



# wwPDB X-ray Structure Validation Summary Report

Mar 12, 2026 – 03:31 PM UTC

PDB ID : 6OF5 / pdb\_00006of5  
Title : The crystal structure of dodecyloxy(naphthalen-1-yl)methylphosphonic acid  
in complex with red kidney bean purple acid phosphatase  
Authors : Feder, D.; Schenk, G.; Guddat, L.W.; Hussein, W.M.; McGeary, R.P.  
Deposited on : 2019-03-28  
Resolution : 2.30 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

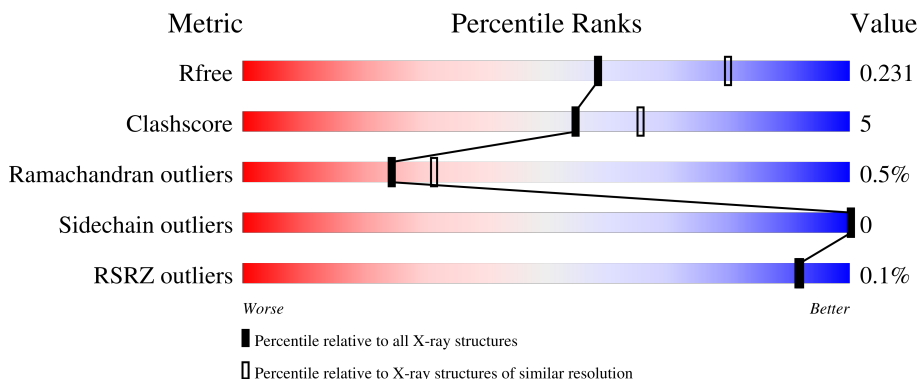
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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





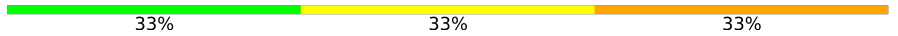
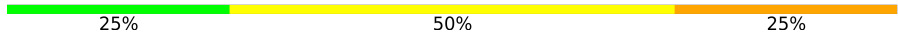
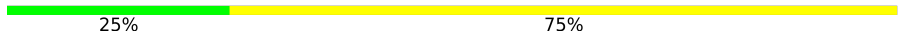

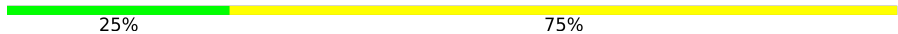
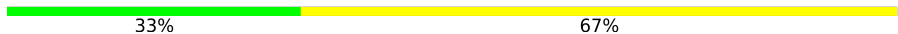

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	426	 90% 9%
1	B	426	 87% 12%
1	C	426	 89% 10% .
1	D	426	 89% 10% .
2	E	3	 67% 33%

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Mol	Chain	Length	Quality of chain
2	H	3	
2	K	3	
2	M	3	
3	F	4	
3	I	4	
3	J	4	
3	N	4	
4	G	6	
5	L	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	SO4	A	519	-	-	X	-
9	SO4	B	516	-	-	X	-
9	SO4	B	517	-	-	X	-

## 2 Entry composition [i](#)

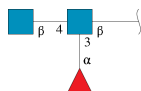
There are 15 unique types of molecules in this entry. The entry contains 15939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

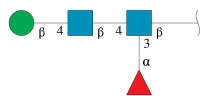
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	Total 3507	C 2251	N 611	O 635	S 10	0	2	0
1	B	425	Total 3531	C 2265	N 616	O 639	S 11	0	4	0
1	D	423	Total 3491	C 2244	N 605	O 632	S 10	0	1	0
1	C	423	Total 3487	C 2240	N 604	O 633	S 10	0	1	0

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



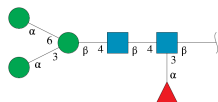
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	Total 38	C 22	N 2	O 14	0	0	0
2	H	3	Total 38	C 22	N 2	O 14	0	0	0
2	K	3	Total 38	C 22	N 2	O 14	0	0	0
2	M	3	Total 38	C 22	N 2	O 14	0	0	0

- Molecule 3 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
			Total	C	N	O			
3	F	4	49	28	2	19	0	0	0
3	I	4	49	28	2	19	0	0	0
3	J	4	49	28	2	19	0	0	0
3	N	4	49	28	2	19	0	0	0

- Molecule 4 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
			Total	C	N	O			
4	G	6	71	40	2	29	0	0	0

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



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0

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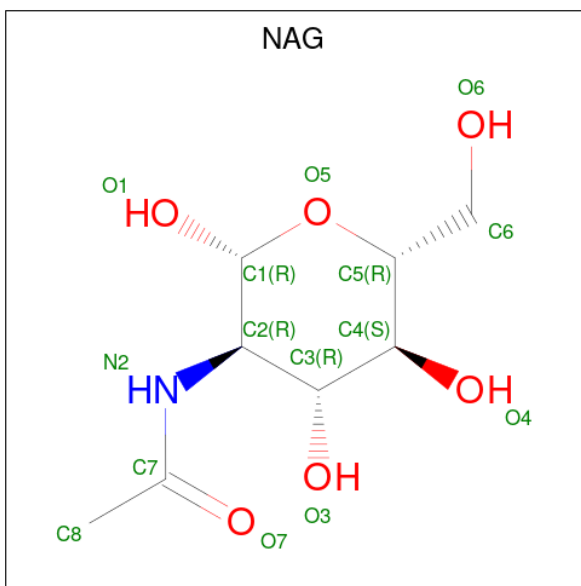
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Zn 1 1	0	0
6	D	1	Total Zn 1 1	0	0
6	C	1	Total Zn 1 1	0	0

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



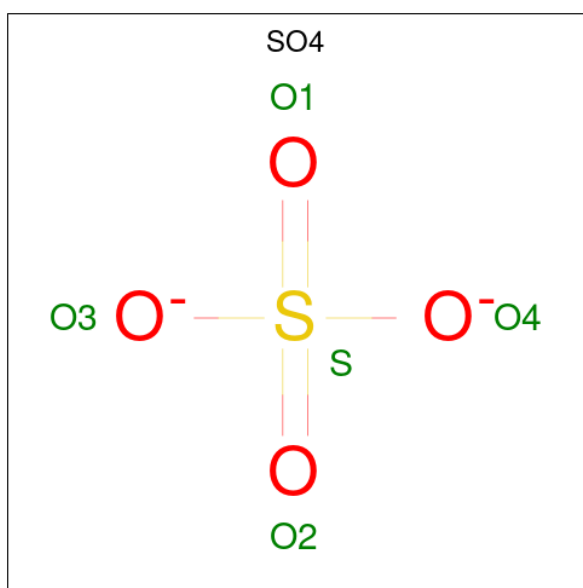
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0

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

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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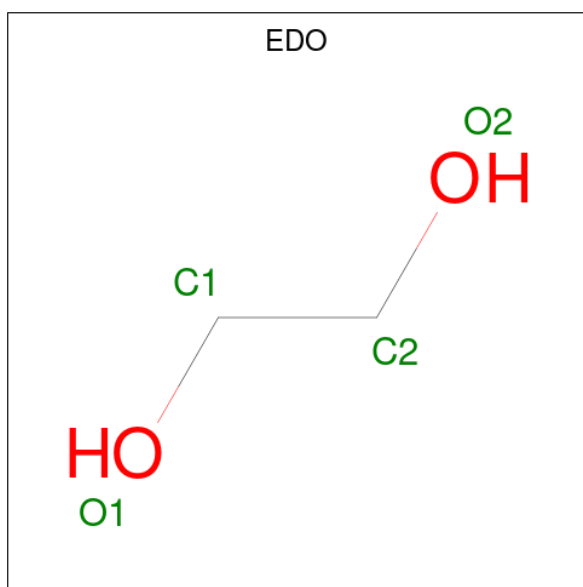
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0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

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

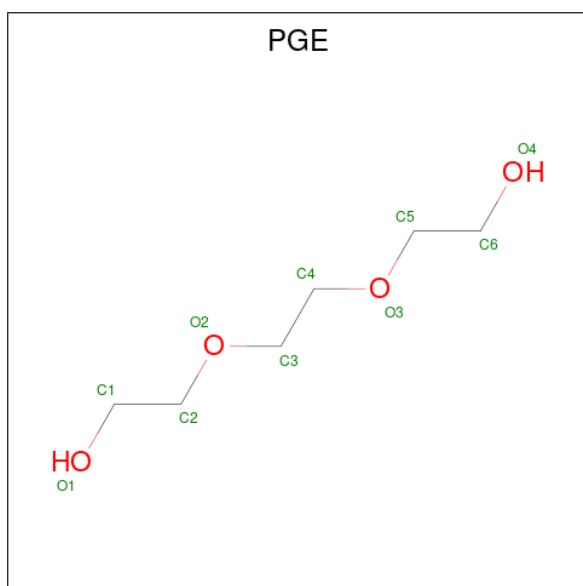
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	Na	0	0
			2	2		
10	D	1	Total	Na	0	0
			1	1		
10	C	2	Total	Na	0	0
			2	2		

- Molecule 11 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 7 4 3	0	0
12	A	1	Total C O 10 6 4	0	0
12	D	1	Total C O 7 4 3	0	0
12	D	1	Total C O 4 2 2	0	0
12	D	1	Total C O 10 6 4	0	0

- Molecule 13 is [(R)-{(2E,4Z,8Z)-dodeca-2,4,8-trien-1-yl}oxy](naphthalen-1-yl)methyl]phosphonic acid (CCD ID: MFJ) (formula:  $C_{23}H_{29}O_4P$ ) (labeled as "Ligand of Interest" by depositor).

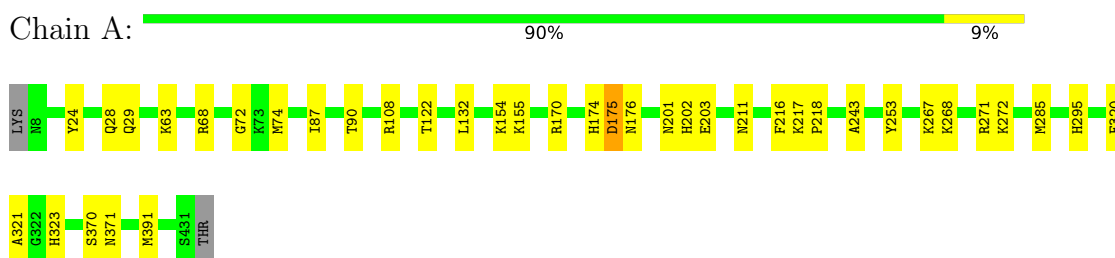


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	316	Total 316	O 316	0	0
15	B	265	Total 265	O 265	0	0
15	D	287	Total 287	O 287	0	0
15	C	278	Total 278	O 278	0	0

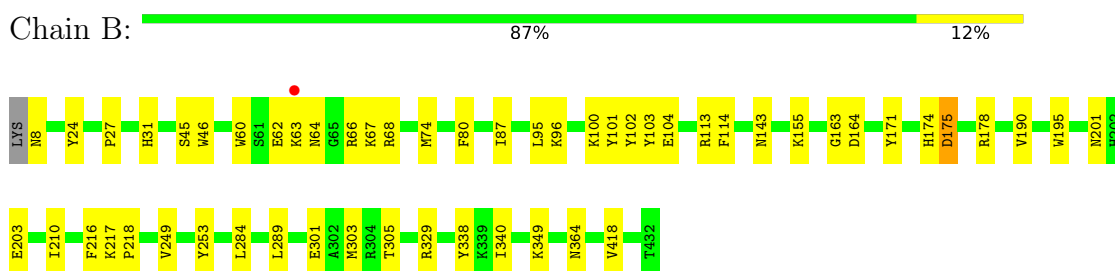
### 3 Residue-property plots [i](#)

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.

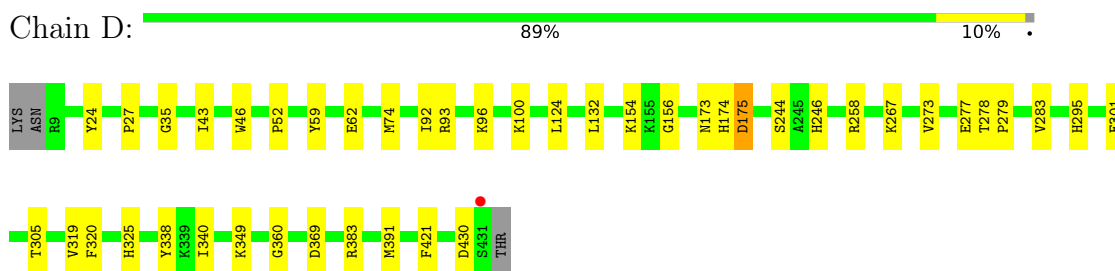
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



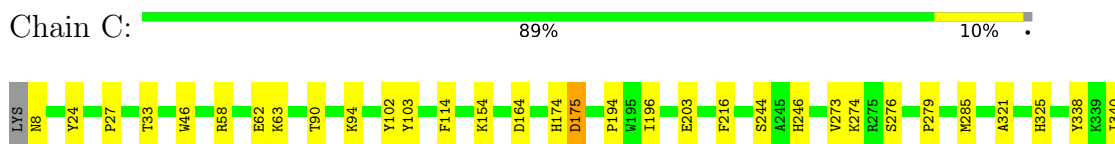
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



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

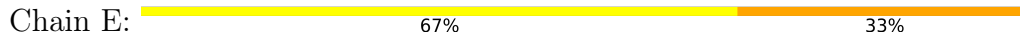


- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase





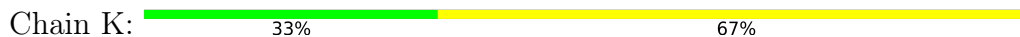
- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



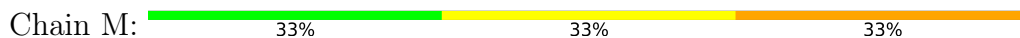
- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 3: 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



- Molecule 3: 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

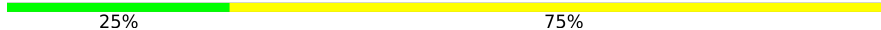


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  50% 50%

MAG1  
MAG2  
BMA3  
FUC4

- Molecule 3: 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:  25% 75%


MAG1  
MAG2  
BMA3  
FUC4

- Molecule 4: 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 G:  33% 67%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
FUC6

- Molecule 5: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%

MAG1  
FUC2

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.81Å 126.81Å 298.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.99-2.30) 97.7 (19.99-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.30Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.179 , 0.231 0.179 , 0.231	Depositor DCC
$R_{free}$ test set	6057 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/3632	0.59	0/4938
1	B	0.37	0/3656	0.55	0/4969
1	C	0.40	0/3609	0.57	0/4909
1	D	0.38	0/3613	0.54	0/4913
All	All	0.39	0/14510	0.56	0/19729

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3507	0	3327	32	0
1	B	3531	0	3353	35	0
1	C	3487	0	3296	30	0
1	D	3491	0	3313	32	0
2	E	38	0	34	1	0
2	H	38	0	34	2	0
2	K	38	0	34	0	0
2	M	38	0	34	1	0
3	F	49	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	49	0	43	0	0
3	J	49	0	43	0	0
3	N	49	0	43	1	0
4	G	71	0	61	0	0
5	L	24	0	22	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	14	0	13	0	0
8	B	14	0	13	1	0
8	C	42	0	39	0	0
8	D	28	0	26	0	0
9	A	20	0	0	2	0
9	B	40	0	0	4	0
9	C	20	0	0	1	0
9	D	15	0	0	1	0
10	A	2	0	0	0	0
10	C	2	0	0	0	0
10	D	1	0	0	0	0
11	A	12	0	18	0	0
11	B	8	0	12	0	0
11	C	20	0	30	0	0
11	D	16	0	24	1	0
12	A	17	0	23	4	0
12	D	21	0	27	1	0
13	A	28	0	0	7	0
14	D	6	0	8	1	0
15	A	316	0	0	4	1
15	B	265	0	0	7	0
15	C	278	0	0	8	0
15	D	287	0	0	8	0
All	All	15939	0	13913	139	1

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 5.

The worst 5 of 139 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NH1	9:A:519:SO4:O4	2.02	0.91
1:C:274:LYS:HE3	1:C:276:SER:H	1.34	0.89
1:D:154:LYS:NZ	15:D:601:HOH:O	2.04	0.89
1:B:96:LYS:NZ	15:B:603:HOH:O	2.19	0.74
15:C:601:HOH:O	2:M:2:FUC:O2	2.08	0.70

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:795:HOH:O	15:A:859:HOH:O[5_554]	2.18	0.02

### 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	424/426 (100%)	400 (94%)	22 (5%)	2 (0%)	24	31
1	B	427/426 (100%)	405 (95%)	19 (4%)	3 (1%)	18	23
1	C	422/426 (99%)	402 (95%)	17 (4%)	3 (1%)	18	23
1	D	422/426 (99%)	403 (96%)	18 (4%)	1 (0%)	43	55
All	All	1695/1704 (100%)	1610 (95%)	76 (4%)	9 (0%)	24	31

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	175	ASP
1	A	175	ASP
1	B	64	ASN
1	B	175	ASP
1	B	364	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	375/375 (100%)	375 (100%)	0	100	100
1	B	378/375 (101%)	378 (100%)	0	100	100
1	C	372/375 (99%)	372 (100%)	0	100	100
1	D	373/375 (100%)	373 (100%)	0	100	100
All	All	1498/1500 (100%)	1498 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	405	ASN
1	D	176	ASN
1	C	424	HIS
1	C	351	GLN
1	C	405	ASN

### 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](#)

36 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	0.66	0	17,19,21	1.10	1 (5%)
2	FUC	E	2	2	10,10,11	0.92	0	14,14,16	1.38	2 (14%)
2	NAG	E	3	2	14,14,15	0.79	1 (7%)	17,19,21	0.43	0
3	NAG	F	1	1,3	14,14,15	0.42	0	17,19,21	0.53	0
3	NAG	F	2	3	14,14,15	0.36	0	17,19,21	0.51	0
3	BMA	F	3	3	11,11,12	1.09	1 (9%)	15,15,17	0.70	0
3	FUC	F	4	3	10,10,11	0.96	1 (10%)	14,14,16	1.23	1 (7%)
4	NAG	G	1	4,1	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
4	NAG	G	2	4	14,14,15	0.41	0	17,19,21	0.67	0
4	BMA	G	3	4	11,11,12	1.49	3 (27%)	15,15,17	0.96	0
4	MAN	G	4	4	11,11,12	0.84	1 (9%)	15,15,17	1.26	2 (13%)
4	MAN	G	5	4	11,11,12	1.52	3 (27%)	15,15,17	1.01	0
4	FUC	G	6	4	10,10,11	0.88	0	14,14,16	0.98	0
2	NAG	H	1	1,2	14,14,15	0.37	0	17,19,21	1.24	1 (5%)
2	FUC	H	2	2	10,10,11	0.71	0	14,14,16	1.51	4 (28%)
2	NAG	H	3	2	14,14,15	0.49	0	17,19,21	0.56	0
3	NAG	I	1	1,3	14,14,15	0.65	1 (7%)	17,19,21	1.51	2 (11%)
3	NAG	I	2	3	14,14,15	0.47	0	17,19,21	0.72	0
3	BMA	I	3	3	11,11,12	1.30	2 (18%)	15,15,17	0.92	1 (6%)
3	FUC	I	4	3	10,10,11	1.55	3 (30%)	14,14,16	1.53	3 (21%)
3	NAG	J	1	1,3	14,14,15	0.36	0	17,19,21	0.55	0
3	NAG	J	2	3	14,14,15	0.49	0	17,19,21	0.56	0
3	BMA	J	3	3	11,11,12	1.28	1 (9%)	15,15,17	0.84	0
3	FUC	J	4	3	10,10,11	1.03	0	14,14,16	1.35	3 (21%)
2	NAG	K	1	1,2	14,14,15	0.62	1 (7%)	17,19,21	0.61	0
2	FUC	K	2	2	10,10,11	0.88	0	14,14,16	1.18	1 (7%)
2	NAG	K	3	2	14,14,15	0.39	0	17,19,21	0.64	0
5	NAG	L	1	1,5	14,14,15	0.31	0	17,19,21	0.82	1 (5%)
5	FUC	L	2	5	10,10,11	1.27	1 (10%)	14,14,16	1.02	1 (7%)
2	NAG	M	1	1,2	14,14,15	0.40	0	17,19,21	0.60	0
2	FUC	M	2	2	10,10,11	1.02	0	14,14,16	1.02	1 (7%)
2	NAG	M	3	2	14,14,15	0.68	1 (7%)	17,19,21	0.47	0
3	NAG	N	1	1,3	14,14,15	0.43	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	N	2	3	14,14,15	0.44	0	17,19,21	0.70	0
3	BMA	N	3	3	11,11,12	1.21	1 (9%)	15,15,17	1.35	1 (6%)
3	FUC	N	4	3	10,10,11	1.06	0	14,14,16	0.88	1 (7%)

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	-	2/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	E	3	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	2/2/19/22	0/1/1/1
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
4	FUC	G	6	4	-	-	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	FUC	H	2	2	-	-	0/1/1/1
2	NAG	H	3	2	-	4/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	FUC	I	4	3	-	-	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	FUC	J	4	3	-	-	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
2	NAG	K	3	2	-	2/6/23/26	0/1/1/1
5	NAG	L	1	1,5	-	2/6/23/26	0/1/1/1
5	FUC	L	2	5	-	-	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1

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

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	3	BMA	C1-C2	3.13	1.59	1.52
3	I	4	FUC	O5-C1	-2.73	1.39	1.43
4	G	3	BMA	C2-C3	2.72	1.56	1.52
4	G	3	BMA	C1-C2	2.62	1.58	1.52
4	G	5	MAN	C2-C3	2.46	1.56	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C1-O5-C5	4.52	118.24	112.19
3	I	1	NAG	O3-C3-C4	4.47	120.91	110.38
2	E	1	NAG	C1-O5-C5	3.88	117.39	112.19
3	N	3	BMA	C1-O5-C5	3.61	117.03	112.19
3	I	1	NAG	C3-C4-C5	-3.32	104.21	110.23

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	3	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	K	3	NAG	C4-C5-C6-O6
2	M	3	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 8 short contacts:

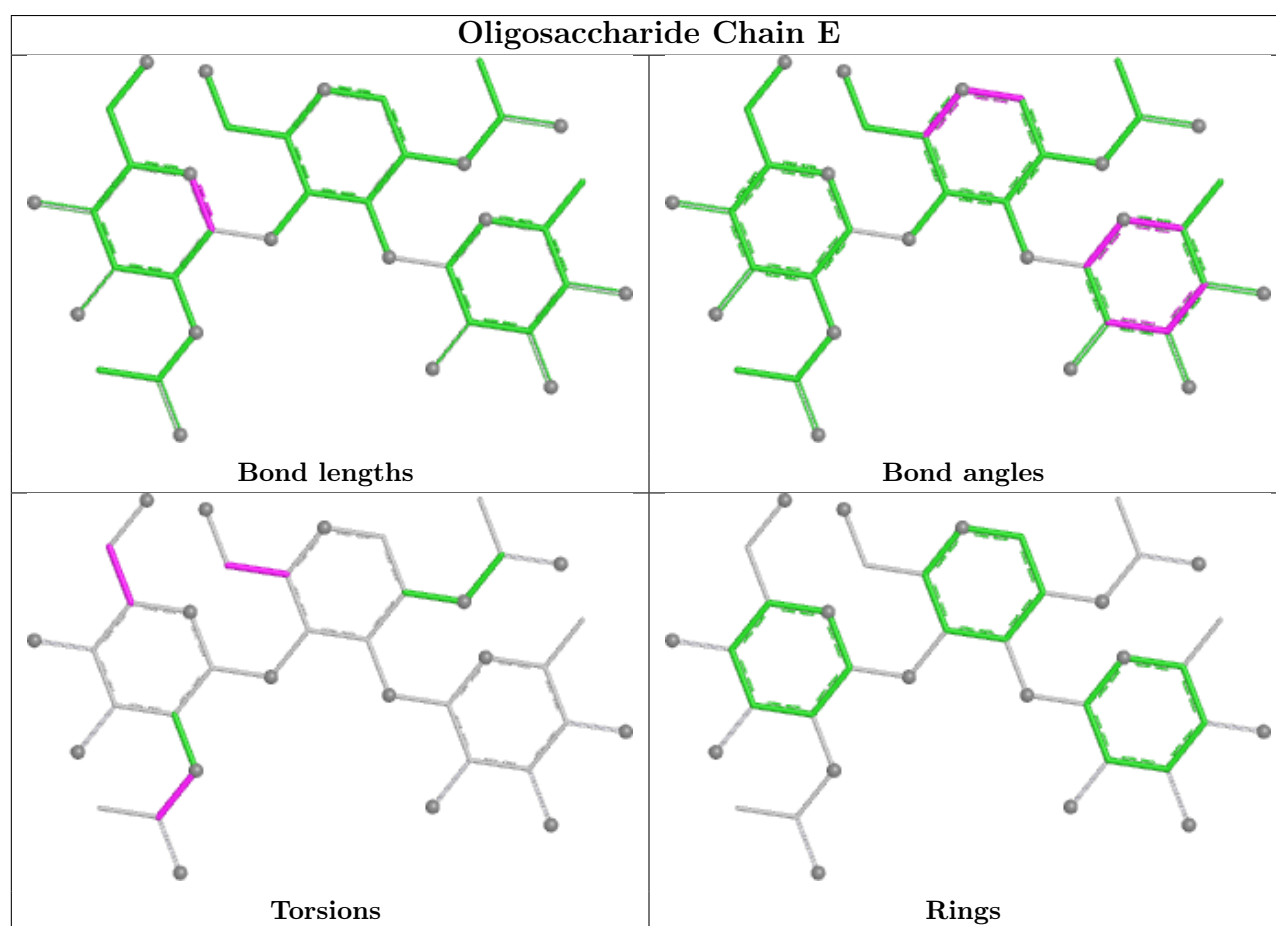
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0

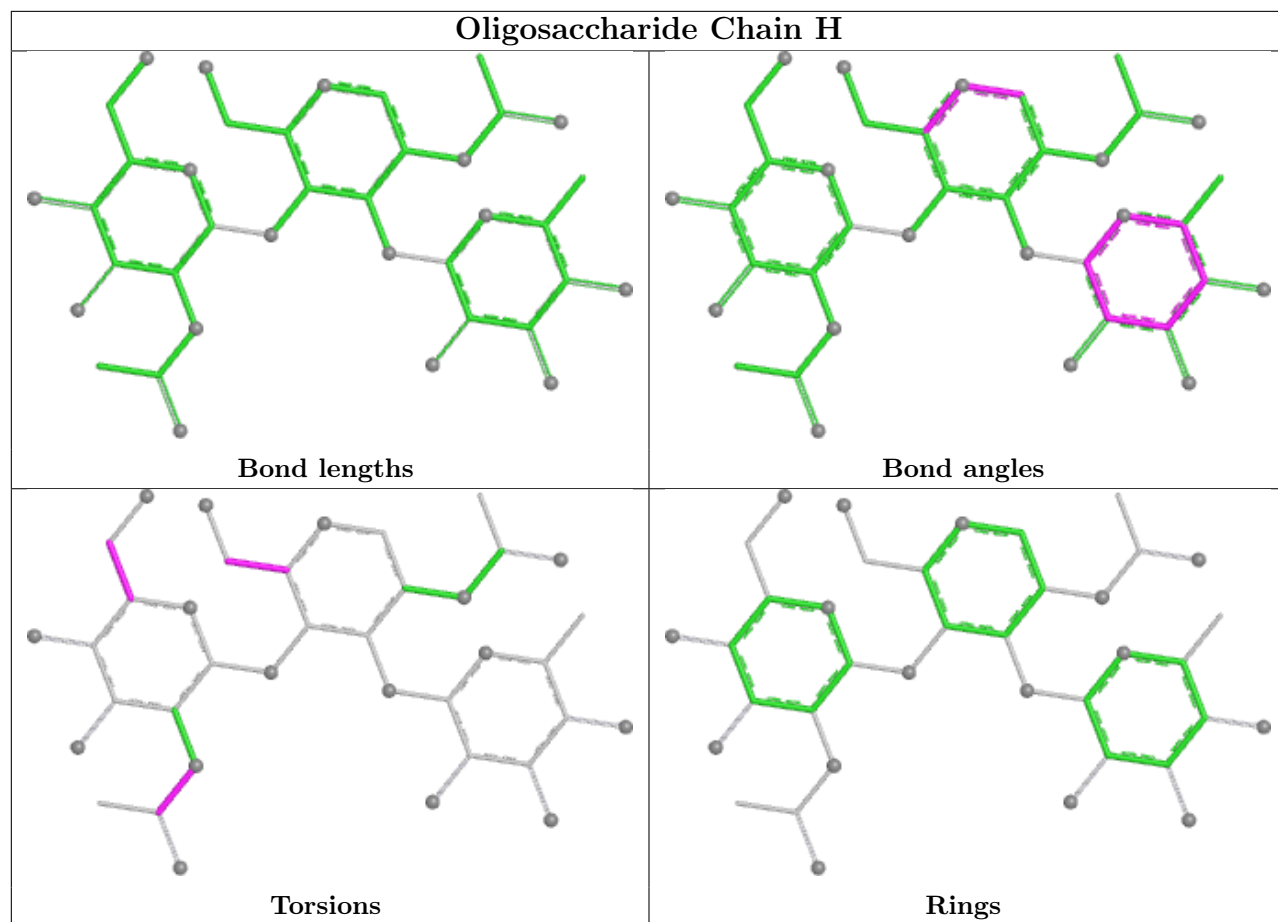
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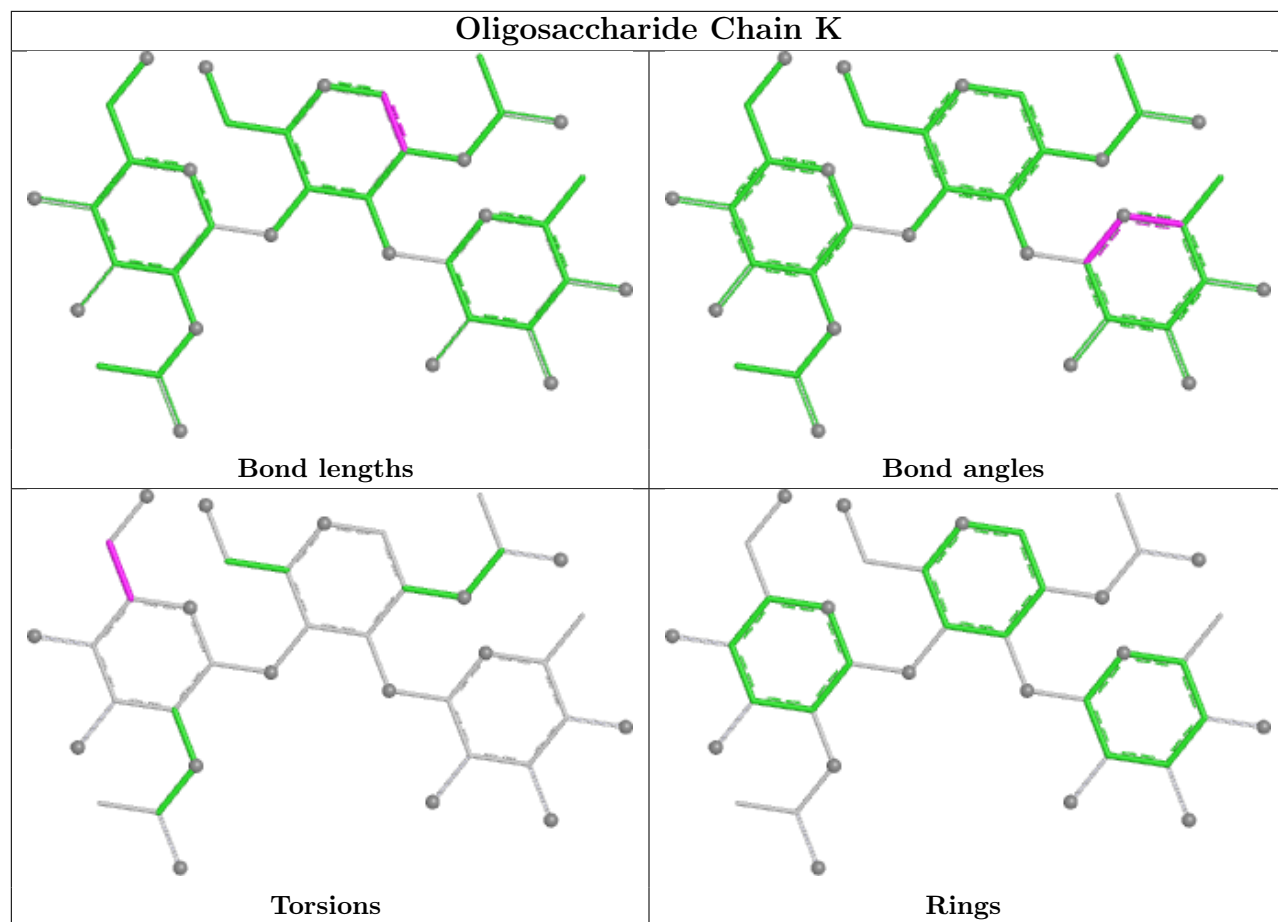
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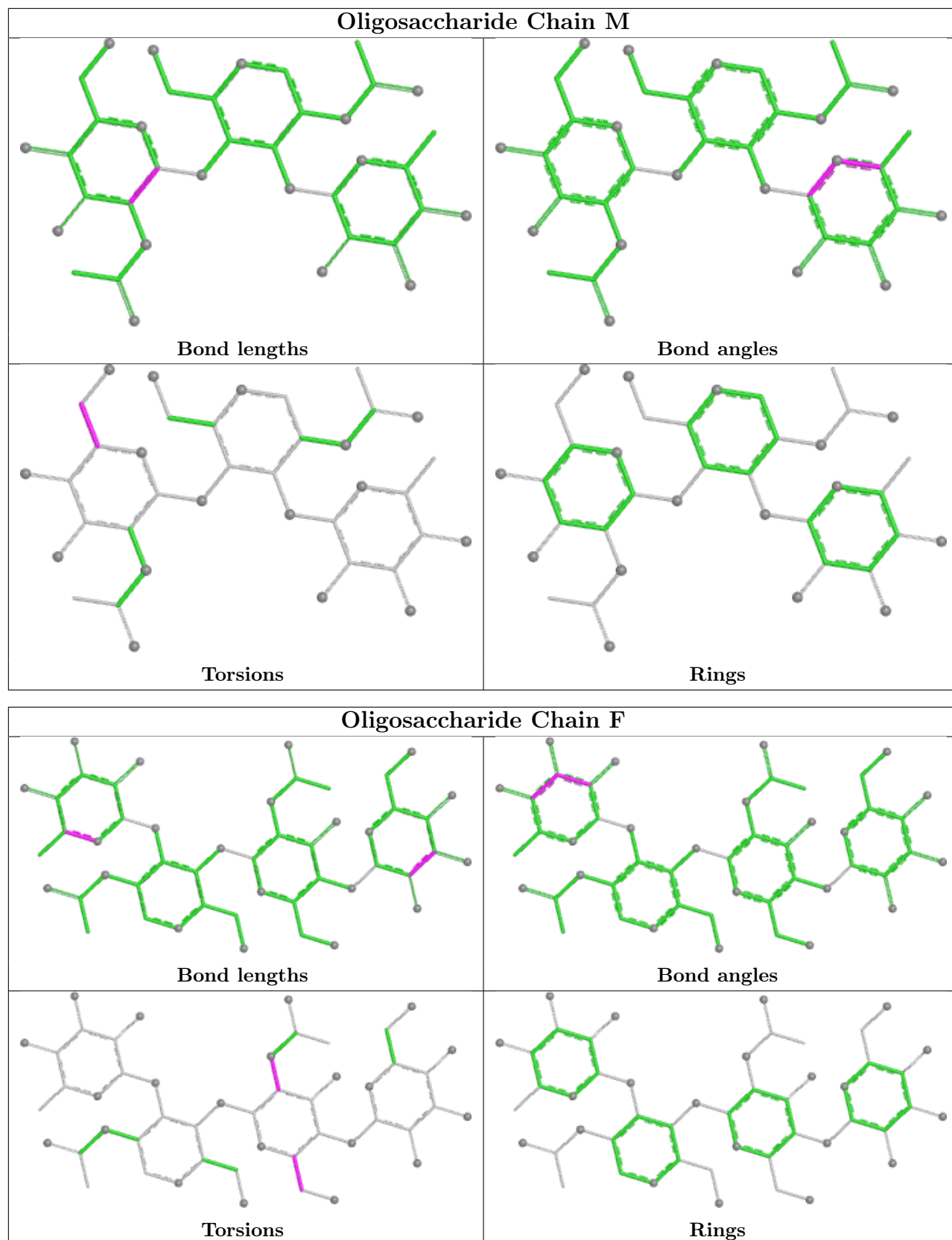
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1	NAG	2	0
2	H	3	NAG	1	0
3	N	1	NAG	1	0
3	F	4	FUC	1	0
3	F	2	NAG	1	0
2	H	2	FUC	1	0
2	M	2	FUC	1	0
2	E	1	NAG	1	0

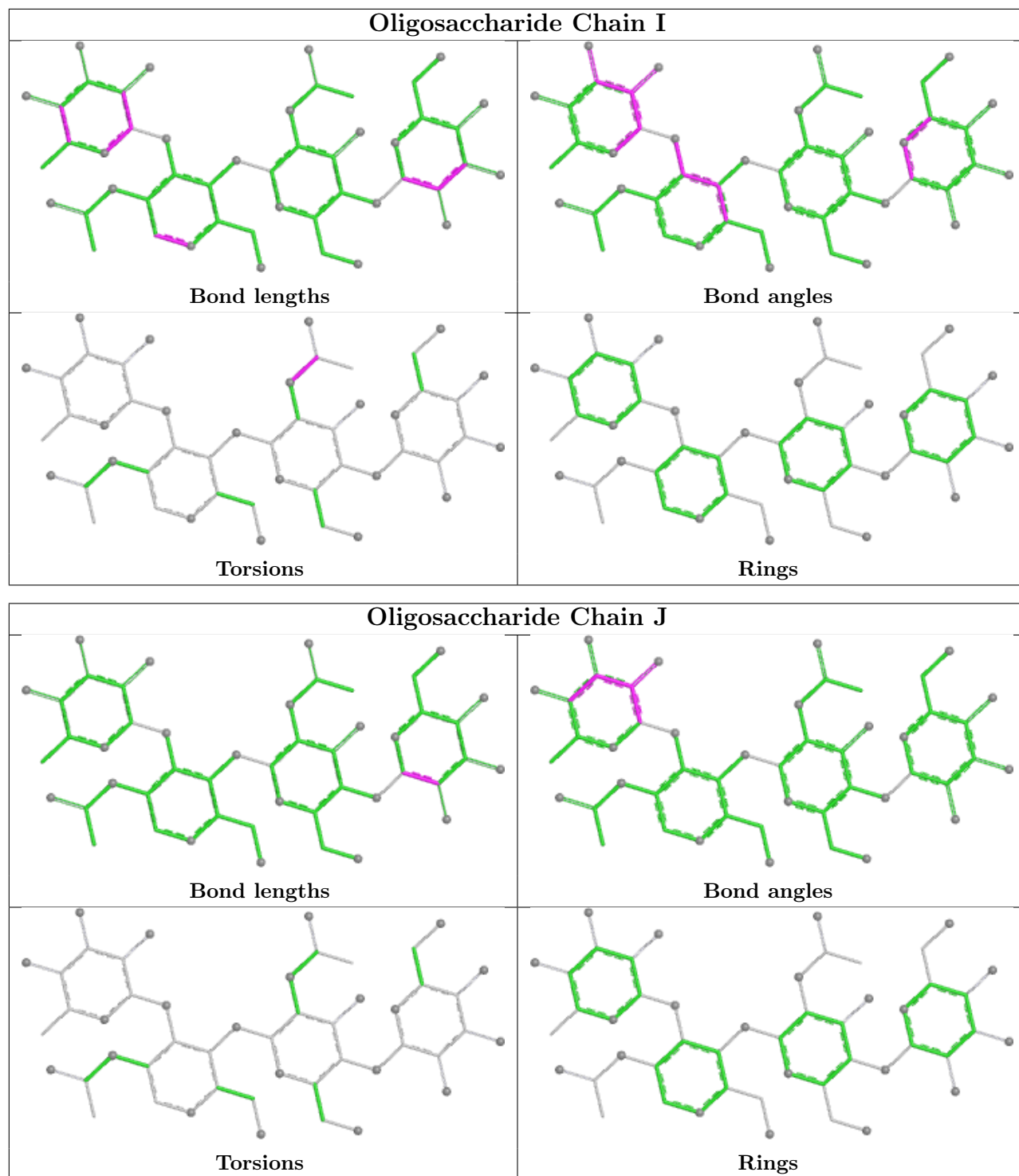
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

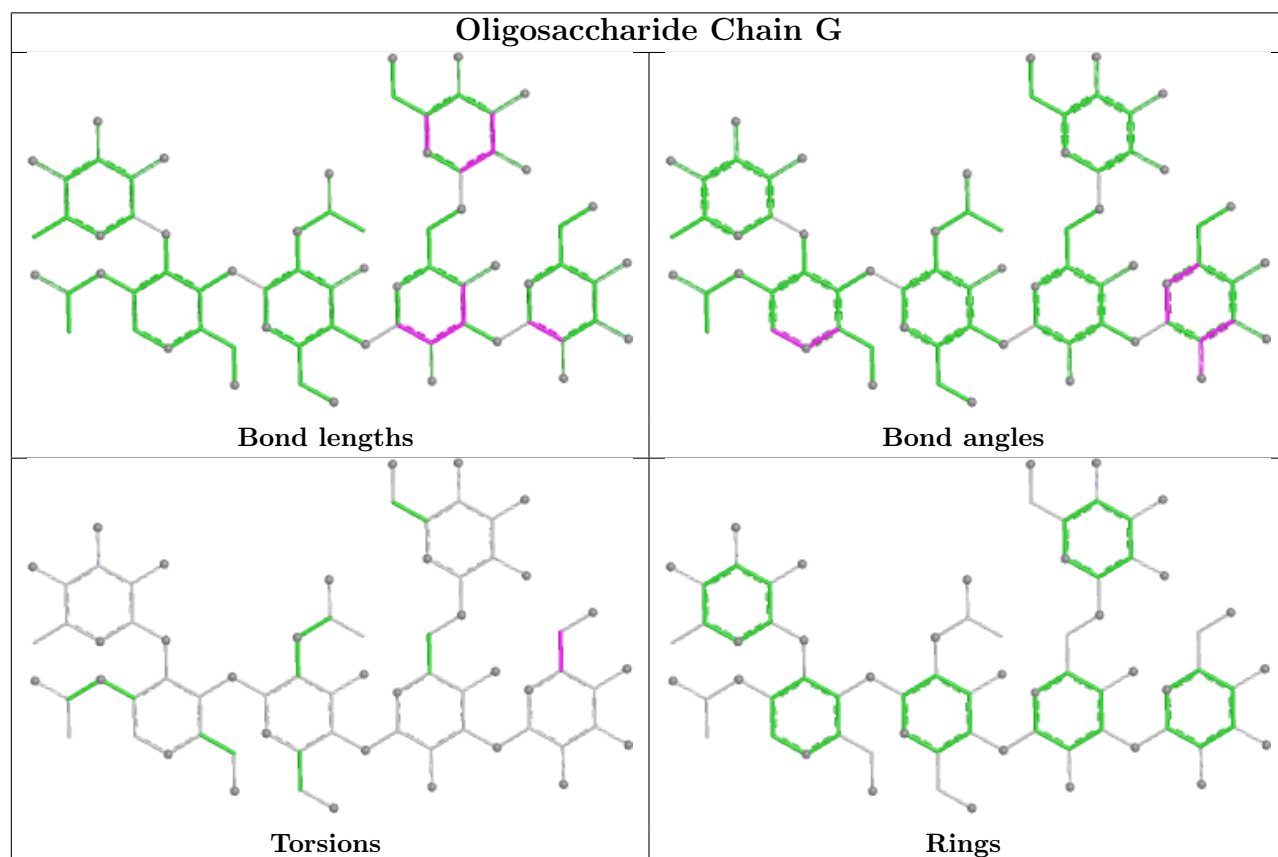
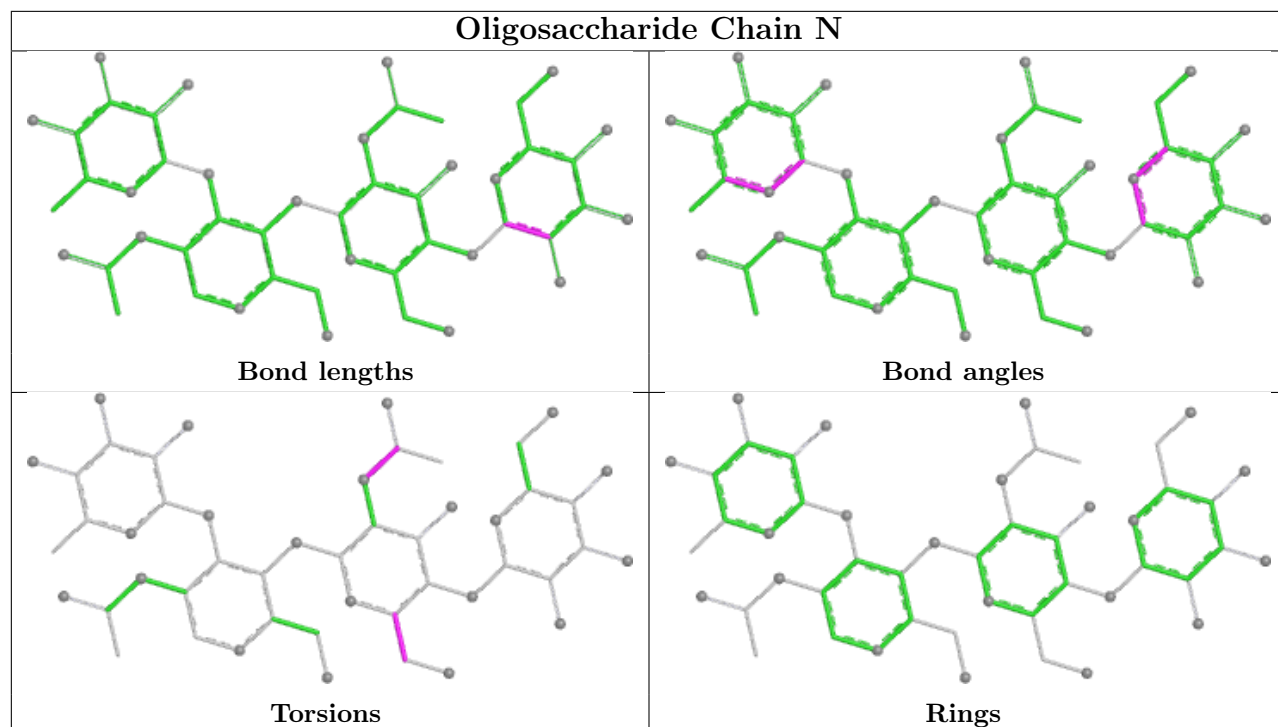


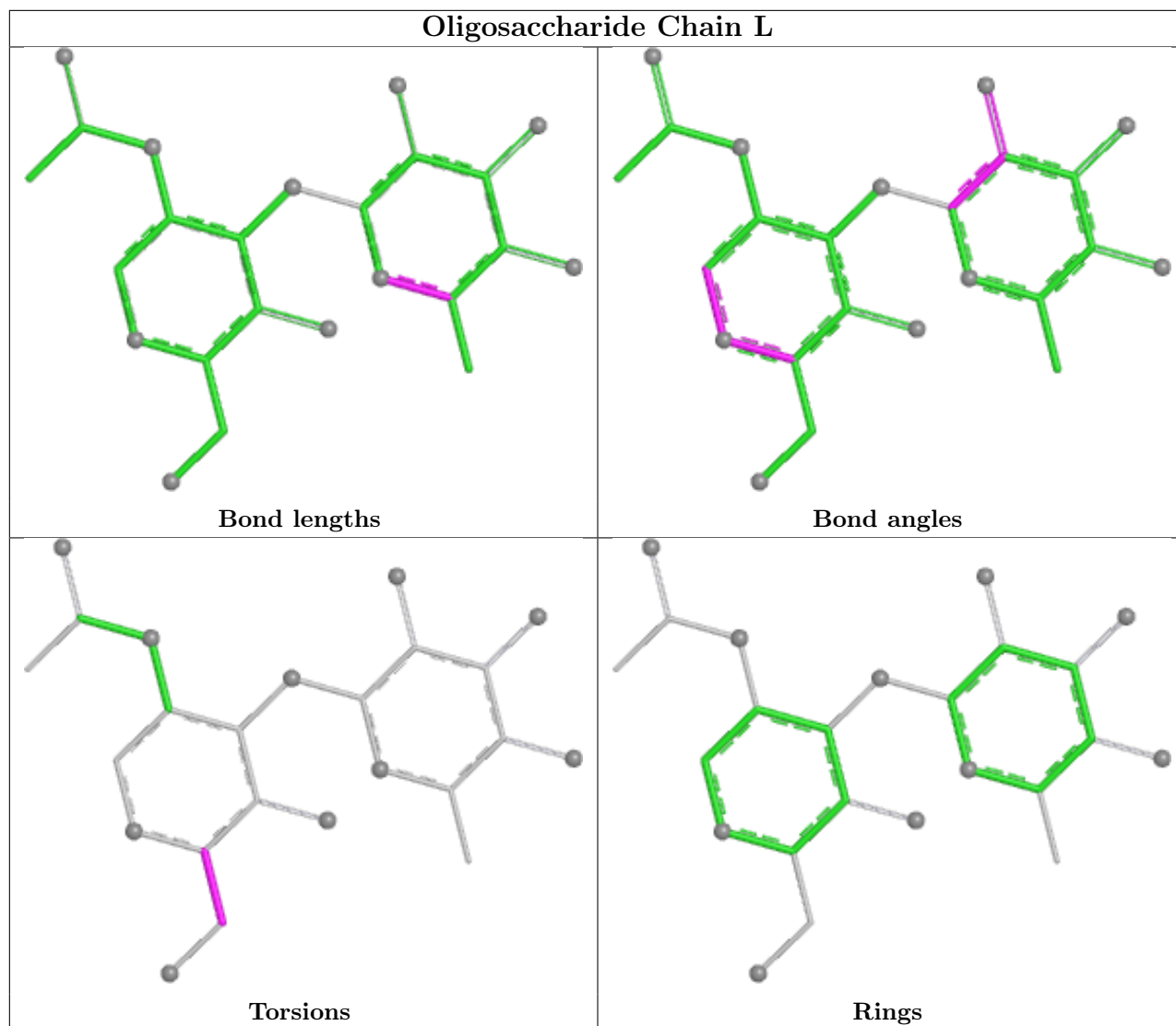












## 5.6 Ligand geometry [\(i\)](#)

Of 60 ligands modelled in this entry, 13 are monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	PGE	A	527	-	9,9,9	0.39	0	8,8,8	0.36	0
9	SO4	B	519	-	4,4,4	0.27	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	A	503	1	14,14,15	0.56	0	17,19,21	0.72	1 (5%)
11	EDO	D	515	-	3,3,3	0.56	0	2,2,2	0.11	0
11	EDO	A	524	-	3,3,3	0.70	0	2,2,2	0.33	0
8	NAG	D	503	1	14,14,15	0.44	0	17,19,21	0.56	0
9	SO4	A	517	-	4,4,4	0.32	0	6,6,6	0.12	0
9	SO4	B	515	-	4,4,4	0.22	0	6,6,6	0.31	0
9	SO4	D	512	-	4,4,4	0.24	0	6,6,6	0.26	0
11	EDO	B	524	-	3,3,3	0.40	0	2,2,2	0.66	0
9	SO4	D	513	-	4,4,4	0.29	0	6,6,6	0.28	0
11	EDO	C	518	-	3,3,3	0.46	0	2,2,2	0.78	0
8	NAG	C	523	1	14,14,15	1.97	2 (14%)	17,19,21	1.69	4 (23%)
14	GOL	D	518	-	5,5,5	0.82	0	5,5,5	1.24	0
11	EDO	A	525	-	3,3,3	0.65	0	2,2,2	0.28	0
9	SO4	C	514	-	4,4,4	0.27	0	6,6,6	0.09	0
11	EDO	B	523	-	3,3,3	0.45	0	2,2,2	0.53	0
11	EDO	D	517	-	3,3,3	0.59	0	2,2,2	0.58	0
11	EDO	C	521	-	3,3,3	0.37	0	2,2,2	0.88	0
9	SO4	B	517	-	4,4,4	0.20	0	6,6,6	0.29	0
9	SO4	B	522	-	4,4,4	0.30	0	6,6,6	0.10	0
9	SO4	C	515	-	4,4,4	0.31	0	6,6,6	0.20	0
12	PGE	D	521	-	9,9,9	0.43	0	8,8,8	0.26	0
9	SO4	A	519	10	4,4,4	0.33	0	6,6,6	0.35	0
9	SO4	B	521	-	4,4,4	0.25	0	6,6,6	0.14	0
8	NAG	D	510	1	14,14,15	0.82	1 (7%)	17,19,21	0.79	1 (5%)
9	SO4	D	511	-	4,4,4	0.29	0	6,6,6	0.29	0
12	PGE	D	520	-	3,3,9	0.33	0	2,2,8	0.48	0
11	EDO	D	504	-	3,3,3	0.56	0	2,2,2	0.30	0
9	SO4	C	513	-	4,4,4	0.31	0	6,6,6	0.21	0
9	SO4	C	512	-	4,4,4	0.30	0	6,6,6	0.20	0
11	EDO	C	522	-	3,3,3	0.48	0	2,2,2	0.44	0
11	EDO	C	519	-	3,3,3	0.47	0	2,2,2	0.49	0
11	EDO	C	520	-	3,3,3	0.42	0	2,2,2	0.78	0
9	SO4	A	518	-	4,4,4	0.32	0	6,6,6	0.37	0
9	SO4	A	520	-	4,4,4	0.29	0	6,6,6	0.09	0
8	NAG	B	503	1	14,14,15	0.40	0	17,19,21	0.80	1 (5%)
12	PGE	A	526	-	6,6,9	0.24	0	5,5,8	0.36	0
13	MFJ	A	528	7,6	27,29,29	2.06	6 (22%)	30,37,37	1.67	8 (26%)
11	EDO	A	523	-	3,3,3	0.60	0	2,2,2	0.27	0
9	SO4	B	518	-	4,4,4	0.34	0	6,6,6	0.35	0
9	SO4	B	516	10	4,4,4	0.31	0	6,6,6	0.15	0
11	EDO	D	516	-	3,3,3	0.44	0	2,2,2	0.48	0
8	NAG	C	507	1	14,14,15	0.61	1 (7%)	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	SO4	B	520	-	4,4,4	0.29	0	6,6,6	0.23	0
8	NAG	C	503	1	14,14,15	0.90	2 (14%)	17,19,21	0.79	0
12	PGE	D	519	-	6,6,9	0.34	0	5,5,8	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGE	A	527	-	-	3/7/7/7	-
8	NAG	A	503	1	-	0/6/23/26	0/1/1/1
11	EDO	D	515	-	-	1/1/1/1	-
11	EDO	A	524	-	-	1/1/1/1	-
8	NAG	D	503	1	-	2/6/23/26	0/1/1/1
11	EDO	B	524	-	-	0/1/1/1	-
11	EDO	C	518	-	-	1/1/1/1	-
8	NAG	C	523	1	-	4/6/23/26	0/1/1/1
14	GOL	D	518	-	-	2/4/4/4	-
11	EDO	A	525	-	-	1/1/1/1	-
11	EDO	B	523	-	-	1/1/1/1	-
11	EDO	D	517	-	-	1/1/1/1	-
11	EDO	C	521	-	-	0/1/1/1	-
12	PGE	D	521	-	-	4/7/7/7	-
8	NAG	D	510	1	-	1/6/23/26	0/1/1/1
12	PGE	D	520	-	-	1/1/1/7	-
11	EDO	D	504	-	-	0/1/1/1	-
11	EDO	C	522	-	-	0/1/1/1	-
11	EDO	C	519	-	-	0/1/1/1	-
11	EDO	C	520	-	-	1/1/1/1	-
8	NAG	B	503	1	-	4/6/23/26	0/1/1/1
12	PGE	A	526	-	-	1/4/4/7	-
13	MFJ	A	528	7,6	-	9/20/23/23	0/2/2/2
11	EDO	A	523	-	-	1/1/1/1	-
11	EDO	D	516	-	-	0/1/1/1	-
8	NAG	C	507	1	-	0/6/23/26	0/1/1/1
8	NAG	C	503	1	-	2/6/23/26	0/1/1/1
12	PGE	D	519	-	-	1/4/4/7	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	523	NAG	C1-C2	-5.54	1.44	1.52
13	A	528	MFJ	CAY-CAX	5.25	1.51	1.33
13	A	528	MFJ	CAZ-CBA	4.66	1.49	1.33
13	A	528	MFJ	PBH-OAC	-4.24	1.48	1.54
8	C	523	NAG	C8-C7	3.91	1.58	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	523	NAG	C1-O5-C5	-3.40	107.63	112.19
13	A	528	MFJ	CAI-CBE-CBF	3.30	123.38	119.12
8	C	523	NAG	C2-N2-C7	3.25	127.26	122.90
13	A	528	MFJ	OAD-PBH-OAB	-3.21	105.39	113.45
13	A	528	MFJ	CAJ-CAG-CAH	-3.07	116.28	121.00

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

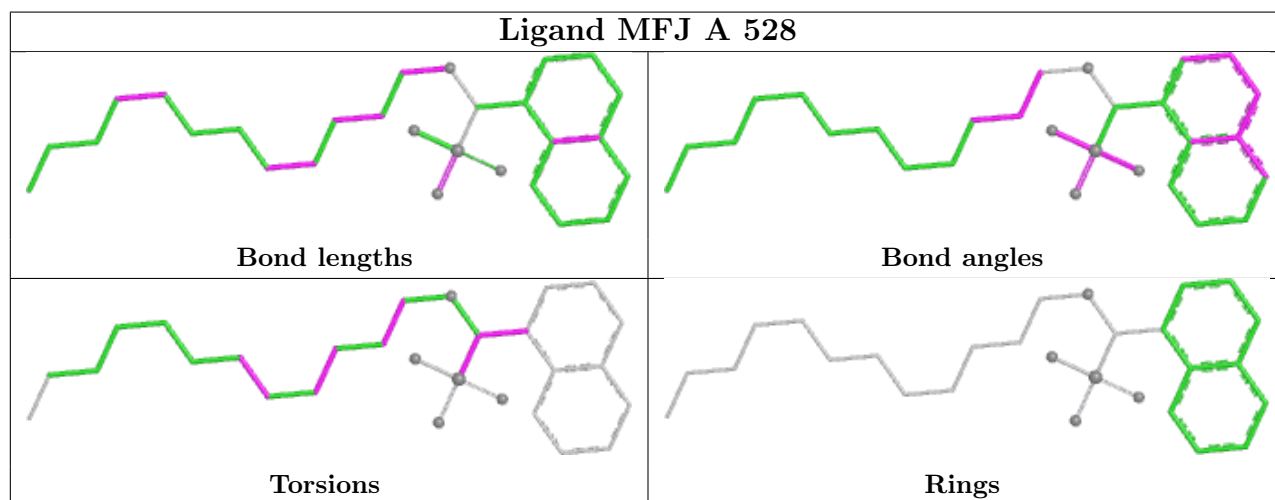
Mol	Chain	Res	Type	Atoms
13	A	528	MFJ	CAX-CAY-CAZ-CBA
13	A	528	MFJ	CAH-CBD-CBG-OBC
13	A	528	MFJ	CAH-CBD-CBG-PBH
13	A	528	MFJ	CBD-CBG-PBH-OAB
13	A	528	MFJ	CBD-CBG-PBH-OAD

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	527	PGE	1	0
9	D	512	SO4	1	0
14	D	518	GOL	1	0
9	B	517	SO4	2	0
9	C	515	SO4	1	0
12	D	521	PGE	1	0
9	A	519	SO4	2	0
8	B	503	NAG	1	0
12	A	526	PGE	3	0
13	A	528	MFJ	7	0
9	B	516	SO4	2	0
11	D	516	EDO	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	424/426 (99%)	-0.70	0 <a href="#">100</a>   <a href="#">100</a>	22, 29, 42, 70	2 (0%)
1	B	425/426 (99%)	-0.59	1 (0%) <a href="#">91</a>   <a href="#">91</a>	18, 33, 47, 73	4 (0%)
1	C	423/426 (99%)	-0.63	0 <a href="#">100</a>   <a href="#">100</a>	23, 31, 45, 76	1 (0%)
1	D	423/426 (99%)	-0.63	1 (0%) <a href="#">91</a>   <a href="#">91</a>	21, 32, 45, 74	1 (0%)
All	All	1695/1704 (99%)	-0.64	2 (0%) <a href="#">92</a>   <a href="#">91</a>	18, 32, 45, 76	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	SER	3.5
1	B	63	LYS	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	FUC	I	4	10/11	0.58	0.15	58,62,67,69	0
3	BMA	J	3	11/12	0.58	0.14	66,72,78,81	0
2	NAG	E	3	14/15	0.60	0.15	67,83,93,94	0
2	NAG	H	3	14/15	0.69	0.15	73,86,97,97	0
3	BMA	N	3	11/12	0.69	0.12	76,83,88,91	0

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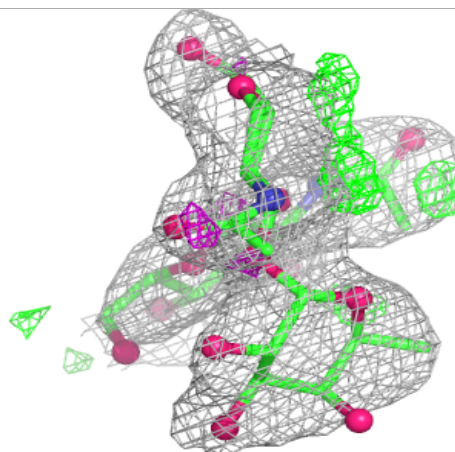
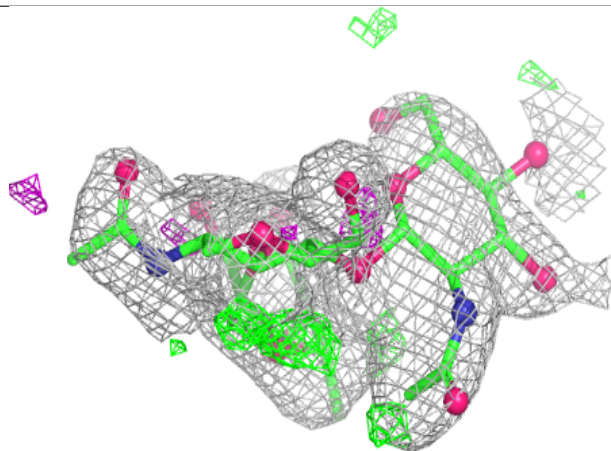
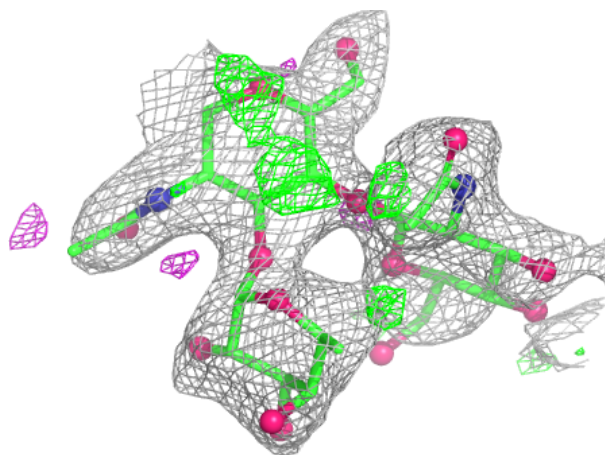
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	G	5	11/12	0.69	0.15	80,81,93,93	0
3	NAG	N	2	14/15	0.71	0.15	66,75,81,83	0
4	BMA	G	3	11/12	0.74	0.13	59,66,80,84	0
3	BMA	F	3	11/12	0.75	0.11	64,76,80,83	0
2	FUC	H	2	10/11	0.76	0.13	72,77,83,87	0
2	NAG	H	1	14/15	0.78	0.12	45,65,75,81	0
2	FUC	E	2	10/11	0.78	0.12	68,71,79,82	0
4	MAN	G	4	11/12	0.79	0.13	60,69,75,75	0
2	NAG	E	1	14/15	0.82	0.12	48,59,76,80	0
3	BMA	I	3	11/12	0.82	0.11	55,62,67,71	0
3	NAG	F	2	14/15	0.82	0.12	46,68,73,77	0
3	NAG	I	2	14/15	0.83	0.12	54,65,70,71	0
5	FUC	L	2	10/11	0.83	0.13	54,62,66,68	0
3	FUC	F	4	10/11	0.84	0.11	63,67,72,75	0
2	FUC	K	2	10/11	0.85	0.10	48,53,59,59	0
3	NAG	I	1	14/15	0.85	0.10	37,49,61,61	0
2	NAG	M	3	14/15	0.86	0.09	39,51,59,63	0
5	NAG	L	1	14/15	0.86	0.11	47,54,60,62	0
3	NAG	N	1	14/15	0.86	0.10	41,58,66,69	0
3	FUC	N	4	10/11	0.87	0.11	51,61,66,66	0
2	FUC	M	2	10/11	0.89	0.09	50,53,55,56	0
3	NAG	J	2	14/15	0.89	0.09	37,47,56,64	0
4	FUC	G	6	10/11	0.91	0.07	38,46,48,54	0
3	FUC	J	4	10/11	0.91	0.08	40,46,54,59	0
2	NAG	K	3	14/15	0.91	0.08	37,50,63,64	0
2	NAG	M	1	14/15	0.92	0.09	39,43,48,52	0
3	NAG	F	1	14/15	0.92	0.09	45,53,60,63	0
2	NAG	K	1	14/15	0.93	0.07	36,40,42,51	0
4	NAG	G	2	14/15	0.93	0.07	34,44,48,52	0
4	NAG	G	1	14/15	0.96	0.06	32,36,42,44	0
3	NAG	J	1	14/15	0.96	0.07	28,41,46,47	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.

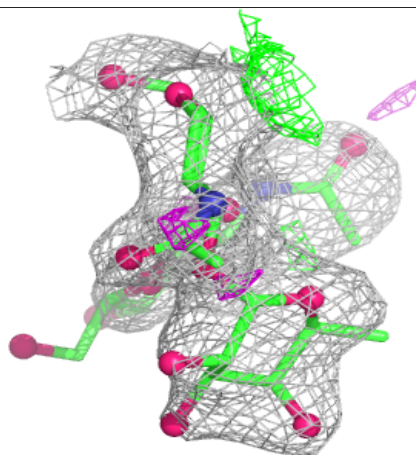
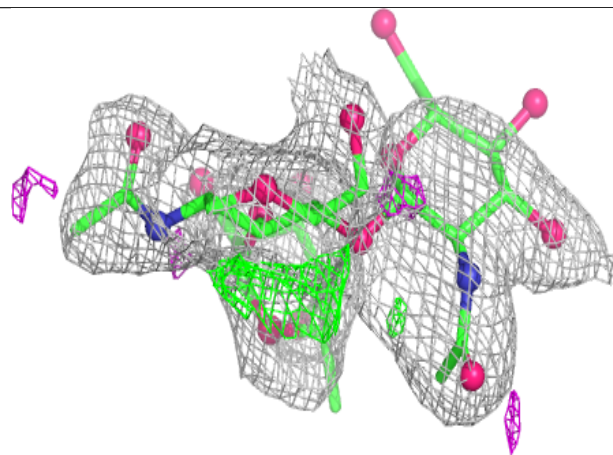
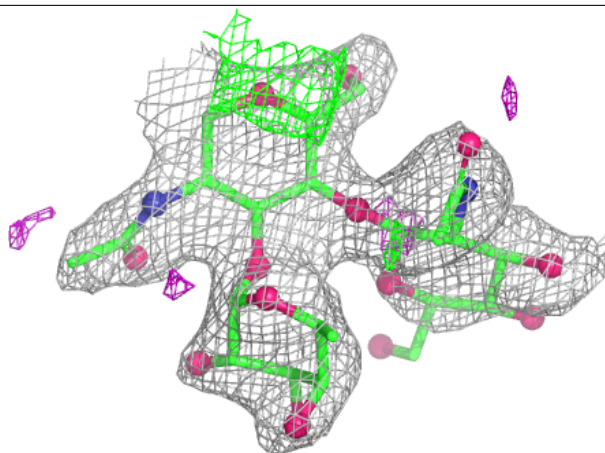
**Electron density around Chain E:**

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



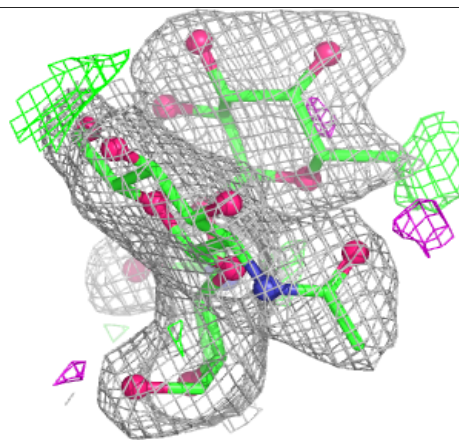
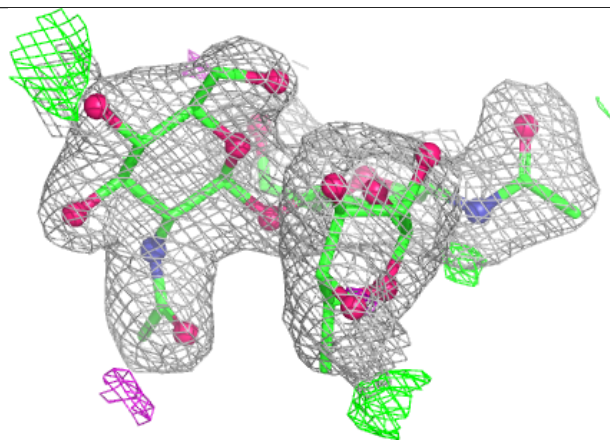
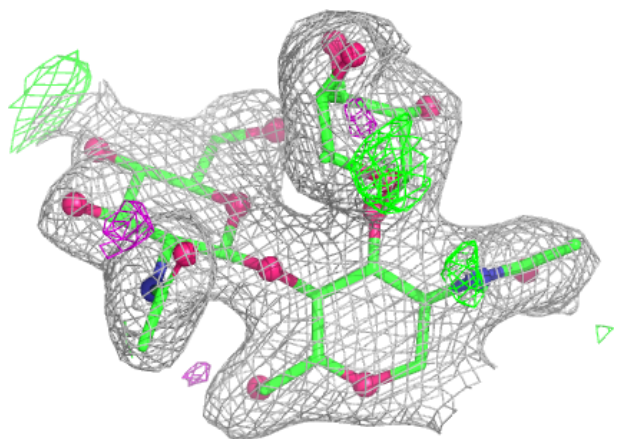
**Electron density around Chain H:**

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



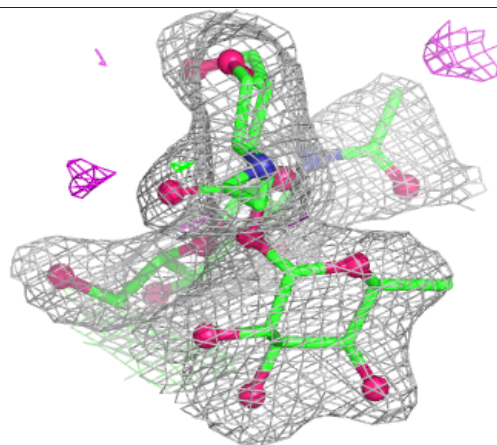
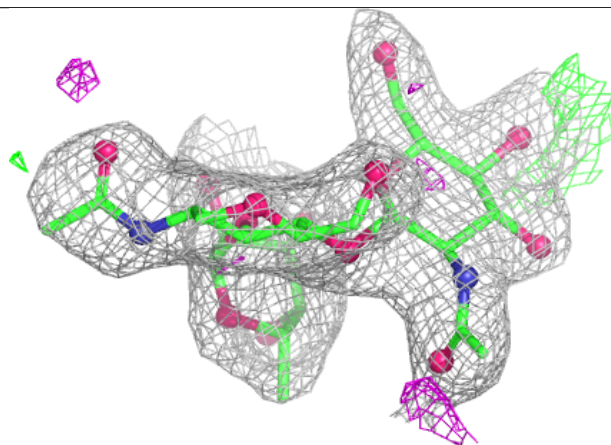
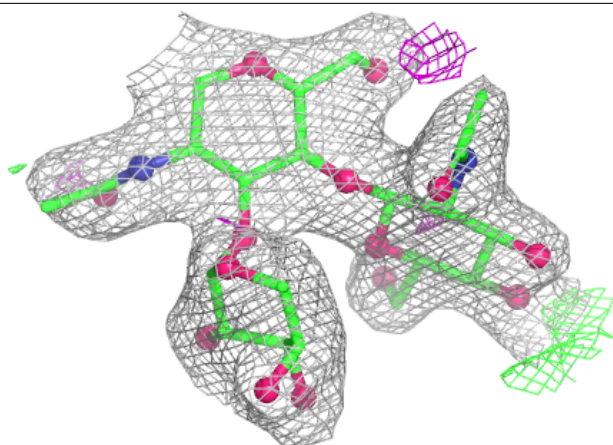
**Electron density around Chain K:**

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

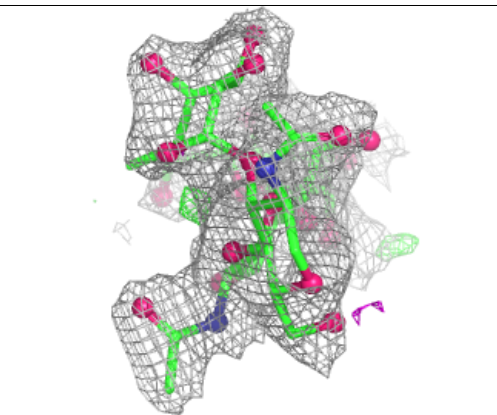
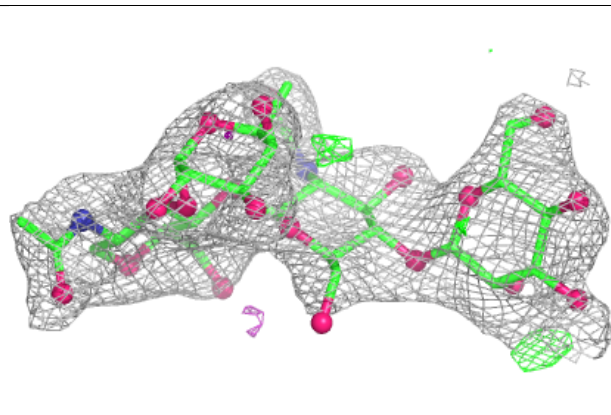
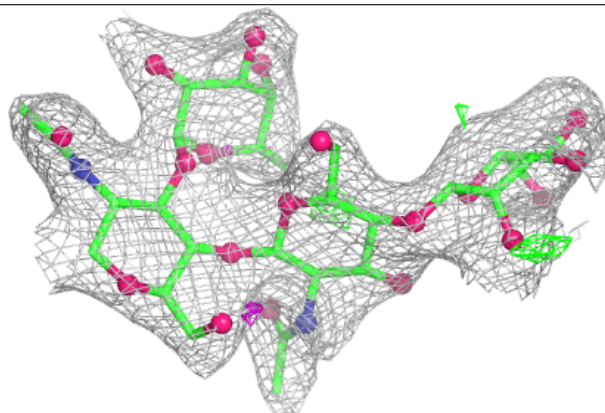


**Electron density around Chain M:**

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

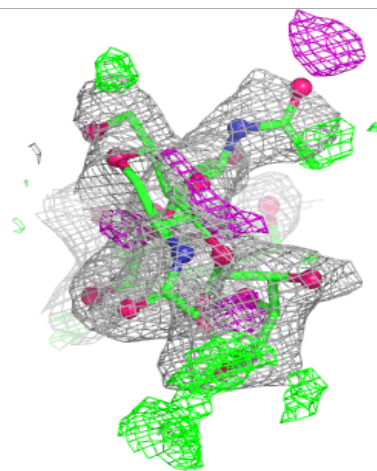
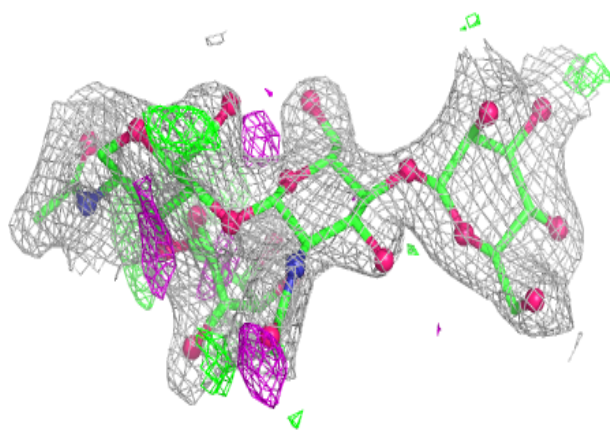
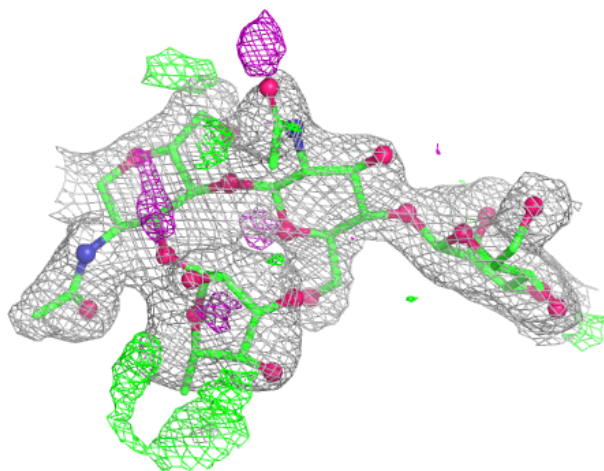
**Electron density around Chain F:**

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and green (positive)



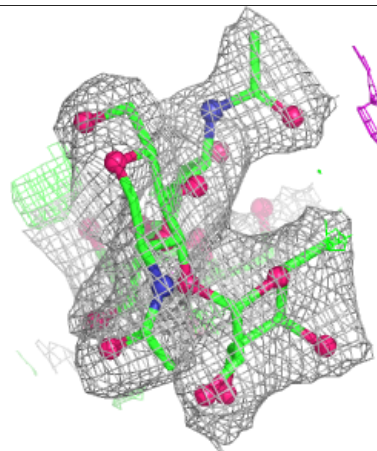
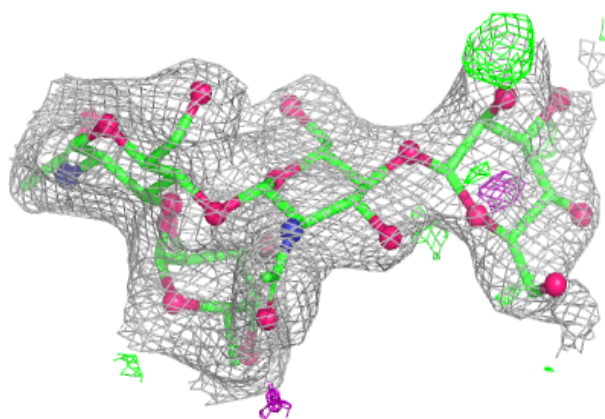
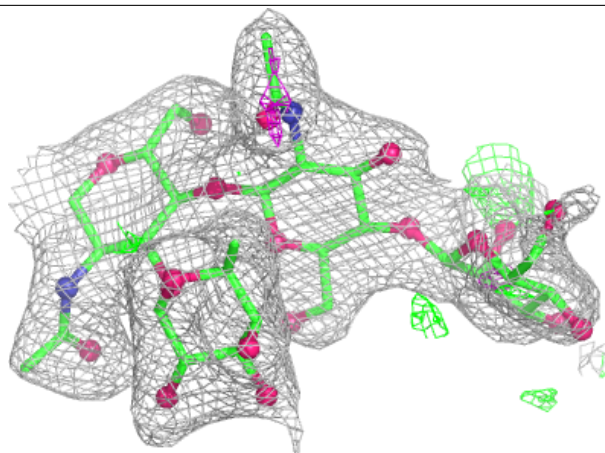
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and green (positive)

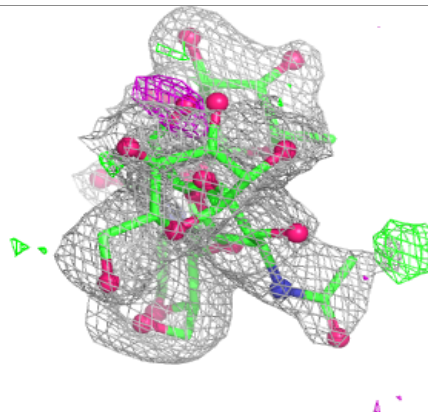
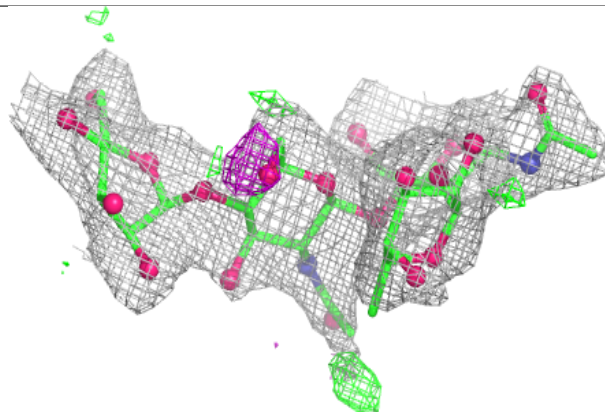
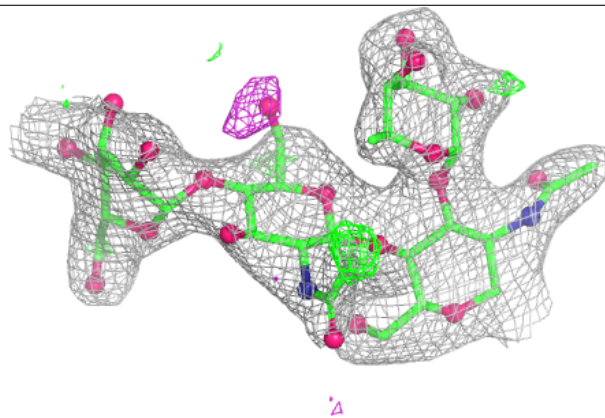


**Electron density around Chain J:**

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and green (positive)

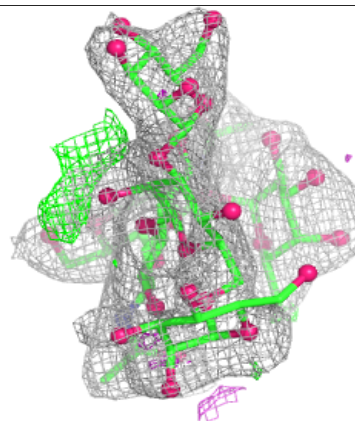
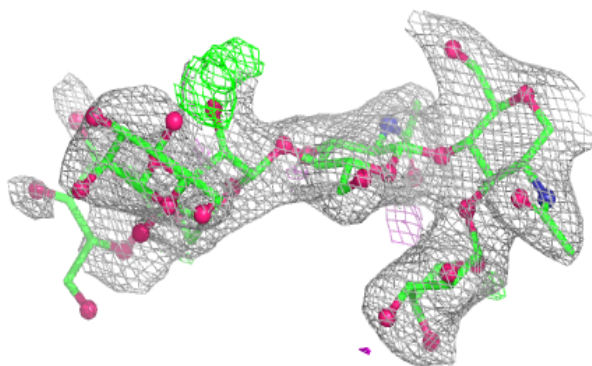
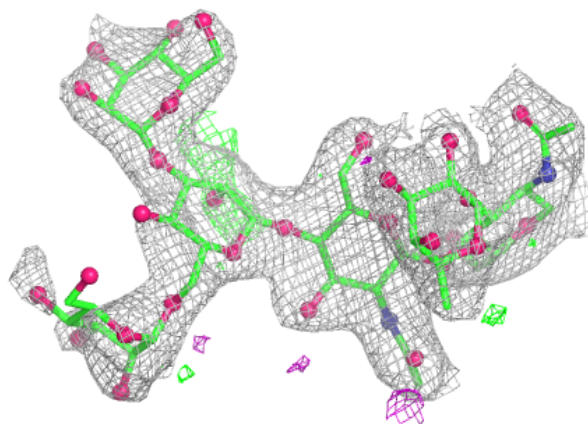
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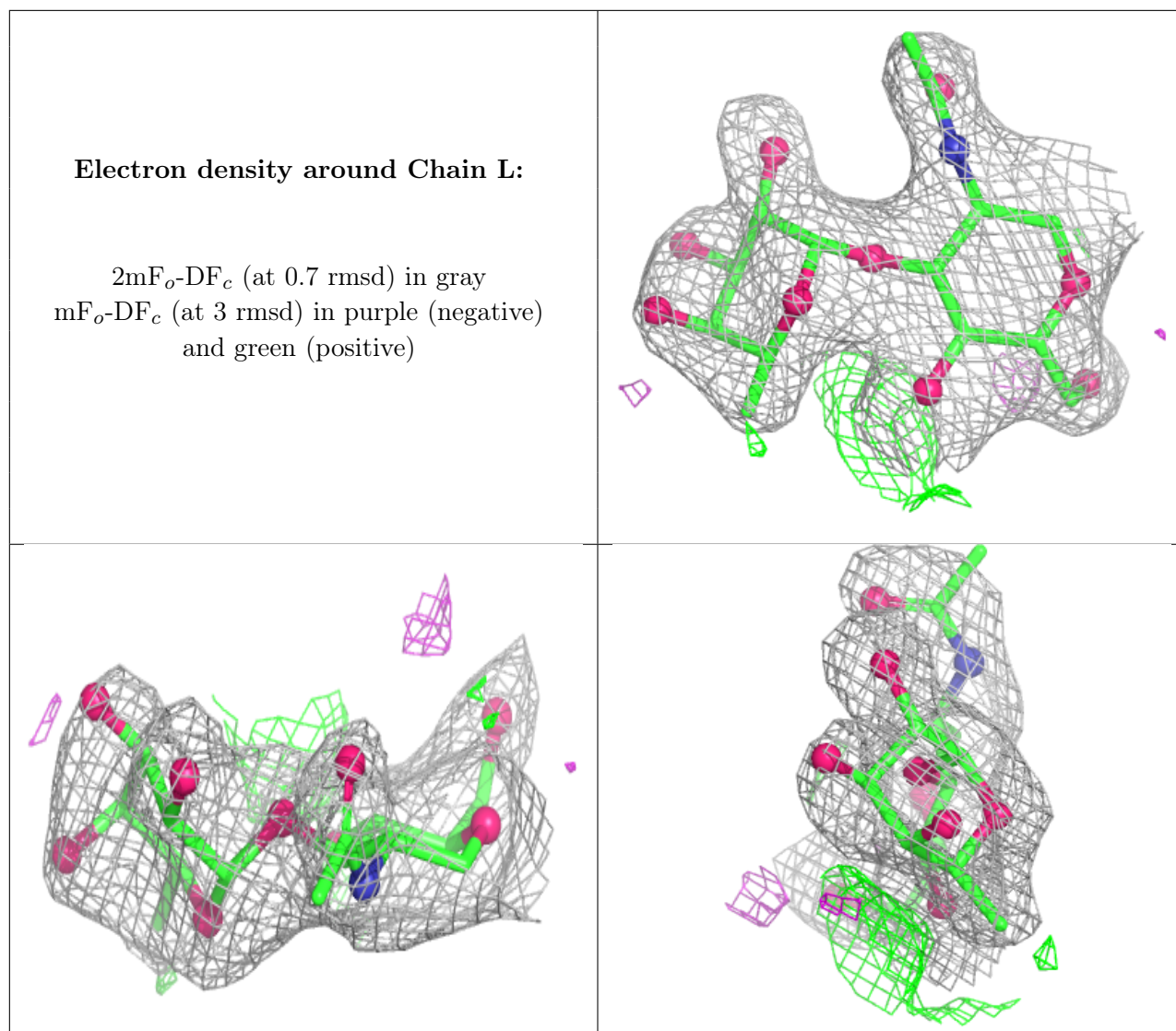
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
8	NAG	C	523	14/15	0.41	0.20	77,90,99,110	0
12	PGE	D	521	10/10	0.51	0.21	62,80,88,91	0
12	PGE	A	527	10/10	0.62	0.20	57,64,70,71	0
9	SO4	B	522	5/5	0.64	0.12	93,94,121,123	0
11	EDO	A	525	4/4	0.69	0.21	58,67,69,70	0
9	SO4	C	512	5/5	0.70	0.17	80,87,97,108	0
12	PGE	D	520	4/10	0.71	0.16	48,48,56,57	0

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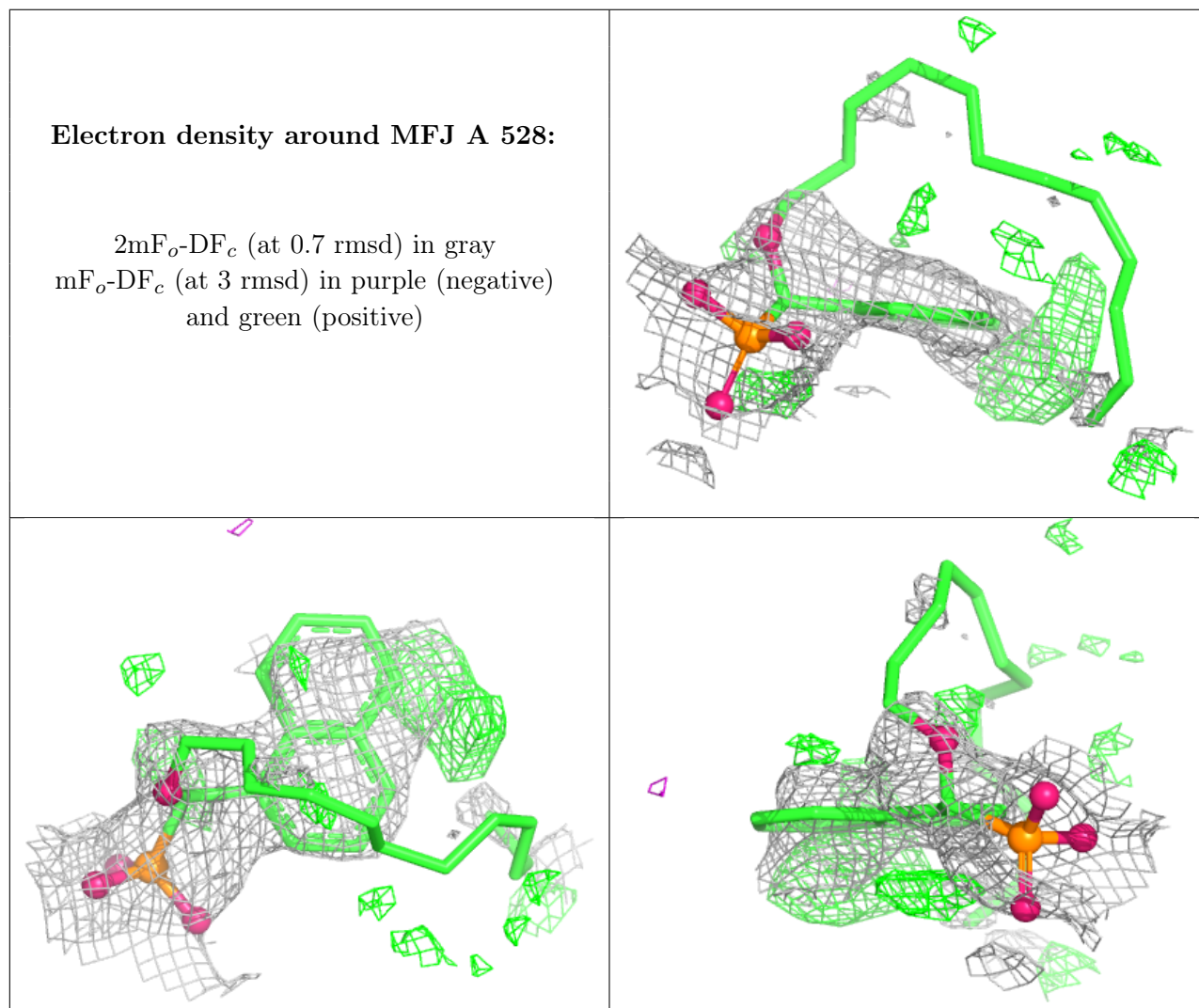
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	SO4	B	521	5/5	0.71	0.10	85,97,109,110	0
11	EDO	C	522	4/4	0.73	0.17	40,49,54,58	0
9	SO4	C	513	5/5	0.74	0.09	85,88,112,112	0
11	EDO	D	515	4/4	0.74	0.21	69,69,69,71	0
11	EDO	D	516	4/4	0.76	0.14	44,45,53,54	0
11	EDO	B	524	4/4	0.77	0.13	46,55,55,57	0
9	SO4	D	513	5/5	0.79	0.19	78,80,93,95	0
9	SO4	A	520	5/5	0.82	0.15	71,72,94,96	0
11	EDO	A	523	4/4	0.82	0.15	45,51,60,64	0
9	SO4	B	518	5/5	0.82	0.12	44,45,55,59	5
11	EDO	C	518	4/4	0.82	0.13	53,54,55,63	0
9	SO4	C	515	5/5	0.84	0.23	61,64,76,87	0
11	EDO	C	519	4/4	0.84	0.12	43,50,53,65	0
12	PGE	A	526	7/10	0.85	0.12	36,47,58,65	0
12	PGE	D	519	7/10	0.85	0.13	47,47,54,55	0
9	SO4	D	512	5/5	0.86	0.18	48,64,85,89	0
8	NAG	D	510	14/15	0.86	0.09	39,52,55,56	0
9	SO4	A	518	5/5	0.87	0.13	36,39,49,56	5
11	EDO	D	504	4/4	0.87	0.11	39,45,48,53	0
11	EDO	B	523	4/4	0.88	0.14	50,53,54,55	0
11	EDO	D	517	4/4	0.88	0.11	36,40,41,45	0
11	EDO	C	521	4/4	0.88	0.13	31,40,43,55	0
13	MFJ	A	528	28/28	0.89	0.20	33,54,64,67	28
8	NAG	D	503	14/15	0.90	0.08	32,41,49,51	0
9	SO4	B	515	5/5	0.90	0.10	45,50,62,63	5
8	NAG	C	507	14/15	0.90	0.08	37,44,48,50	0
9	SO4	B	519	5/5	0.90	0.11	44,45,51,52	5
9	SO4	B	520	5/5	0.90	0.13	51,58,64,75	0
8	NAG	A	503	14/15	0.91	0.08	33,36,43,48	0
8	NAG	C	503	14/15	0.91	0.09	36,42,52,57	0
11	EDO	A	524	4/4	0.91	0.10	32,32,34,37	0
11	EDO	C	520	4/4	0.91	0.13	37,39,51,55	0
14	GOL	D	518	6/6	0.91	0.09	39,47,49,51	0
8	NAG	B	503	14/15	0.92	0.08	37,43,49,55	0
9	SO4	C	514	5/5	0.92	0.23	71,72,93,96	0
9	SO4	B	517	5/5	0.92	0.12	31,37,41,42	5
9	SO4	A	517	5/5	0.93	0.08	41,47,54,55	5
9	SO4	D	511	5/5	0.94	0.09	34,35,36,44	5
7	FE	D	502	1/1	0.96	0.04	46,46,46,46	1
7	FE	B	502	1/1	0.96	0.03	38,38,38,38	1
10	NA	C	516	1/1	0.97	0.06	33,33,33,33	0
10	NA	A	522	1/1	0.98	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	SO4	A	519	5/5	0.98	0.04	37,40,48,53	0
10	NA	C	517	1/1	0.98	0.04	17,17,17,17	0
9	SO4	B	516	5/5	0.98	0.13	20,27,29,33	5
7	FE	C	502	1/1	0.98	0.03	40,40,40,40	1
10	NA	A	521	1/1	0.98	0.05	19,19,19,19	0
10	NA	D	514	1/1	0.99	0.10	21,21,21,21	0
6	ZN	C	501	1/1	0.99	0.02	31,31,31,31	1
6	ZN	D	501	1/1	0.99	0.02	35,35,35,35	0
6	ZN	B	501	1/1	1.00	0.02	39,39,39,39	0
7	FE	A	502	1/1	1.00	0.01	30,30,30,30	1
6	ZN	A	501	1/1	1.00	0.01	28,28,28,28	1

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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.