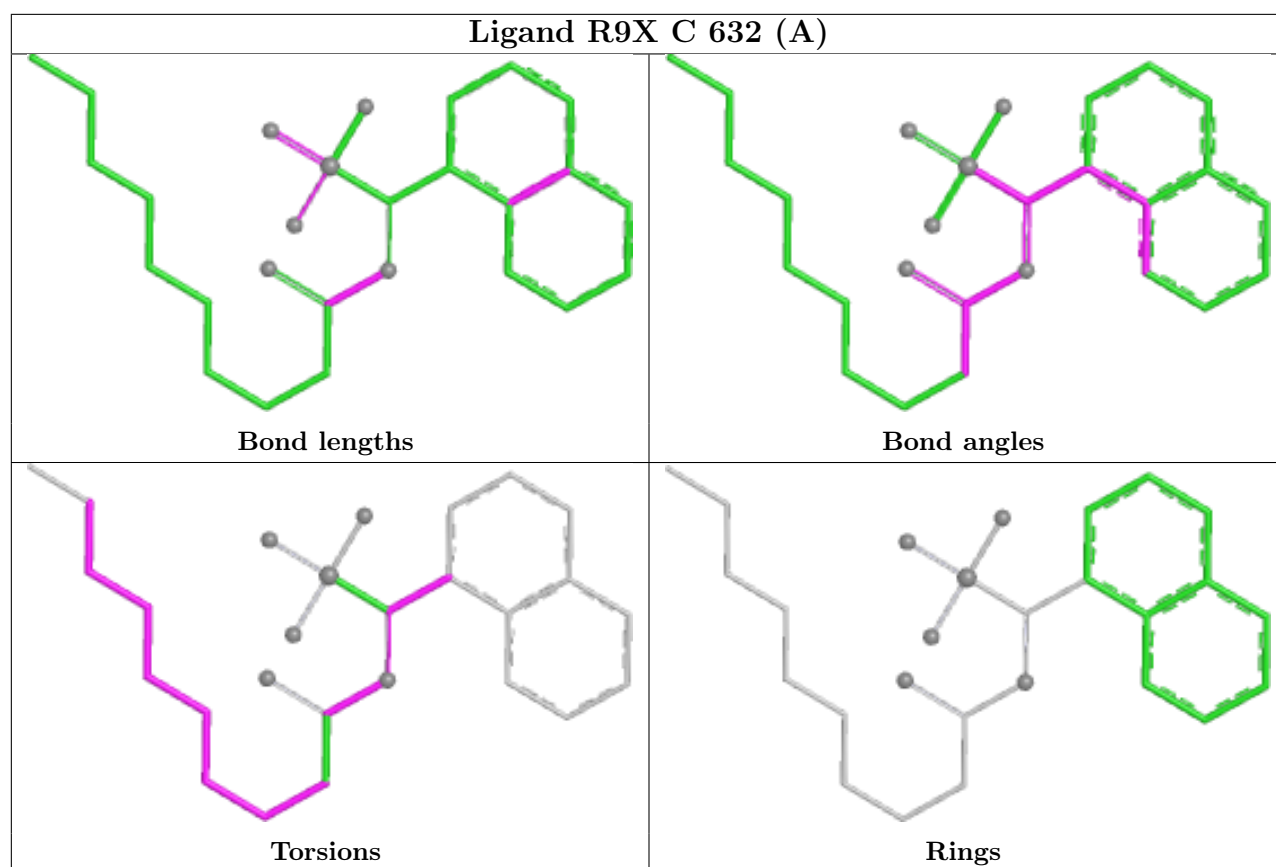


Ligand R9X C 633 (B)



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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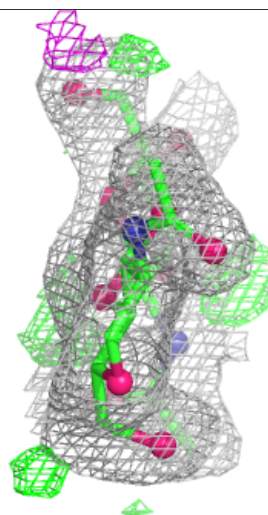
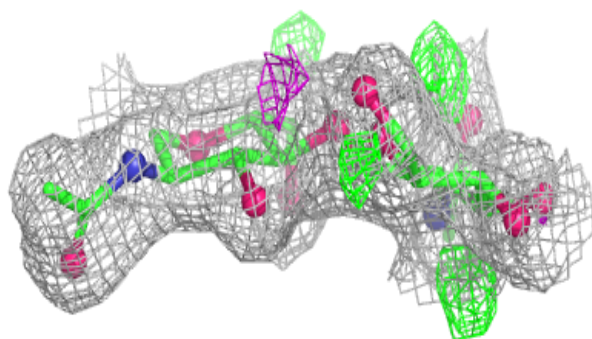
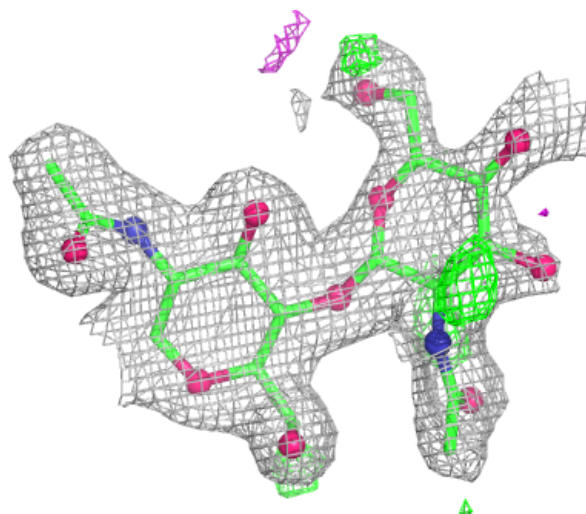
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	I	1	14/15	0.90	0.09	35,44,57,61	0
5	BMA	H	3	11/12	0.90	0.08	25,32,39,42	11
3	NAG	F	2	14/15	0.91	0.08	35,39,44,44	14
4	NAG	S	1	14/15	0.91	0.08	30,39,44,46	14
4	NAG	G	1	14/15	0.91	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.

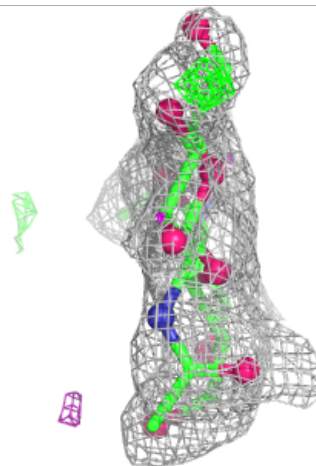
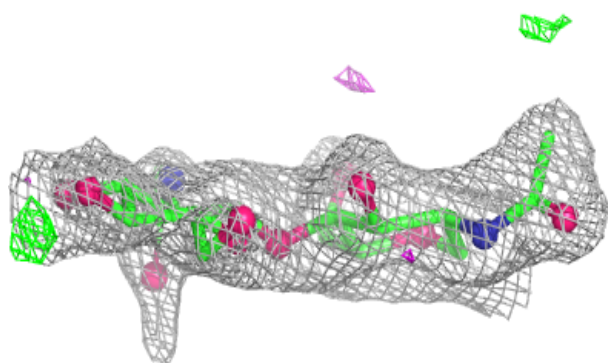
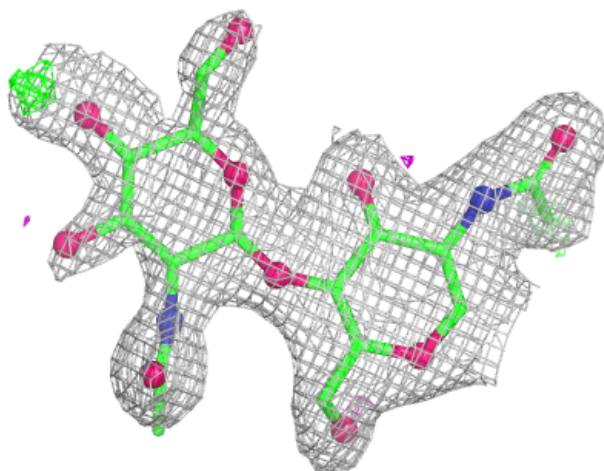
Electron density around Chain E:

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



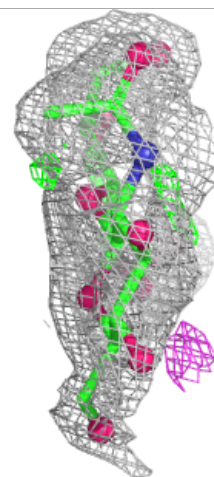
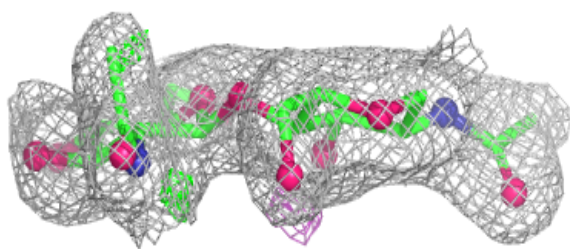
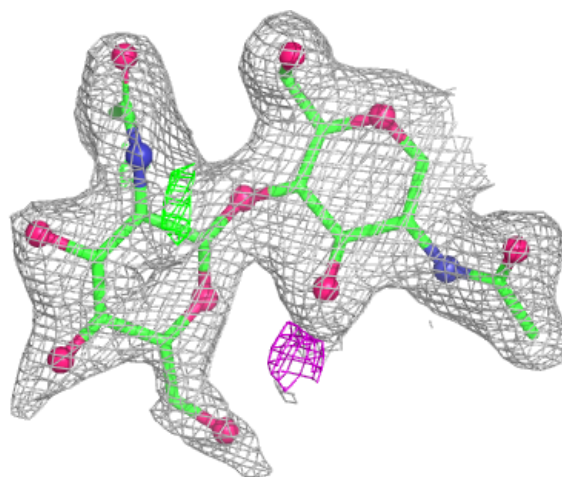
Electron density around Chain K:

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



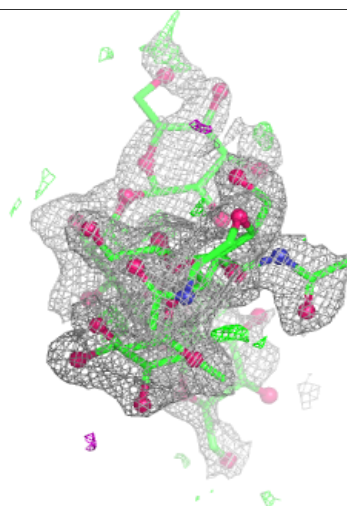
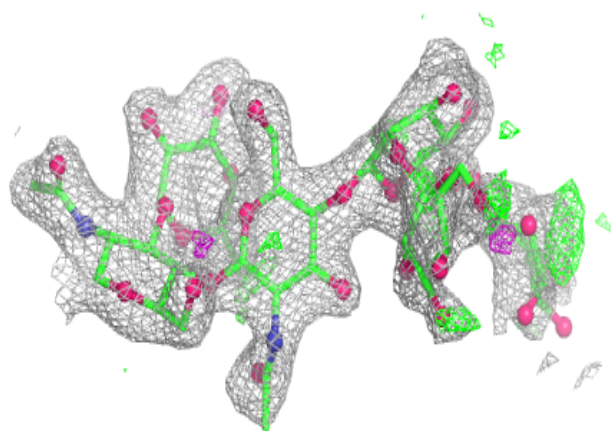
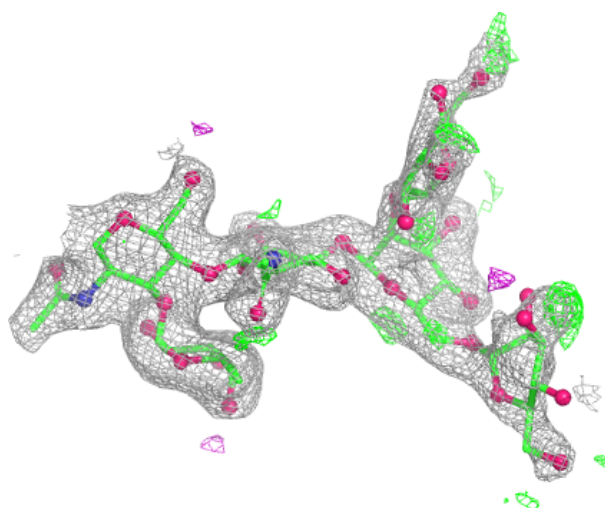
Electron density around Chain Q:

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



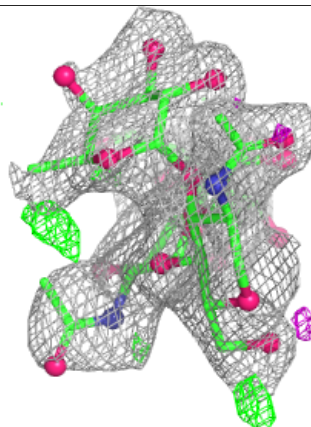
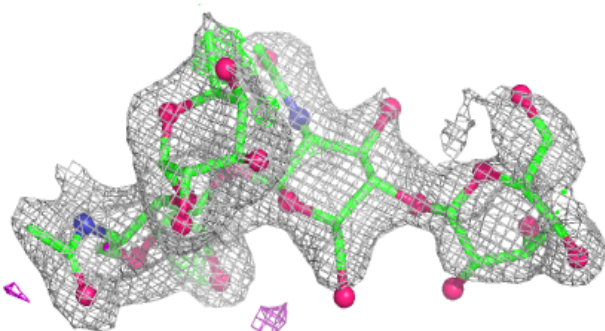
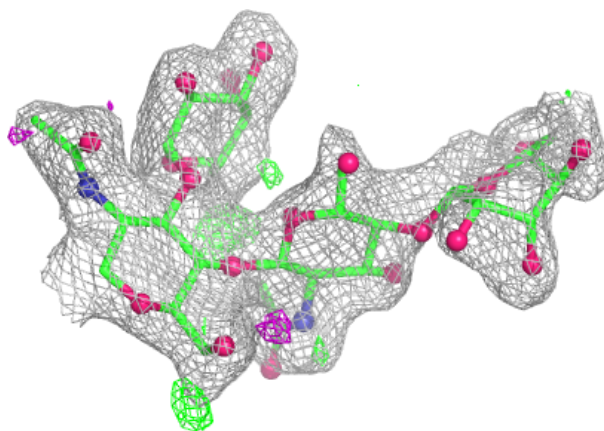
Electron density around Chain F:

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

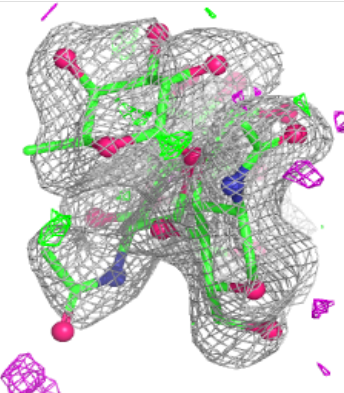
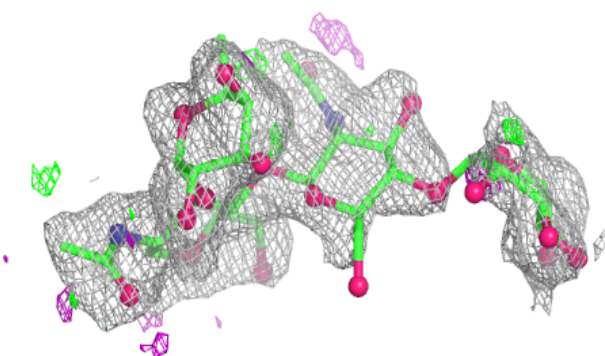
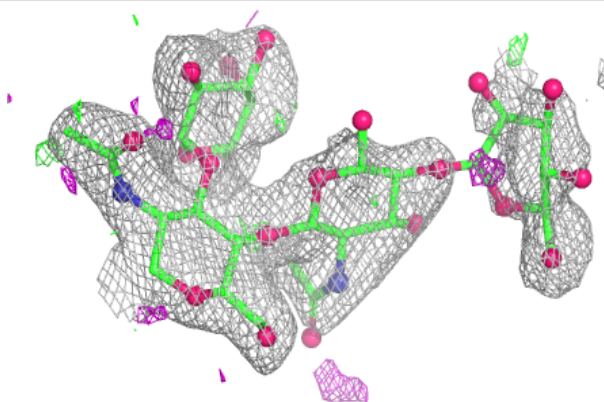


Electron density around Chain G:

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

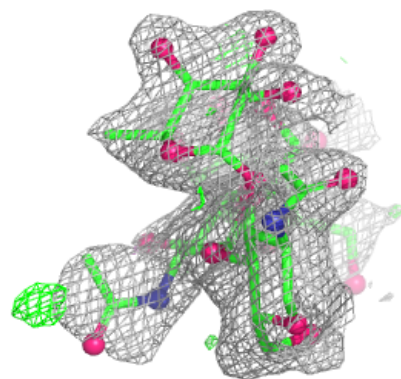
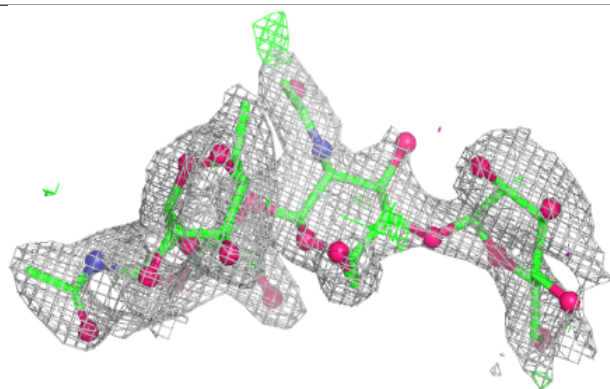
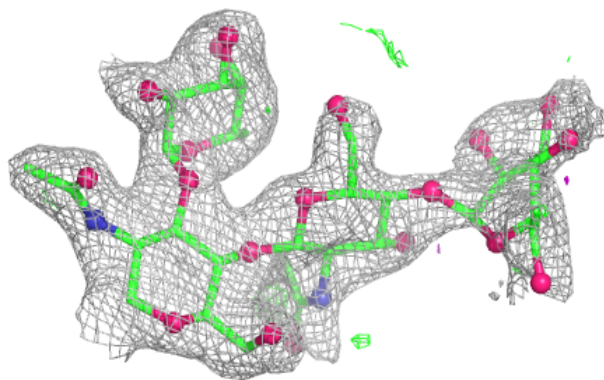
**Electron density around Chain I:**

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

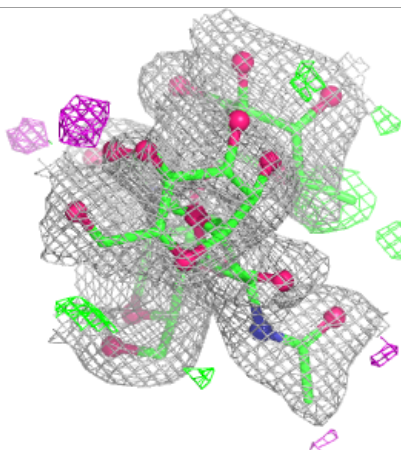
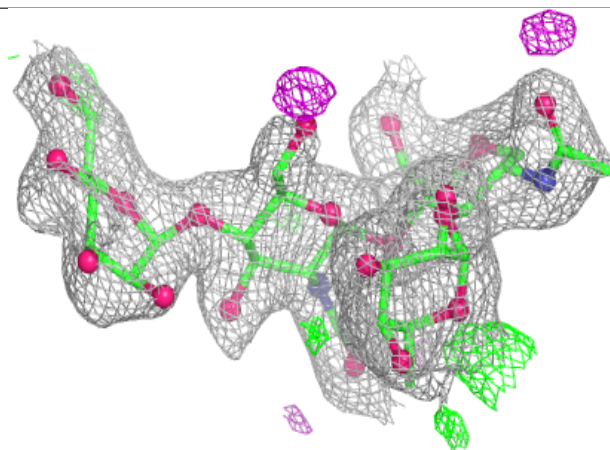
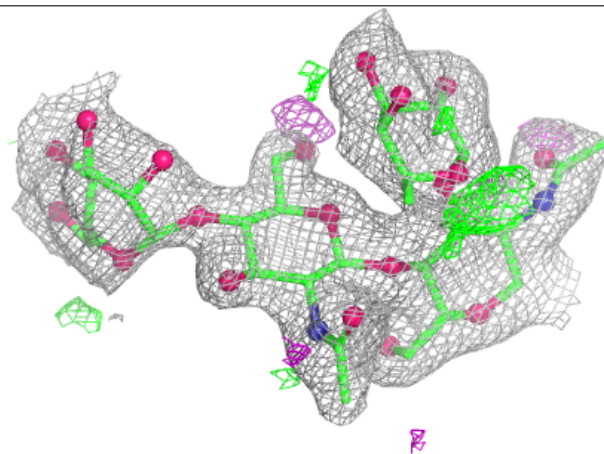


Electron density around Chain N:

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

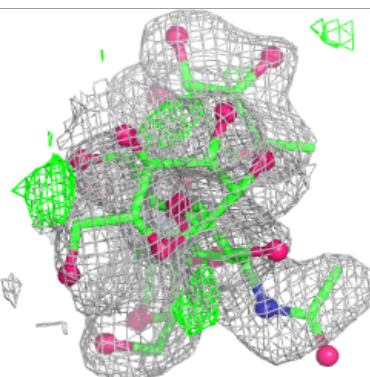
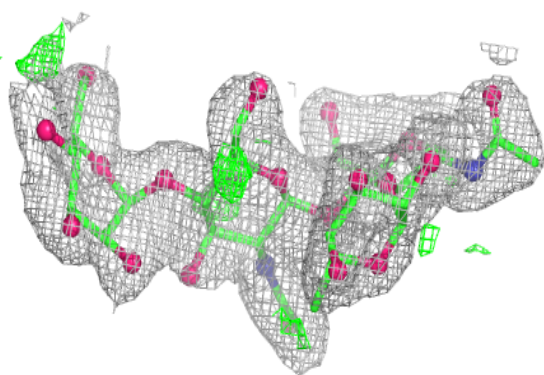
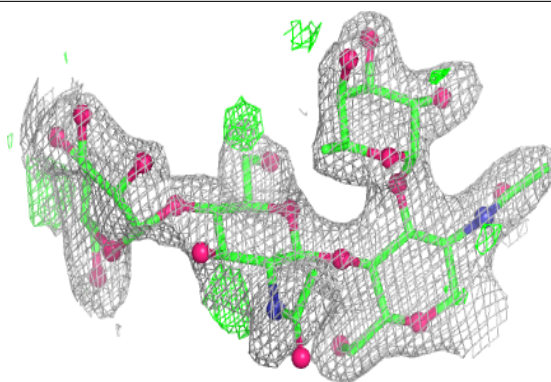
**Electron density around Chain P:**

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

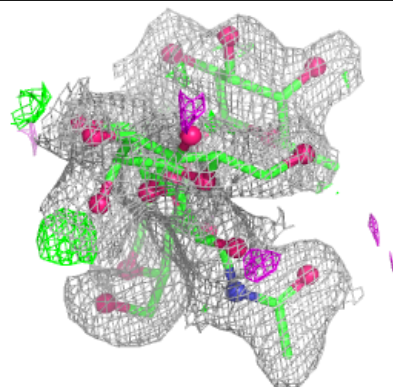
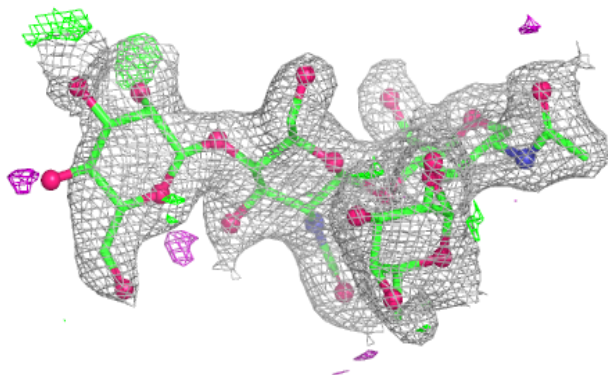
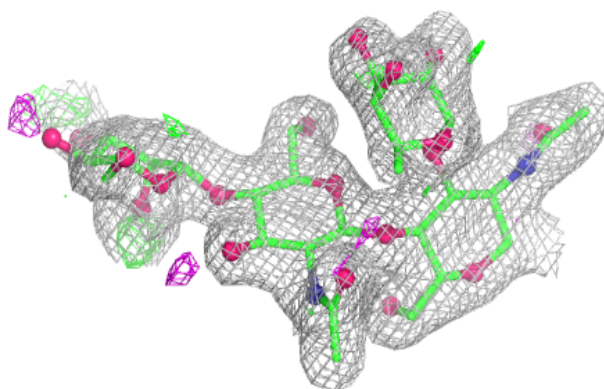


Electron density around Chain S:

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

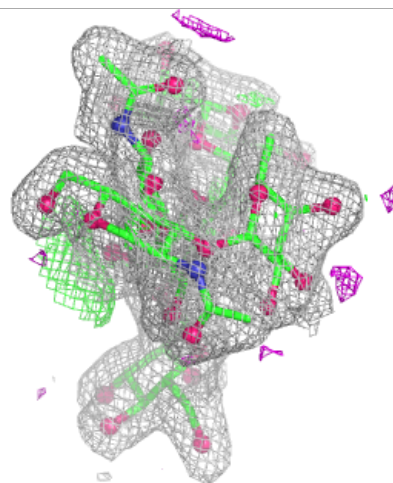
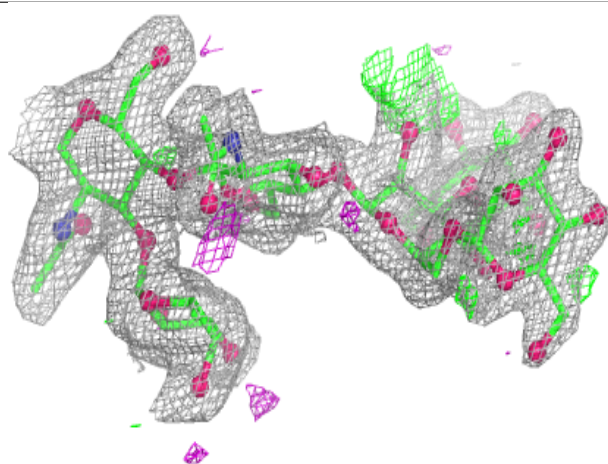
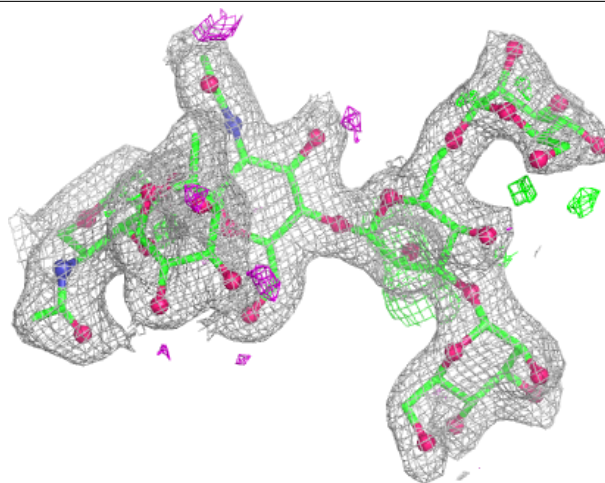
**Electron density around Chain V:**

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



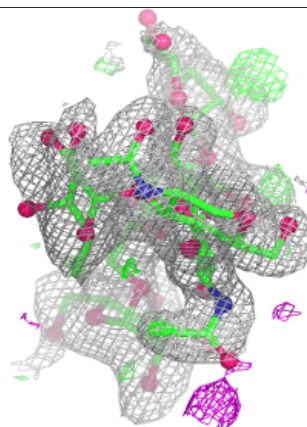
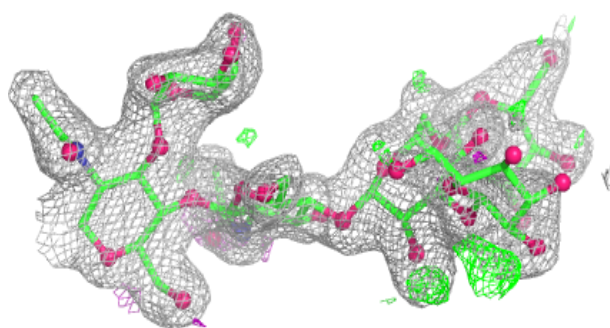
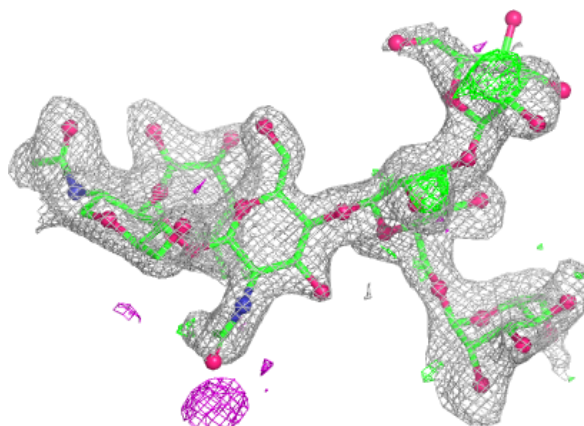
Electron density around Chain H:

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

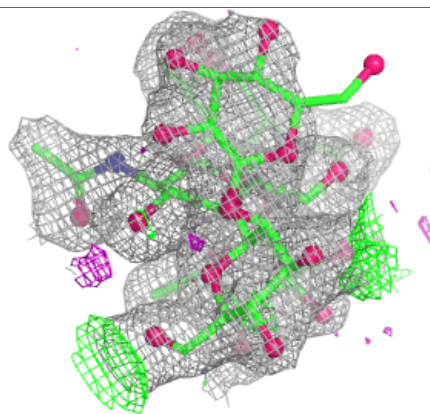
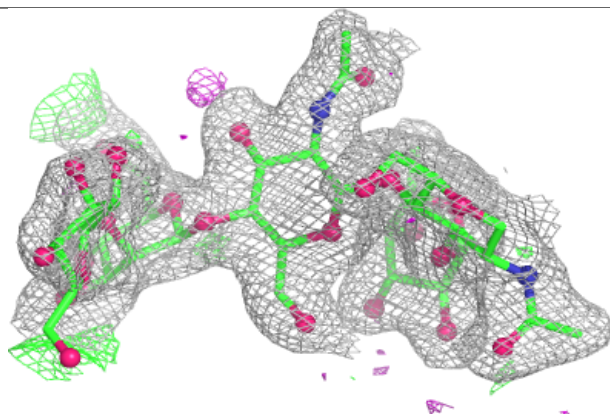
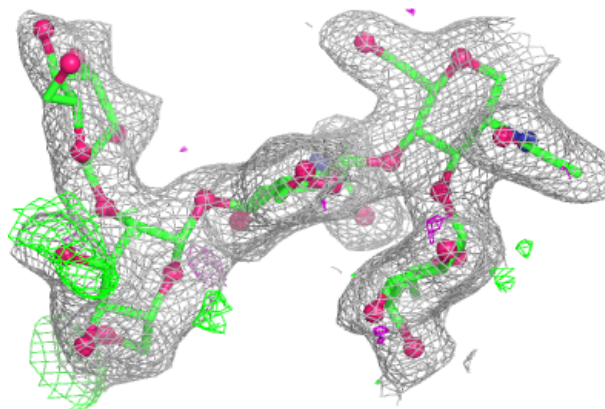


Electron density around Chain J:

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

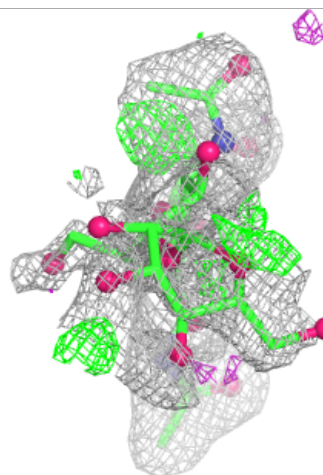
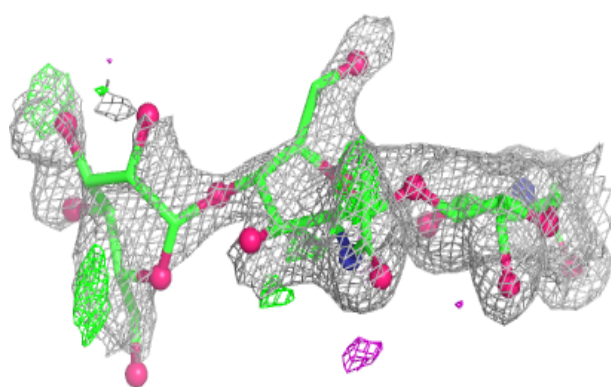
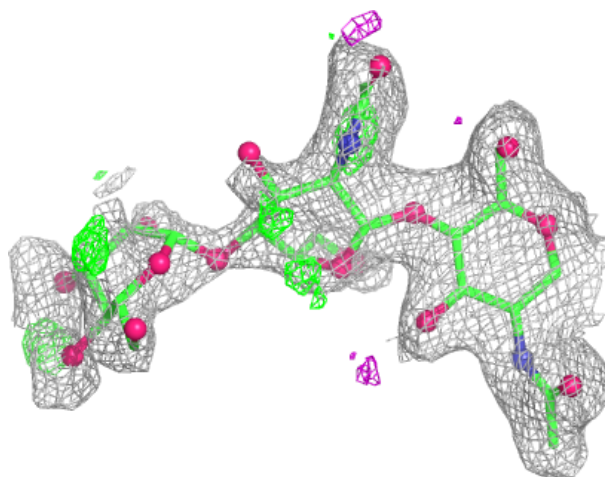
**Electron density around Chain L:**

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



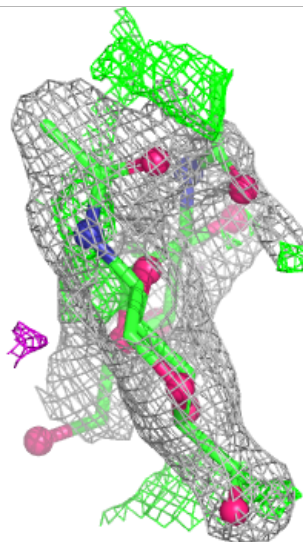
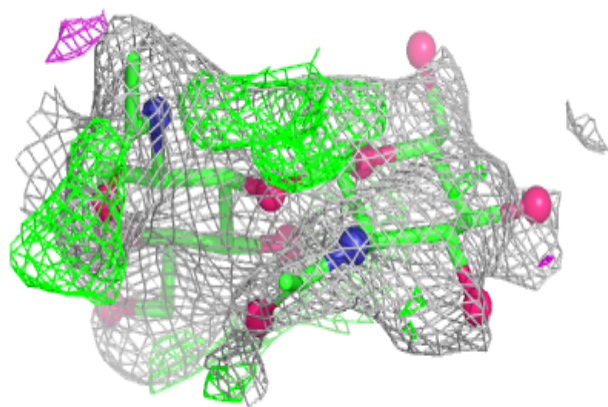
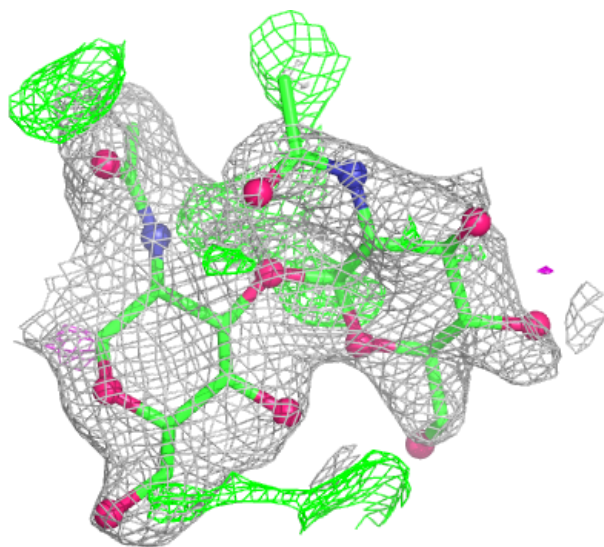
Electron density around Chain M:

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



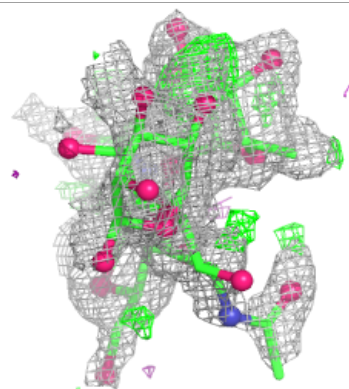
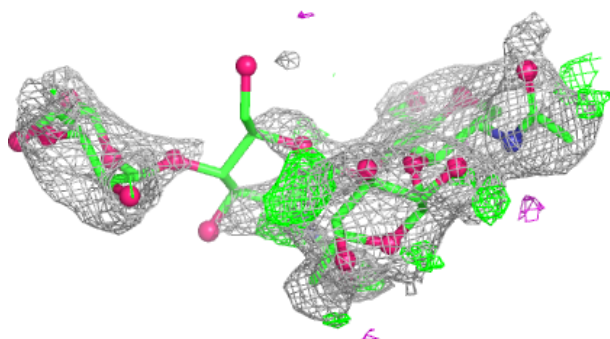
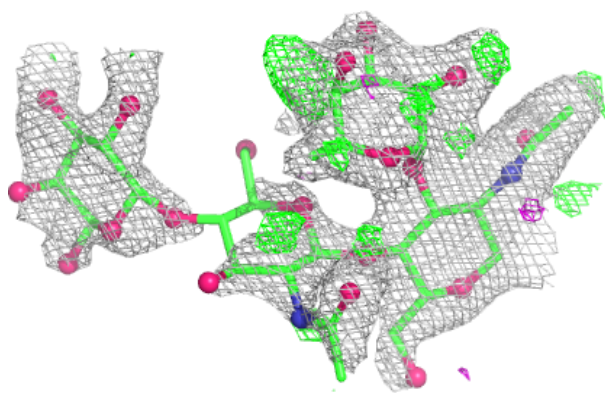
Electron density around Chain O:

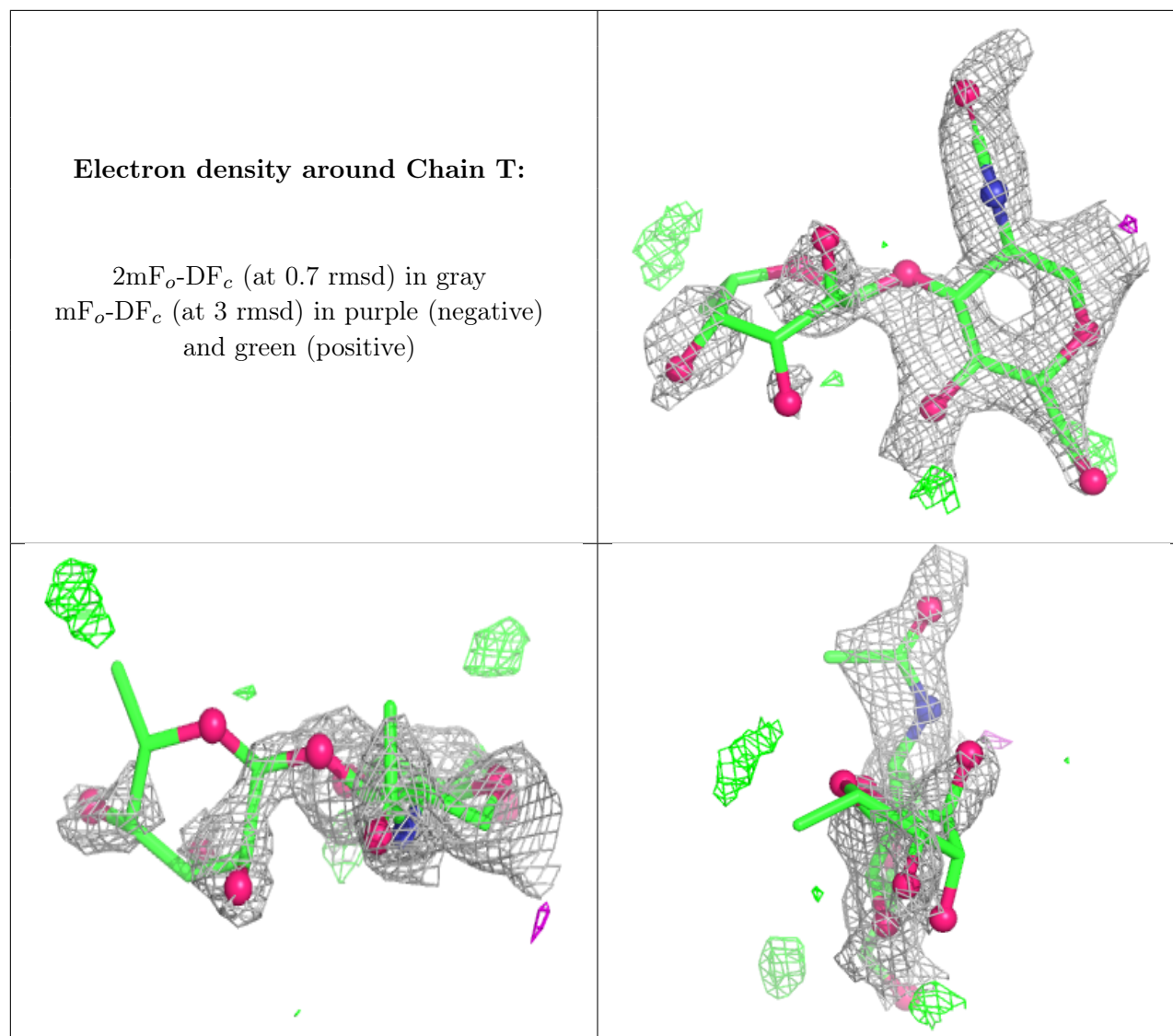
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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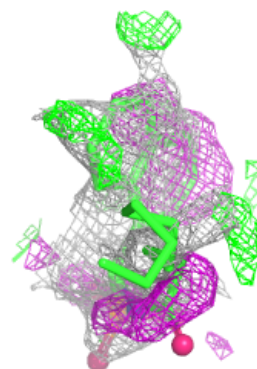
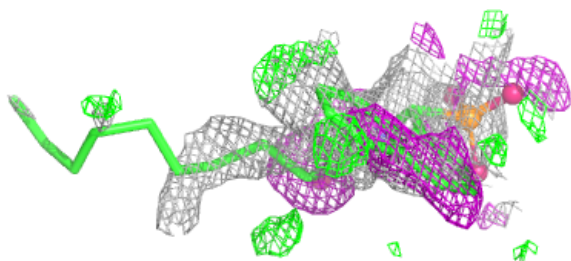
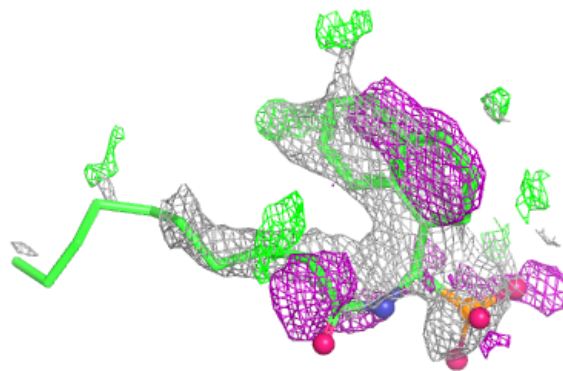
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	CL	D	530	1/1	1.00	0.04	19,19,19,19	0

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.

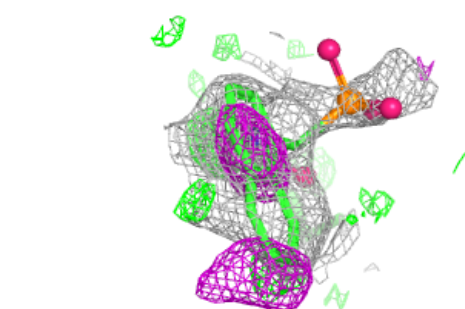
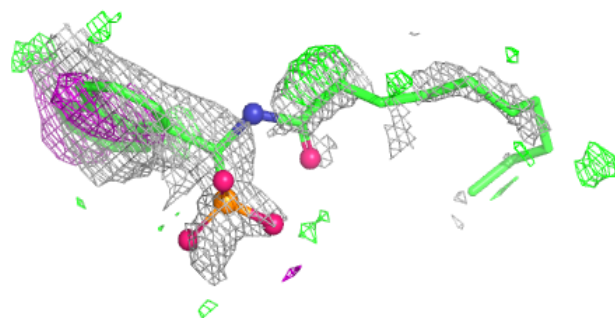
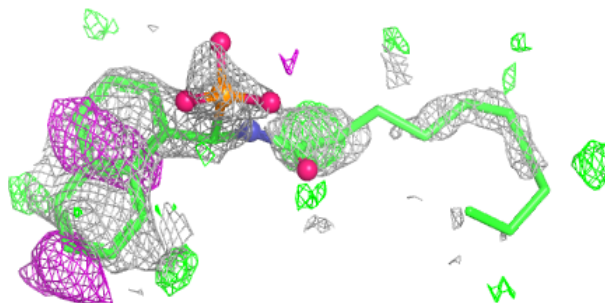
Electron density around R9X C 632 (A):

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

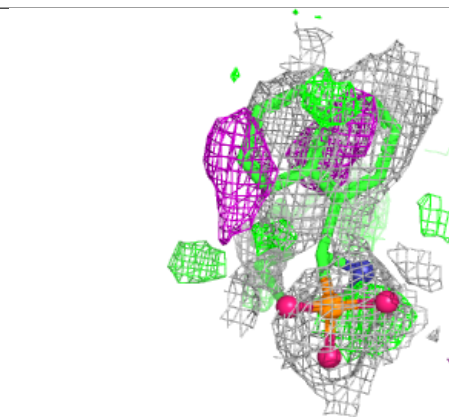
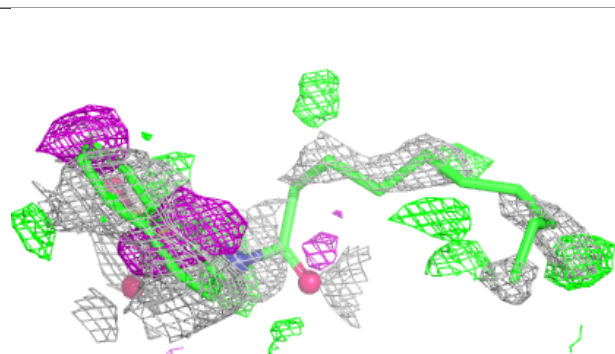
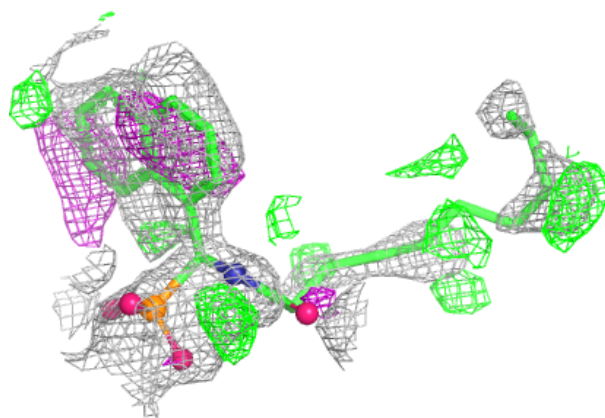


Electron density around R9X A 532 (B):

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

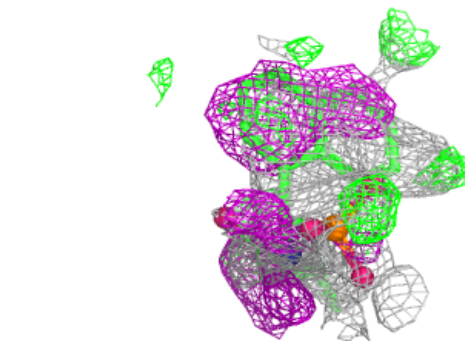
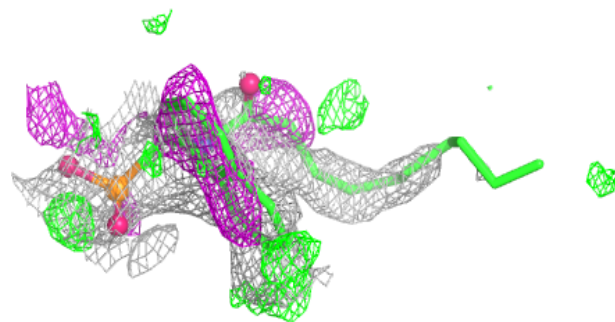
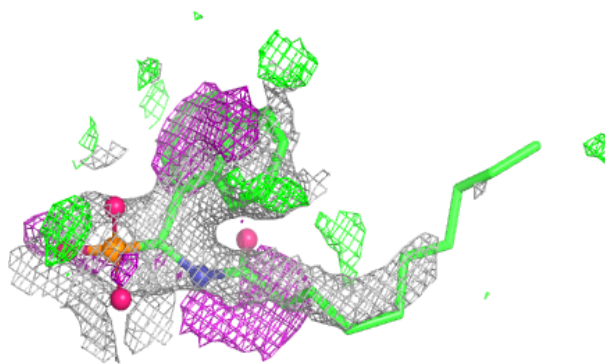
**Electron density around R9X A 532 (A):**

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



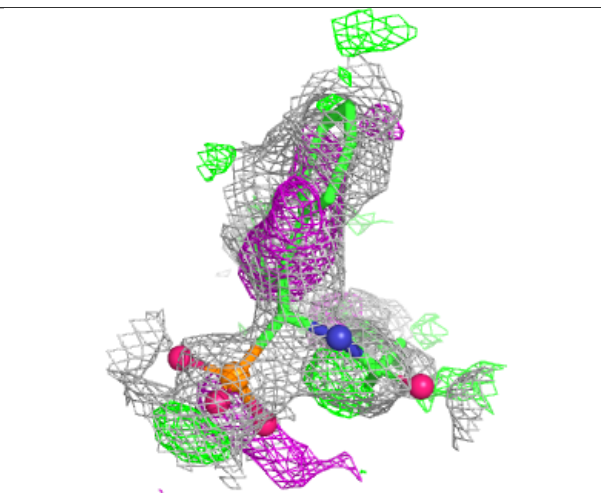
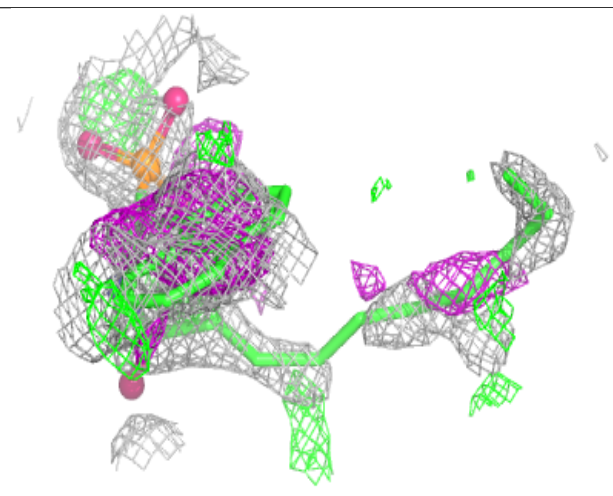
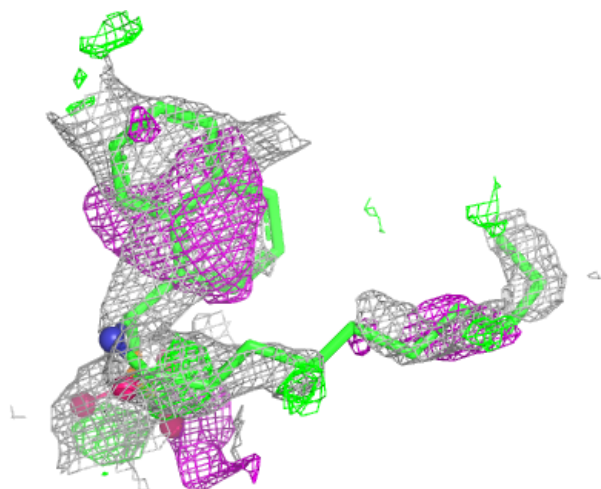
Electron density around R9X C 633 (B):

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



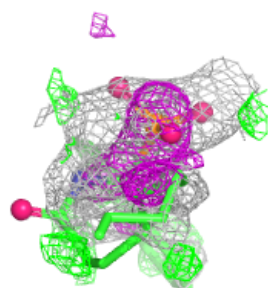
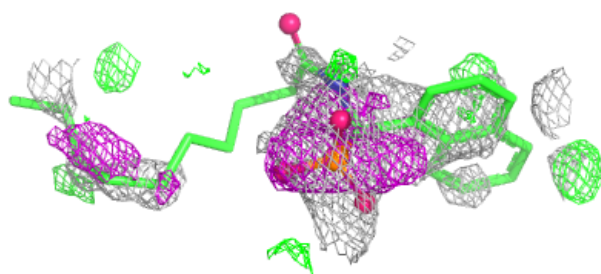
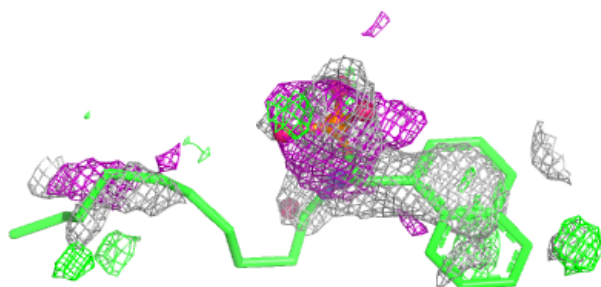
Electron density around R9X B 531 (A):

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



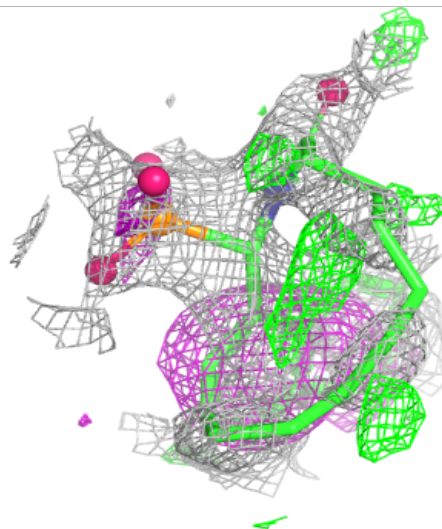
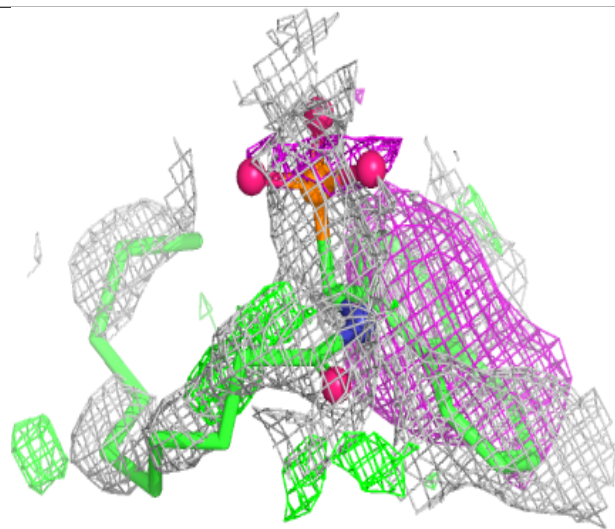
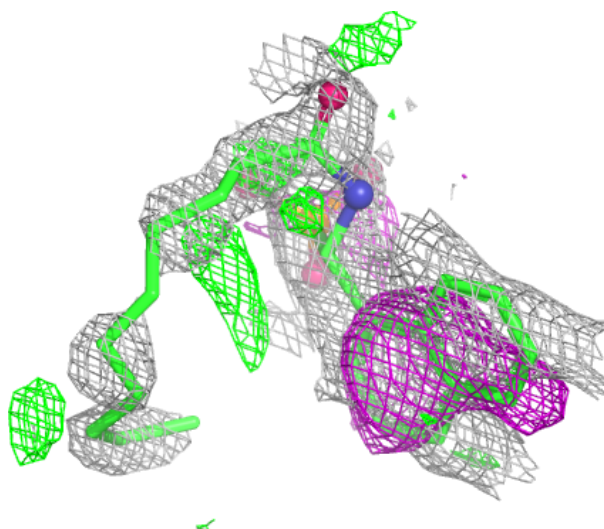
Electron density around R9X B 531 (B):

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



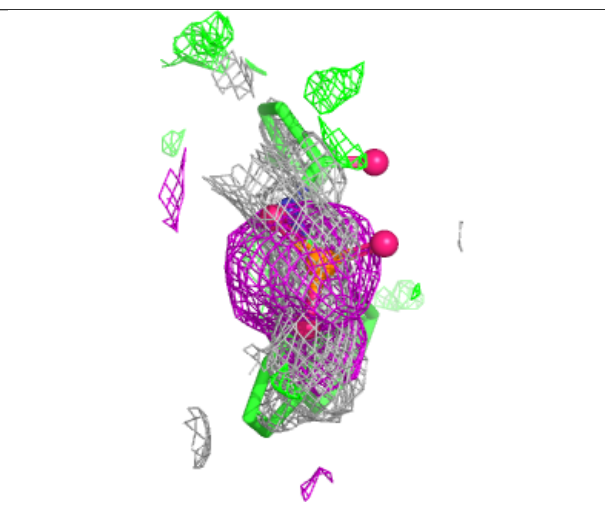
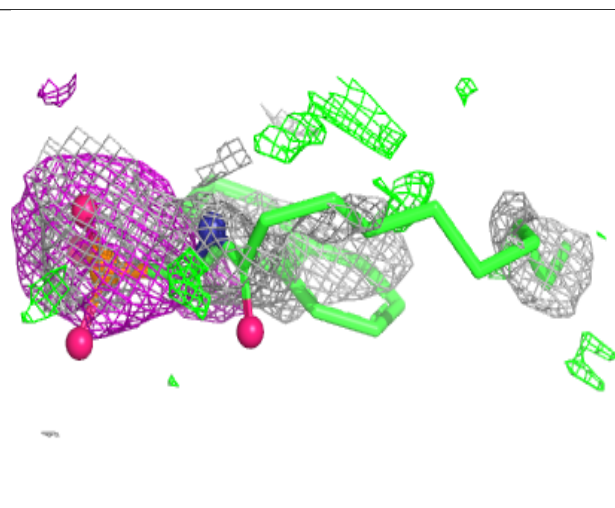
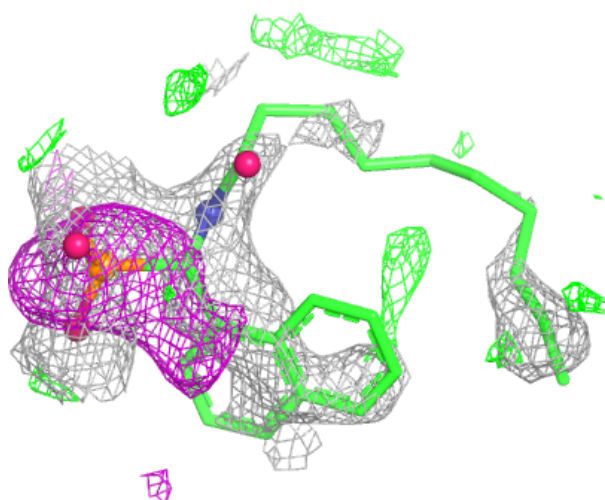
Electron density around R9X D 535 (A):

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.