Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2023 – 04:45 pm BST

PDB ID	:	8BRN
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:

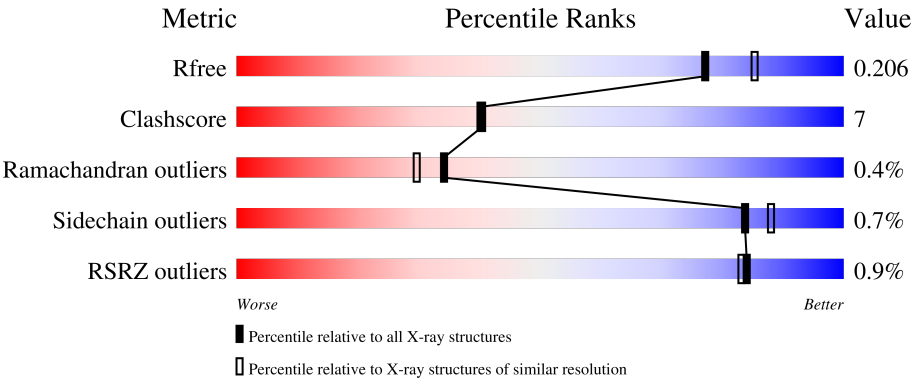
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	89% 10%
1	B	428	89% 11%
1	C	428	90% 9%
1	D	428	89% 10%
2	E	2	100%

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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	50% 50%
4	I	4	25% 50% 25%
4	N	4	50% 50%
4	P	4	75% 25%
4	S	4	75% 25%
4	V	4	75% 25%
5	H	6	33% 67%
5	J	6	33% 67%
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	-	-
13	FLC	D	503	-	-	X	-
14	PGE	B	508	-	-	-	X
14	PGE	D	504	-	-	X	-
16	SO4	A	510	-	-	X	-
16	SO4	A	512	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SO4	C	608	-	-	X	-
16	SO4	C	613	-	-	X	-
18	GOL	A	526	-	-	-	X
18	GOL	A	531	-	-	X	-
18	GOL	D	522	-	-	X	-
20	R9X	A	532[A]	X	-	-	-
20	R9X	A	532[B]	X	-	-	-
20	R9X	C	632[A]	-	-	-	X
20	R9X	C	633[B]	X	-	-	X
20	R9X	D	535[A]	X	-	-	-
20	R9X	D	535[B]	X	-	-	-
4	BMA	I	3	-	-	-	X
4	BMA	N	3	-	-	-	X
7	BMA	M	3	-	-	-	X
9	BMA	R	3	X	-	-	-

2 Entry composition

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.

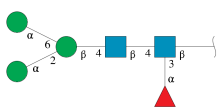
- Molecule 1 is a protein called Fe(3+)-Zn(2+) purple acid phosphatase.

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.

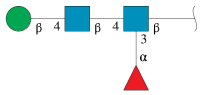
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



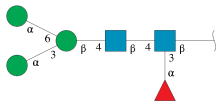
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	6	Total C N O 71 40 2 29	0	0	0

- 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.



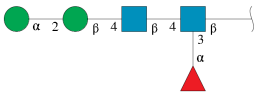
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	4	Total C N O 49 28 2 19	0	0	0
4	I	4	Total C N O 49 28 2 19	0	0	0
4	N	4	Total C N O 49 28 2 19	0	0	0
4	P	4	Total C N O 49 28 2 19	0	0	0
4	S	4	Total C N O 49 28 2 19	0	0	0
4	V	4	Total C N O 49 28 2 19	0	0	0

- 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.



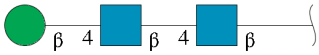
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	H	6	Total C N O 71 40 2 29	0	0	0
5	J	6	Total C N O 71 40 2 29	0	0	0

- 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 24 14 1 9	0	0	0

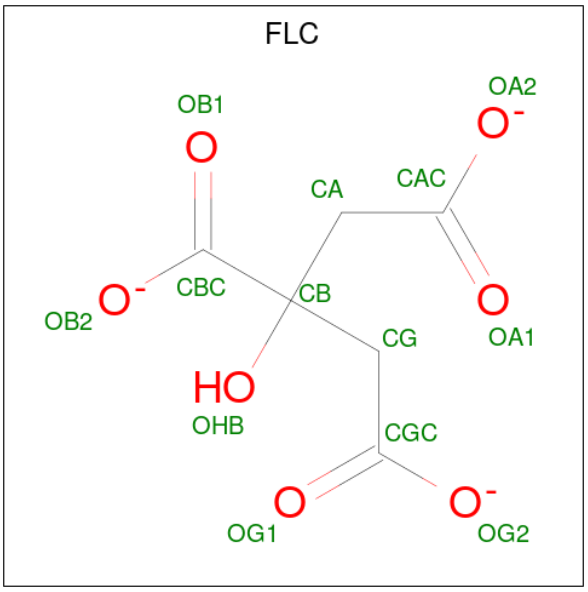
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

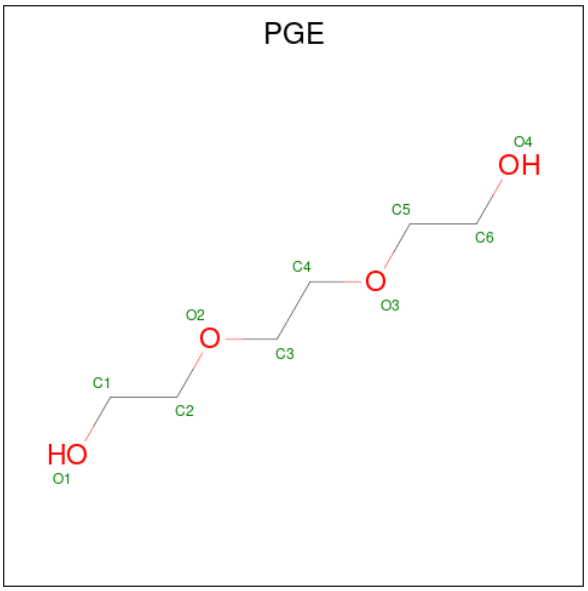
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Fe 1 1	0	0
12	B	1	Total Fe 1 1	0	0
12	C	1	Total Fe 1 1	0	0
12	D	1	Total Fe 1 1	0	0

- Molecule 13 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



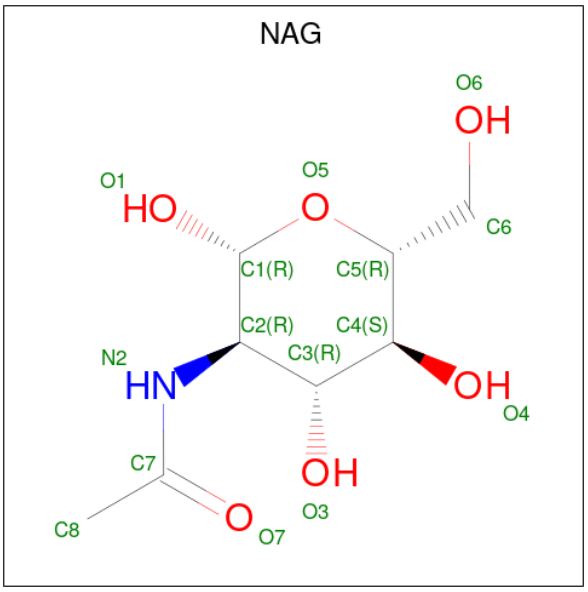
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 13 6 7	0	0
13	A	1	Total C O 13 6 7	0	0
13	A	1	Total C O 13 6 7	0	0
13	B	1	Total C O 13 6 7	0	0
13	B	1	Total C O 13 6 7	0	0
13	B	1	Total C O 13 6 7	0	0
13	B	1	Total C O 13 6 7	0	0
13	C	1	Total C O 13 6 7	0	0
13	C	1	Total C O 13 6 7	0	0
13	C	1	Total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

- Molecule 14 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



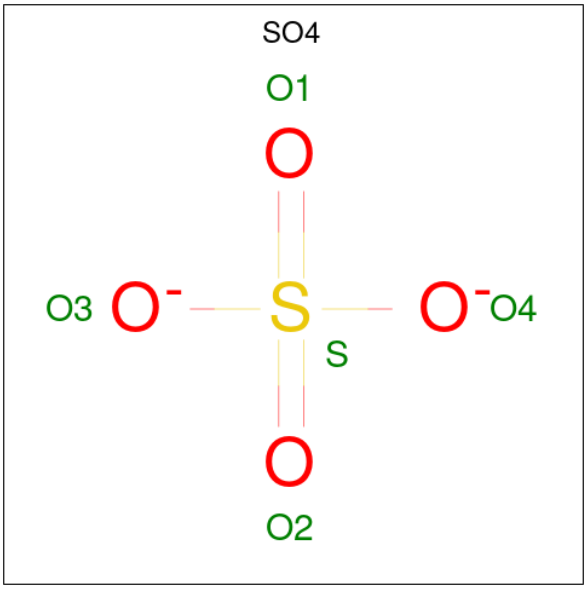
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C O 10 6 4	0	0
14	A	1	Total C O 7 4 3	0	0
14	B	1	Total C O 10 6 4	0	0
14	B	1	Total C O 10 6 4	0	0
14	C	1	Total C O 10 6 4	0	0
14	D	1	Total C O 10 6 4	0	0

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



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

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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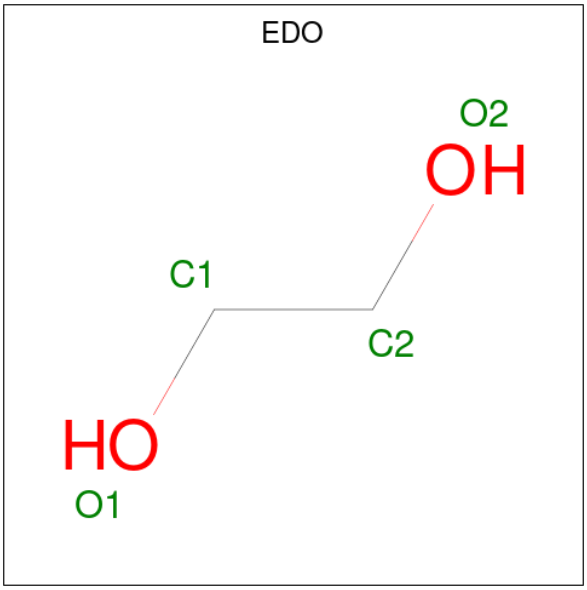
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total O S 5 4 1	0	0
16	D	1	Total O S 5 4 1	0	0
16	D	1	Total O S 5 4 1	0	0
16	D	1	Total O S 5 4 1	0	0
16	D	1	Total O S 5 4 1	0	0
16	D	1	Total O S 5 4 1	0	0
16	D	1	Total O S 5 4 1	0	0
16	D	1	Total O S 5 4 1	0	0
16	D	1	Total O S 5 4 1	0	0
16	D	1	Total O S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

- Molecule 17 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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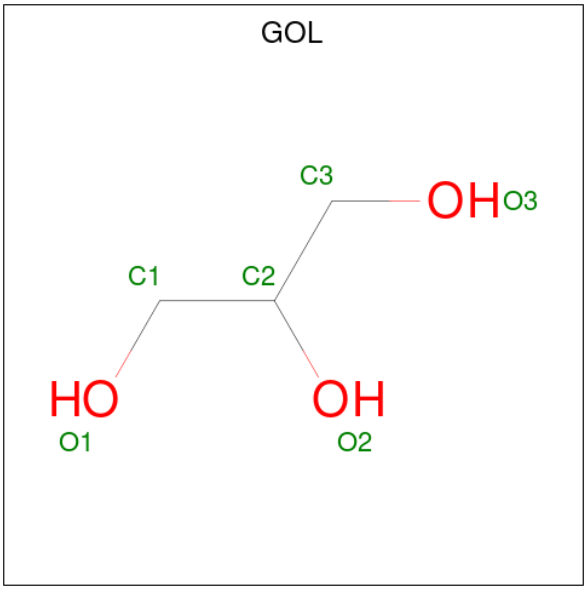
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total C O 4 2 2	0	0
17	C	1	Total C O 4 2 2	0	0
17	D	1	Total C O 4 2 2	0	0

- Molecule 18 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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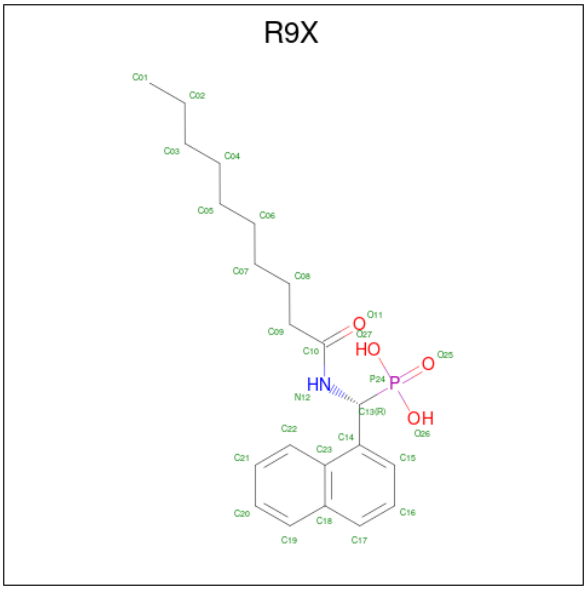
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	C	1	Total C O 6 3 3	0	0
18	C	1	Total C O 6 3 3	0	0
18	C	1	Total C O 6 3 3	0	0
18	C	1	Total C O 6 3 3	0	0
18	C	1	Total C O 6 3 3	0	0
18	C	1	Total C O 6 3 3	0	0
18	D	1	Total C O 6 3 3	0	0
18	D	1	Total C O 6 3 3	0	0
18	D	1	Total C O 6 3 3	0	0
18	D	1	Total C O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

- Molecule 19 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 20 is [(R)-(decanoylamino)-naphthalen-1-yl-methyl]phosphonic acid (three-letter code: R9X) (formula: $C_{21}H_{30}NO_4P$) (labeled as "Ligand of Interest" by depositor).

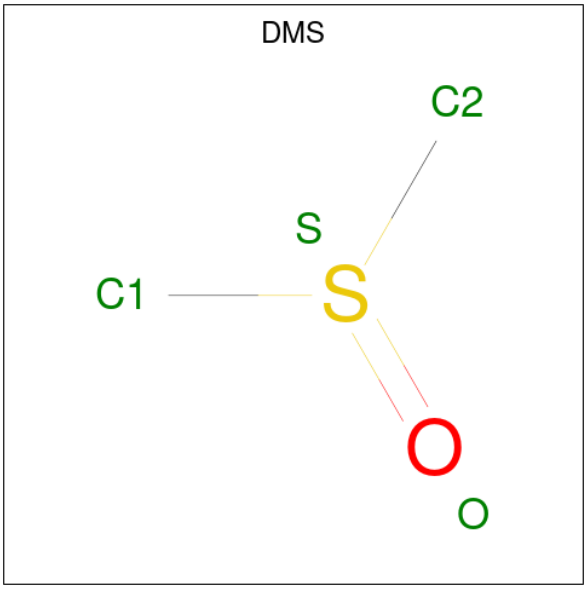


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C N O P 54 42 2 8 2	0	1
20	B	1	Total C N O P 54 42 2 8 2	0	1
20	C	1	Total C N O P 27 21 1 4 1	0	1
20	C	1	Total C N O P 27 21 1 4 1	0	1
20	D	1	Total C N O P 54 42 2 8 2	0	1

- Molecule 21 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 22 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 23 is water.

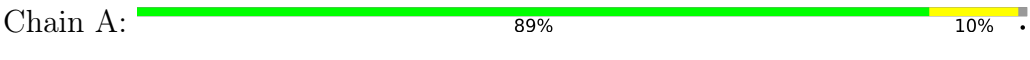
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	711	Total O 720 720	1	9
23	B	644	Total O 658 658	1	14
23	C	674	Total O 682 682	0	8
23	D	634	Total O 646 646	2	12

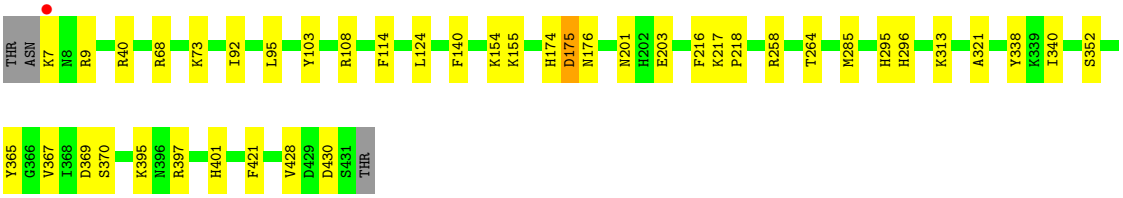
3 Residue-property plots (i)

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

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

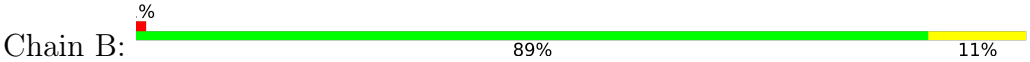
Chain A:

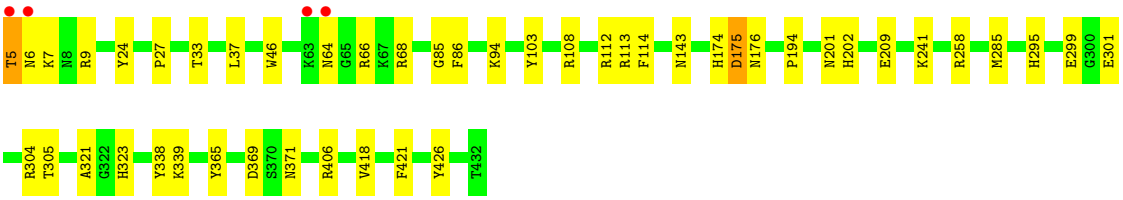




• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

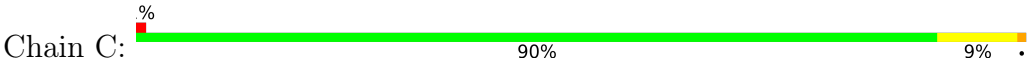
Chain B:

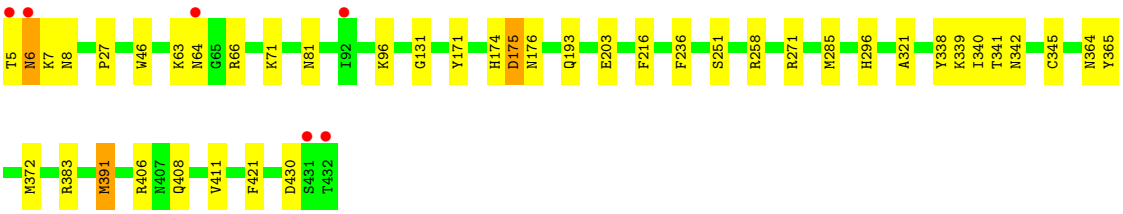




• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

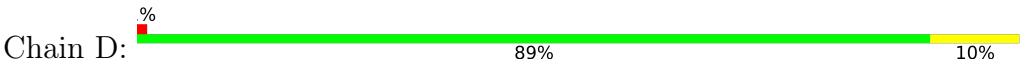
Chain C:

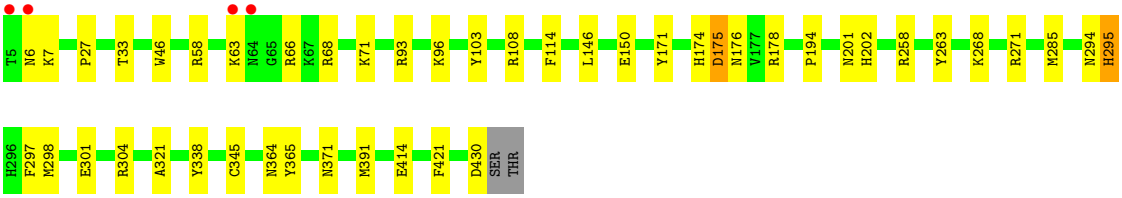




• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

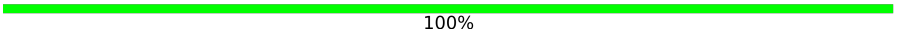
Chain D:





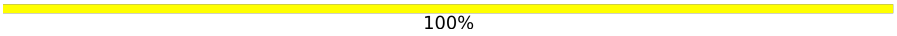
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



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

Chain K:



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

Chain Q:

• 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

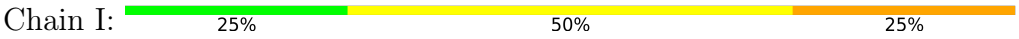
Chain F:

• 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:

• 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:



• 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:

• 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:

• 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:

• 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

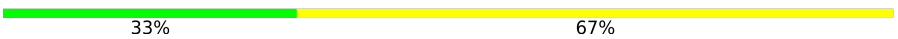
Chain V:

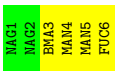
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• 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

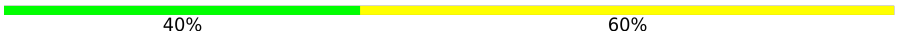
Chain J:





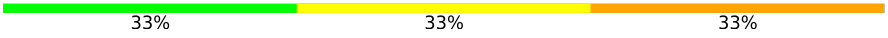
• Molecule 6: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



• 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:



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

Chain O:

• 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:

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

Chain T:

4 Data and refinement statistics (i)

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) 98.6 (19.96-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [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 (5.01%)	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)	0.31 , 59.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FLC, R9X, GOL, PGE, BMA, ZN, SO4, NA, FE, FUC, EDO, DMS, MAN, 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	0.40	0/3722	0.59	0/5057
1	B	0.39	0/3687	0.59	0/5011
1	C	0.39	0/3734	0.60	0/5076
1	D	0.39	0/3736	0.60	0/5076
All	All	0.39	0/14879	0.60	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

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	44	0
1	B	3558	0	3379	51	0
1	C	3584	0	3423	39	0
1	D	3586	0	3442	43	0
2	E	28	0	25	0	0
2	K	28	0	25	1	0
2	Q	28	0	25	1	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	6	0
14	A	17	0	23	6	0
14	B	20	0	28	3	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	4	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	13	0
18	B	60	0	80	7	0
18	C	66	0	88	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	D	90	0	120	11	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	7	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	1	0
23	A	720	0	0	12	0
23	B	658	0	0	15	0
23	C	682	0	0	19	0
23	D	646	0	0	12	0
All	All	18800	0	15003	224	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 (224) 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)
20:B:531[A]:R9X:O26	23:B:601:HOH:O	1.78	1.01
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
18:B:527:GOL:O2	23:B:603:HOH:O	2.09	0.70
1:A:7:LYS:HE3	18:A:531:GOL:H11	1.73	0.70
1:D:271[B]:ARG:NH1	16:D:508:SO4:O2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
18:A:523:GOL:HO2	18:A:531:GOL:HO1	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:D:294[B]:ASN:HB3	13:D:503:FLC:HA1	1.78	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
1:A:367[B]:VAL:HG11	18:A:531:GOL:H2	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:131:GLY:HA2	1:C:391[B]:MET:HE3	1.86	0.58
1:B:258[A]:ARG:NH1	23:B:624:HOH:O	2.37	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
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
1:A:295:HIS:HE1	20:A:532[A]:R9X:C16	2.19	0.54
16:C:615:SO4:O1	18:C:625:GOL:O3	2.25	0.54
1:B:338:TYR:CD2	14:D:504:PGE:H12	2.41	0.54
1:B:241:LYS:NZ	23:B:622:HOH:O	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:341:THR:OG1	18:C:620:GOL:H12	2.12	0.49
1:D:294[B]:ASN:OD1	18:D:534:GOL:O3	2.17	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: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
13:D:503:FLC:HG1	23:D:631[B]:HOH:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:HIS:CE1	20:B:531[A]:R9X:C22	2.99	0.46
1:B:258[A]:ARG:NH2	18:B:527:GOL:H12	2.31	0.46
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:C:174:HIS:O	1:C:175:ASP:C	2.55	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:D:174:HIS:O	1:D:175:ASP:C	2.55	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
1:A:174:HIS:O	1:A:175:ASP:C	2.56	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:D:295[A]:HIS:HB2	13:D:503:FLC:HG2	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:174:HIS:O	1:B:175:ASP:C	2.57	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: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:B:94:LYS:NZ	23:B:640:HOH:O	2.54	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: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:HG23	23:C:950:HOH:O	2.21	0.40
1:C:5:THR:O	1:C:6:ASN:HB2	2.22	0.40
1:C:63:LYS:NZ	23:C:708:HOH:O	2.37	0.40
1:C:236:PHE:O	1:C:251:SER:HB2	2.21	0.40
1:D:298:MET:HE2	1:D:301:GLU:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	47	44
1	B	431/428 (101%)	412 (96%)	18 (4%)	1 (0%)	47	44
1	C	437/428 (102%)	415 (95%)	20 (5%)	2 (0%)	29	23
1	D	436/428 (102%)	414 (95%)	20 (5%)	2 (0%)	29	23
All	All	1739/1712 (102%)	1658 (95%)	75 (4%)	6 (0%)	34	37

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%)	384 (100%)	2 (0%)	88 92
1	B	382/377 (101%)	378 (99%)	4 (1%)	76 81
1	C	388/377 (103%)	385 (99%)	3 (1%)	81 86
1	D	387/377 (103%)	383 (99%)	4 (1%)	76 81
All	All	1543/1508 (102%)	1530 (99%)	13 (1%)	84 86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	LEU
1	A	176	ASN
1	B	5	THR
1	B	7	LYS
1	B	64	ASN
1	B	176	ASN
1	C	176	ASN
1	C	391[A]	MET
1	C	391[B]	MET
1	D	66	ARG
1	D	176	ASN
1	D	295[A]	HIS
1	D	295[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	HIS
1	B	295	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.57	0	17,19,21	0.54	0
2	NAG	E	2	2	14,14,15	0.47	0	17,19,21	0.52	0
3	NAG	F	1	1,3	14,14,15	0.34	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.44	0	17,19,21	0.56	0
3	BMA	F	3	3	11,11,12	1.70	3 (27%)	15,15,17	1.47	3 (20%)
3	MAN	F	4	3	11,11,12	1.49	2 (18%)	15,15,17	1.89	5 (33%)
3	MAN	F	5	3	11,11,12	1.00	1 (9%)	15,15,17	1.27	2 (13%)
3	FUC	F	6	3	10,10,11	0.77	0	14,14,16	0.73	0
4	NAG	G	1	1,4	14,14,15	0.50	0	17,19,21	0.64	0
4	NAG	G	2	4	14,14,15	0.49	0	17,19,21	0.76	1 (5%)
4	BMA	G	3	4	11,11,12	0.78	0	15,15,17	0.82	0
4	FUC	G	4	4	10,10,11	0.60	0	14,14,16	1.02	1 (7%)
5	NAG	H	1	1,5	14,14,15	0.47	0	17,19,21	0.68	0
5	NAG	H	2	5	14,14,15	0.28	0	17,19,21	0.50	0
5	BMA	H	3	5	11,11,12	1.17	0	15,15,17	1.01	1 (6%)
5	MAN	H	4	5	11,11,12	0.63	0	15,15,17	1.36	2 (13%)
5	MAN	H	5	5	11,11,12	0.99	1 (9%)	15,15,17	1.21	2 (13%)
5	FUC	H	6	5	10,10,11	0.92	0	14,14,16	0.90	0
4	NAG	I	1	1,4	14,14,15	0.39	0	17,19,21	0.73	1 (5%)
4	NAG	I	2	4	14,14,15	0.38	0	17,19,21	0.54	0
4	BMA	I	3	4	11,11,12	1.65	2 (18%)	15,15,17	1.86	4 (26%)
4	FUC	I	4	4	10,10,11	0.55	0	14,14,16	1.08	1 (7%)
5	NAG	J	1	1,5	14,14,15	0.50	0	17,19,21	0.57	0
5	NAG	J	2	5	14,14,15	0.44	0	17,19,21	0.53	0
5	BMA	J	3	5	11,11,12	1.18	2 (18%)	15,15,17	1.22	3 (20%)
5	MAN	J	4	5	11,11,12	1.11	1 (9%)	15,15,17	1.35	3 (20%)
5	MAN	J	5	5	11,11,12	0.83	0	15,15,17	1.21	1 (6%)
5	FUC	J	6	5	10,10,11	0.96	0	14,14,16	1.16	1 (7%)
2	NAG	K	1	1,2	14,14,15	0.49	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	K	2	2	14,14,15	0.17	0	17,19,21	0.88	1 (5%)
6	NAG	L	1	1,6	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
6	NAG	L	2	6	14,14,15	0.31	0	17,19,21	0.55	0
6	BMA	L	3	6	11,11,12	0.97	0	15,15,17	0.87	0
6	MAN	L	4	6	11,11,12	1.17	2 (18%)	15,15,17	1.15	2 (13%)
6	FUC	L	5	6	10,10,11	0.74	0	14,14,16	0.95	1 (7%)
7	NAG	M	1	1,7	14,14,15	0.36	0	17,19,21	0.63	0
7	NAG	M	2	7	14,14,15	0.92	1 (7%)	17,19,21	1.53	1 (5%)
7	BMA	M	3	7	11,11,12	1.74	3 (27%)	15,15,17	1.99	4 (26%)
4	NAG	N	1	1,4	14,14,15	0.55	0	17,19,21	0.66	0
4	NAG	N	2	4	14,14,15	0.41	0	17,19,21	0.70	0
4	BMA	N	3	4	11,11,12	1.63	3 (27%)	15,15,17	1.83	3 (20%)
4	FUC	N	4	4	10,10,11	0.66	0	14,14,16	1.14	1 (7%)
8	NAG	O	1	1,8	14,14,15	0.79	1 (7%)	17,19,21	1.04	2 (11%)
8	NAG	O	2	8	14,14,15	0.54	0	17,19,21	0.62	0
4	NAG	P	1	1,4	14,14,15	0.48	0	17,19,21	0.66	0
4	NAG	P	2	4	14,14,15	0.60	0	17,19,21	0.67	0
4	BMA	P	3	4	11,11,12	1.38	2 (18%)	15,15,17	1.71	2 (13%)
4	FUC	P	4	4	10,10,11	0.56	0	14,14,16	0.73	0
2	NAG	Q	1	1,2	14,14,15	0.30	0	17,19,21	0.53	0
2	NAG	Q	2	2	14,14,15	0.24	0	17,19,21	0.65	1 (5%)
9	NAG	R	1	9,1	14,14,15	0.51	0	17,19,21	0.59	0
9	NAG	R	2	9	14,14,15	0.40	0	17,19,21	0.56	0
9	BMA	R	3	9	10,10,12	0.87	0	14,14,17	0.88	0
9	FUC	R	4	9	10,10,11	0.88	0	14,14,16	1.04	0
4	NAG	S	1	1,4	14,14,15	0.58	0	17,19,21	0.56	0
4	NAG	S	2	4	14,14,15	0.54	0	17,19,21	0.70	0
4	BMA	S	3	4	11,11,12	1.45	2 (18%)	15,15,17	1.47	1 (6%)
4	FUC	S	4	4	10,10,11	0.81	0	14,14,16	0.84	0
10	NAG	T	1	1,10	14,14,15	0.46	0	17,19,21	0.65	0
10	FUC	T	2	10	10,10,11	1.36	2 (20%)	14,14,16	1.87	3 (21%)
4	NAG	V	1	1,4	14,14,15	0.46	0	17,19,21	0.57	0
4	NAG	V	2	4	14,14,15	0.40	0	17,19,21	0.55	0
4	BMA	V	3	4	11,11,12	0.77	1 (9%)	15,15,17	0.97	0
4	FUC	V	4	4	10,10,11	0.50	0	14,14,16	0.74	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	1/2/19/22	1/1/1/1
3	FUC	F	6	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
4	FUC	G	4	4	-	-	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	FUC	H	6	5	-	-	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1
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	9,1	-	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 (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	3	BMA	C1-C2	4.01	1.61	1.52
7	M	3	BMA	C1-C2	3.80	1.60	1.52
4	I	3	BMA	C1-C2	3.79	1.60	1.52
3	F	4	MAN	C2-C3	3.71	1.58	1.52
3	F	3	BMA	C1-C2	3.65	1.60	1.52
4	P	3	BMA	C1-C2	3.32	1.59	1.52
7	M	2	NAG	O5-C1	3.26	1.48	1.43
7	M	3	BMA	O5-C1	3.20	1.48	1.43
4	S	3	BMA	C1-C2	2.99	1.59	1.52
10	T	2	FUC	C4-C5	2.94	1.59	1.52
4	I	3	BMA	O5-C1	2.88	1.48	1.43
8	O	1	NAG	O5-C1	2.83	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	C2-C3	2.79	1.56	1.52
4	P	3	BMA	O5-C1	2.55	1.47	1.43
3	F	3	BMA	O2-C2	2.53	1.48	1.43
3	F	4	MAN	C1-C2	2.51	1.57	1.52
5	H	5	MAN	C1-C2	2.49	1.57	1.52
4	N	3	BMA	O5-C1	2.49	1.47	1.43
6	L	4	MAN	C1-C2	2.48	1.57	1.52
5	J	4	MAN	C1-C2	2.34	1.57	1.52
7	M	3	BMA	C2-C3	2.21	1.55	1.52
3	F	5	MAN	C1-C2	2.20	1.57	1.52
4	V	3	BMA	C1-C2	2.18	1.57	1.52
5	J	3	BMA	C1-C2	2.18	1.57	1.52
6	L	4	MAN	O5-C5	2.17	1.47	1.43
10	T	2	FUC	O5-C5	2.16	1.48	1.43
5	J	3	BMA	C4-C3	2.08	1.57	1.52
4	N	3	BMA	O5-C5	2.03	1.47	1.43
4	S	3	BMA	O5-C1	2.02	1.46	1.43

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	3	BMA	C1-O5-C5	5.88	120.16	112.19
7	M	2	NAG	C1-O5-C5	5.81	120.07	112.19
4	P	3	BMA	C1-O5-C5	5.29	119.36	112.19
4	I	3	BMA	C1-O5-C5	5.11	119.11	112.19
4	N	3	BMA	C1-O5-C5	5.08	119.07	112.19
3	F	4	MAN	C1-C2-C3	4.89	115.67	109.67
10	T	2	FUC	O5-C5-C4	4.67	117.90	109.52
4	S	3	BMA	C1-O5-C5	4.58	118.39	112.19
5	H	4	MAN	C1-O5-C5	4.36	118.10	112.19
5	J	5	MAN	C1-O5-C5	3.60	117.07	112.19
10	T	2	FUC	C3-C4-C5	3.57	115.33	109.77
2	K	2	NAG	C1-O5-C5	3.33	116.71	112.19
3	F	3	BMA	C1-C2-C3	3.27	113.68	109.67
3	F	3	BMA	O2-C2-C1	3.10	115.49	109.15
8	O	1	NAG	O3-C3-C2	-2.98	103.31	109.47
4	I	3	BMA	C1-C2-C3	2.92	113.25	109.67
5	J	4	MAN	C1-C2-C3	-2.91	106.09	109.67
5	J	3	BMA	C1-O5-C5	2.78	115.96	112.19
4	N	3	BMA	C1-C2-C3	2.76	113.06	109.67
10	T	2	FUC	C1-O5-C5	2.76	119.03	112.78
3	F	5	MAN	C1-C2-C3	-2.66	106.40	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4	MAN	C2-C3-C4	2.60	115.40	110.89
7	M	3	BMA	C1-C2-C3	2.55	112.81	109.67
5	H	5	MAN	C1-O5-C5	2.54	115.63	112.19
5	H	4	MAN	O2-C2-C3	-2.51	105.10	110.14
4	P	3	BMA	C1-C2-C3	2.43	112.65	109.67
5	J	4	MAN	O2-C2-C1	2.39	114.05	109.15
3	F	5	MAN	O2-C2-C1	2.38	114.01	109.15
4	I	3	BMA	O5-C1-C2	2.33	114.38	110.77
7	M	3	BMA	O5-C1-C2	2.33	114.36	110.77
3	F	4	MAN	O2-C2-C3	-2.30	105.52	110.14
6	L	4	MAN	O2-C2-C3	-2.30	105.52	110.14
6	L	5	FUC	C1-O5-C5	2.30	117.99	112.78
3	F	4	MAN	C1-O5-C5	2.29	115.30	112.19
6	L	4	MAN	C1-O5-C5	2.28	115.28	112.19
8	O	1	NAG	C1-O5-C5	2.27	115.26	112.19
5	J	4	MAN	O2-C2-C3	-2.26	105.61	110.14
7	M	3	BMA	C3-C4-C5	-2.25	106.22	110.24
4	I	1	NAG	C1-O5-C5	2.23	115.21	112.19
5	H	3	BMA	C1-O5-C5	2.19	115.15	112.19
4	G	2	NAG	O4-C4-C3	-2.18	105.32	110.35
5	H	5	MAN	O2-C2-C3	-2.15	105.82	110.14
3	F	3	BMA	C2-C3-C4	2.13	114.58	110.89
5	J	3	BMA	O5-C1-C2	2.13	114.06	110.77
4	N	3	BMA	O5-C1-C2	2.12	114.05	110.77
4	N	4	FUC	C1-O5-C5	2.10	117.55	112.78
4	I	3	BMA	C3-C4-C5	-2.10	106.49	110.24
5	J	6	FUC	O2-C2-C1	2.09	113.44	109.15
3	F	4	MAN	O5-C1-C2	2.08	113.98	110.77
2	Q	2	NAG	C1-O5-C5	2.07	115.00	112.19
6	L	1	NAG	C1-O5-C5	2.05	114.97	112.19
4	I	4	FUC	C1-O5-C5	2.04	117.39	112.78
4	G	4	FUC	C1-O5-C5	2.03	117.38	112.78
5	J	3	BMA	O2-C2-C1	2.02	113.28	109.15

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
3	F	3	BMA	C4-C5-C6-O6
4	G	2	NAG	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
9	R	2	NAG	C4-C5-C6-O6
10	T	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
6	L	4	MAN	C4-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
4	I	2	NAG	O5-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
4	V	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
10	T	1	NAG	O5-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	K	2	NAG	O5-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
4	V	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-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
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:

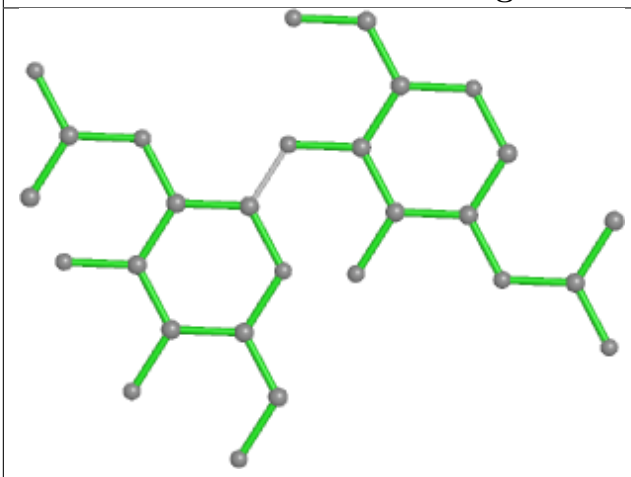
Mol	Chain	Res	Type	Atoms
4	S	3	BMA	C1-C2-C3-C4-C5-O5
6	L	4	MAN	C1-C2-C3-C4-C5-O5
3	F	5	MAN	C1-C2-C3-C4-C5-O5
5	J	4	MAN	C1-C2-C3-C4-C5-O5

8 monomers are involved in 9 short contacts:

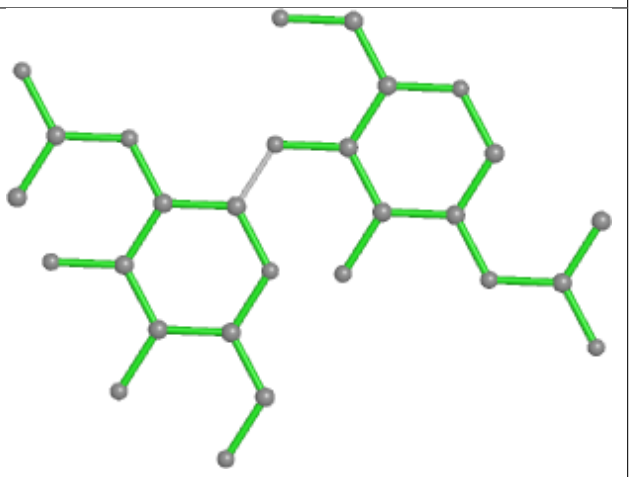
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
2	Q	2	NAG	1	0
4	I	1	NAG	2	0
7	M	2	NAG	1	0
2	K	1	NAG	1	0
3	F	4	MAN	1	0
9	R	2	NAG	1	0
9	R	1	NAG	1	0

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

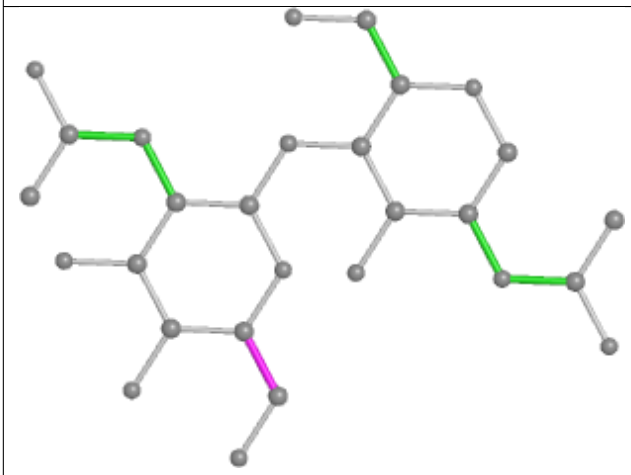
Oligosaccharide Chain E



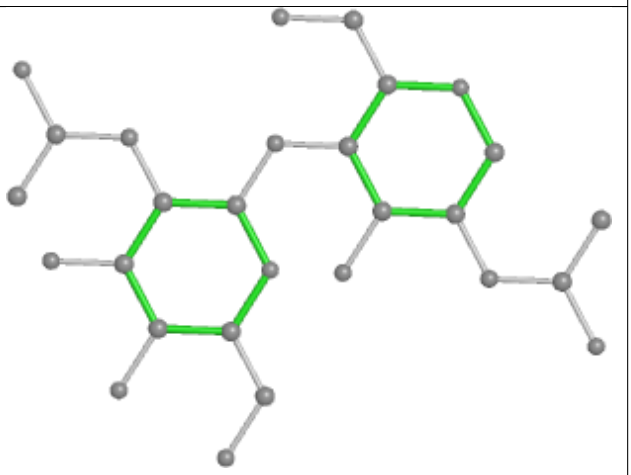
Bond lengths



Bond angles

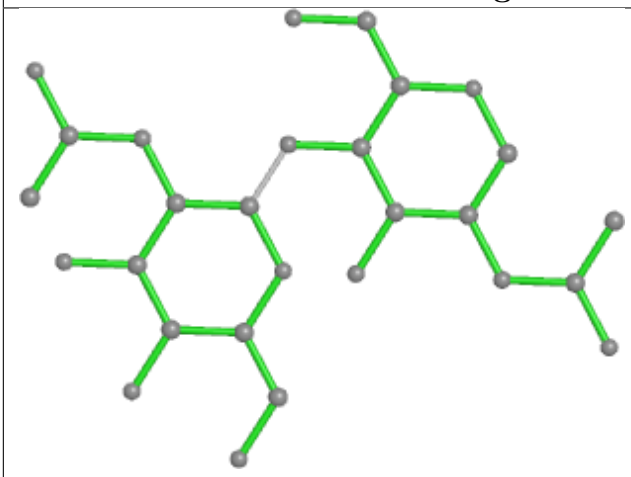


Torsions

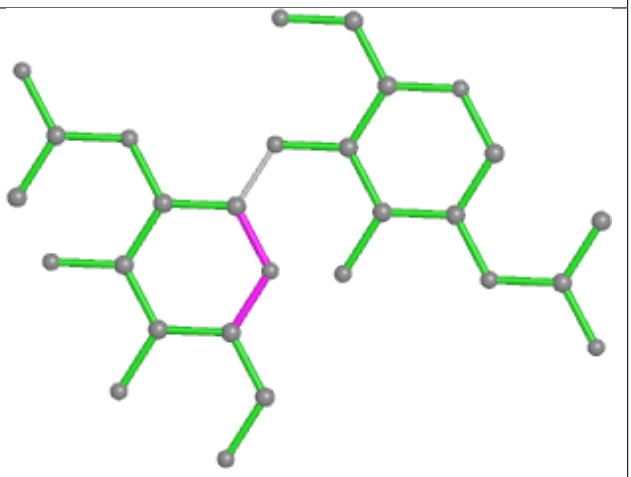


Rings

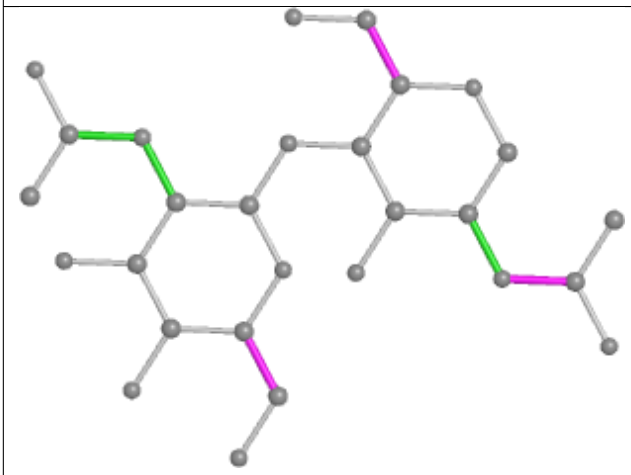
Oligosaccharide Chain K



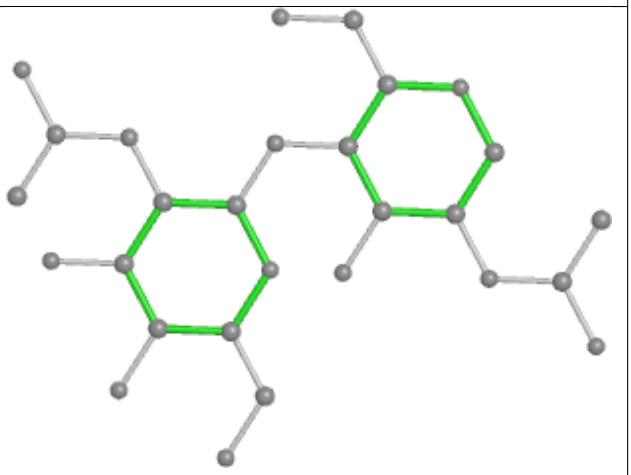
Bond lengths



Bond angles

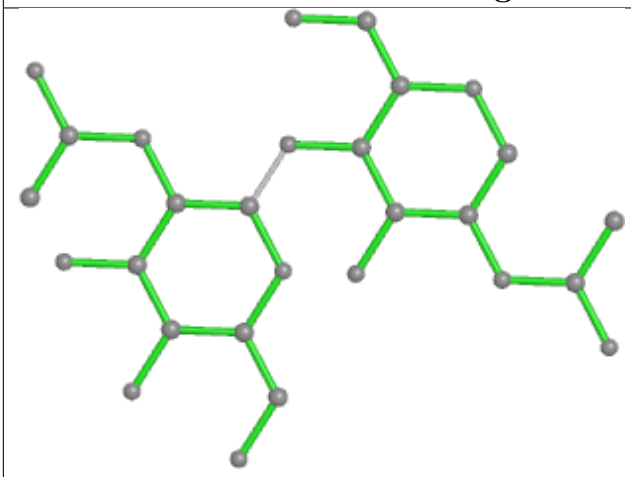


Torsions



Rings

Oligosaccharide Chain Q



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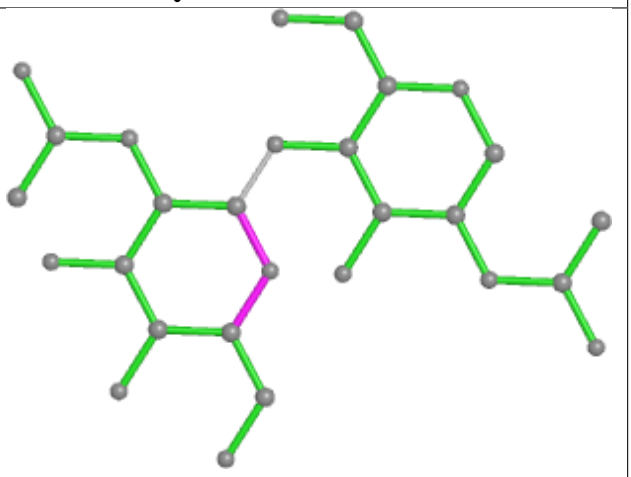
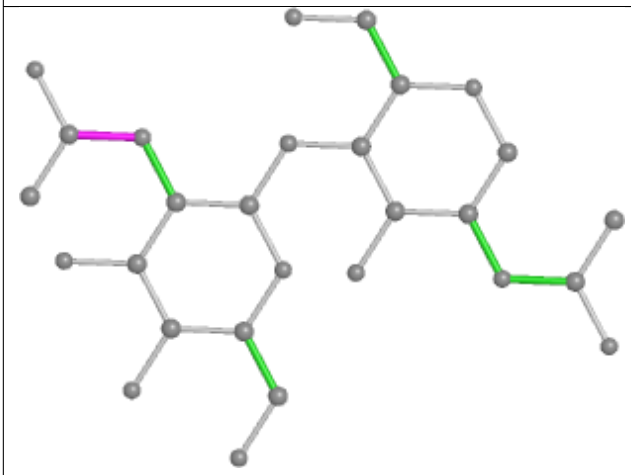


Bond angles



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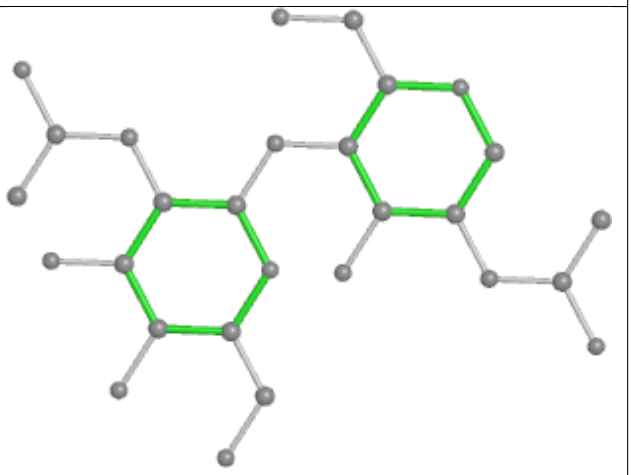
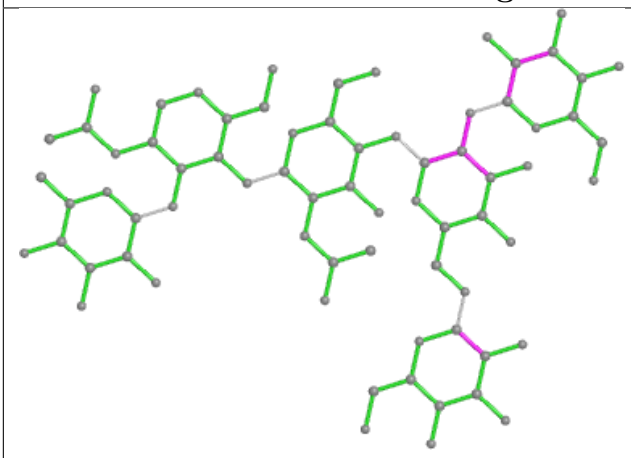


Rings

Oligosaccharide Chain F



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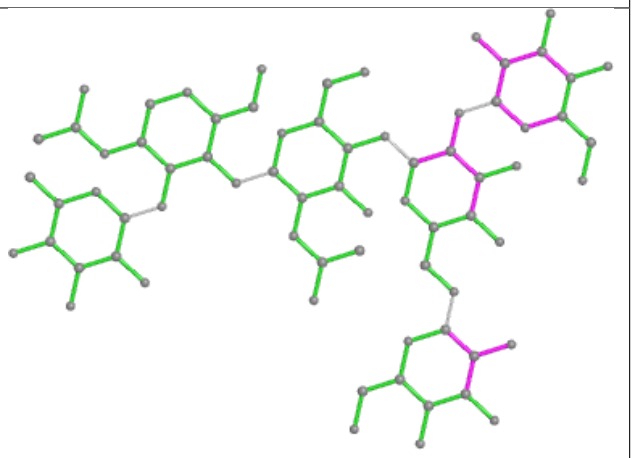
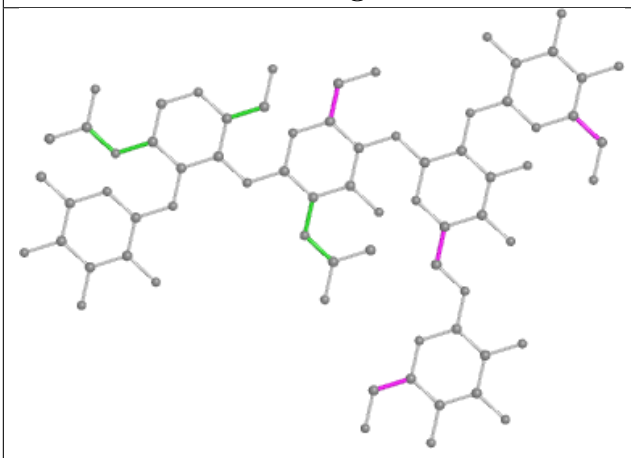


Bond angles



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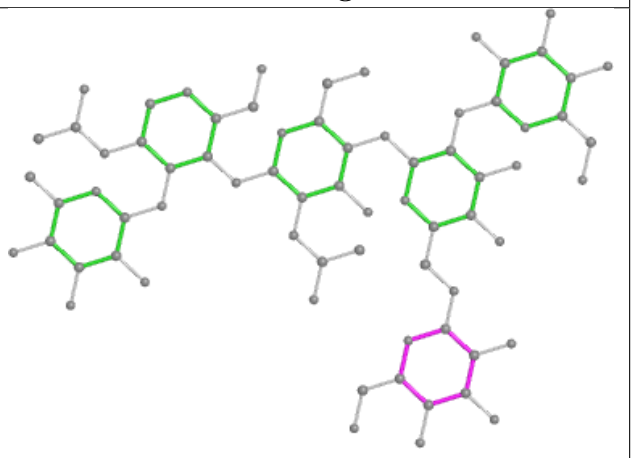
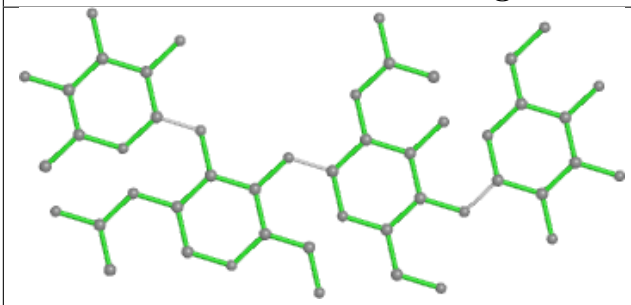
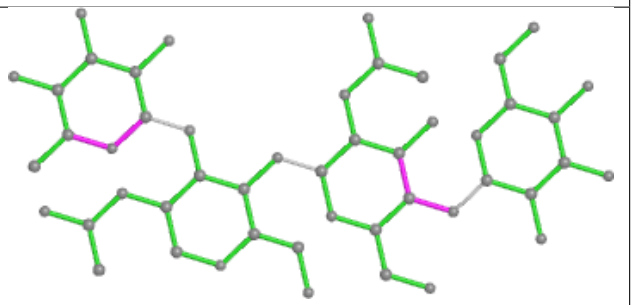


Rings

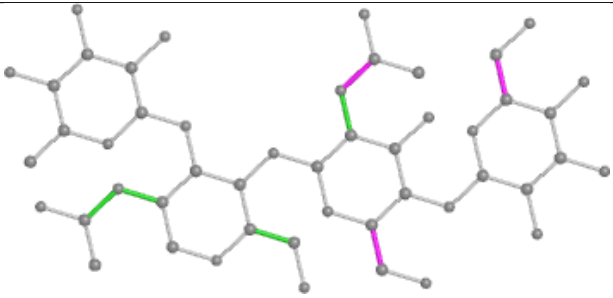
Oligosaccharide Chain G



Bond lengths



Bond angles



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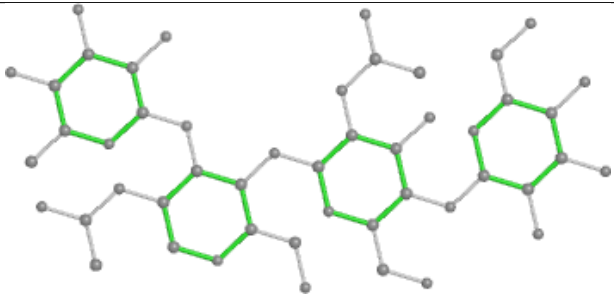
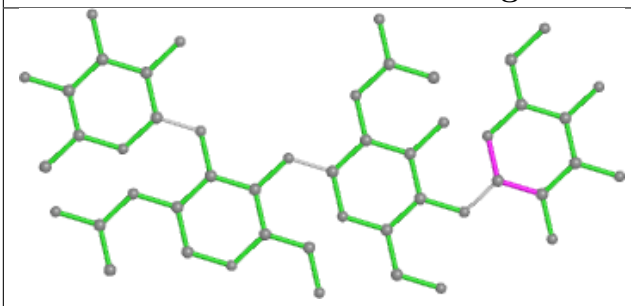


Rings

Oligosaccharide Chain I



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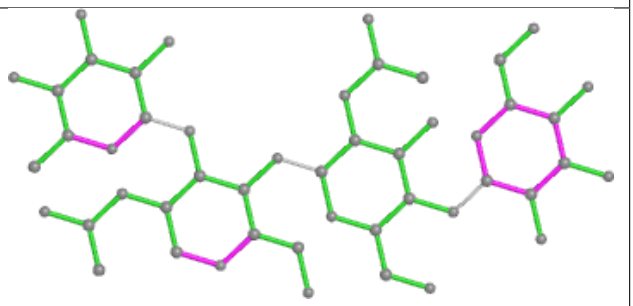

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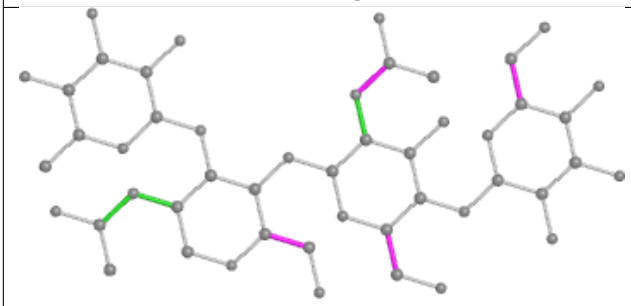

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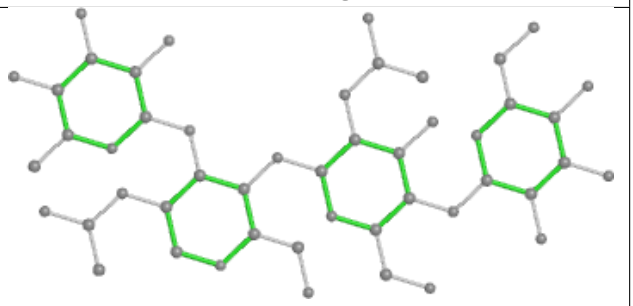
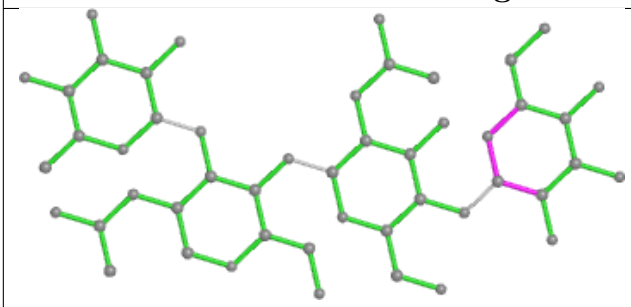


Rings

Oligosaccharide Chain N



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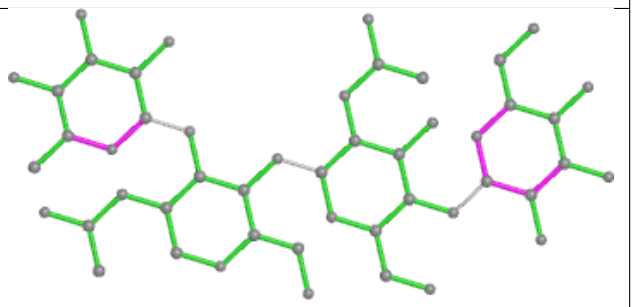
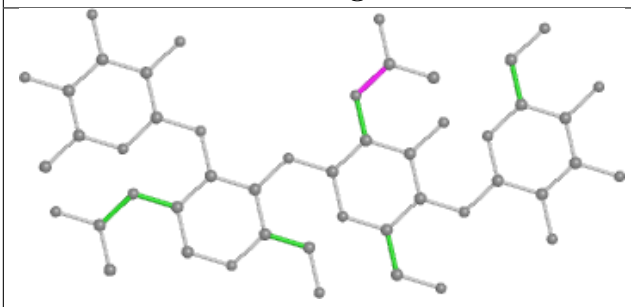


Bond angles



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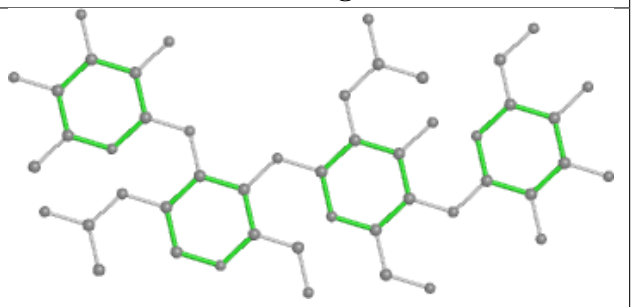
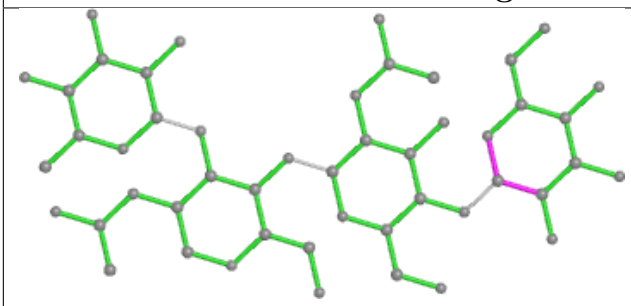
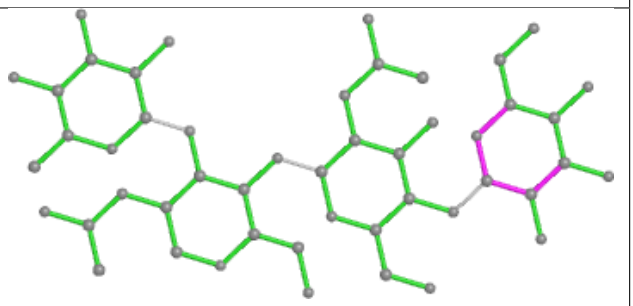


Rings

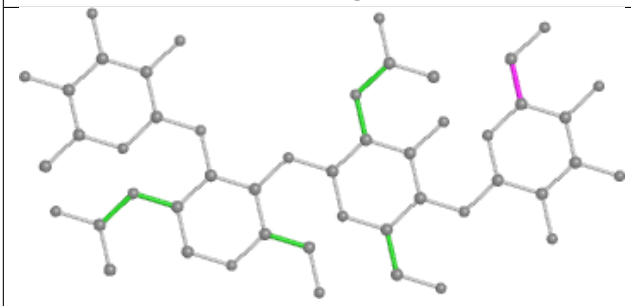
Oligosaccharide Chain P



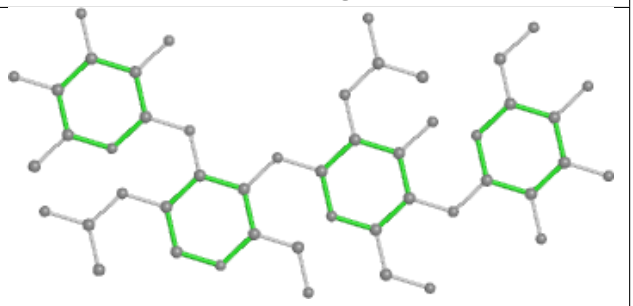
Bond lengths



Bond angles

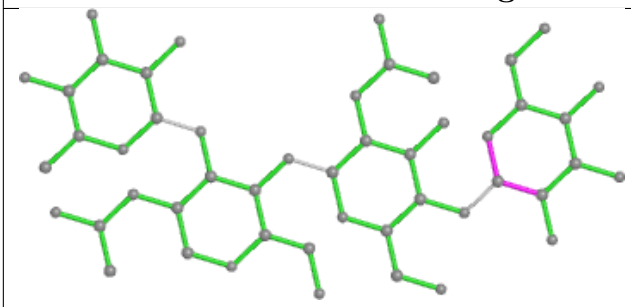


Torsions



Rings

Oligosaccharide Chain S



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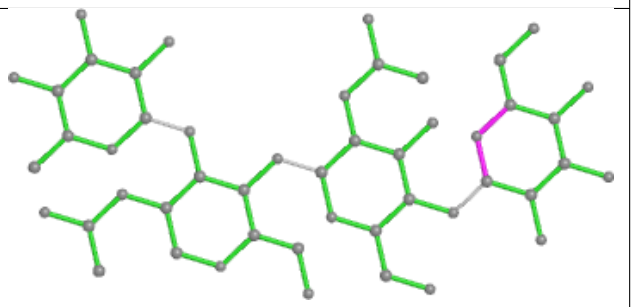
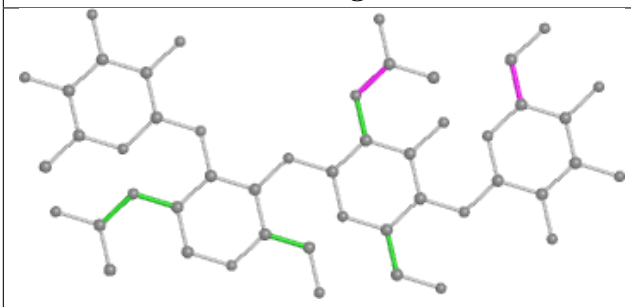
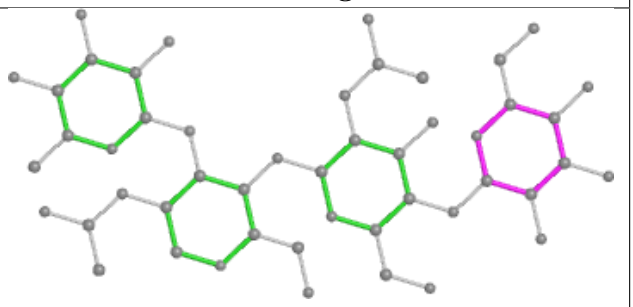


Bond angles

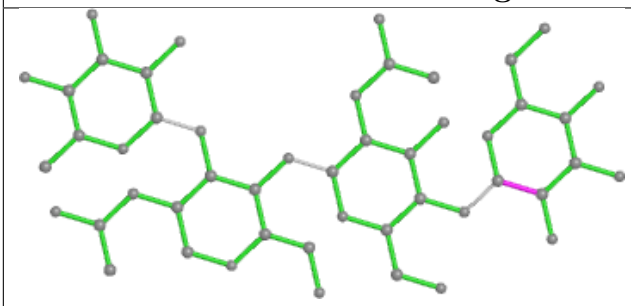


Torsions



Rings

Oligosaccharide Chain V



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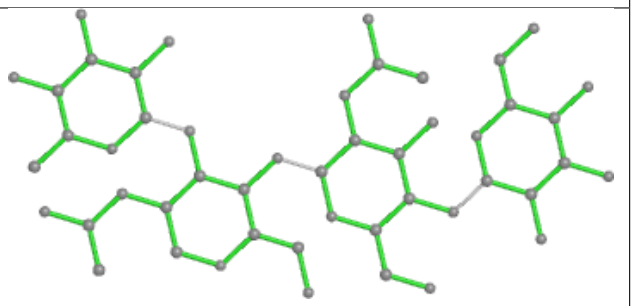
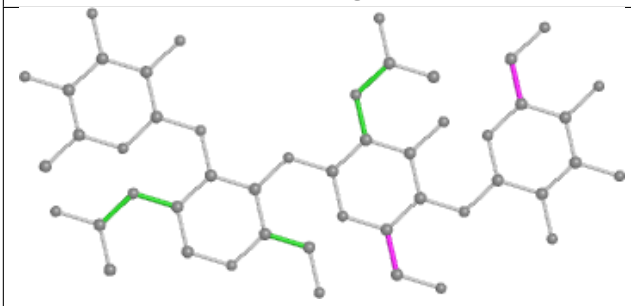


Bond angles



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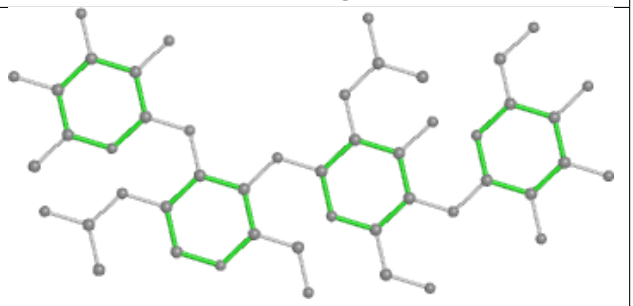
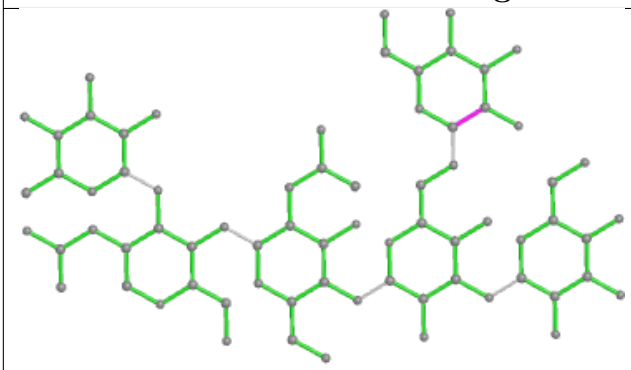


Rings

Oligosaccharide Chain H



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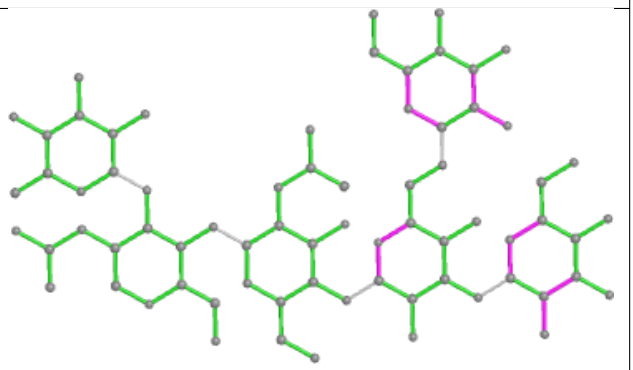
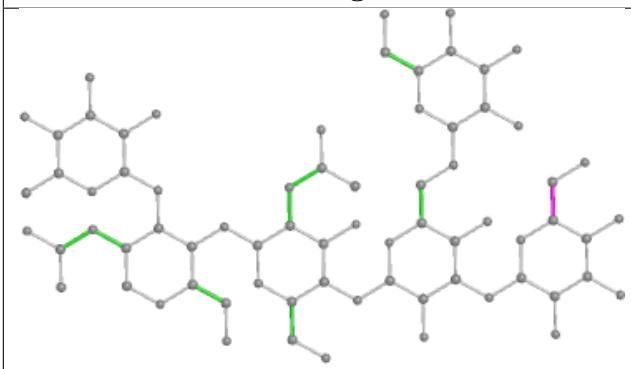


Bond angles



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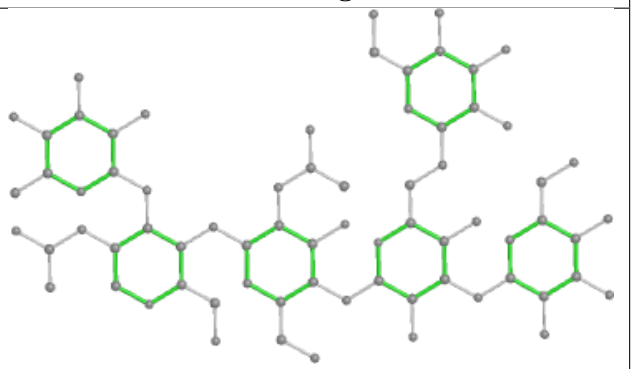
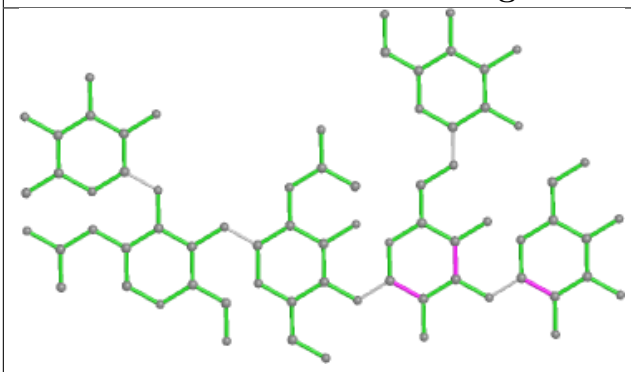


Rings

Oligosaccharide Chain J



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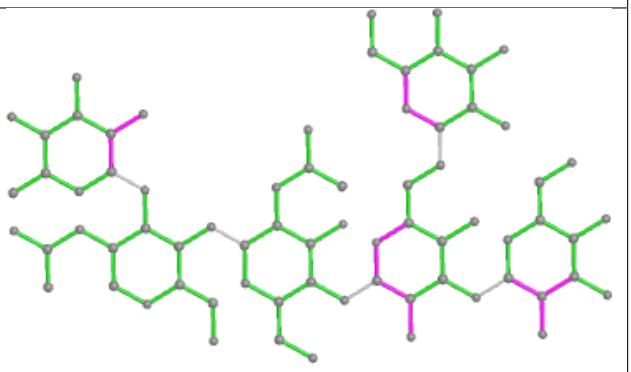
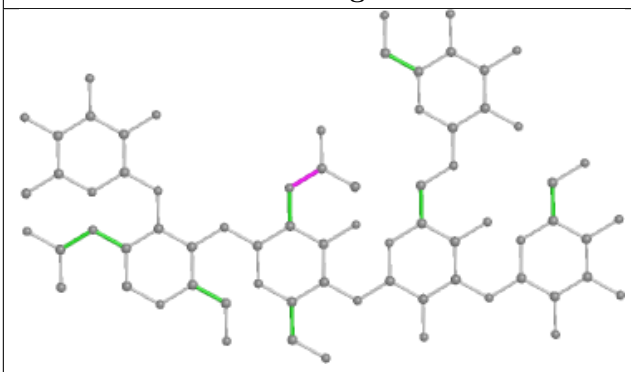


Bond angles



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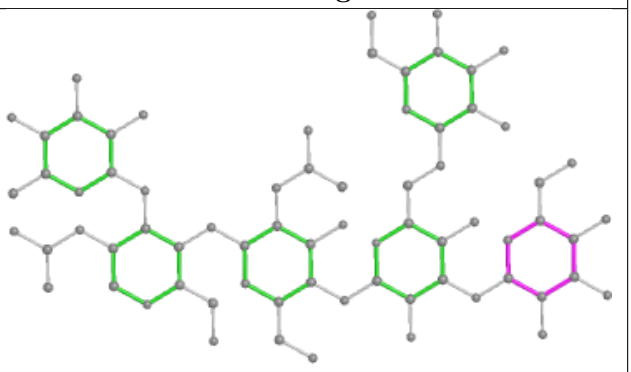
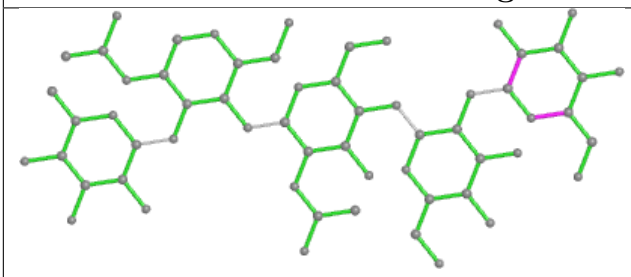


Rings

Oligosaccharide Chain L



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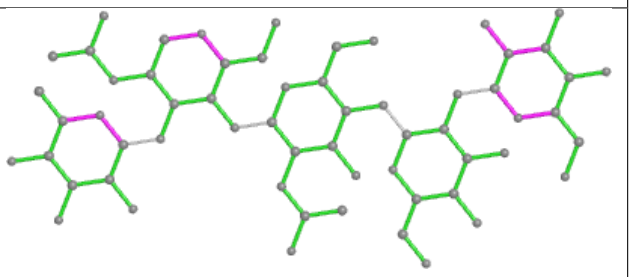
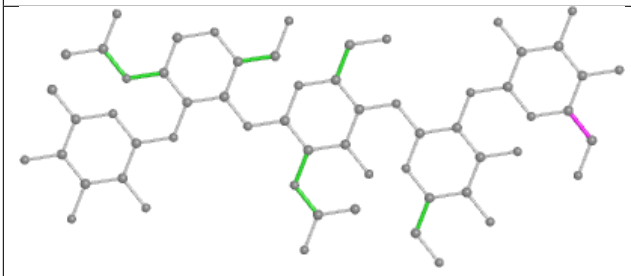


Bond angles



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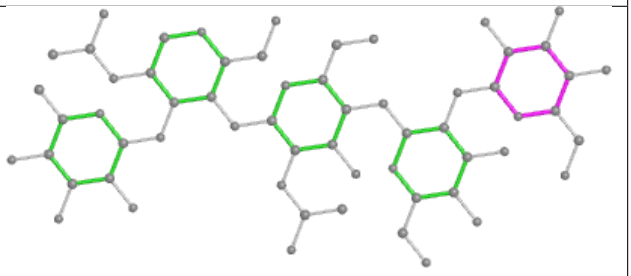
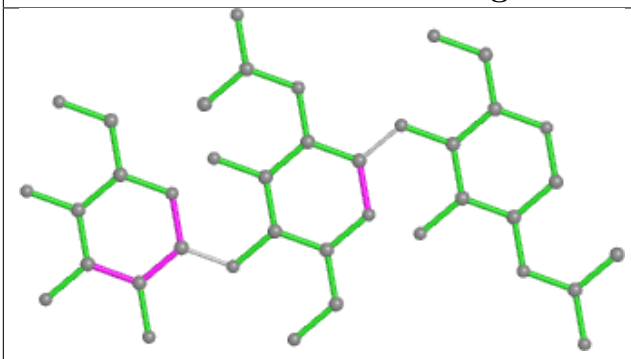
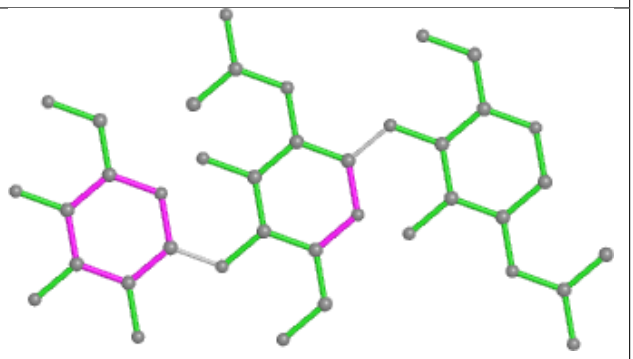


Rings

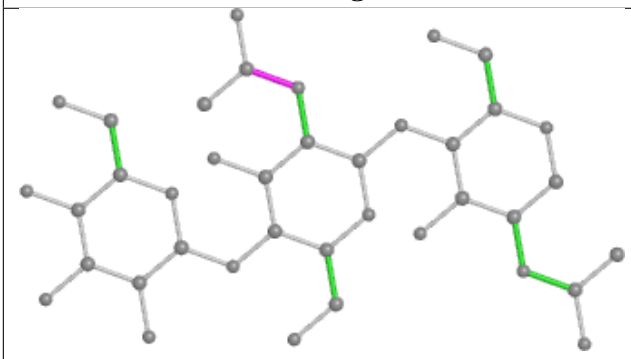
Oligosaccharide Chain M



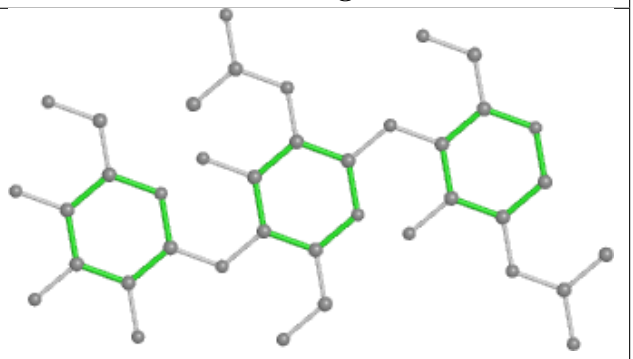
Bond lengths



Bond angles

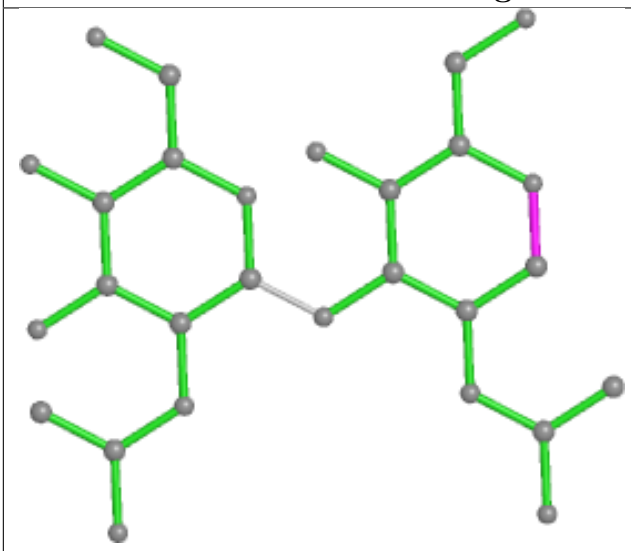


Torsions

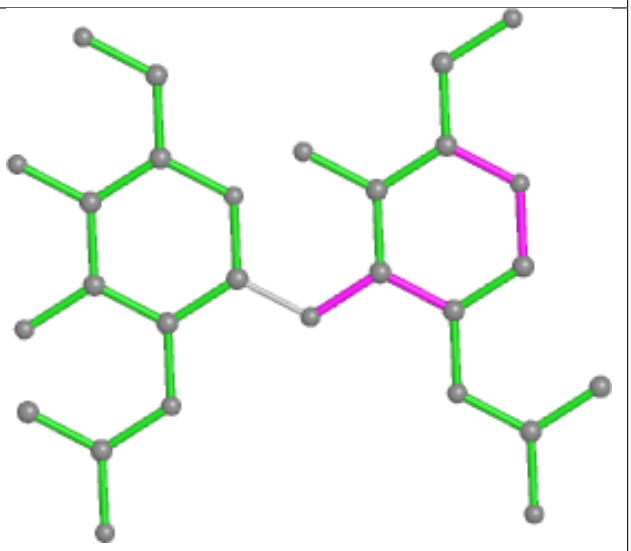


Rings

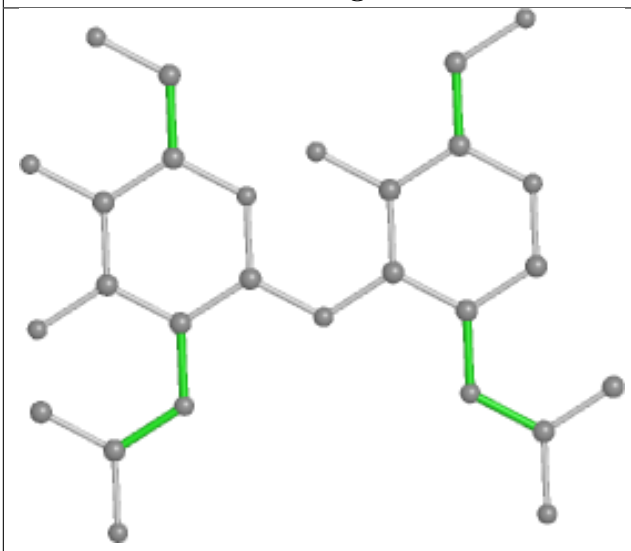
Oligosaccharide Chain O



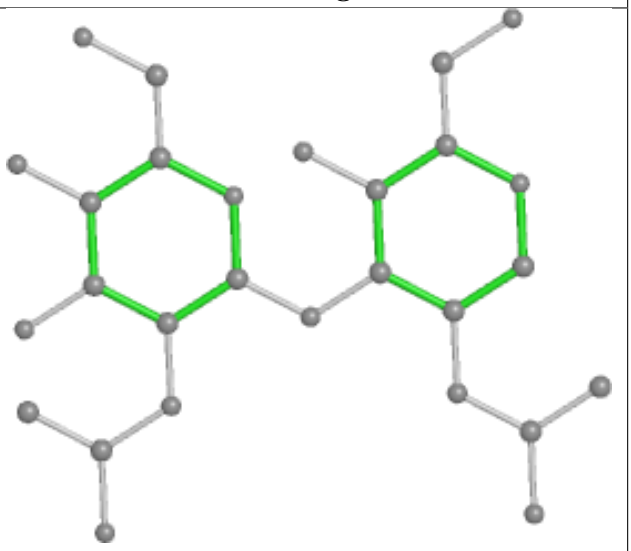
Bond lengths



Bond angles

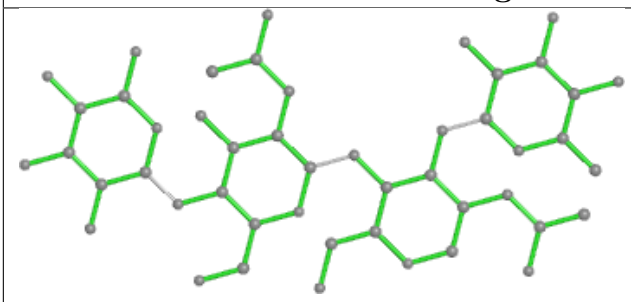


Torsions

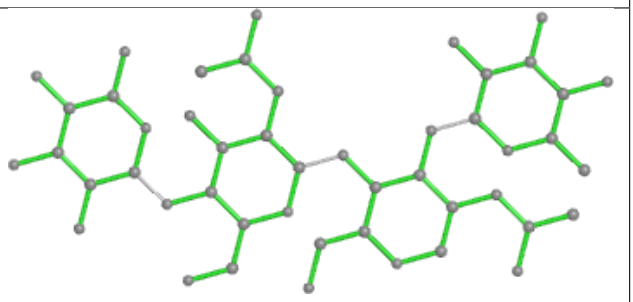


Rings

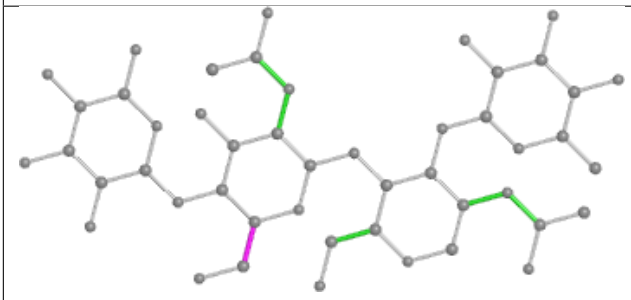
Oligosaccharide Chain R



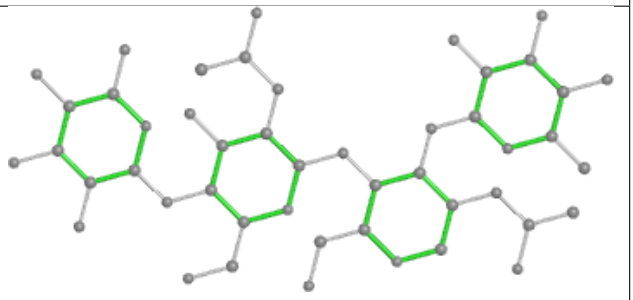
Bond lengths



Bond angles

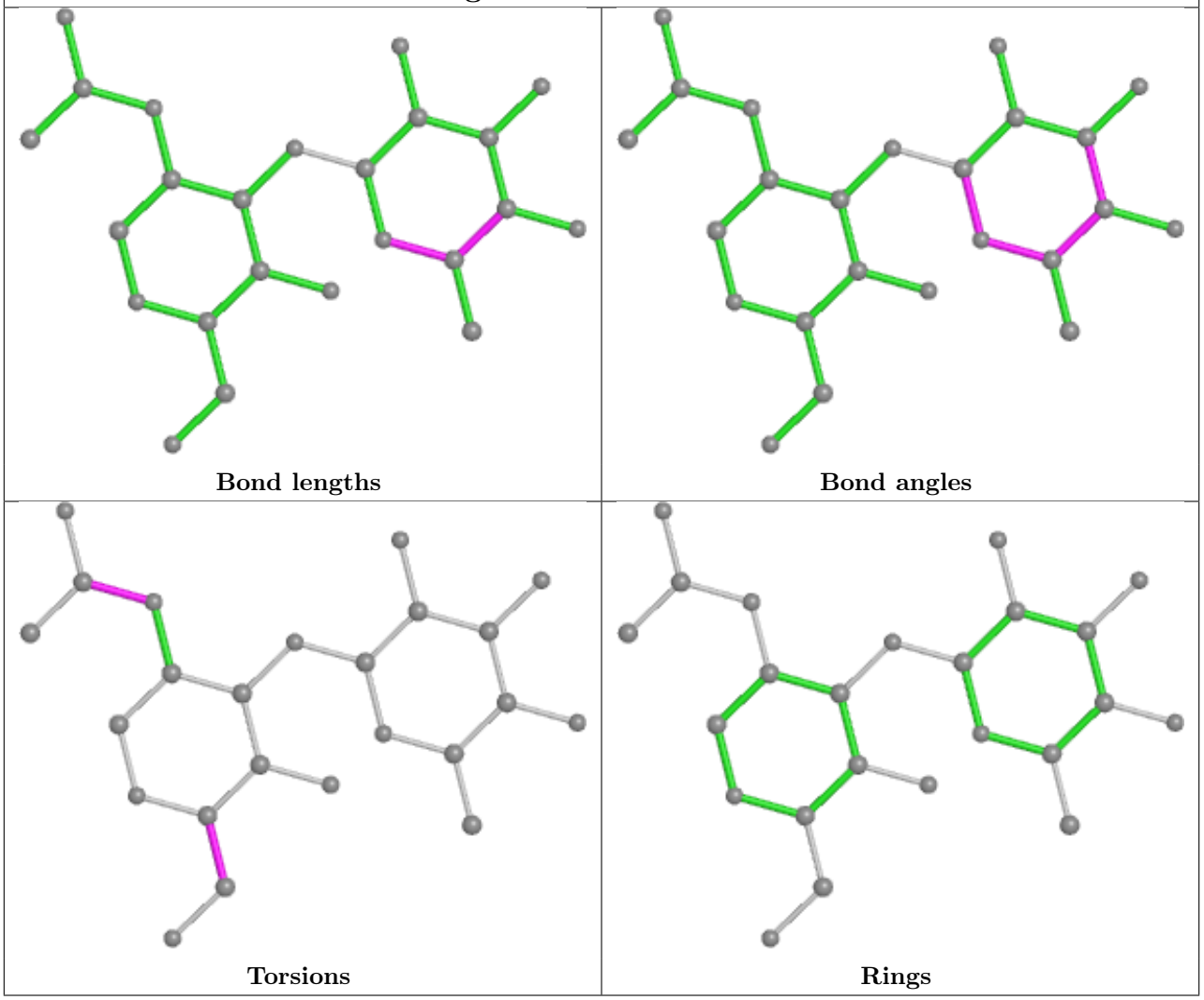


Torsions



Rings

Oligosaccharide Chain T



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	$\#\|Z\| > 2$
17	EDO	A	514	-	3,3,3	0.37	0	2,2,2	0.44	0
18	GOL	B	521	-	5,5,5	1.08	1 (20%)	5,5,5	1.00	0
16	SO4	A	510	-	4,4,4	0.12	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	R9X	A	532[A]	-	28,28,28	1.59	5 (17%)	35,37,37	2.64	9 (25%)
16	SO4	C	608	-	4,4,4	0.19	0	6,6,6	0.44	0
18	GOL	B	524	-	5,5,5	0.77	0	5,5,5	1.04	0
16	SO4	D	508	-	4,4,4	0.14	0	6,6,6	0.19	0
18	GOL	D	523	-	5,5,5	0.85	0	5,5,5	1.04	0
16	SO4	A	508	-	4,4,4	0.17	0	6,6,6	0.25	0
16	SO4	B	514	-	4,4,4	0.14	0	6,6,6	0.07	0
16	SO4	C	610	-	4,4,4	0.15	0	6,6,6	0.12	0
16	SO4	A	511	-	4,4,4	0.15	0	6,6,6	0.10	0
18	GOL	B	528	-	5,5,5	0.89	0	5,5,5	1.01	0
13	FLC	C	628	-	12,12,12	1.51	4 (33%)	17,17,17	2.28	4 (23%)
18	GOL	C	620	-	5,5,5	1.37	2 (40%)	5,5,5	0.90	0
16	SO4	C	615	-	4,4,4	0.16	0	6,6,6	0.15	0
18	GOL	C	619	-	5,5,5	0.90	0	5,5,5	0.90	0
13	FLC	C	602	-	12,12,12	1.03	2 (16%)	17,17,17	2.07	2 (11%)
18	GOL	A	518	-	5,5,5	0.89	0	5,5,5	1.20	1 (20%)
18	GOL	C	625	-	5,5,5	0.98	0	5,5,5	1.07	1 (20%)
14	PGE	B	504	-	9,9,9	0.26	0	8,8,8	0.38	0
18	GOL	C	618	-	5,5,5	1.07	0	5,5,5	1.09	1 (20%)
20	R9X	B	531[B]	-	28,28,28	1.51	3 (10%)	35,37,37	2.01	6 (17%)
15	NAG	C	616	1	14,14,15	0.28	0	17,19,21	0.50	0
18	GOL	C	621	-	5,5,5	0.97	0	5,5,5	0.97	0
18	GOL	D	520	-	5,5,5	1.06	1 (20%)	5,5,5	1.07	0
16	SO4	D	512	-	4,4,4	0.20	0	6,6,6	0.17	0
18	GOL	D	528	-	5,5,5	0.80	0	5,5,5	1.14	0
18	GOL	D	529	-	5,5,5	0.92	0	5,5,5	0.96	0
16	SO4	B	511	-	4,4,4	0.12	0	6,6,6	0.12	0
18	GOL	A	520	-	5,5,5	0.77	0	5,5,5	1.01	0
16	SO4	D	513	-	4,4,4	0.13	0	6,6,6	0.09	0
20	R9X	A	532[B]	-	28,28,28	1.53	6 (21%)	35,37,37	1.21	3 (8%)
18	GOL	D	534	-	5,5,5	0.91	0	5,5,5	1.01	0
18	GOL	A	527	-	5,5,5	0.91	0	5,5,5	0.90	0
18	GOL	A	521	-	5,5,5	0.93	0	5,5,5	1.04	0
16	SO4	B	509	-	4,4,4	0.14	0	6,6,6	0.13	0
16	SO4	D	509	-	4,4,4	0.13	0	6,6,6	0.06	0
13	FLC	B	507	-	12,12,12	1.56	4 (33%)	17,17,17	2.35	4 (23%)
18	GOL	A	524	-	5,5,5	0.82	0	5,5,5	0.96	0
16	SO4	D	515	-	4,4,4	0.15	0	6,6,6	0.13	0
16	SO4	D	514	-	4,4,4	0.12	0	6,6,6	0.13	0
15	NAG	A	506	1	14,14,15	1.11	1 (7%)	17,19,21	1.25	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	GOL	A	519	-	5,5,5	1.34	1 (20%)	5,5,5	0.82	0
14	PGE	B	508	-	9,9,9	0.29	0	8,8,8	0.45	0
18	GOL	D	522	-	5,5,5	0.86	0	5,5,5	0.92	0
14	PGE	C	604	-	9,9,9	0.31	0	8,8,8	0.29	0
16	SO4	C	613	-	4,4,4	0.14	0	6,6,6	0.05	0
13	FLC	B	506	-	12,12,12	1.15	2 (16%)	17,17,17	1.39	2 (11%)
16	SO4	B	513	-	4,4,4	0.13	0	6,6,6	0.09	0
14	PGE	D	504	-	9,9,9	0.27	0	8,8,8	0.57	0
13	FLC	A	503	-	12,12,12	0.23	0	17,17,17	0.56	0
13	FLC	C	627	-	12,12,12	1.89	6 (50%)	17,17,17	2.77	8 (47%)
18	GOL	A	523	-	5,5,5	0.83	0	5,5,5	1.15	0
13	FLC	B	503	-	12,12,12	1.49	4 (33%)	17,17,17	2.33	4 (23%)
18	GOL	D	525	-	5,5,5	0.80	0	5,5,5	1.02	0
18	GOL	D	533	-	5,5,5	0.81	0	5,5,5	1.16	0
16	SO4	A	509	-	4,4,4	0.16	0	6,6,6	0.24	0
20	R9X	D	535[B]	-	28,28,28	1.69	4 (14%)	35,37,37	1.13	3 (8%)
16	SO4	D	511	-	4,4,4	0.13	0	6,6,6	0.16	0
20	R9X	D	535[A]	-	28,28,28	1.43	4 (14%)	35,37,37	1.90	7 (20%)
13	FLC	C	603	-	12,12,12	1.50	4 (33%)	17,17,17	2.37	4 (23%)
16	SO4	B	512	-	4,4,4	0.20	0	6,6,6	0.18	0
13	FLC	A	530	-	12,12,12	1.58	4 (33%)	17,17,17	1.36	4 (23%)
15	NAG	D	506	1	14,14,15	0.50	0	17,19,21	0.43	0
16	SO4	A	513	-	4,4,4	0.15	0	6,6,6	0.08	0
18	GOL	B	525	-	5,5,5	0.84	0	5,5,5	1.02	0
14	PGE	A	507	-	6,6,9	0.23	0	5,5,8	0.84	0
18	GOL	A	522	-	5,5,5	0.90	0	5,5,5	0.95	0
18	GOL	C	630	-	5,5,5	1.06	0	5,5,5	1.02	0
18	GOL	A	531	-	5,5,5	0.91	0	5,5,5	1.19	0
18	GOL	B	526	-	5,5,5	0.90	0	5,5,5	1.04	0
16	SO4	A	512	-	4,4,4	0.16	0	6,6,6	0.23	0
18	GOL	D	527	-	5,5,5	1.15	0	5,5,5	1.18	1 (20%)
16	SO4	D	510	-	4,4,4	0.10	0	6,6,6	0.15	0
18	GOL	D	521	-	5,5,5	0.83	0	5,5,5	1.02	0
16	SO4	B	515	-	4,4,4	0.14	0	6,6,6	0.06	0
13	FLC	A	505	-	12,12,12	1.51	4 (33%)	17,17,17	2.31	4 (23%)
18	GOL	D	519	-	5,5,5	1.08	0	5,5,5	0.85	0
18	GOL	A	515	-	5,5,5	1.01	0	5,5,5	0.88	0
18	GOL	C	623	-	5,5,5	0.94	0	5,5,5	1.04	0
17	EDO	D	517	-	3,3,3	0.50	0	2,2,2	0.26	0
16	SO4	C	609	-	4,4,4	0.14	0	6,6,6	0.10	0
18	GOL	C	624	-	5,5,5	0.86	0	5,5,5	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	EDO	C	617	-	3,3,3	0.49	0	2,2,2	0.25	0
16	SO4	B	510	-	4,4,4	0.12	0	6,6,6	0.29	0
18	GOL	D	526	-	5,5,5	0.86	0	5,5,5	1.05	0
18	GOL	C	629	-	5,5,5	0.90	0	5,5,5	0.93	0
18	GOL	D	518	-	5,5,5	0.87	0	5,5,5	1.01	0
18	GOL	C	622	-	5,5,5	0.94	0	5,5,5	1.03	0
16	SO4	C	614	-	4,4,4	0.14	0	6,6,6	0.11	0
18	GOL	B	527	-	5,5,5	1.00	0	5,5,5	0.86	0
13	FLC	C	601	-	12,12,12	1.19	2 (16%)	17,17,17	1.03	2 (11%)
18	GOL	A	517	-	5,5,5	0.85	0	5,5,5	0.98	0
18	GOL	A	516	-	5,5,5	1.04	1 (20%)	5,5,5	0.89	0
15	NAG	C	605	1	14,14,15	1.09	1 (7%)	17,19,21	1.66	1 (5%)
18	GOL	A	525	-	5,5,5	0.88	0	5,5,5	0.98	0
20	R9X	C	633[B]	-	28,28,28	1.67	4 (14%)	35,37,37	1.78	7 (20%)
20	R9X	C	632[A]	-	28,28,28	1.60	4 (14%)	35,37,37	2.75	7 (20%)
15	NAG	D	516	1	14,14,15	0.28	0	17,19,21	0.64	1 (5%)
18	GOL	D	524	-	5,5,5	0.93	0	5,5,5	1.01	0
18	GOL	A	526	-	5,5,5	0.88	0	5,5,5	1.05	0
17	EDO	B	518	-	3,3,3	0.46	0	2,2,2	0.38	0
22	DMS	D	505	-	3,3,3	0.69	0	3,3,3	0.51	0
16	SO4	C	611	-	4,4,4	0.11	0	6,6,6	0.12	0
18	GOL	C	631	-	5,5,5	0.87	0	5,5,5	1.01	0
16	SO4	C	612	-	4,4,4	0.12	0	6,6,6	0.16	0
13	FLC	B	505	-	12,12,12	0.15	0	17,17,17	0.32	0
18	GOL	B	523	-	5,5,5	0.74	0	5,5,5	1.12	0
16	SO4	D	507	-	4,4,4	0.16	0	6,6,6	0.15	0
18	GOL	B	519	-	5,5,5	0.82	0	5,5,5	1.02	0
16	SO4	B	517	-	4,4,4	0.13	0	6,6,6	0.06	0
14	PGE	A	504	-	9,9,9	0.31	0	8,8,8	0.26	0
20	R9X	B	531[A]	-	28,28,28	1.69	7 (25%)	35,37,37	1.55	6 (17%)
18	GOL	D	532	-	5,5,5	0.84	0	5,5,5	1.01	0
13	FLC	D	503	-	12,12,12	1.49	4 (33%)	17,17,17	2.36	4 (23%)
18	GOL	B	522	-	5,5,5	0.95	0	5,5,5	1.16	1 (20%)
16	SO4	B	516	-	4,4,4	0.13	0	6,6,6	0.11	0
18	GOL	B	520	-	5,5,5	0.93	0	5,5,5	0.95	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
17	EDO	A	514	-	-	0/1/1/1	-
18	GOL	B	521	-	-	3/4/4/4	-
20	R9X	A	532[A]	-	1/1/3/4	10/23/23/23	0/2/2/2
18	GOL	B	524	-	-	4/4/4/4	-
18	GOL	D	523	-	-	2/4/4/4	-
18	GOL	B	528	-	-	4/4/4/4	-
13	FLC	C	628	-	-	9/16/16/16	-
18	GOL	C	620	-	-	2/4/4/4	-
18	GOL	C	619	-	-	1/4/4/4	-
13	FLC	C	602	-	-	3/16/16/16	-
18	GOL	A	518	-	-	0/4/4/4	-
18	GOL	C	625	-	-	3/4/4/4	-
14	PGE	B	504	-	-	6/7/7/7	-
18	GOL	C	618	-	-	0/4/4/4	-
20	R9X	B	531[B]	-	-	7/23/23/23	0/2/2/2
15	NAG	C	616	1	-	4/6/23/26	0/1/1/1
18	GOL	C	621	-	-	0/4/4/4	-
18	GOL	D	520	-	-	0/4/4/4	-
18	GOL	D	528	-	-	0/4/4/4	-
18	GOL	D	529	-	-	1/4/4/4	-
18	GOL	A	520	-	-	2/4/4/4	-
20	R9X	A	532[B]	-	1/1/3/4	9/23/23/23	0/2/2/2
18	GOL	D	534	-	-	2/4/4/4	-
18	GOL	A	527	-	-	1/4/4/4	-
18	GOL	A	521	-	-	2/4/4/4	-
13	FLC	B	507	-	-	9/16/16/16	-
18	GOL	A	524	-	-	2/4/4/4	-
15	NAG	A	506	1	-	2/6/23/26	0/1/1/1
18	GOL	A	519	-	-	2/4/4/4	-
14	PGE	B	508	-	-	3/7/7/7	-
18	GOL	D	522	-	-	4/4/4/4	-
14	PGE	C	604	-	-	5/7/7/7	-
13	FLC	B	506	-	-	10/16/16/16	-
14	PGE	D	504	-	-	6/7/7/7	-
13	FLC	A	503	-	-	6/16/16/16	-
13	FLC	C	627	-	-	11/16/16/16	-
18	GOL	A	523	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FLC	B	503	-	-	11/16/16/16	-
18	GOL	D	525	-	-	2/4/4/4	-
18	GOL	D	533	-	-	2/4/4/4	-
20	R9X	D	535[B]	-	1/1/3/4	14/23/23/23	0/2/2/2
20	R9X	D	535[A]	-	1/1/3/4	17/23/23/23	0/2/2/2
13	FLC	C	603	-	-	3/16/16/16	-
13	FLC	A	530	-	-	10/16/16/16	-
15	NAG	D	506	1	-	3/6/23/26	0/1/1/1
18	GOL	B	525	-	-	2/4/4/4	-
14	PGE	A	507	-	-	3/4/4/7	-
18	GOL	A	522	-	-	2/4/4/4	-
18	GOL	C	630	-	-	2/4/4/4	-
18	GOL	A	531	-	-	2/4/4/4	-
18	GOL	B	526	-	-	2/4/4/4	-
18	GOL	D	527	-	-	2/4/4/4	-
18	GOL	D	521	-	-	2/4/4/4	-
13	FLC	A	505	-	-	14/16/16/16	-
18	GOL	D	519	-	-	0/4/4/4	-
18	GOL	A	515	-	-	0/4/4/4	-
18	GOL	C	623	-	-	0/4/4/4	-
17	EDO	D	517	-	-	1/1/1/1	-
18	GOL	C	624	-	-	2/4/4/4	-
17	EDO	C	617	-	-	1/1/1/1	-
18	GOL	D	526	-	-	0/4/4/4	-
18	GOL	C	629	-	-	4/4/4/4	-
18	GOL	D	518	-	-	0/4/4/4	-
18	GOL	C	622	-	-	1/4/4/4	-
18	GOL	B	527	-	-	1/4/4/4	-
13	FLC	C	601	-	-	2/16/16/16	-
18	GOL	A	517	-	-	3/4/4/4	-
18	GOL	A	516	-	-	1/4/4/4	-
15	NAG	C	605	1	-	4/6/23/26	0/1/1/1
18	GOL	A	525	-	-	2/4/4/4	-
20	R9X	C	633[B]	-	1/1/3/4	14/23/23/23	0/2/2/2
20	R9X	C	632[A]	-	-	13/23/23/23	0/2/2/2
15	NAG	D	516	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	GOL	D	524	-	-	3/4/4/4	-
18	GOL	A	526	-	-	1/4/4/4	-
17	EDO	B	518	-	-	0/1/1/1	-
18	GOL	C	631	-	-	2/4/4/4	-
13	FLC	B	505	-	-	9/16/16/16	-
18	GOL	B	523	-	-	0/4/4/4	-
18	GOL	B	519	-	-	2/4/4/4	-
14	PGE	A	504	-	-	3/7/7/7	-
20	R9X	B	531[A]	-	-	10/23/23/23	0/2/2/2
18	GOL	D	532	-	-	0/4/4/4	-
13	FLC	D	503	-	-	4/16/16/16	-
18	GOL	B	522	-	-	2/4/4/4	-
18	GOL	B	520	-	-	0/4/4/4	-

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	633[B]	R9X	C10-N12	6.42	1.47	1.34
20	C	632[A]	R9X	C10-N12	5.92	1.46	1.34
20	A	532[B]	R9X	C10-N12	5.62	1.46	1.34
20	D	535[B]	R9X	C10-N12	5.54	1.45	1.34
20	B	531[B]	R9X	C10-N12	5.53	1.45	1.34
20	B	531[A]	R9X	C10-N12	5.38	1.45	1.34
20	D	535[A]	R9X	C10-N12	4.95	1.44	1.34
20	A	532[A]	R9X	C10-N12	4.09	1.42	1.34
20	A	532[A]	R9X	C13-N12	-4.09	1.42	1.46
15	C	605	NAG	O5-C1	3.96	1.50	1.43
15	A	506	NAG	O5-C1	3.93	1.50	1.43
20	D	535[B]	R9X	P24-C13	3.78	1.88	1.83
20	B	531[A]	R9X	C14-C13	3.72	1.55	1.52
13	C	601	FLC	OG2-CGC	-3.10	1.20	1.30
13	C	628	FLC	OG1-CGC	2.89	1.31	1.22
13	A	530	FLC	OA1-CAC	2.87	1.31	1.22
20	D	535[B]	R9X	C23-C18	-2.86	1.37	1.43
20	C	633[B]	R9X	C23-C18	-2.84	1.37	1.43
20	C	632[A]	R9X	C23-C18	-2.84	1.37	1.43
13	B	507	FLC	OB1-CBC	2.83	1.31	1.22
13	C	628	FLC	OB1-CBC	2.82	1.31	1.22
13	A	505	FLC	OB1-CBC	2.82	1.31	1.22
13	A	530	FLC	OG1-CGC	2.81	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	603	FLC	OB1-CBC	2.80	1.31	1.22
13	B	507	FLC	OA1-CAC	2.79	1.31	1.22
13	C	603	FLC	OG1-CGC	2.79	1.31	1.22
13	C	627	FLC	OA2-CAC	-2.78	1.21	1.30
13	C	627	FLC	OB1-CBC	2.78	1.31	1.22
18	A	519	GOL	O2-C2	-2.77	1.35	1.43
13	D	503	FLC	OB1-CBC	2.76	1.31	1.22
13	A	505	FLC	OG1-CGC	2.76	1.31	1.22
13	B	506	FLC	OA1-CAC	2.75	1.31	1.22
13	B	503	FLC	OB1-CBC	2.75	1.31	1.22
13	C	627	FLC	OA1-CAC	2.75	1.31	1.22
13	B	503	FLC	OG1-CGC	2.75	1.31	1.22
20	B	531[B]	R9X	C23-C18	-2.74	1.38	1.43
13	C	627	FLC	OG1-CGC	2.73	1.31	1.22
13	C	602	FLC	OB1-CBC	2.72	1.30	1.22
13	B	507	FLC	OA2-CAC	-2.72	1.21	1.30
13	B	506	FLC	OA2-CAC	-2.71	1.21	1.30
13	A	505	FLC	OG2-CGC	-2.68	1.21	1.30
20	A	532[A]	R9X	O11-C10	-2.63	1.17	1.23
13	C	601	FLC	OG1-CGC	2.63	1.30	1.22
20	A	532[B]	R9X	C23-C18	-2.61	1.38	1.43
13	C	603	FLC	OG2-CGC	-2.61	1.22	1.30
13	A	530	FLC	OG2-CGC	-2.60	1.22	1.30
13	A	530	FLC	OA2-CAC	-2.58	1.22	1.30
13	D	503	FLC	OG1-CGC	2.57	1.30	1.22
13	C	628	FLC	OG2-CGC	-2.56	1.22	1.30
20	B	531[A]	R9X	P24-O27	-2.55	1.50	1.54
20	B	531[A]	R9X	C23-C18	-2.53	1.38	1.43
20	A	532[A]	R9X	P24-O26	-2.50	1.50	1.54
20	C	632[A]	R9X	P24-O27	-2.47	1.50	1.54
20	D	535[B]	R9X	C14-C13	2.47	1.54	1.52
13	C	627	FLC	OG2-CGC	-2.47	1.22	1.30
13	D	503	FLC	OG2-CGC	-2.46	1.22	1.30
13	B	503	FLC	OG2-CGC	-2.45	1.22	1.30
20	A	532[A]	R9X	C23-C18	-2.45	1.38	1.43
20	D	535[A]	R9X	P24-O27	-2.39	1.51	1.54
20	C	633[B]	R9X	P24-O27	-2.37	1.51	1.54
13	C	627	FLC	OB2-CBC	-2.33	1.21	1.30
20	C	633[B]	R9X	P24-C13	2.27	1.86	1.83
20	B	531[A]	R9X	O11-C10	-2.24	1.18	1.23
13	B	503	FLC	OB2-CBC	-2.24	1.21	1.30
20	B	531[A]	R9X	P24-C13	2.23	1.86	1.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	602	FLC	OB2-CBC	-2.22	1.22	1.30
20	C	632[A]	R9X	P24-O26	-2.22	1.51	1.54
13	D	503	FLC	OB2-CBC	-2.21	1.22	1.30
13	B	507	FLC	OB2-CBC	-2.18	1.22	1.30
13	A	505	FLC	OB2-CBC	-2.16	1.22	1.30
20	A	532[B]	R9X	P24-O26	-2.16	1.51	1.54
18	C	620	GOL	O2-C2	-2.14	1.37	1.43
13	C	628	FLC	OB2-CBC	-2.12	1.22	1.30
20	A	532[B]	R9X	P24-C13	2.11	1.86	1.83
20	D	535[A]	R9X	C23-C18	-2.11	1.39	1.43
20	B	531[B]	R9X	O11-C10	-2.09	1.19	1.23
13	C	603	FLC	OB2-CBC	-2.07	1.22	1.30
20	B	531[A]	R9X	P24-O26	-2.07	1.51	1.54
18	C	620	GOL	C3-C2	2.05	1.60	1.51
20	D	535[A]	R9X	O11-C10	-2.04	1.19	1.23
20	A	532[B]	R9X	P24-O27	-2.03	1.51	1.54
18	D	520	GOL	O2-C2	-2.03	1.37	1.43
18	B	521	GOL	O2-C2	-2.02	1.37	1.43
18	A	516	GOL	O2-C2	-2.02	1.37	1.43
20	A	532[B]	R9X	O11-C10	-2.02	1.19	1.23

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	632[A]	R9X	C13-N12-C10	10.95	136.25	121.19
20	A	532[A]	R9X	C14-C13-N12	-9.26	103.01	114.52
20	B	531[B]	R9X	C14-C13-N12	-8.16	104.38	114.52
20	C	632[A]	R9X	P24-C13-N12	-7.70	92.58	108.01
20	C	633[B]	R9X	C14-C13-N12	-6.90	105.95	114.52
13	B	503	FLC	OB1-CBC-CB	-6.67	112.80	122.25
13	A	505	FLC	OB1-CBC-CB	-6.51	113.03	122.25
13	C	603	FLC	OB1-CBC-CB	-6.47	113.09	122.25
13	D	503	FLC	OB1-CBC-CB	-6.44	113.13	122.25
15	C	605	NAG	C1-O5-C5	6.42	120.89	112.19
13	C	602	FLC	OB1-CBC-CB	-6.40	113.20	122.25
20	A	532[A]	R9X	P24-C13-N12	-6.29	95.41	108.01
13	C	628	FLC	OB1-CBC-CB	-6.27	113.37	122.25
13	B	507	FLC	OB1-CBC-CB	-6.21	113.46	122.25
20	A	532[A]	R9X	P24-C13-C14	6.04	121.28	111.52
13	C	627	FLC	OB1-CBC-CB	-5.93	113.85	122.25
20	D	535[A]	R9X	P24-C13-N12	-5.83	96.32	108.01
13	B	507	FLC	OB2-CBC-CB	5.80	123.13	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	632[A]	R9X	C09-C10-N12	5.60	125.55	115.83
13	C	603	FLC	OB2-CBC-CB	5.60	122.77	113.05
13	A	505	FLC	OB2-CBC-CB	5.59	122.75	113.05
13	C	628	FLC	OB2-CBC-CB	5.55	122.69	113.05
13	C	602	FLC	OB2-CBC-CB	5.48	122.57	113.05
13	B	503	FLC	OB2-CBC-CB	5.46	122.53	113.05
13	D	503	FLC	OB2-CBC-CB	5.39	122.42	113.05
13	C	627	FLC	OB2-CBC-CB	5.35	122.34	113.05
15	A	506	NAG	C1-O5-C5	4.80	118.70	112.19
20	D	535[A]	R9X	C13-N12-C10	-4.59	114.88	121.19
20	A	532[A]	R9X	O11-C10-N12	-4.46	115.42	122.95
20	B	531[A]	R9X	C09-C10-N12	4.35	123.38	115.83
20	C	632[A]	R9X	O11-C10-N12	-4.18	115.90	122.95
20	B	531[A]	R9X	C13-N12-C10	3.90	126.55	121.19
20	D	535[A]	R9X	C15-C14-C13	-3.73	116.48	121.00
13	C	627	FLC	OG1-CGC-CG	-3.61	112.39	122.94
13	D	503	FLC	OG1-CGC-CG	-3.55	112.58	122.94
20	D	535[A]	R9X	C13-C14-C23	3.53	125.49	120.36
20	D	535[A]	R9X	O25-P24-C13	-3.45	105.21	111.07
20	B	531[A]	R9X	O11-C10-N12	-3.44	117.14	122.95
13	B	506	FLC	OA1-CAC-CA	-3.44	112.89	122.94
20	A	532[B]	R9X	C14-C13-N12	-3.41	110.28	114.52
20	B	531[B]	R9X	C15-C14-C13	-3.41	116.86	121.00
13	C	627	FLC	OA1-CAC-CA	-3.38	113.08	122.94
20	A	532[A]	R9X	C22-C23-C14	-3.34	119.52	123.40
20	B	531[B]	R9X	C09-C10-N12	3.23	121.43	115.83
20	B	531[B]	R9X	P24-C13-N12	-3.19	101.61	108.01
13	C	628	FLC	OG1-CGC-CG	-3.17	113.69	122.94
13	A	505	FLC	OG1-CGC-CG	-3.14	113.77	122.94
20	B	531[A]	R9X	O26-P24-O25	-3.11	105.63	113.45
13	C	627	FLC	OA2-CAC-CA	3.10	124.30	114.35
13	B	507	FLC	OA1-CAC-CA	-3.09	113.91	122.94
13	D	503	FLC	OG2-CGC-CG	3.07	124.22	114.35
13	C	603	FLC	OG1-CGC-CG	-3.06	114.00	122.94
13	B	506	FLC	OA2-CAC-CA	3.06	124.17	114.35
20	D	535[A]	R9X	O26-P24-O25	-3.04	105.80	113.45
13	C	627	FLC	CA-CB-CBC	3.00	116.55	110.11
20	C	633[B]	R9X	P24-C13-N12	2.99	114.00	108.01
20	C	633[B]	R9X	O27-P24-O25	-2.98	105.95	113.45
13	A	530	FLC	OA1-CAC-CA	-2.97	114.27	122.94
13	B	503	FLC	OG1-CGC-CG	-2.95	114.33	122.94
20	C	632[A]	R9X	C22-C23-C14	-2.93	119.99	123.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	530	FLC	OG1-CGC-CG	-2.92	114.41	122.94
13	C	627	FLC	OG2-CGC-CG	2.88	123.60	114.35
20	A	532[A]	R9X	C09-C10-N12	2.88	120.82	115.83
20	A	532[B]	R9X	C22-C23-C14	-2.83	120.11	123.40
20	B	531[B]	R9X	C13-N12-C10	2.81	125.06	121.19
13	C	627	FLC	CB-CA-CAC	-2.79	107.05	113.81
20	C	633[B]	R9X	C15-C14-C13	-2.79	117.62	121.00
20	D	535[B]	R9X	C14-C13-N12	-2.73	111.13	114.52
13	C	601	FLC	OG1-CGC-CG	-2.72	114.99	122.94
20	A	532[A]	R9X	C13-N12-C10	-2.72	117.45	121.19
20	C	633[B]	R9X	C09-C10-N12	2.72	120.55	115.83
20	B	531[A]	R9X	C14-C13-N12	2.71	117.89	114.52
20	C	633[B]	R9X	O26-P24-O25	-2.70	106.66	113.45
13	B	507	FLC	OA2-CAC-CA	2.66	122.88	114.35
13	C	628	FLC	OG2-CGC-CG	2.65	122.87	114.35
20	B	531[B]	R9X	O11-C10-N12	-2.65	118.48	122.95
13	C	603	FLC	OG2-CGC-CG	2.65	122.85	114.35
13	A	505	FLC	OG2-CGC-CG	2.59	122.66	114.35
20	A	532[B]	R9X	C09-C10-N12	2.56	120.27	115.83
13	A	530	FLC	OG2-CGC-CG	2.54	122.52	114.35
13	B	503	FLC	OG2-CGC-CG	2.50	122.36	114.35
13	A	530	FLC	OA2-CAC-CA	2.47	122.30	114.35
20	A	532[A]	R9X	C15-C14-C13	-2.46	118.02	121.00
20	B	531[A]	R9X	C22-C23-C14	-2.43	120.58	123.40
13	C	601	FLC	OG2-CGC-CG	2.41	122.10	114.35
18	A	518	GOL	C3-C2-C1	-2.36	102.51	111.70
20	C	632[A]	R9X	P24-C13-C14	-2.31	107.78	111.52
20	C	632[A]	R9X	C14-C13-N12	2.29	117.36	114.52
20	C	633[B]	R9X	O11-C10-C09	-2.28	117.85	122.02
18	B	522	GOL	C3-C2-C1	-2.17	103.27	111.70
15	D	516	NAG	C1-O5-C5	2.15	115.11	112.19
20	D	535[A]	R9X	C19-C18-C17	-2.14	118.19	123.19
20	A	532[A]	R9X	C22-C23-C18	2.13	120.64	117.89
20	D	535[B]	R9X	C09-C10-N12	2.08	119.43	115.83
20	D	535[B]	R9X	O27-P24-O25	-2.04	108.32	113.45
18	C	625	GOL	C3-C2-C1	-2.03	103.80	111.70
18	D	527	GOL	C3-C2-C1	-2.02	103.86	111.70
18	C	618	GOL	C3-C2-C1	-2.01	103.90	111.70

All (5) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
20	A	532[A]	R9X	C13
20	A	532[B]	R9X	C13
20	C	633[B]	R9X	C13
20	D	535[A]	R9X	C13
20	D	535[B]	R9X	C13

All (316) 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-CG
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	CA-CB-CG-CGC
13	B	506	FLC	CBC-CB-CG-CGC
13	B	506	FLC	OHB-CB-CG-CGC
13	B	507	FLC	CAC-CA-CB-CBC
13	B	507	FLC	CAC-CA-CB-CG
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	602	FLC	CA-CB-CG-CGC
13	C	602	FLC	CBC-CB-CG-CGC
13	C	602	FLC	OHB-CB-CG-CGC

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Mol	Chain	Res	Type	Atoms
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	CA-CB-CG-CGC
13	C	628	FLC	CBC-CB-CG-CGC
13	C	628	FLC	OHB-CB-CG-CGC
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	519	GOL	O1-C1-C2-C3
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	C14-C13-N12-C10
20	A	532[B]	R9X	P24-C13-N12-C10
20	B	531[A]	R9X	N12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
20	B	531[A]	R9X	P24-C13-C14-C23
20	B	531[A]	R9X	P24-C13-C14-C15
20	B	531[A]	R9X	C14-C13-N12-C10
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-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
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[A]	R9X	C14-C13-P24-O27
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

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Mol	Chain	Res	Type	Atoms
20	D	535[A]	R9X	O11-C10-N12-C13
15	C	616	NAG	O5-C5-C6-O6
14	D	504	PGE	O2-C3-C4-O3
20	C	633[B]	R9X	C05-C06-C07-C08
15	C	605	NAG	O5-C5-C6-O6
14	B	504	PGE	O2-C3-C4-O3
20	A	532[A]	R9X	C02-C03-C04-C05
14	D	504	PGE	C6-C5-O3-C4
14	A	507	PGE	O2-C3-C4-O3
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
13	A	505	FLC	CBC-CB-CG-CGC
13	A	505	FLC	OHB-CB-CG-CGC
15	D	506	NAG	C4-C5-C6-O6
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	B	504	PGE	O1-C1-C2-O2
14	D	504	PGE	O1-C1-C2-O2
15	C	605	NAG	C4-C5-C6-O6
20	C	632[A]	R9X	C07-C08-C09-C10
14	A	504	PGE	O1-C1-C2-O2
14	B	508	PGE	O1-C1-C2-O2
20	B	531[A]	R9X	C06-C07-C08-C09
13	A	503	FLC	CAC-CA-CB-CBC
20	D	535[B]	R9X	C02-C03-C04-C05
20	C	632[A]	R9X	C06-C07-C08-C09
20	A	532[A]	R9X	C04-C05-C06-C07
18	A	517	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	625	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

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Mol	Chain	Res	Type	Atoms
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
20	B	531[B]	R9X	C06-C07-C08-C09
14	C	604	PGE	O3-C5-C6-O4
20	C	632[A]	R9X	C02-C03-C04-C05
20	B	531[B]	R9X	C02-C03-C04-C05
20	A	532[B]	R9X	C02-C03-C04-C05
20	C	633[B]	R9X	C06-C07-C08-C09
20	D	535[A]	R9X	C04-C05-C06-C07
13	A	505	FLC	CG-CB-CBC-OB2
13	A	530	FLC	CG-CB-CBC-OB2
13	C	628	FLC	CA-CB-CBC-OB1
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
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	A	532[B]	R9X	C05-C06-C07-C08
14	B	504	PGE	O3-C5-C6-O4
17	C	617	EDO	O1-C1-C2-O2
20	C	632[A]	R9X	C03-C04-C05-C06
20	C	632[A]	R9X	C04-C05-C06-C07
20	D	535[A]	R9X	C01-C02-C03-C04
20	D	535[A]	R9X	N12-C13-P24-O25
13	A	503	FLC	OHB-CB-CG-CGC
13	A	505	FLC	CA-CB-CG-CGC
13	B	503	FLC	CBC-CB-CG-CGC
20	A	532[B]	R9X	C03-C04-C05-C06
20	D	535[A]	R9X	C02-C03-C04-C05
14	D	504	PGE	O3-C5-C6-O4
20	C	633[B]	R9X	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
20	D	535[B]	R9X	C05-C06-C07-C08
20	C	632[A]	R9X	C01-C02-C03-C04
20	A	532[A]	R9X	C01-C02-C03-C04
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	633[B]	R9X	C01-C02-C03-C04
15	A	506	NAG	C4-C5-C6-O6
18	B	527	GOL	O1-C1-C2-C3
20	D	535[A]	R9X	C06-C07-C08-C09
20	B	531[B]	R9X	C04-C05-C06-C07
20	A	532[B]	R9X	C06-C07-C08-C09
20	D	535[B]	R9X	C04-C05-C06-C07
13	A	505	FLC	OHB-CB-CBC-OB1
13	C	628	FLC	OHB-CB-CBC-OB2
13	A	505	FLC	CA-CB-CBC-OB1
13	A	505	FLC	CA-CB-CBC-OB2
13	B	506	FLC	CG-CB-CBC-OB2
13	B	507	FLC	CA-CB-CBC-OB1
13	B	507	FLC	CA-CB-CBC-OB2
13	C	603	FLC	CG-CB-CBC-OB1
13	C	627	FLC	CA-CB-CBC-OB2
13	C	628	FLC	CA-CB-CBC-OB2
18	A	520	GOL	O1-C1-C2-O2
13	A	505	FLC	CAC-CA-CB-CBC
20	A	532[A]	R9X	C06-C07-C08-C09
20	D	535[A]	R9X	N12-C13-P24-O26
20	D	535[A]	R9X	N12-C13-P24-O27
20	C	632[A]	R9X	N12-C13-C14-C15
20	B	531[B]	R9X	C01-C02-C03-C04
20	A	532[B]	R9X	C01-C02-C03-C04
14	B	508	PGE	C4-C3-O2-C2
14	C	604	PGE	C1-C2-O2-C3
14	A	504	PGE	C3-C4-O3-C5
14	A	504	PGE	C6-C5-O3-C4
14	B	504	PGE	C4-C3-O2-C2
13	B	506	FLC	CAC-CA-CB-OHB
13	C	603	FLC	OHB-CB-CG-CGC
14	D	504	PGE	C1-C2-O2-C3
20	A	532[A]	R9X	C05-C06-C07-C08
13	B	503	FLC	CB-CA-CAC-OA1
13	B	503	FLC	CB-CA-CAC-OA2

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Mol	Chain	Res	Type	Atoms
14	C	604	PGE	C3-C4-O3-C5
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	A	507	PGE	O1-C1-C2-O2
18	A	526	GOL	O1-C1-C2-C3
18	C	631	GOL	C1-C2-C3-O3
14	D	504	PGE	C4-C3-O2-C2
20	B	531[A]	R9X	C14-C13-P24-O26
20	C	633[B]	R9X	C14-C13-P24-O26
15	A	506	NAG	C1-C2-N2-C7
20	B	531[A]	R9X	C03-C04-C05-C06
13	A	505	FLC	CG-CB-CBC-OB1
13	A	530	FLC	CA-CB-CBC-OB2
13	B	506	FLC	CA-CB-CBC-OB1
13	B	506	FLC	CG-CB-CBC-OB1
13	C	603	FLC	CG-CB-CBC-OB2
13	C	627	FLC	CA-CB-CBC-OB1
13	C	628	FLC	CG-CB-CBC-OB2
20	D	535[A]	R9X	C05-C06-C07-C08
18	C	629	GOL	O1-C1-C2-O2
20	C	632[A]	R9X	C05-C06-C07-C08
13	B	506	FLC	CB-CA-CAC-OA2
20	B	531[B]	R9X	C05-C06-C07-C08
13	A	503	FLC	CAC-CA-CB-CG
13	A	505	FLC	CAC-CA-CB-OHB
13	B	503	FLC	CAC-CA-CB-CBC
13	C	601	FLC	CB-CA-CAC-OA2
20	D	535[B]	R9X	C01-C02-C03-C04
14	B	508	PGE	C6-C5-O3-C4
18	A	527	GOL	C1-C2-C3-O3
13	A	503	FLC	CA-CB-CG-CGC
13	B	503	FLC	CAC-CA-CB-CG
13	B	506	FLC	CB-CA-CAC-OA1
13	A	505	FLC	OHB-CB-CBC-OB2
13	A	503	FLC	CA-CB-CBC-OB2
13	B	506	FLC	CA-CB-CBC-OB2
13	C	628	FLC	CG-CB-CBC-OB1
13	B	505	FLC	CB-CG-CGC-OG2

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Mol	Chain	Res	Type	Atoms
14	A	507	PGE	C4-C3-O2-C2
13	A	530	FLC	CBC-CB-CG-CGC
13	C	601	FLC	CB-CA-CAC-OA1
14	C	604	PGE	O2-C3-C4-O3
14	B	504	PGE	C3-C4-O3-C5
14	C	604	PGE	O1-C1-C2-O2
15	D	506	NAG	C1-C2-N2-C7
18	A	516	GOL	O1-C1-C2-C3
18	A	523	GOL	C1-C2-C3-O3
18	B	526	GOL	C1-C2-C3-O3
13	A	530	FLC	OHB-CB-CG-CGC
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
13	A	505	FLC	CB-CA-CAC-OA1
13	A	505	FLC	CB-CA-CAC-OA2
20	A	532[B]	R9X	C14-C13-P24-O25
20	C	633[B]	R9X	C08-C09-C10-O11
13	B	505	FLC	CB-CG-CGC-OG1
13	A	505	FLC	CAC-CA-CB-CG
13	C	627	FLC	CAC-CA-CB-CG
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-N12
20	D	535[A]	R9X	C14-C13-P24-O25
18	B	521	GOL	O1-C1-C2-C3
18	D	524	GOL	O1-C1-C2-C3
13	A	503	FLC	CAC-CA-CB-OHB
13	C	627	FLC	CAC-CA-CB-CBC
17	D	517	EDO	O1-C1-C2-O2

There are no ring outliers.

66 monomers are involved in 143 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	521	GOL	1	0
16	A	510	SO4	2	0
20	A	532[A]	R9X	7	0
16	C	608	SO4	2	0
18	B	524	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	508	SO4	1	0
16	C	610	SO4	1	0
13	C	628	FLC	2	0
18	C	620	GOL	3	0
16	C	615	SO4	1	0
13	C	602	FLC	1	0
18	A	518	GOL	3	0
18	C	625	GOL	1	0
14	B	504	PGE	3	0
18	C	618	GOL	1	0
18	C	621	GOL	2	0
18	D	529	GOL	1	0
20	A	532[B]	R9X	5	0
18	D	534	GOL	1	0
16	B	509	SO4	1	0
13	B	507	FLC	2	0
18	A	524	GOL	1	0
16	D	515	SO4	1	0
16	D	514	SO4	1	0
18	A	519	GOL	1	0
18	D	522	GOL	4	0
14	C	604	PGE	1	0
16	C	613	SO4	2	0
13	B	506	FLC	3	0
14	D	504	PGE	8	0
13	A	503	FLC	3	0
13	C	627	FLC	2	0
18	A	523	GOL	2	0
18	D	533	GOL	1	0
16	A	509	SO4	1	0
20	D	535[B]	R9X	2	0
20	D	535[A]	R9X	6	0
13	C	603	FLC	1	0
16	B	512	SO4	1	0
15	D	506	NAG	3	0
18	B	525	GOL	1	0
14	A	507	PGE	4	0
18	A	531	GOL	4	0
16	A	512	SO4	3	0
18	D	527	GOL	3	0
13	A	505	FLC	2	0
18	C	623	GOL	1	0

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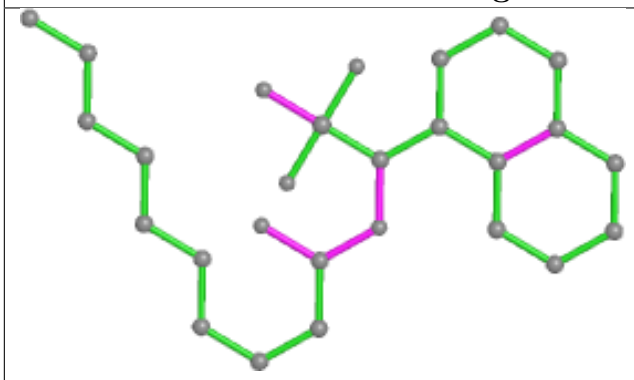
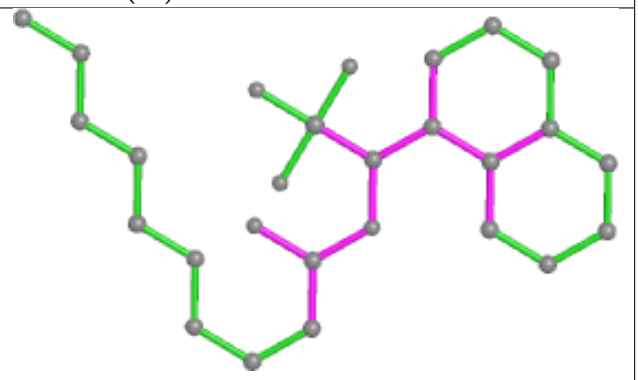
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	624	GOL	1	0
17	C	617	EDO	1	0
16	B	510	SO4	1	0
18	C	622	GOL	1	0
18	B	527	GOL	2	0
18	A	516	GOL	2	0
15	C	605	NAG	1	0
20	C	633[B]	R9X	6	0
20	C	632[A]	R9X	2	0
18	D	524	GOL	1	0
18	A	526	GOL	1	0
22	D	505	DMS	1	0
13	B	505	FLC	4	0
16	D	507	SO4	1	0
18	B	519	GOL	1	0
14	A	504	PGE	2	0
20	B	531[A]	R9X	7	0
13	D	503	FLC	6	0
18	B	522	GOL	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 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 then 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.

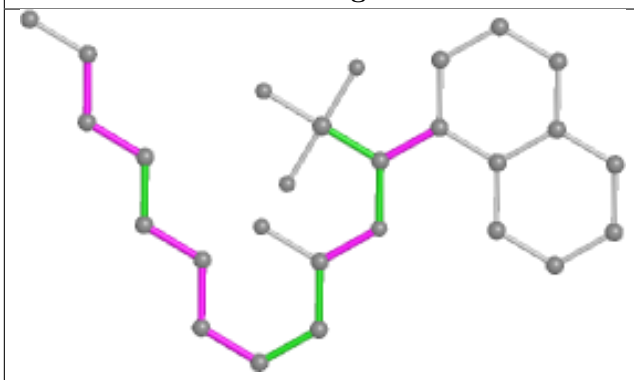
Ligand R9X A 532 (A)



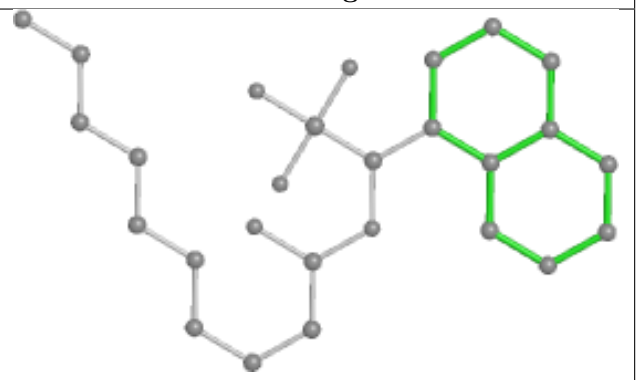
Bond lengths



Bond angles

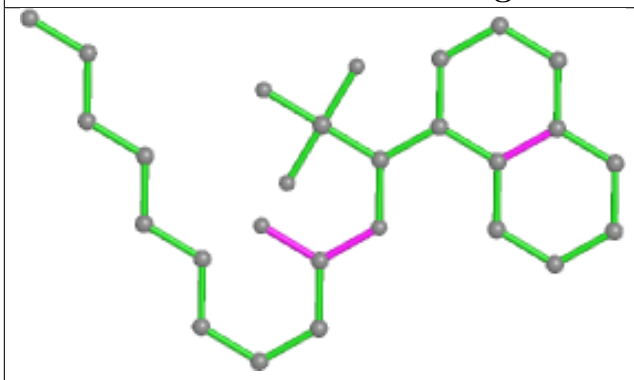


Torsions

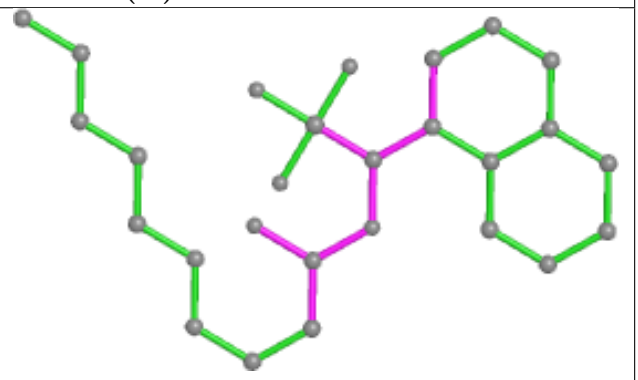


Rings

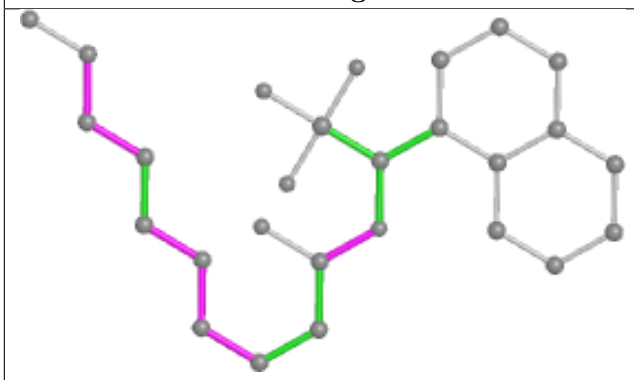
Ligand R9X B 531 (B)



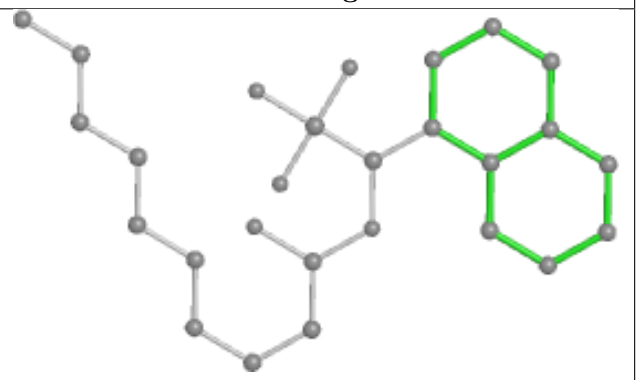
Bond lengths



Bond angles

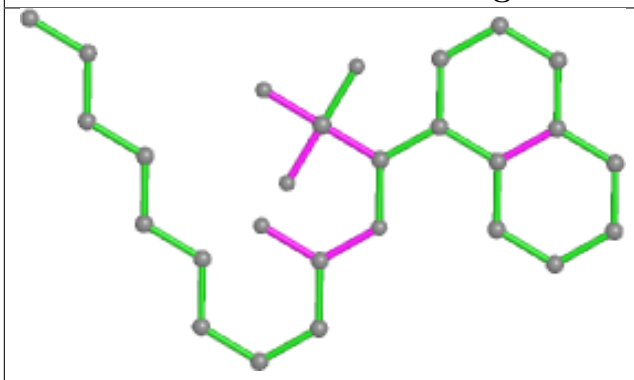


Torsions

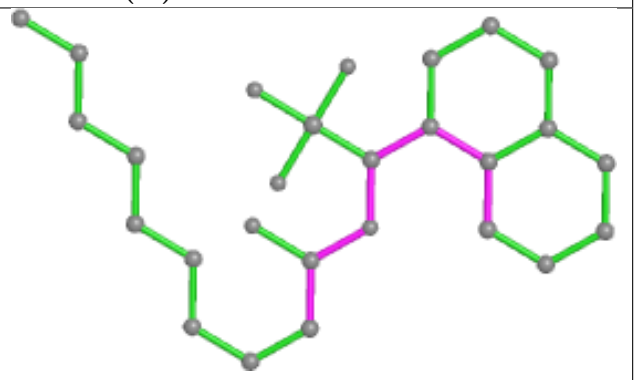


Rings

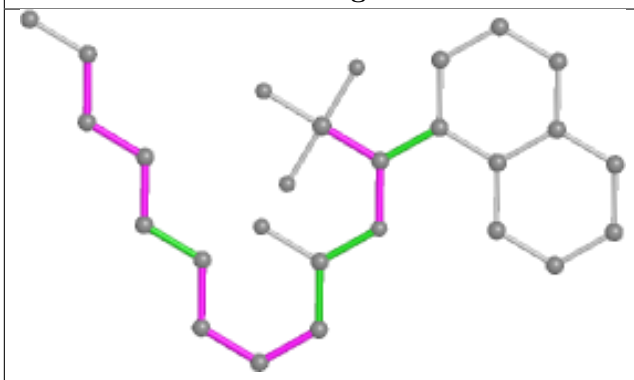
Ligand R9X A 532 (B)



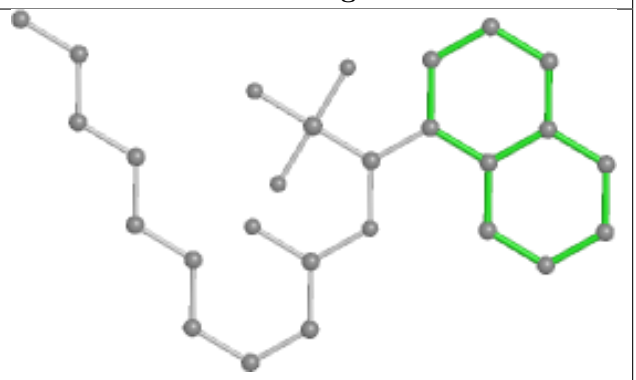
Bond lengths



Bond angles

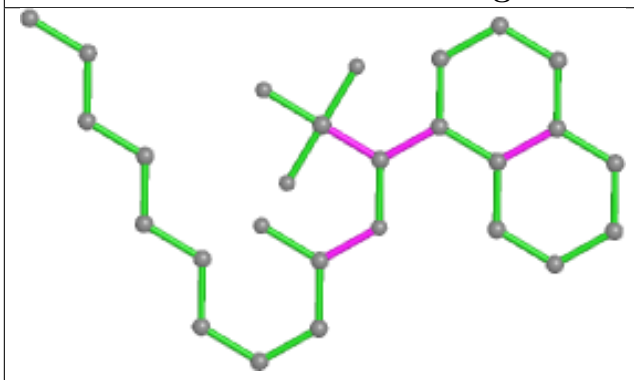


Torsions

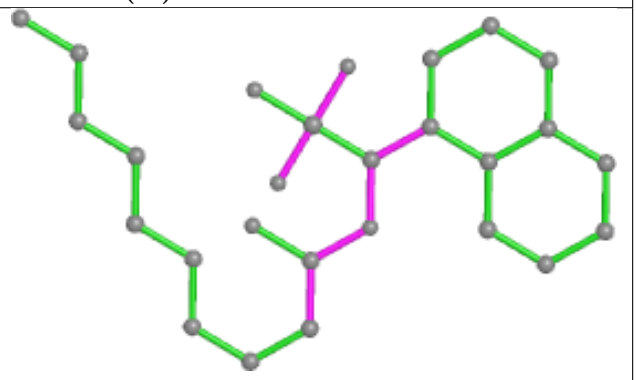


Rings

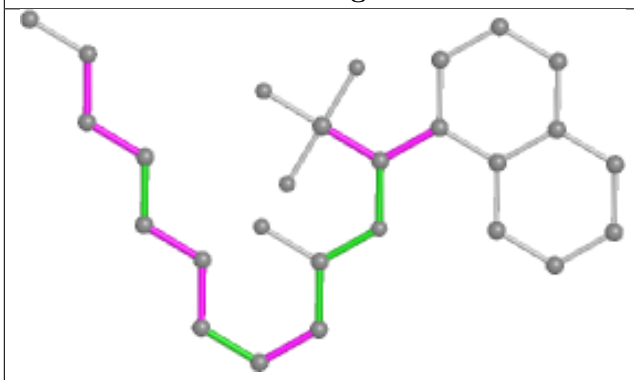
Ligand R9X D 535 (B)



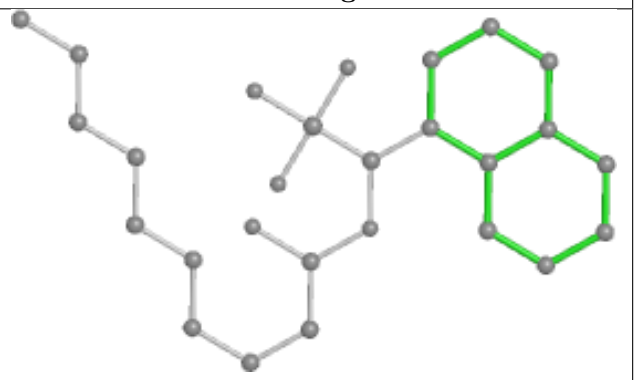
Bond lengths



Bond angles

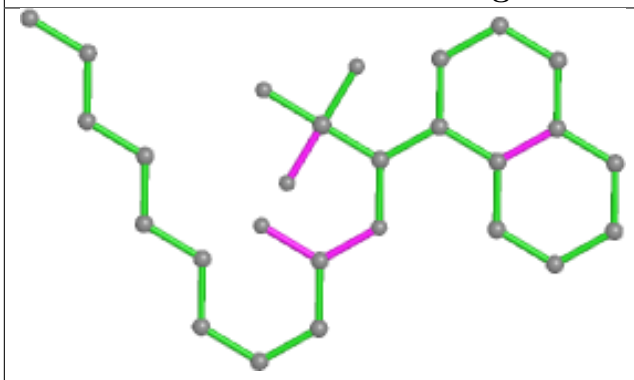


Torsions

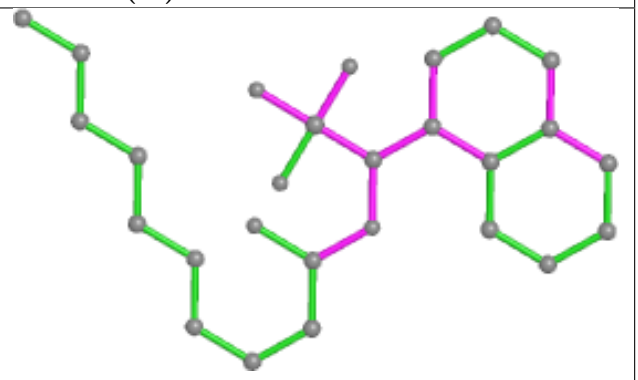


Rings

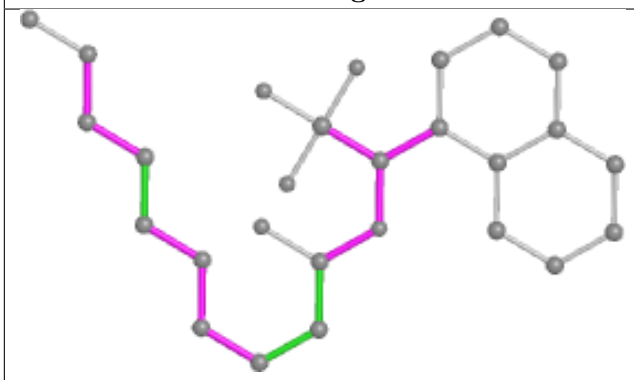
Ligand R9X D 535 (A)



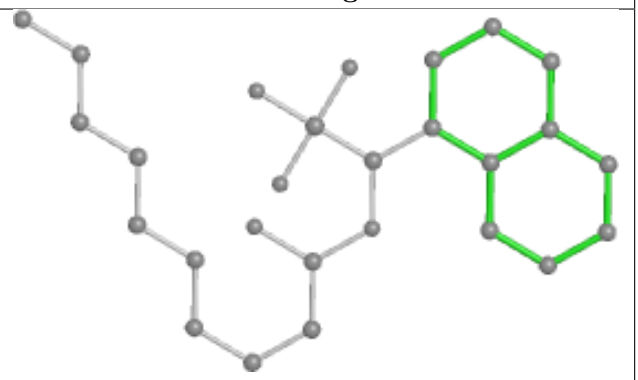
Bond lengths



Bond angles

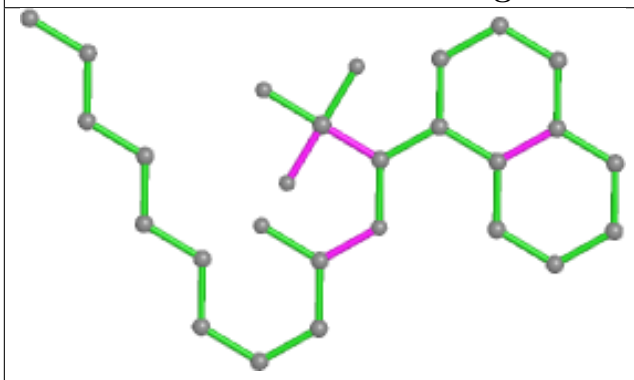


Torsions

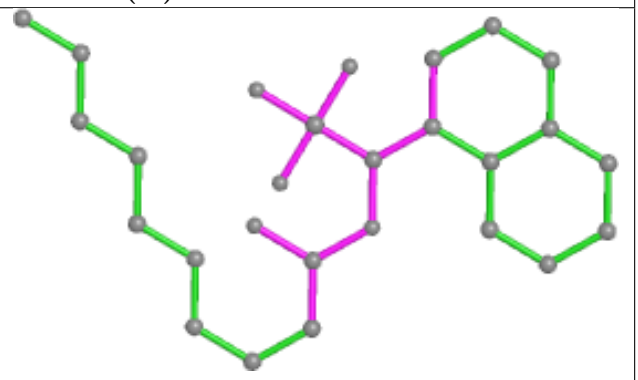


Rings

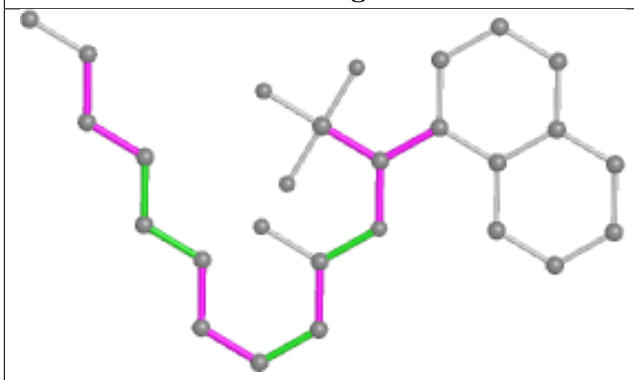
Ligand R9X C 633 (B)



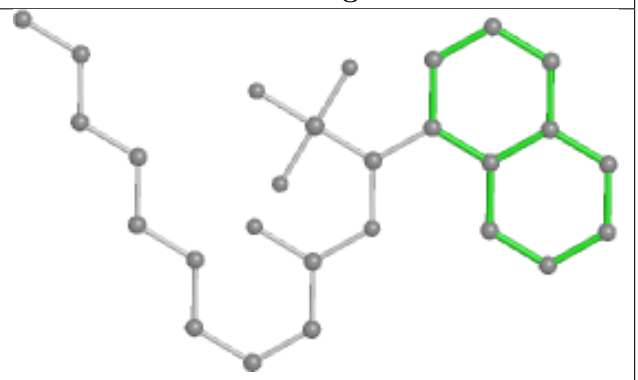
Bond lengths



Bond angles

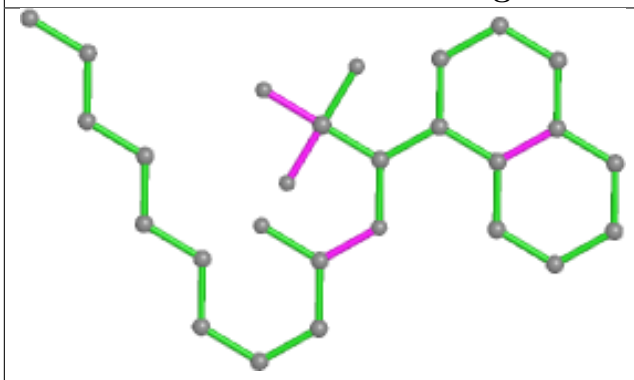


Torsions

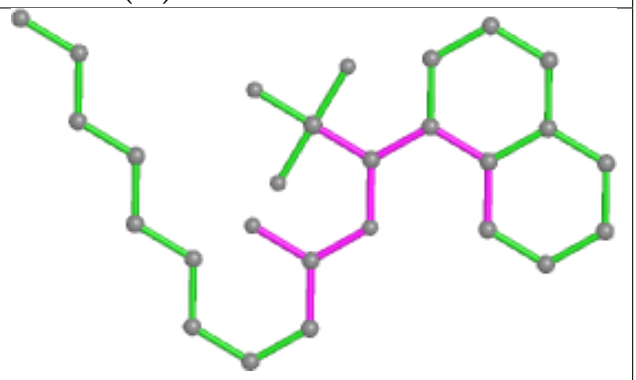


Rings

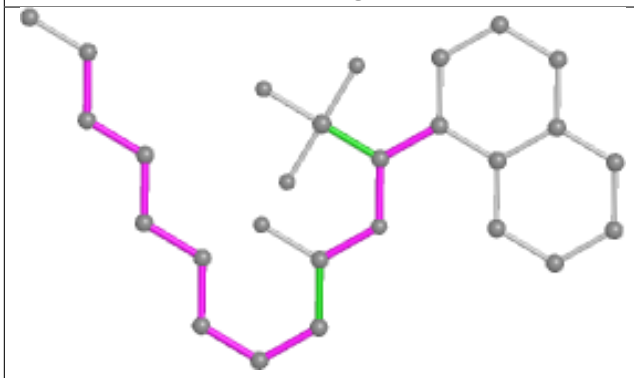
Ligand R9X C 632 (A)



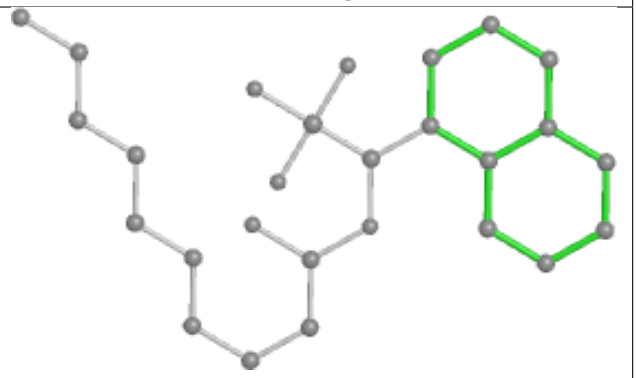
Bond lengths



Bond angles

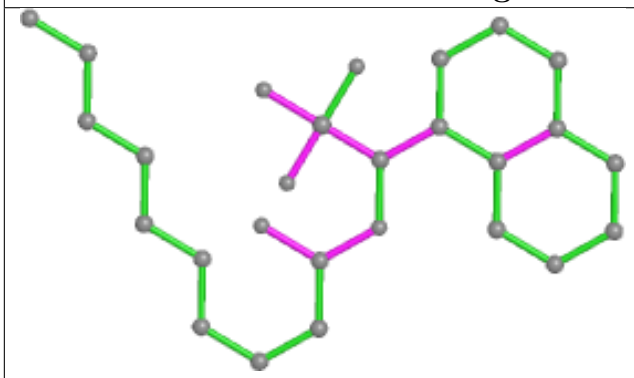


Torsions

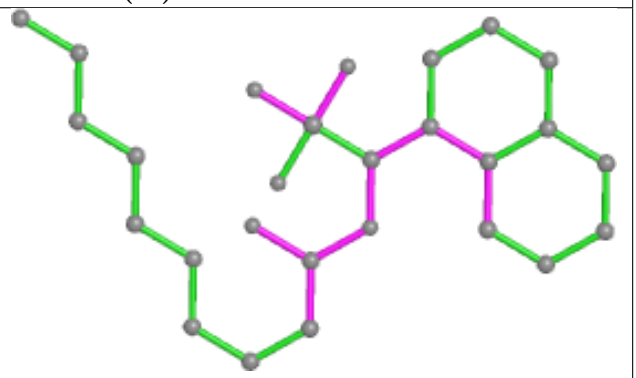


Rings

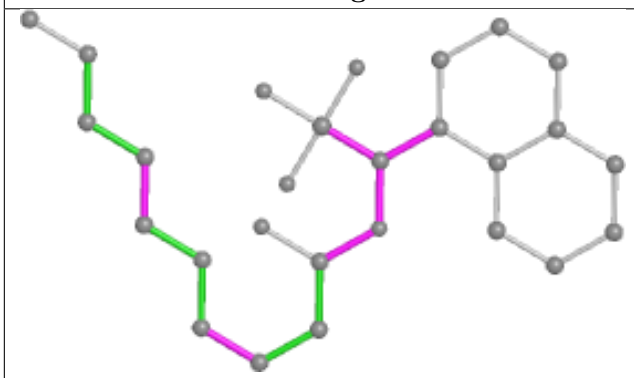
Ligand R9X B 531 (A)



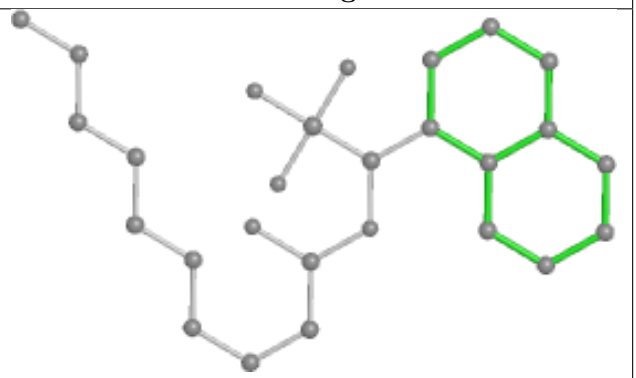
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	-0.89	1 (0%)	95	94	13, 20, 33, 58	0
1	B	428/428 (100%)	-0.81	4 (0%)	84	83	15, 22, 37, 93	0
1	C	428/428 (100%)	-0.80	6 (1%)	75	74	14, 21, 36, 79	0
1	D	426/428 (99%)	-0.83	4 (0%)	84	83	14, 21, 35, 77	1 (0%)
All	All	1707/1712 (99%)	-0.83	15 (0%)	84	83	13, 21, 35, 93	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	THR	6.3
1	B	6	ASN	4.9
1	C	64	ASN	4.6
1	C	5	THR	4.3
1	B	64	ASN	4.2
1	D	5	THR	3.8
1	C	432	THR	3.6
1	D	64	ASN	3.3
1	A	7	LYS	2.9
1	D	63	LYS	2.8
1	C	6	ASN	2.7
1	B	63	LYS	2.5
1	C	92[A]	ILE	2.3
1	C	431	SER	2.3
1	D	6	ASN	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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	0.58	0.42	68,72,75,79	11
4	BMA	G	3	11/12	0.61	0.36	68,82,88,88	11
4	BMA	I	3	11/12	0.63	0.45	83,100,103,108	0
4	BMA	N	3	11/12	0.65	0.44	59,62,68,70	11
4	BMA	V	3	11/12	0.70	0.35	48,60,68,85	11
2	NAG	E	2	14/15	0.71	0.28	30,41,48,49	14
9	NAG	R	2	14/15	0.72	0.33	38,50,61,63	14
9	FUC	R	4	10/11	0.72	0.22	47,50,56,58	10
4	BMA	S	3	11/12	0.74	0.31	59,70,74,75	11
5	MAN	J	4	11/12	0.75	0.35	40,54,64,69	11
3	MAN	F	4	11/12	0.76	0.22	43,48,51,51	11
8	NAG	O	2	14/15	0.77	0.32	41,46,52,58	14
4	NAG	N	2	14/15	0.77	0.31	43,49,57,59	14
5	BMA	J	3	11/12	0.77	0.19	42,44,52,57	11
3	MAN	F	5	11/12	0.78	0.29	48,51,59,60	11
7	NAG	M	2	14/15	0.78	0.25	40,48,60,65	14
9	BMA	R	3	10/12	0.79	0.34	64,67,70,71	10
4	NAG	I	2	14/15	0.81	0.34	60,73,82,92	14
5	MAN	J	5	11/12	0.81	0.16	39,48,52,54	11
10	NAG	T	1	14/15	0.82	0.28	43,48,53,53	14
10	FUC	T	2	10/11	0.82	0.41	46,50,53,55	10
4	NAG	S	2	14/15	0.83	0.25	39,52,60,61	14
2	NAG	Q	2	14/15	0.83	0.26	27,43,49,50	14
2	NAG	K	2	14/15	0.84	0.30	38,46,47,48	14
4	NAG	G	2	14/15	0.85	0.25	51,61,74,78	14
4	FUC	G	4	10/11	0.85	0.20	44,48,55,59	10
4	BMA	P	3	11/12	0.86	0.28	65,75,82,83	0
6	MAN	L	4	11/12	0.86	0.34	40,52,67,72	11
5	BMA	H	3	11/12	0.87	0.16	25,32,39,42	11
8	NAG	O	1	14/15	0.87	0.13	32,35,47,54	14
4	FUC	S	4	10/11	0.87	0.19	30,43,46,47	10
3	BMA	F	3	11/12	0.87	0.17	45,49,57,62	11
5	NAG	J	2	14/15	0.88	0.20	31,37,42,45	14
6	BMA	L	3	11/12	0.88	0.16	39,45,51,57	11
4	FUC	V	4	10/11	0.88	0.14	34,39,47,48	10
4	FUC	I	4	10/11	0.88	0.21	45,60,68,71	0
5	FUC	J	6	10/11	0.89	0.23	35,43,47,56	10

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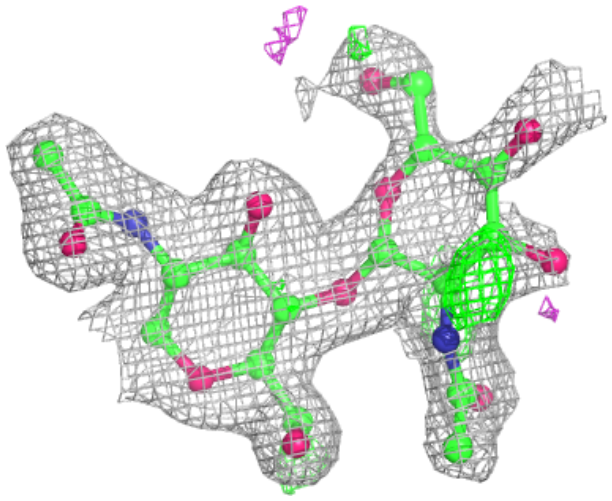
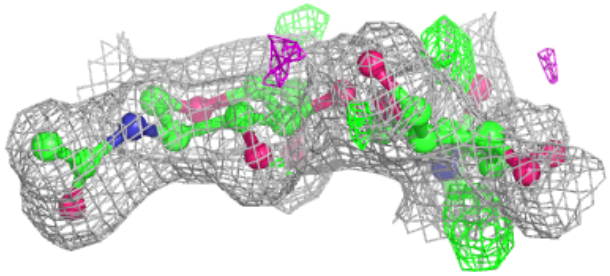
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FUC	N	4	10/11	0.89	0.15	40,44,49,50	10
5	MAN	H	5	11/12	0.89	0.28	39,44,49,50	11
4	NAG	V	2	14/15	0.90	0.18	21,38,44,53	14
4	NAG	I	1	14/15	0.91	0.15	35,44,57,61	0
4	FUC	P	4	10/11	0.91	0.12	37,46,51,51	0
3	NAG	F	2	14/15	0.92	0.13	35,39,44,44	14
4	NAG	N	1	14/15	0.92	0.12	28,43,49,51	14
4	NAG	P	2	14/15	0.92	0.19	29,40,52,62	0
3	FUC	F	6	10/11	0.92	0.18	39,43,51,53	10
9	NAG	R	1	14/15	0.92	0.11	34,40,52,53	14
4	NAG	S	1	14/15	0.93	0.11	30,39,44,46	14
3	NAG	F	1	14/15	0.95	0.09	31,34,39,44	0
4	NAG	G	1	14/15	0.95	0.10	30,38,51,55	0
5	NAG	J	1	14/15	0.95	0.07	27,32,36,37	0
4	NAG	V	1	14/15	0.95	0.09	19,25,30,30	0
6	NAG	L	2	14/15	0.96	0.07	22,28,38,39	0
2	NAG	K	1	14/15	0.96	0.09	22,31,38,46	0
5	MAN	H	4	11/12	0.96	0.13	27,34,36,40	11
7	NAG	M	1	14/15	0.96	0.07	17,28,38,39	0
2	NAG	E	1	14/15	0.96	0.07	22,28,34,39	0
5	FUC	H	6	10/11	0.96	0.12	26,30,33,47	0
5	NAG	H	2	14/15	0.96	0.10	22,27,30,31	0
5	NAG	H	1	14/15	0.97	0.07	17,22,27,32	0
4	NAG	P	1	14/15	0.97	0.08	25,30,38,42	0
2	NAG	Q	1	14/15	0.97	0.09	28,31,39,41	0
6	FUC	L	5	10/11	0.97	0.08	23,29,33,40	0
6	NAG	L	1	14/15	0.97	0.06	19,24,30,31	0

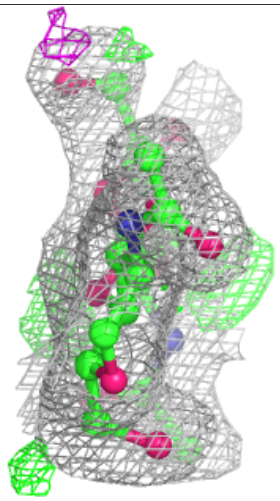
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

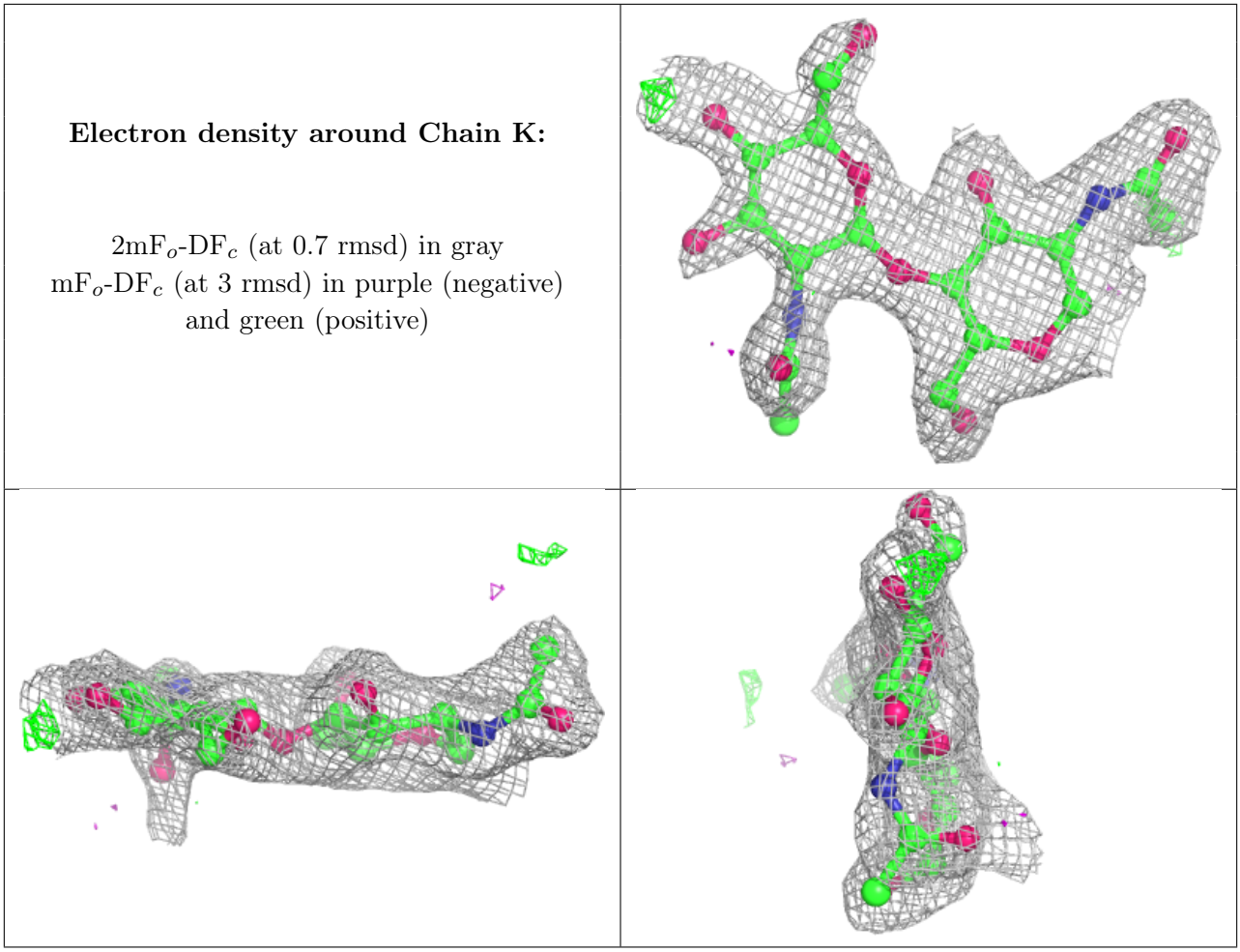






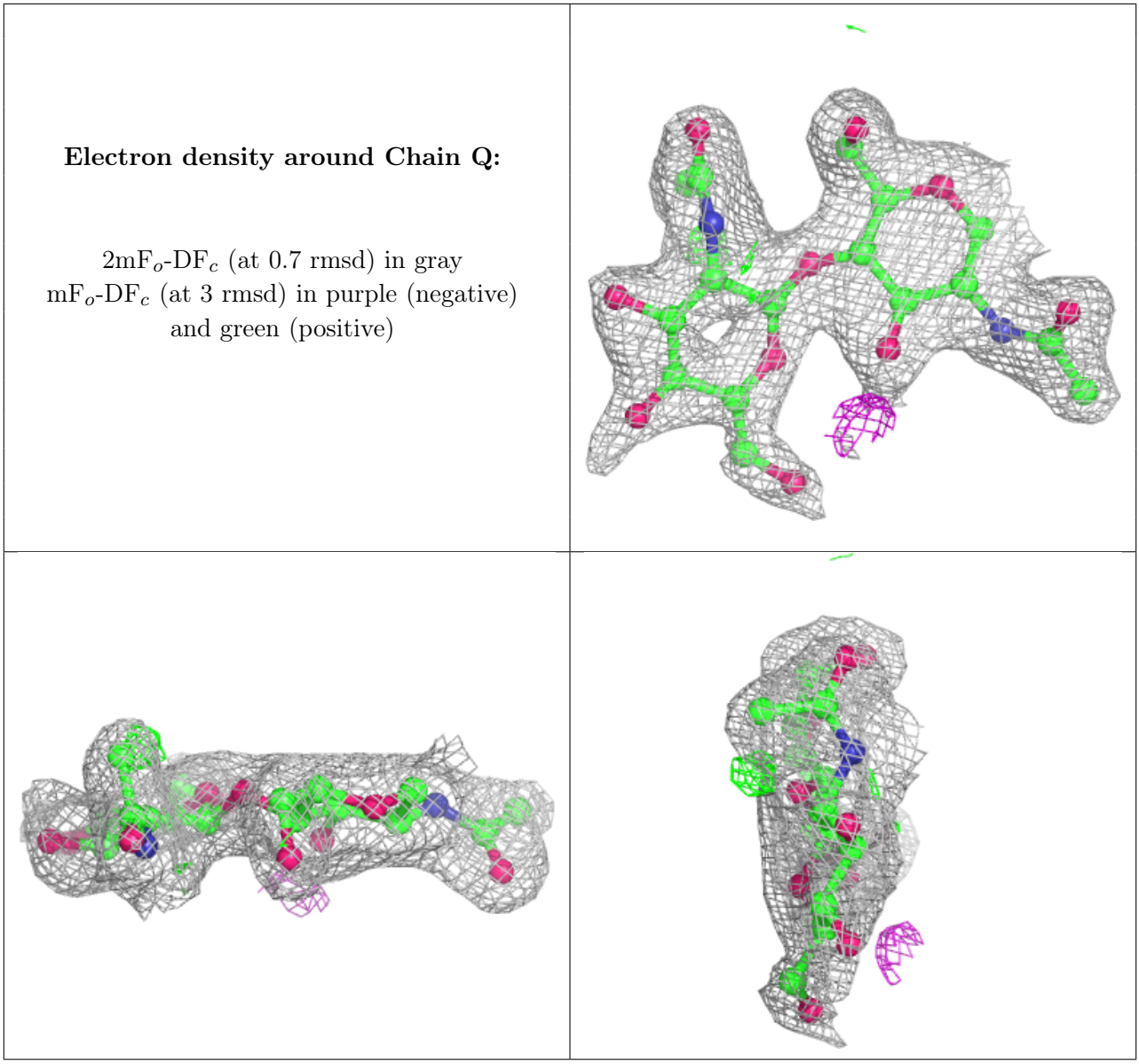
Electron density around Chain K:

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



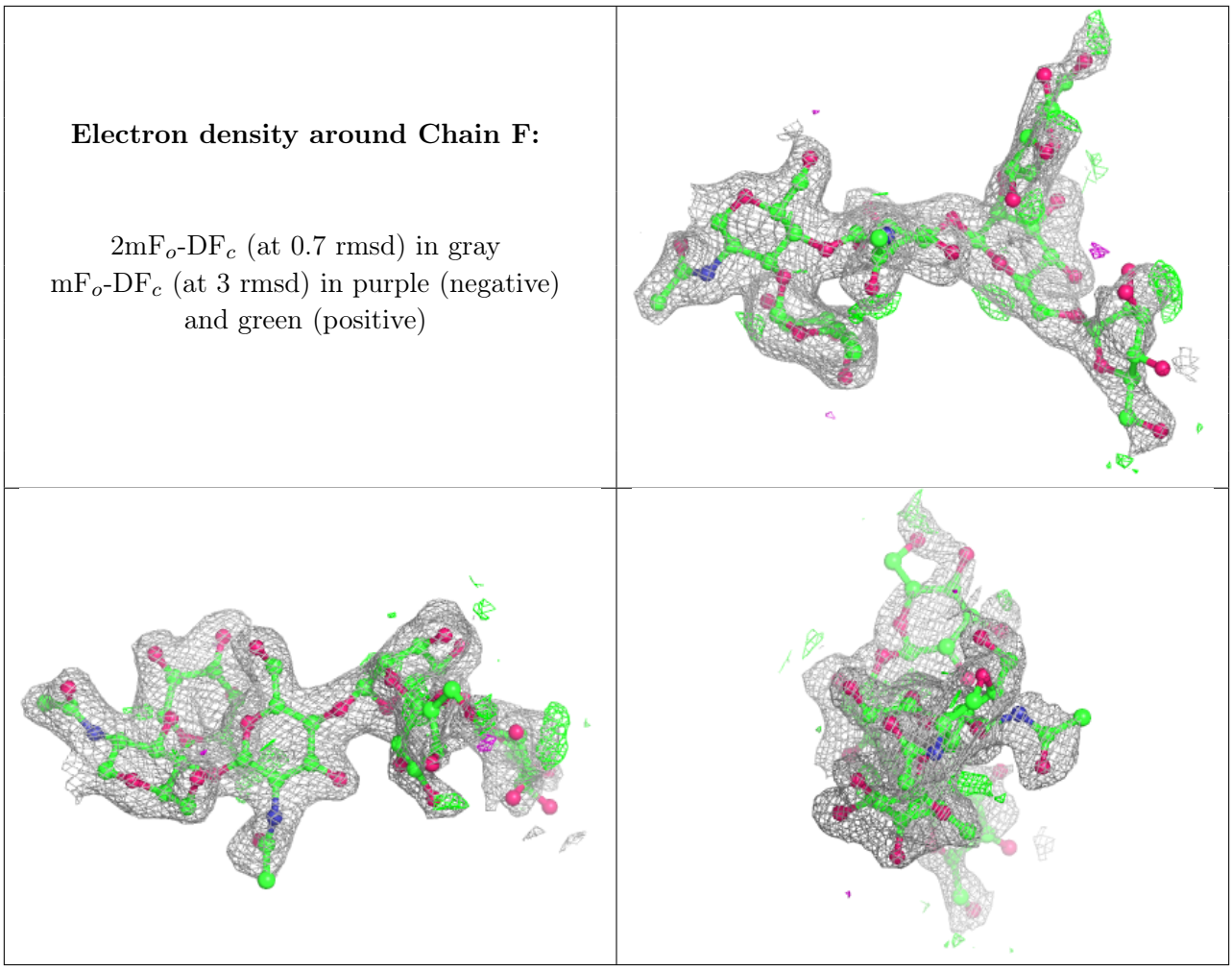
Electron density around Chain Q:

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



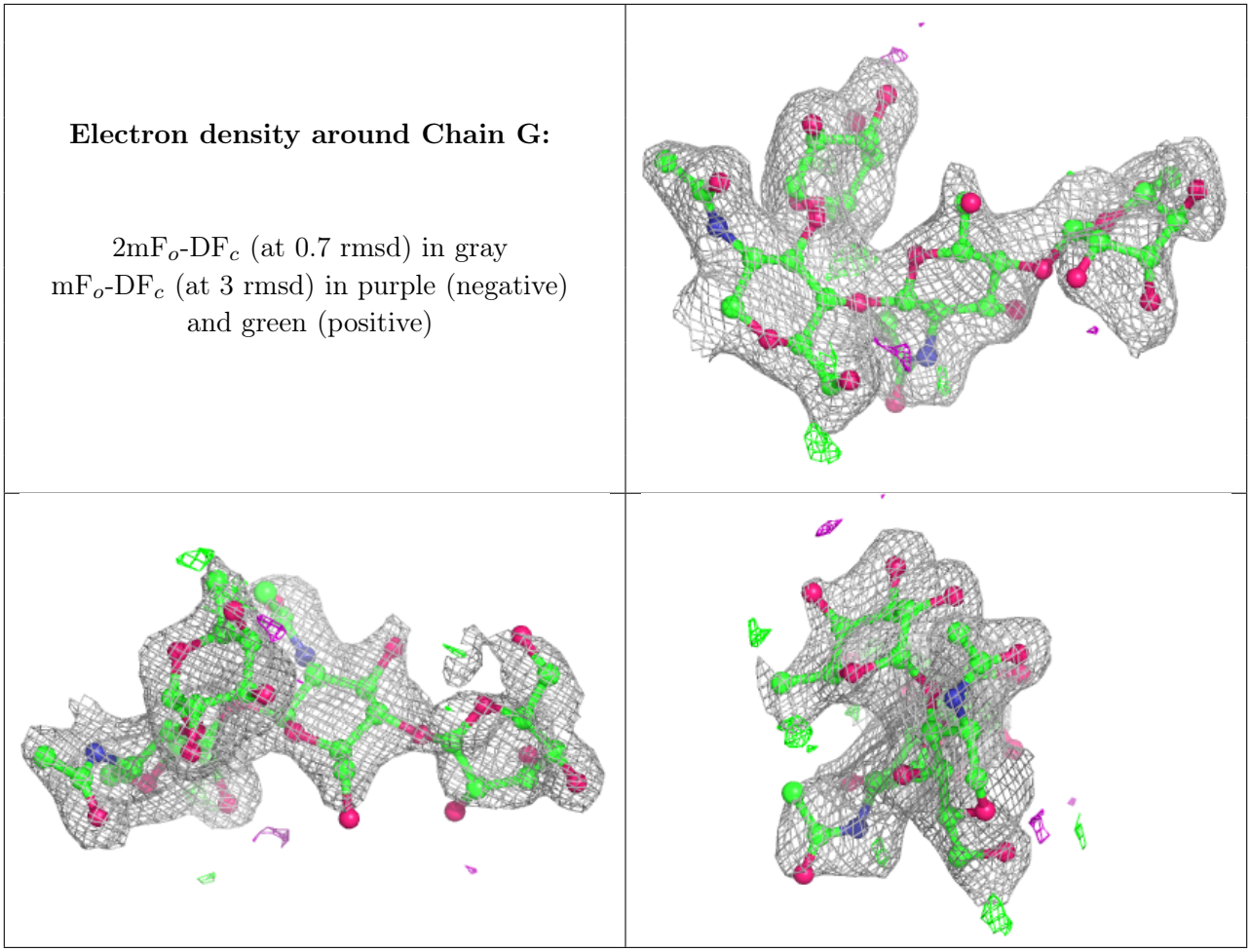
Electron density around Chain F:

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



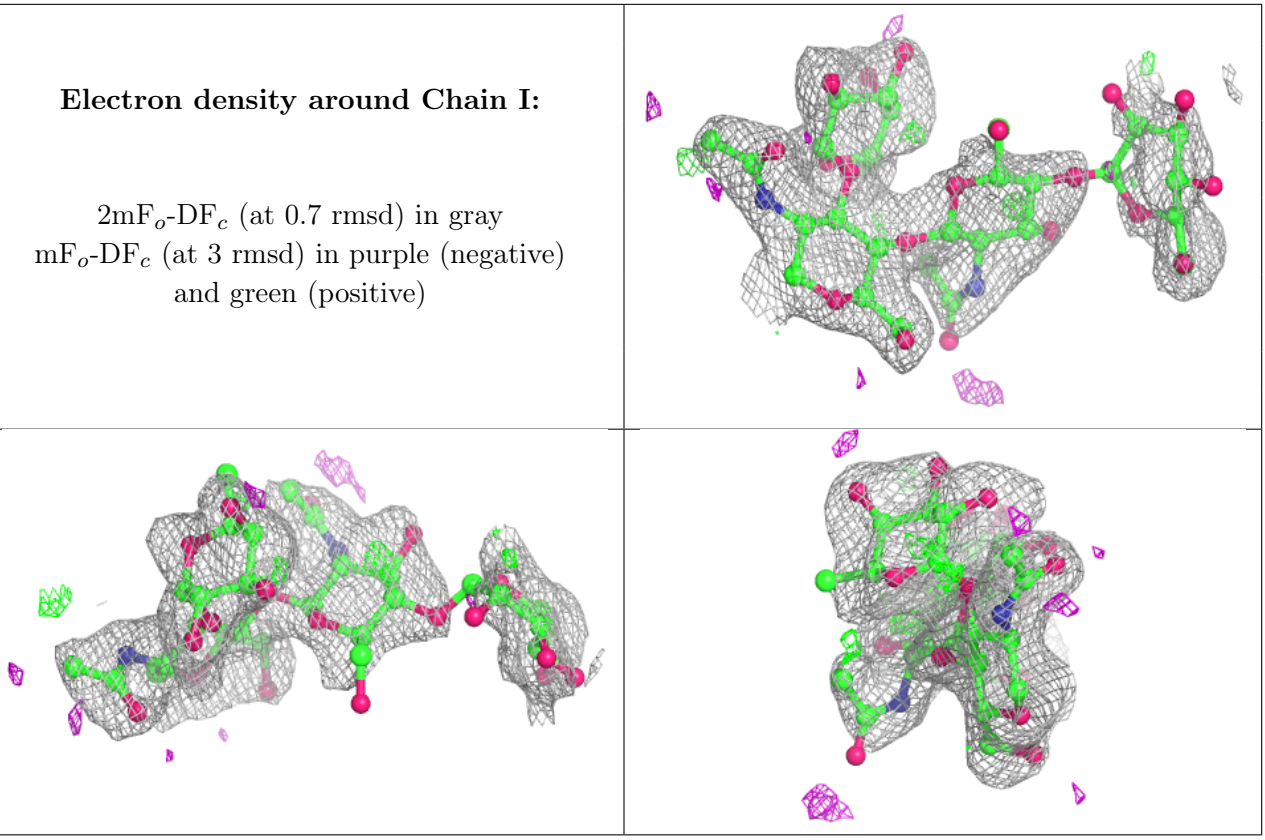
Electron density around Chain G:

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



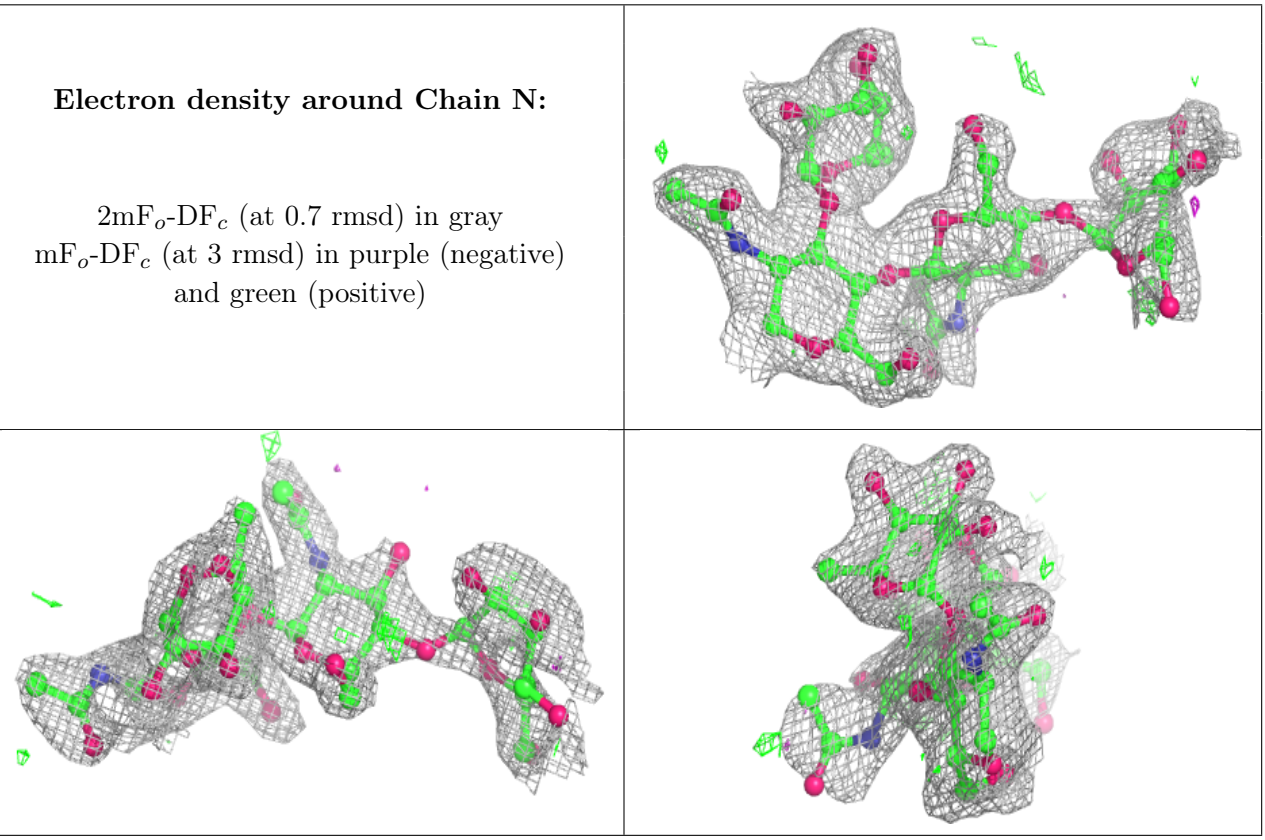
Electron density around Chain I:

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



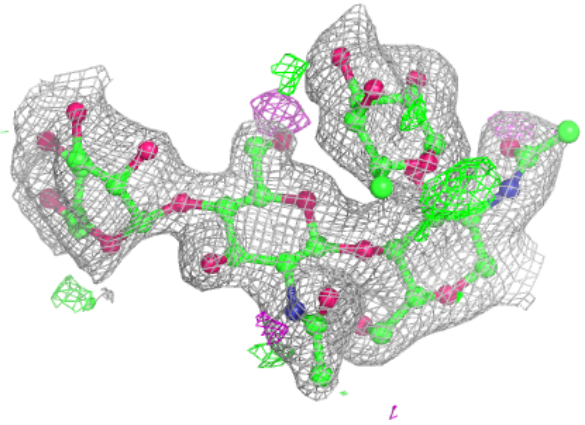
Electron density around Chain N:

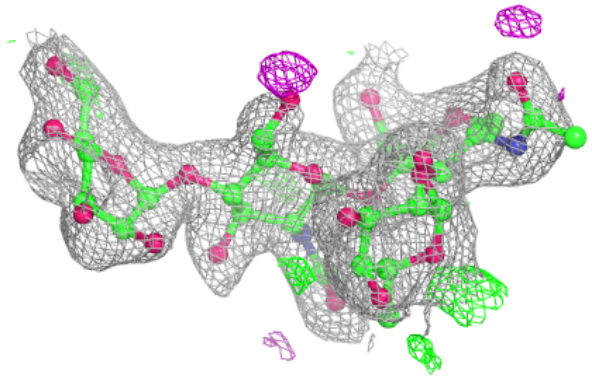
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

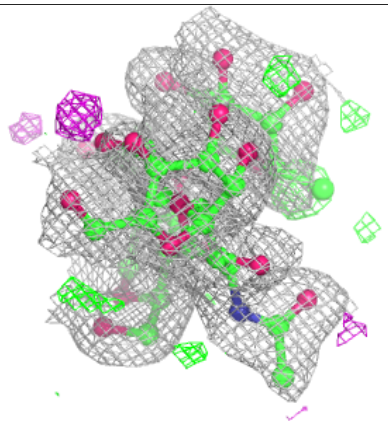


Electron density around Chain P:

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

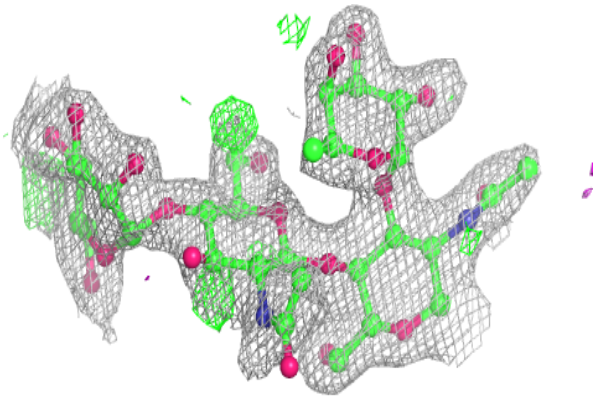


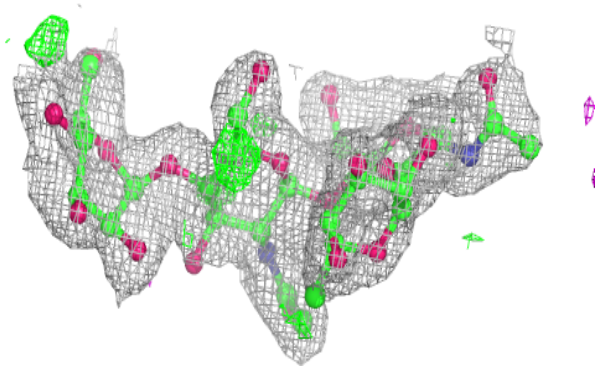


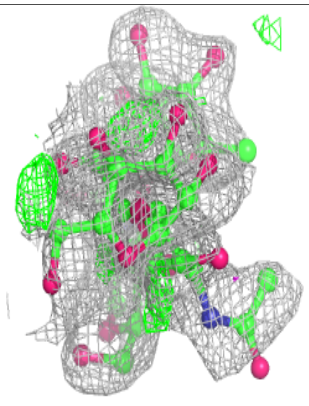


Electron density around Chain S:

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

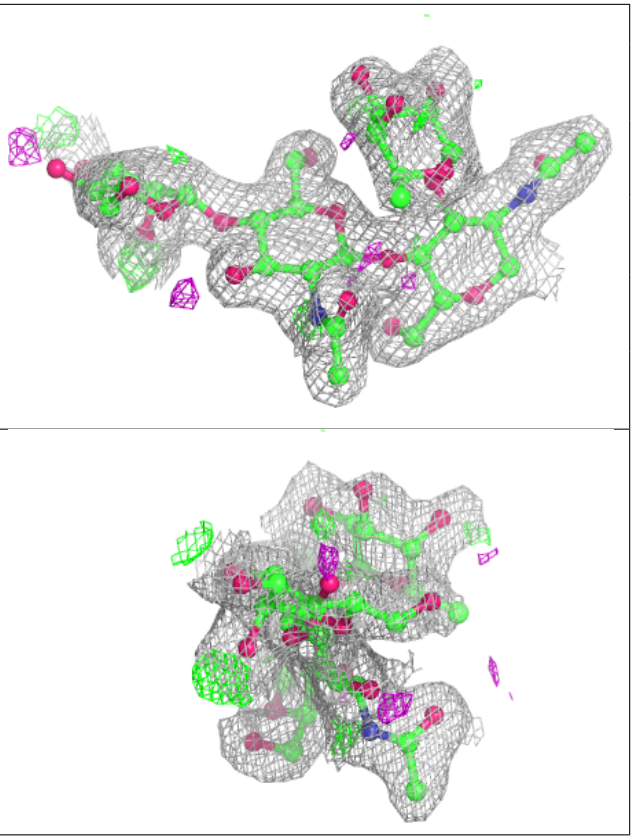


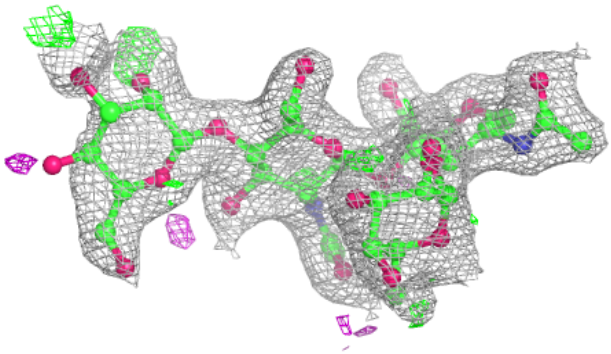




Electron density around Chain V:

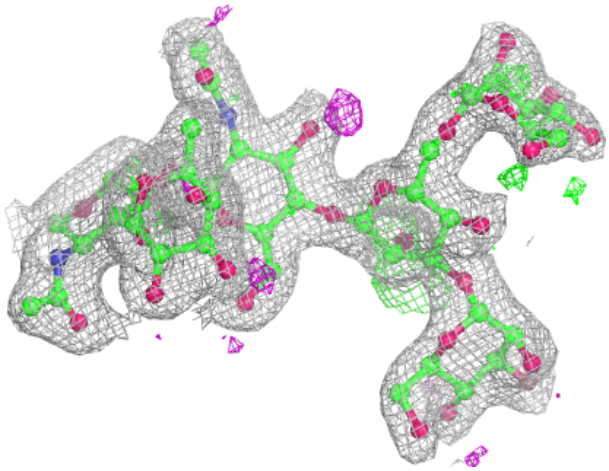
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

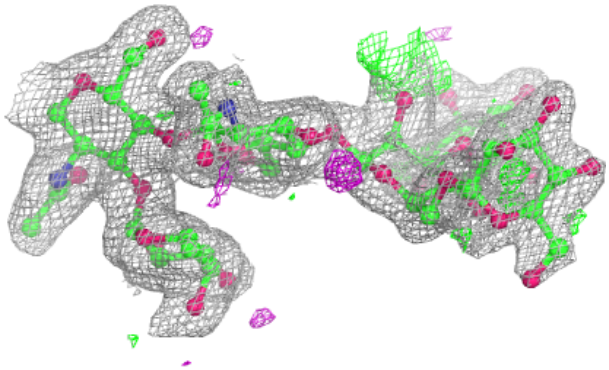


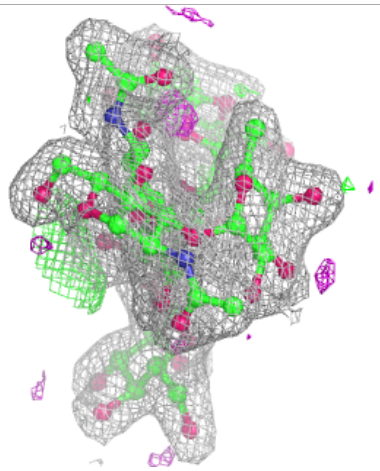


Electron density around Chain H:

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

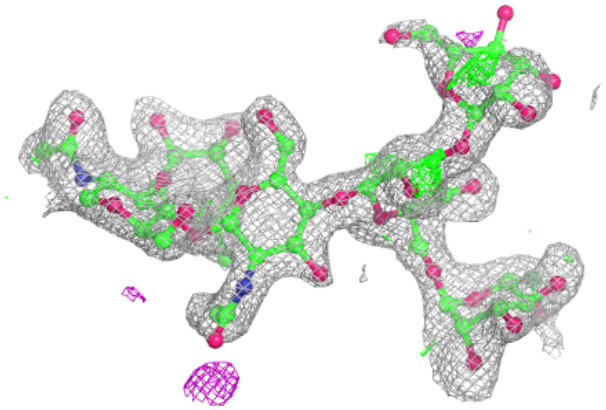


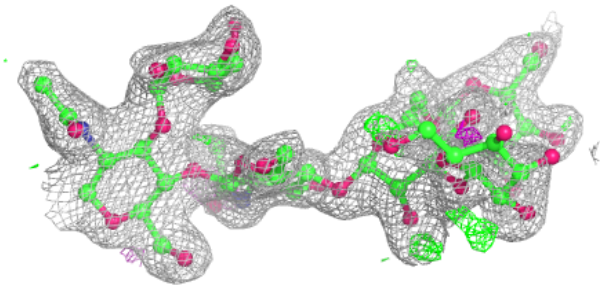


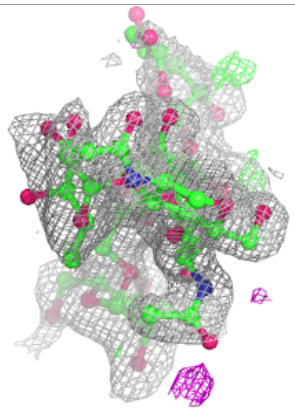


Electron density around Chain J:

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

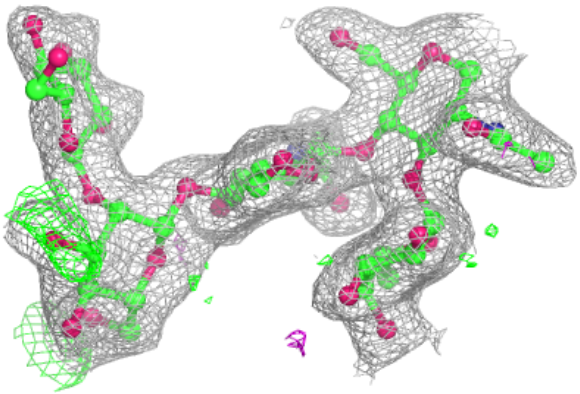


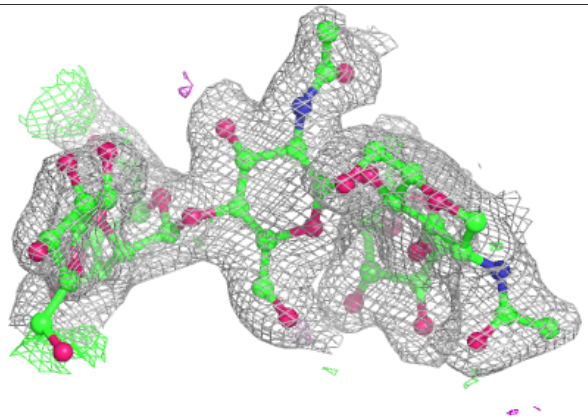


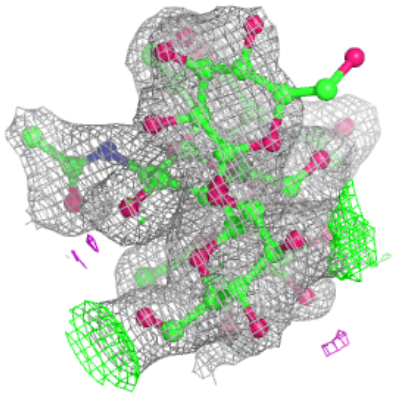


Electron density around Chain L:

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

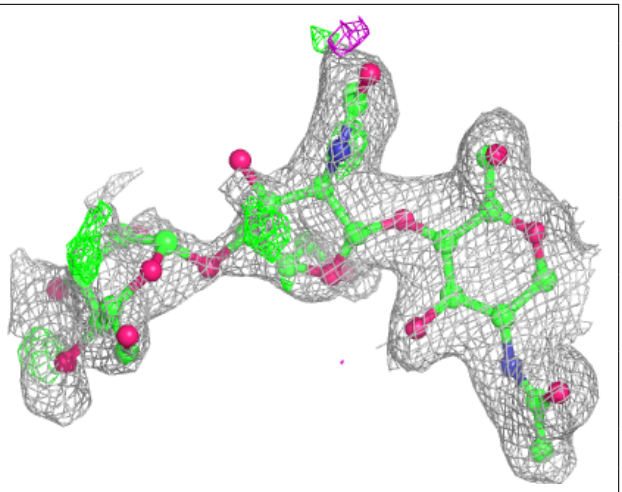


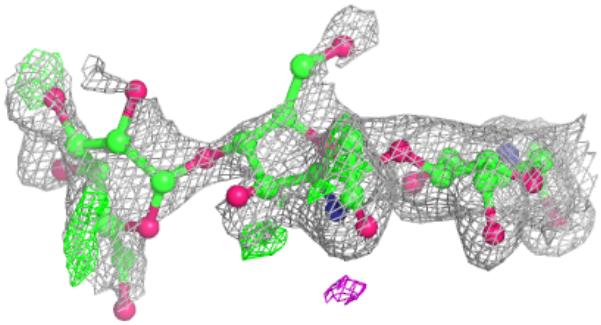


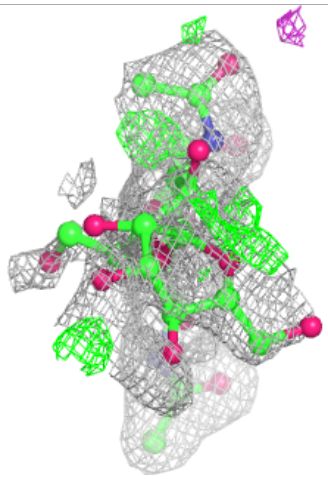


Electron density around Chain M:

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

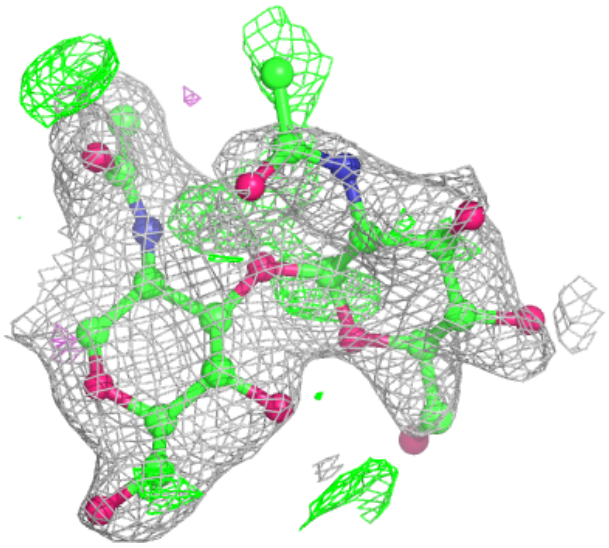


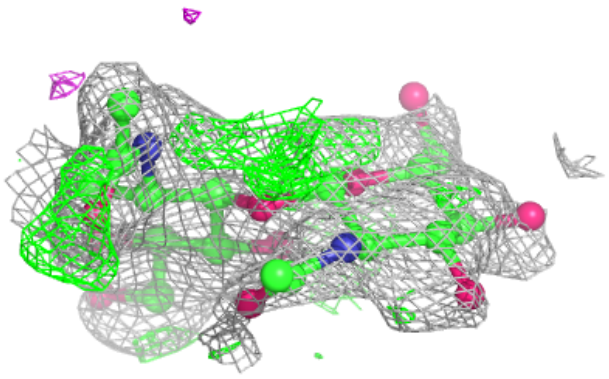


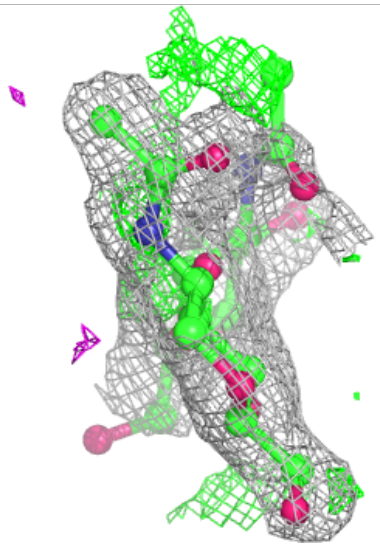


Electron density around Chain O:

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

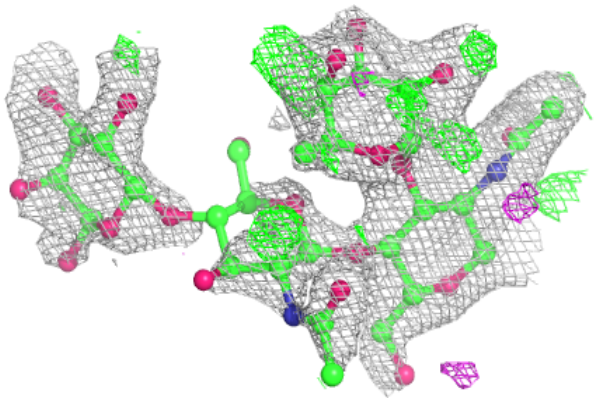


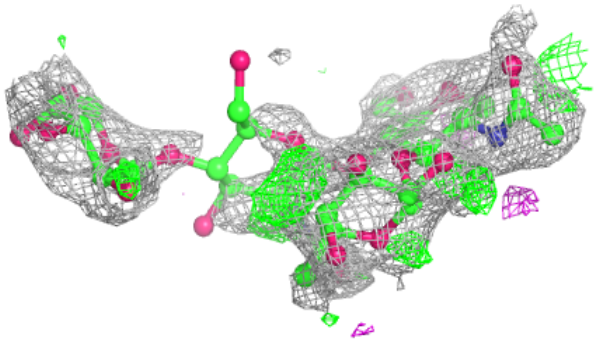


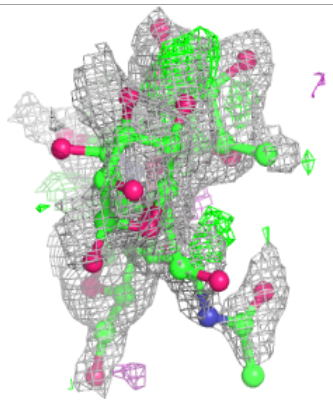


Electron density around Chain R:

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

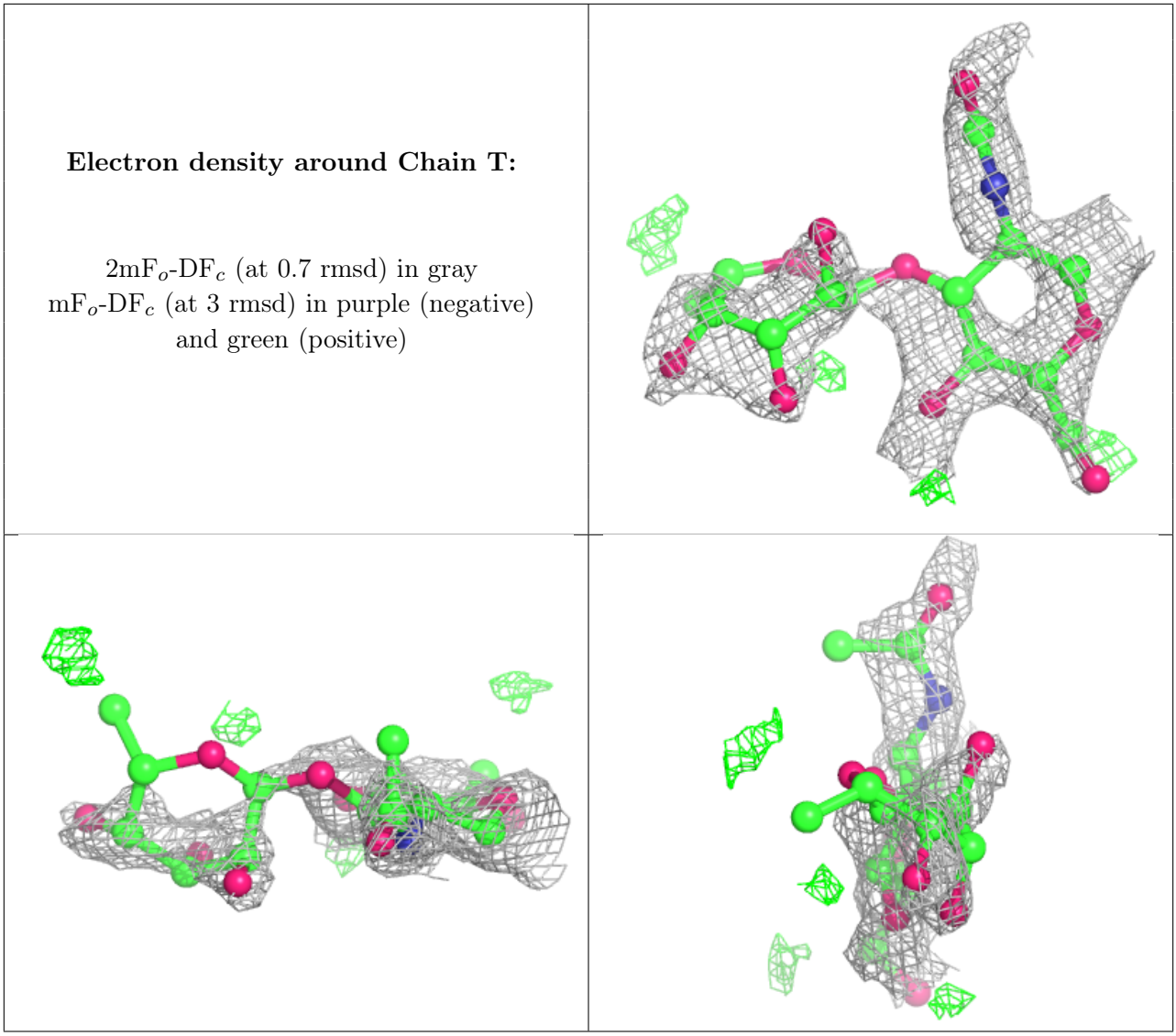






Electron density around Chain T:

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



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, 95^{th} 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
14	PGE	B	508	10/10	0.57	0.46	37,43,48,49	10
13	FLC	B	507	13/13	0.59	0.39	17,32,38,38	13
15	NAG	D	506	14/15	0.63	0.34	53,60,74,80	14
13	FLC	C	603	13/13	0.68	0.33	30,35,48,54	13
18	GOL	A	526	6/6	0.68	0.41	45,50,51,52	6
20	R9X	D	535[A]	27/27	0.68	0.39	21,37,44,45	27
20	R9X	D	535[B]	27/27	0.68	0.39	36,40,45,51	27

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	NAG	A	506	14/15	0.69	0.27	33,44,47,55	14
13	FLC	A	505	13/13	0.70	0.34	40,44,49,57	13
20	R9X	A	532[A]	27/27	0.71	0.36	29,43,48,49	27
20	R9X	A	532[B]	27/27	0.71	0.36	23,44,50,57	27
13	FLC	C	602	13/13	0.71	0.34	25,35,44,49	13
15	NAG	C	605	14/15	0.71	0.25	30,43,51,55	14
13	FLC	D	503	13/13	0.72	0.31	26,33,38,43	13
20	R9X	C	633[B]	27/27	0.72	0.41	36,46,50,52	27
20	R9X	C	632[A]	27/27	0.73	0.41	31,45,48,50	27
18	GOL	C	631	6/6	0.73	0.30	51,55,59,60	6
13	FLC	B	503	13/13	0.73	0.26	28,39,48,54	13
15	NAG	C	616	14/15	0.73	0.27	42,47,52,61	14
13	FLC	A	530	13/13	0.74	0.29	30,39,45,50	13
16	SO4	B	517	5/5	0.74	0.26	42,43,49,53	5
13	FLC	A	503	13/13	0.74	0.31	25,32,40,42	13
13	FLC	B	505	13/13	0.74	0.30	33,41,46,50	13
13	FLC	B	506	13/13	0.74	0.32	47,54,68,68	13
20	R9X	B	531[A]	27/27	0.75	0.36	25,40,44,46	27
20	R9X	B	531[B]	27/27	0.75	0.36	35,42,46,49	27
13	FLC	C	628	13/13	0.77	0.30	43,48,54,54	13
18	GOL	A	527	6/6	0.77	0.28	39,44,50,52	6
18	GOL	C	624	6/6	0.77	0.22	31,37,42,43	6
18	GOL	A	517	6/6	0.77	0.23	27,32,36,37	6
17	EDO	C	617	4/4	0.79	0.25	39,41,44,46	4
18	GOL	B	520	6/6	0.80	0.23	36,39,43,46	6
18	GOL	D	534	6/6	0.80	0.28	36,37,40,41	6
18	GOL	D	532	6/6	0.81	0.26	40,51,54,57	6
18	GOL	C	629	6/6	0.81	0.14	51,53,56,56	6
18	GOL	B	524	6/6	0.82	0.26	33,39,41,50	6
18	GOL	D	524	6/6	0.82	0.32	30,32,35,36	6
18	GOL	C	623	6/6	0.82	0.32	30,39,46,49	6
14	PGE	A	504	10/10	0.82	0.27	31,36,43,44	10
16	SO4	B	516	5/5	0.82	0.29	40,41,45,47	5
18	GOL	C	630	6/6	0.82	0.26	33,41,43,45	6
18	GOL	B	523	6/6	0.83	0.29	31,38,41,41	6
18	GOL	A	524	6/6	0.83	0.20	24,34,39,41	6
13	FLC	C	627	13/13	0.83	0.19	28,33,39,52	13
17	EDO	B	518	4/4	0.84	0.34	28,31,32,37	4
18	GOL	D	533	6/6	0.85	0.35	26,29,32,33	6
18	GOL	A	522	6/6	0.85	0.17	33,38,41,41	6
18	GOL	D	526	6/6	0.85	0.32	32,36,42,43	6
18	GOL	D	529	6/6	0.85	0.36	25,28,34,34	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	PGE	A	507	7/10	0.85	0.28	25,27,34,38	7
18	GOL	C	622	6/6	0.86	0.21	22,28,30,35	6
18	GOL	A	531	6/6	0.86	0.28	37,41,43,46	6
14	PGE	D	504	10/10	0.86	0.24	20,22,26,28	10
16	SO4	C	611	5/5	0.86	0.25	51,52,67,69	5
14	PGE	B	504	10/10	0.86	0.26	17,25,33,33	10
18	GOL	B	526	6/6	0.86	0.23	32,36,39,41	6
18	GOL	D	520	6/6	0.86	0.16	35,38,44,47	6
18	GOL	A	525	6/6	0.87	0.20	36,41,45,47	6
16	SO4	C	615	5/5	0.87	0.20	38,43,46,49	5
18	GOL	B	527	6/6	0.87	0.23	27,31,37,41	6
18	GOL	B	528	6/6	0.87	0.28	43,44,45,46	6
15	NAG	D	516	14/15	0.87	0.14	37,45,47,51	14
18	GOL	A	523	6/6	0.88	0.23	56,58,60,60	6
18	GOL	A	519	6/6	0.88	0.18	22,33,39,39	6
16	SO4	D	513	5/5	0.88	0.28	41,44,46,55	5
18	GOL	C	619	6/6	0.89	0.20	24,25,28,34	6
16	SO4	A	513	5/5	0.89	0.22	44,49,51,56	5
16	SO4	A	511	5/5	0.89	0.29	36,46,63,63	5
18	GOL	B	522	6/6	0.89	0.20	17,34,36,37	6
18	GOL	A	520	6/6	0.89	0.14	29,36,43,46	6
18	GOL	D	527	6/6	0.89	0.23	17,26,32,38	6
14	PGE	C	604	10/10	0.90	0.22	25,33,37,42	10
16	SO4	D	515	5/5	0.90	0.21	47,48,52,62	5
18	GOL	B	525	6/6	0.90	0.24	40,52,54,56	0
17	EDO	D	517	4/4	0.90	0.27	30,30,34,37	4
18	GOL	D	523	6/6	0.90	0.22	30,36,40,45	6
18	GOL	A	516	6/6	0.90	0.20	23,26,31,34	6
18	GOL	D	525	6/6	0.90	0.13	37,47,49,51	6
18	GOL	B	519	6/6	0.91	0.17	27,28,33,35	6
13	FLC	C	601	13/13	0.91	0.13	21,35,45,48	13
18	GOL	C	620	6/6	0.91	0.19	15,27,28,29	6
18	GOL	C	621	6/6	0.91	0.23	20,29,38,48	6
22	DMS	D	505	4/4	0.91	0.27	41,47,53,74	4
18	GOL	D	528	6/6	0.92	0.18	42,44,47,47	0
18	GOL	D	522	6/6	0.92	0.15	25,34,38,40	6
18	GOL	B	521	6/6	0.93	0.17	26,30,35,37	6
16	SO4	D	512	5/5	0.93	0.25	33,36,41,42	5
16	SO4	B	515	5/5	0.93	0.31	55,63,69,70	5
18	GOL	A	521	6/6	0.93	0.17	15,26,27,31	6
18	GOL	C	618	6/6	0.93	0.13	28,29,36,43	6
18	GOL	C	625	6/6	0.94	0.22	22,36,42,45	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	SO4	D	514	5/5	0.94	0.18	55,56,62,63	5
16	SO4	C	608	5/5	0.94	0.13	26,28,30,33	5
18	GOL	A	518	6/6	0.94	0.11	19,23,33,34	6
18	GOL	D	519	6/6	0.94	0.18	23,26,31,34	6
16	SO4	D	509	5/5	0.94	0.20	38,44,56,56	5
18	GOL	D	521	6/6	0.94	0.17	27,33,40,43	6
16	SO4	A	512	5/5	0.94	0.31	26,30,31,34	5
16	SO4	C	613	5/5	0.94	0.31	56,58,59,63	5
16	SO4	C	610	5/5	0.95	0.15	22,24,36,42	5
16	SO4	D	510	5/5	0.95	0.16	27,37,39,43	5
16	SO4	C	609	5/5	0.95	0.19	40,43,54,55	5
16	SO4	D	511	5/5	0.96	0.20	28,37,39,50	5
16	SO4	B	510	5/5	0.96	0.12	18,28,31,32	5
16	SO4	D	508	5/5	0.96	0.17	26,28,32,34	5
16	SO4	B	514	5/5	0.96	0.09	24,28,35,37	5
16	SO4	C	614	5/5	0.96	0.20	35,36,45,51	5
17	EDO	A	514	4/4	0.96	0.13	19,22,28,28	4
16	SO4	C	612	5/5	0.97	0.07	25,34,36,39	5
16	SO4	B	513	5/5	0.97	0.20	40,46,50,51	5
18	GOL	A	515	6/6	0.97	0.07	17,22,24,24	0
16	SO4	B	509	5/5	0.97	0.20	36,42,48,52	5
16	SO4	A	509	5/5	0.97	0.08	25,30,40,40	5
16	SO4	D	507	5/5	0.97	0.09	26,35,40,43	5
18	GOL	D	518	6/6	0.98	0.06	16,20,22,25	0
16	SO4	B	512	5/5	0.98	0.14	26,26,32,37	5
16	SO4	A	508	5/5	0.98	0.08	22,27,27,28	5
19	CL	A	528	1/1	0.99	0.04	24,24,24,24	0
19	CL	C	626	1/1	0.99	0.02	19,19,19,19	0
19	CL	D	531	1/1	0.99	0.04	30,30,30,30	0
16	SO4	B	511	5/5	0.99	0.08	27,29,31,40	5
16	SO4	A	510	5/5	0.99	0.07	28,35,36,38	0
12	FE	B	502	1/1	0.99	0.02	27,27,27,27	1
11	ZN	B	501	1/1	1.00	0.03	24,24,24,24	0
11	ZN	C	606	1/1	1.00	0.01	23,23,23,23	0
11	ZN	D	501	1/1	1.00	0.01	22,22,22,22	0
12	FE	A	502	1/1	1.00	0.02	22,22,22,22	1
11	ZN	A	501	1/1	1.00	0.02	22,22,22,22	0
12	FE	C	607	1/1	1.00	0.01	25,25,25,25	1
19	CL	A	529	1/1	1.00	0.02	19,19,19,19	0
19	CL	B	529	1/1	1.00	0.06	19,19,19,19	0
12	FE	D	502	1/1	1.00	0.02	24,24,24,24	1
21	NA	B	530	1/1	1.00	0.22	21,21,21,21	0

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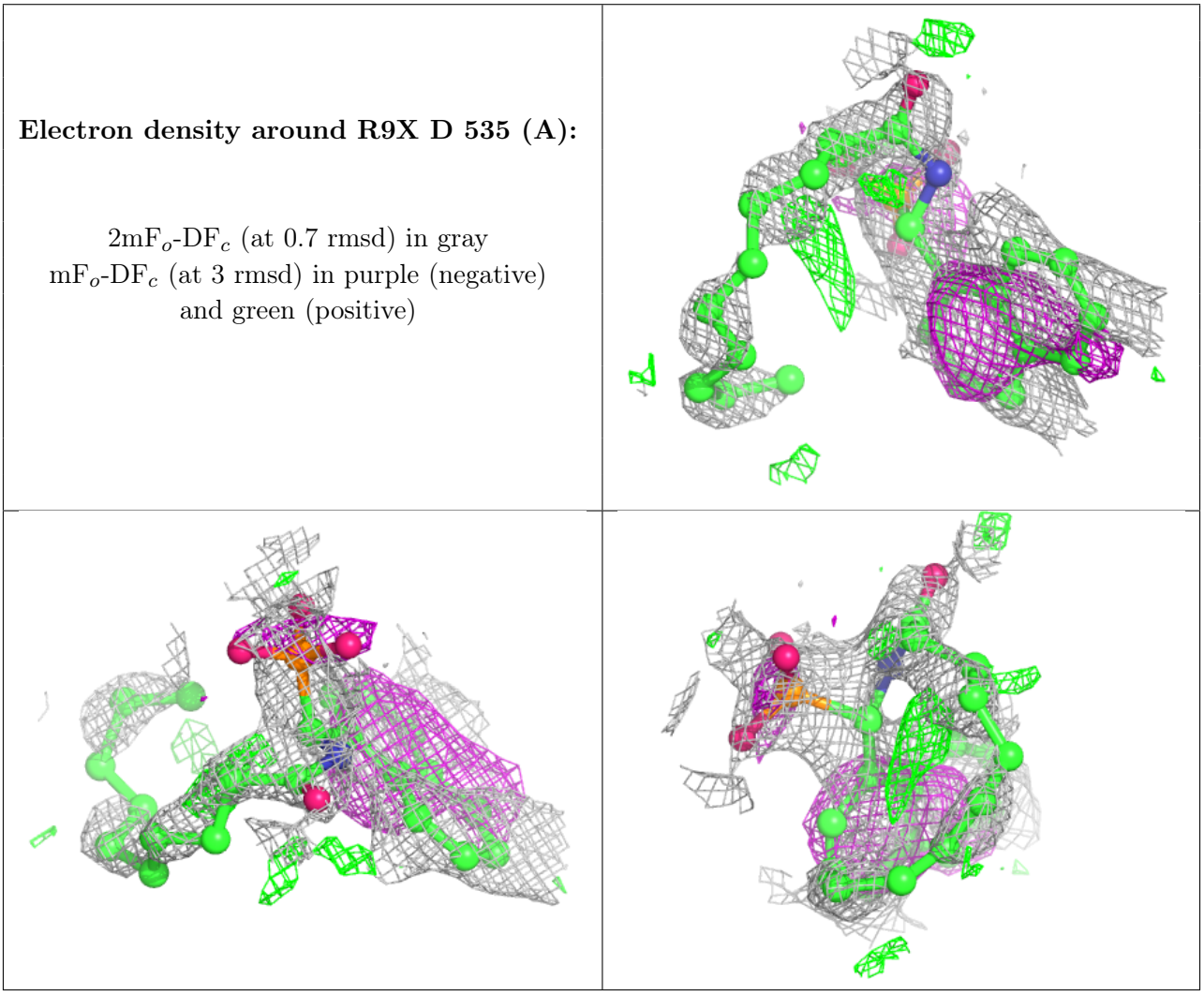
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	CL	D	530	1/1	1.00	0.02	19,19,19,19	0

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.

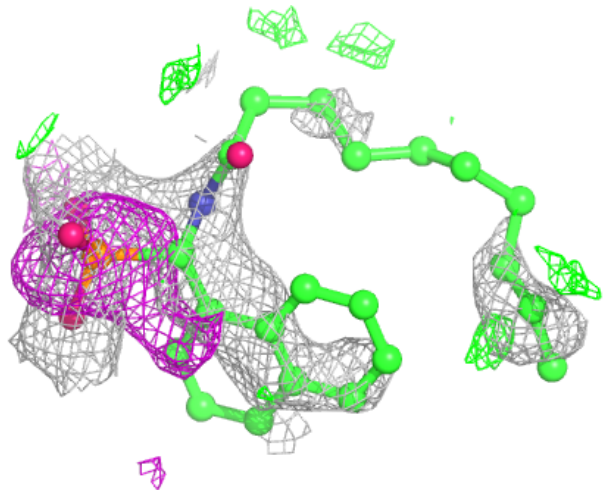
Electron density around R9X D 535 (A):

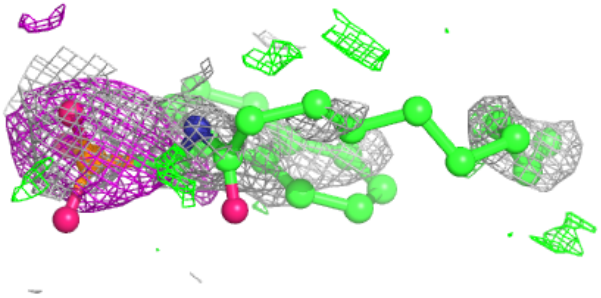
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

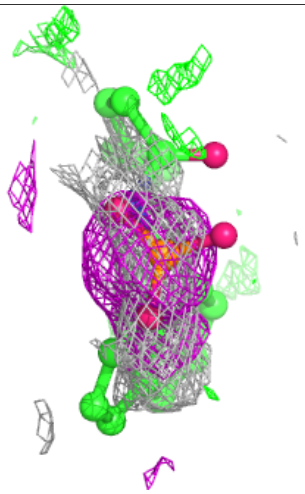


Electron density around R9X D 535 (B):

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

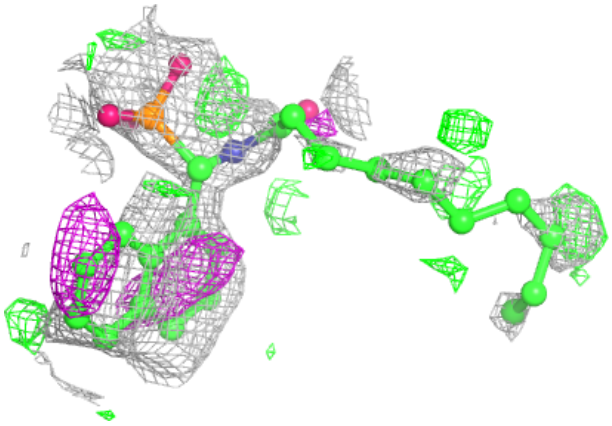


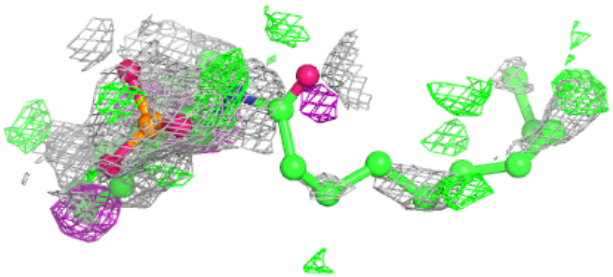


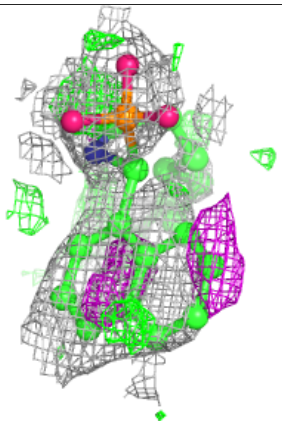


Electron density around R9X A 532 (A):

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

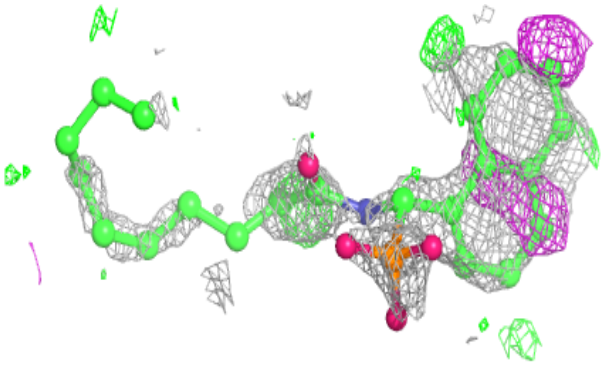


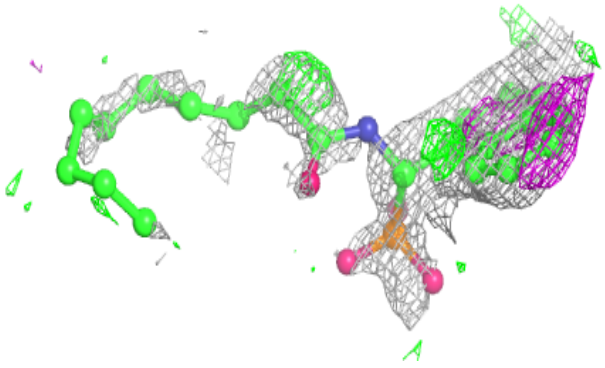


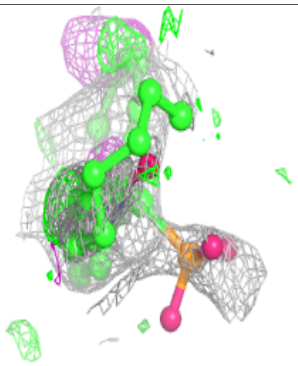


Electron density around R9X A 532 (B):

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

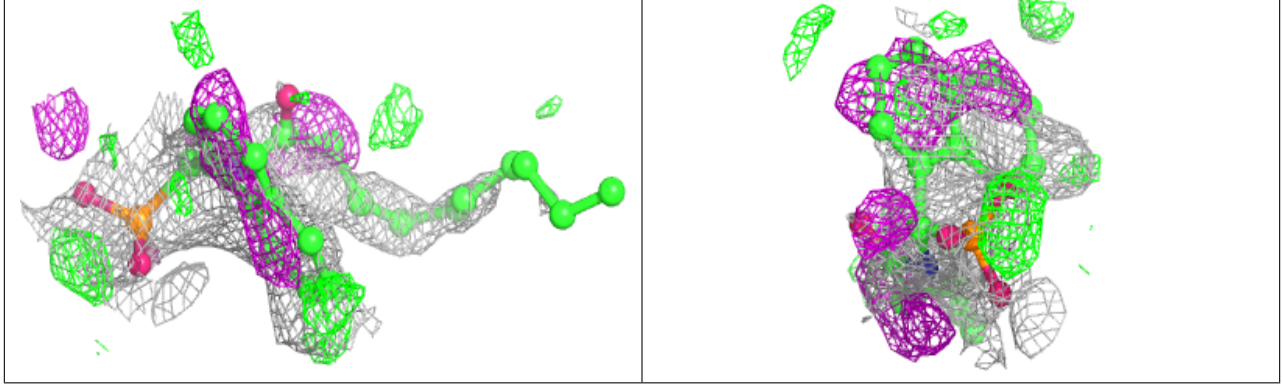






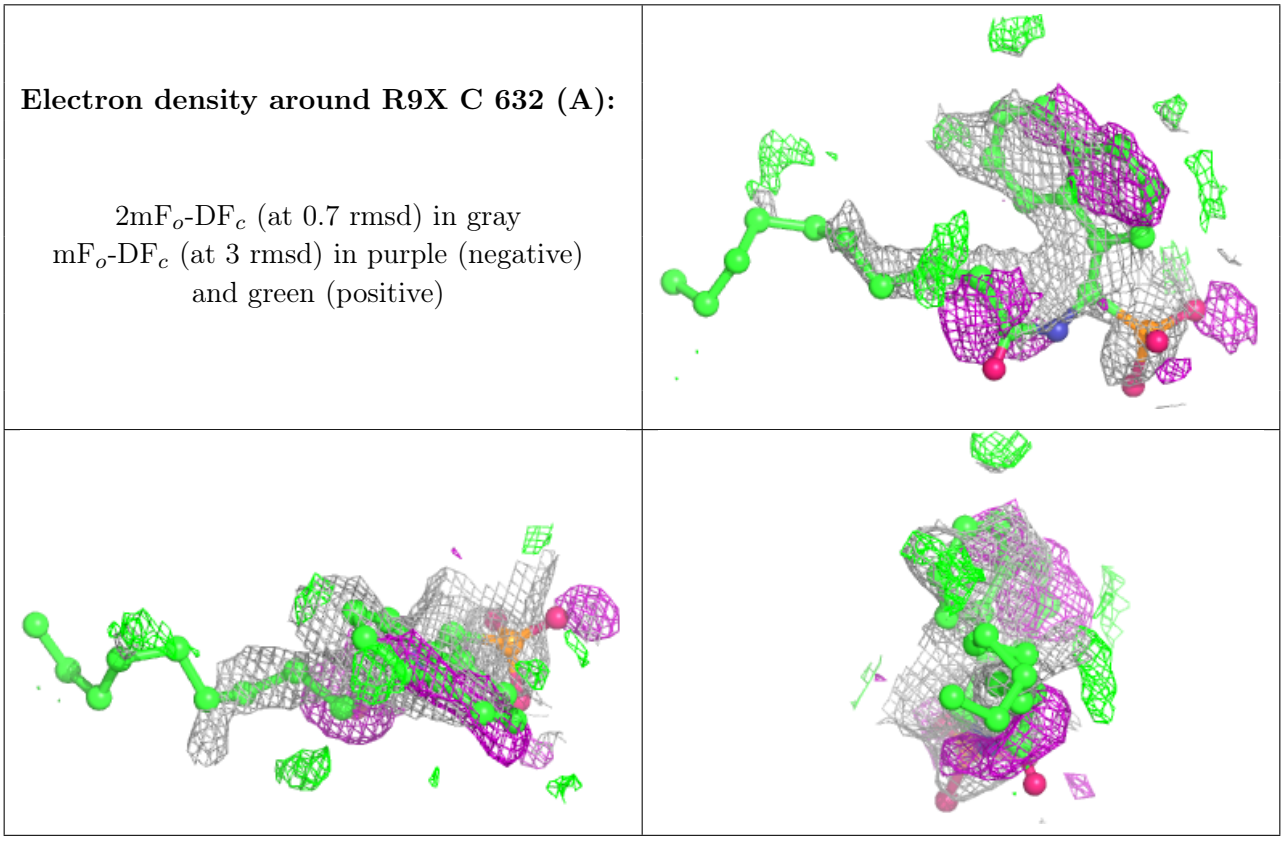
Electron density around R9X C 633 (B):

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



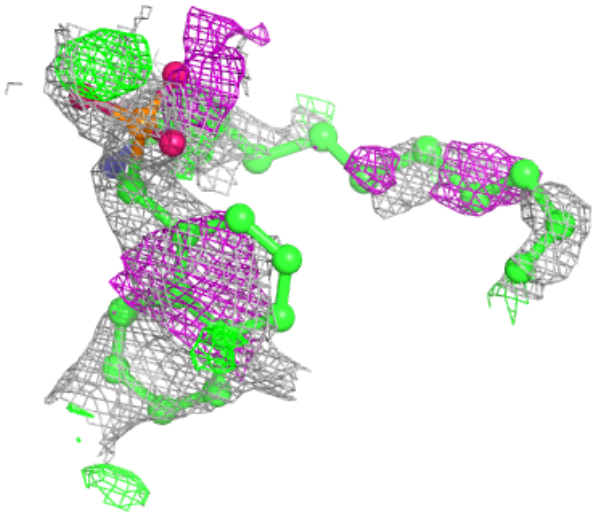
Electron density around R9X C 632 (A):

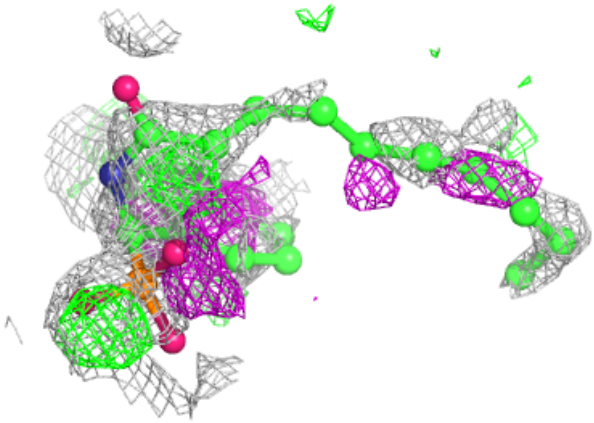
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

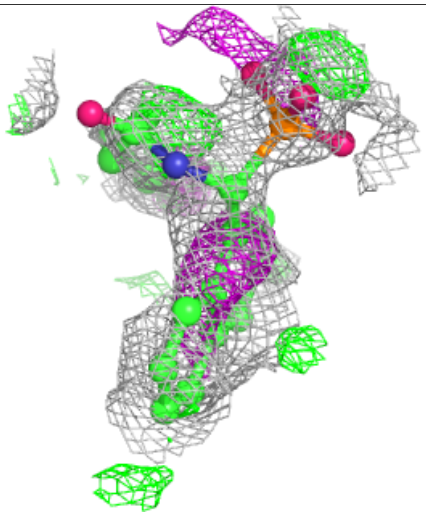


Electron density around R9X B 531 (A):

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

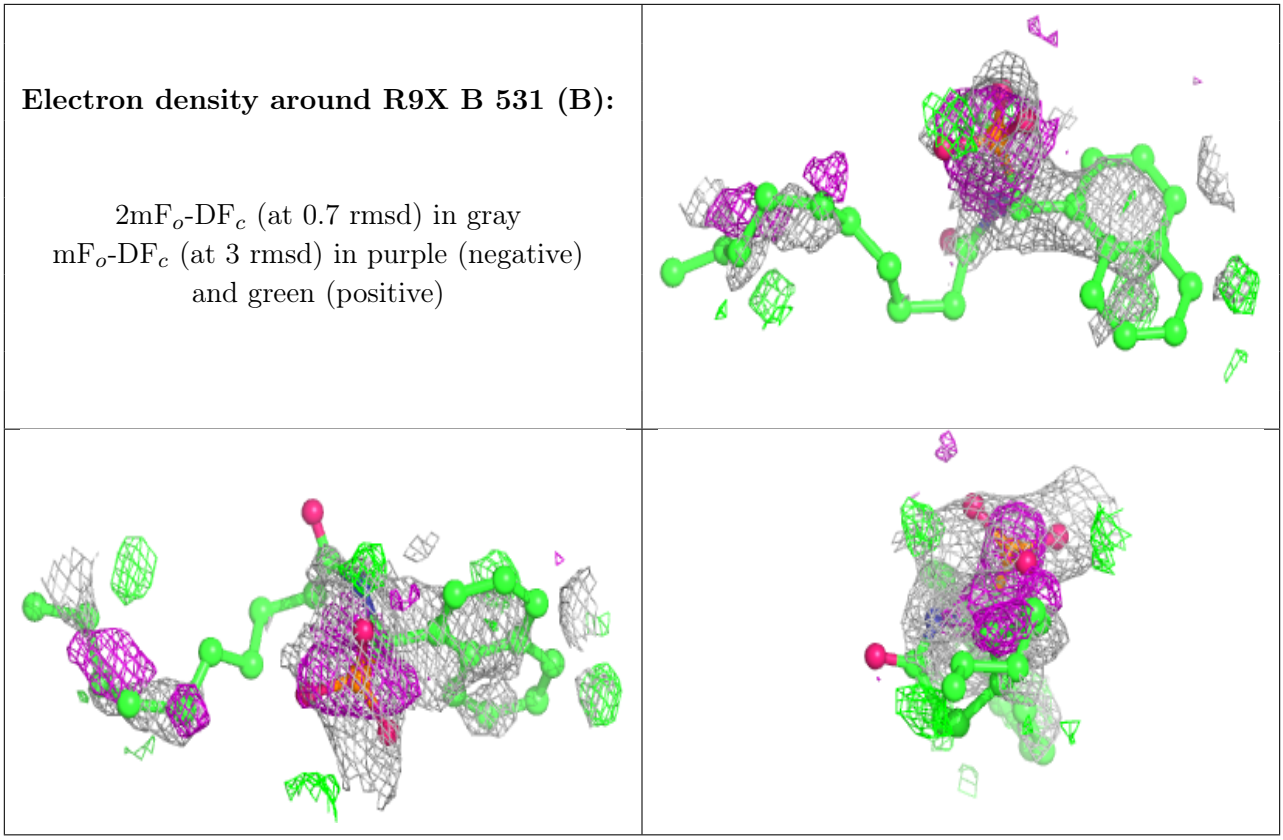






Electron density around R9X B 531 (B):

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



6.5 Other polymers

There are no such residues in this entry.