



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2026 – 10:22 AM EDT

PDB ID : 10TY / pdb\_000010ty  
Title : Tissue Non-specific Alkaline Phosphatase -S110A bound to PPi with ethylene glycol  
Authors : Krishnan, S.S.; Carroll, B.L.; Guarne, A.  
Deposited on : 2026-02-09  
Resolution : 2.28 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](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)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

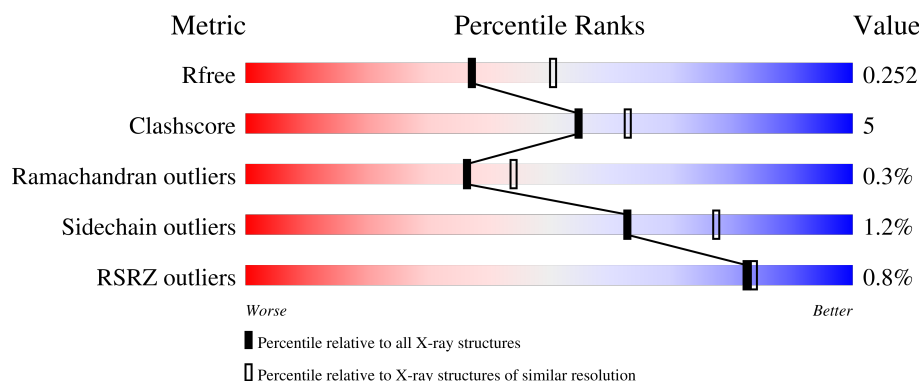
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	493	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	493	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	493	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	493	<div> <div></div> <div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
2	E	5	<div> <div></div> <div> <div>80%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	5	 100%
3	F	5	 60%40%
4	G	2	 100%
4	J	2	 100%
4	K	2	 50%50%
4	M	2	 100%
5	I	3	 100%
6	L	4	 75%25%

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16246 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 Alkaline phosphatase, tissue-nonspecific isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3732	2334	664	714	20			
1	B	481	Total	C	N	O	S	0	1	0
			3731	2330	665	717	19			
1	C	480	Total	C	N	O	S	0	1	0
			3729	2330	664	715	20			
1	D	479	Total	C	N	O	S	0	0	0
			3715	2322	662	711	20			

There are 36 discrepancies between the modelled and reference sequences:

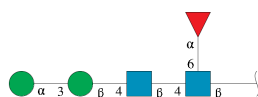
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASP	-	expression tag	UNP P09242
A	16	GLY	-	expression tag	UNP P09242
A	110	ALA	SER	engineered mutation	UNP P09242
A	502	HIS	-	expression tag	UNP P09242
A	503	HIS	-	expression tag	UNP P09242
A	504	HIS	-	expression tag	UNP P09242
A	505	HIS	-	expression tag	UNP P09242
A	506	HIS	-	expression tag	UNP P09242
A	507	HIS	-	expression tag	UNP P09242
B	15	ASP	-	expression tag	UNP P09242
B	16	GLY	-	expression tag	UNP P09242
B	110	ALA	SER	engineered mutation	UNP P09242
B	502	HIS	-	expression tag	UNP P09242
B	503	HIS	-	expression tag	UNP P09242
B	504	HIS	-	expression tag	UNP P09242
B	505	HIS	-	expression tag	UNP P09242
B	506	HIS	-	expression tag	UNP P09242
B	507	HIS	-	expression tag	UNP P09242
C	15	ASP	-	expression tag	UNP P09242
C	16	GLY	-	expression tag	UNP P09242
C	110	ALA	SER	engineered mutation	UNP P09242

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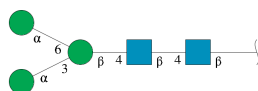
Chain	Residue	Modelled	Actual	Comment	Reference
C	502	HIS	-	expression tag	UNP P09242
C	503	HIS	-	expression tag	UNP P09242
C	504	HIS	-	expression tag	UNP P09242
C	505	HIS	-	expression tag	UNP P09242
C	506	HIS	-	expression tag	UNP P09242
C	507	HIS	-	expression tag	UNP P09242
D	15	ASP	-	expression tag	UNP P09242
D	16	GLY	-	expression tag	UNP P09242
D	110	ALA	SER	engineered mutation	UNP P09242
D	502	HIS	-	expression tag	UNP P09242
D	503	HIS	-	expression tag	UNP P09242
D	504	HIS	-	expression tag	UNP P09242
D	505	HIS	-	expression tag	UNP P09242
D	506	HIS	-	expression tag	UNP P09242
D	507	HIS	-	expression tag	UNP P09242

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



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

- Molecule 3 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



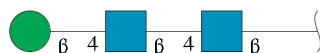
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 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
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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.



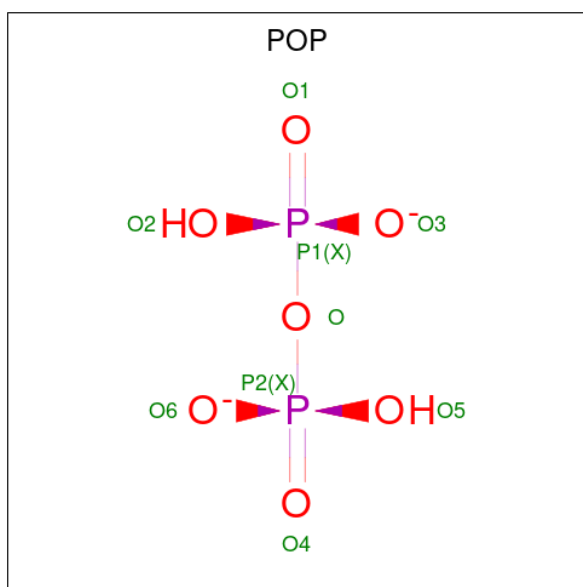
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
6	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			9	7	2		
7	B	1	Total	O	P	0	0
			9	7	2		
7	C	1	Total	O	P	0	0
			9	7	2		
7	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Mg 1	0	0
9	C	1	Total 1	Mg 1	0	0
9	D	1	Total 1	Mg 1	0	0

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total 1	Ca 1	0	0
10	B	1	Total 1	Ca 1	0	0
10	C	1	Total 1	Ca 1	0	0
10	D	1	Total 1	Ca 1	0	0

- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na).

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

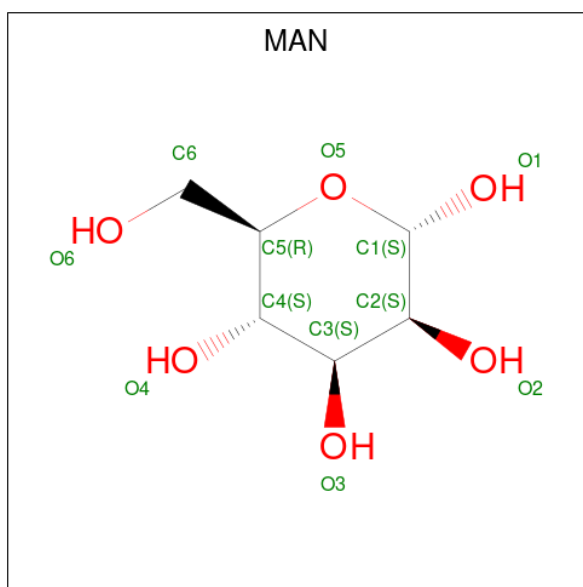
- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





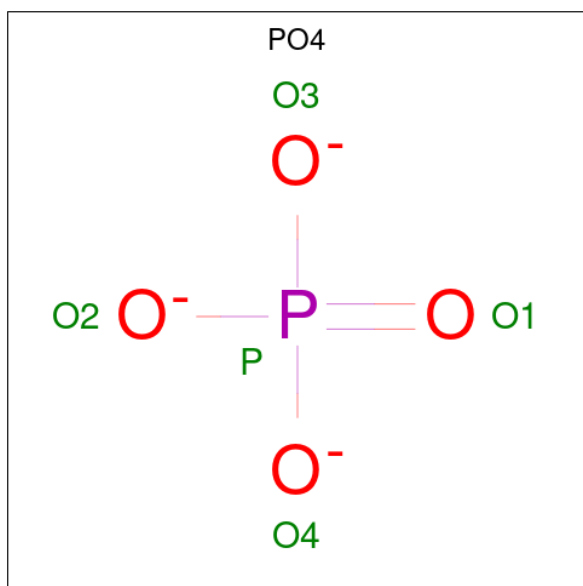
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	C	1	Total	C	N	O	0	0
			14	8	1	5		
12	D	1	Total	C	N	O	0	0
			14	8	1	5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

- Molecule 13 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



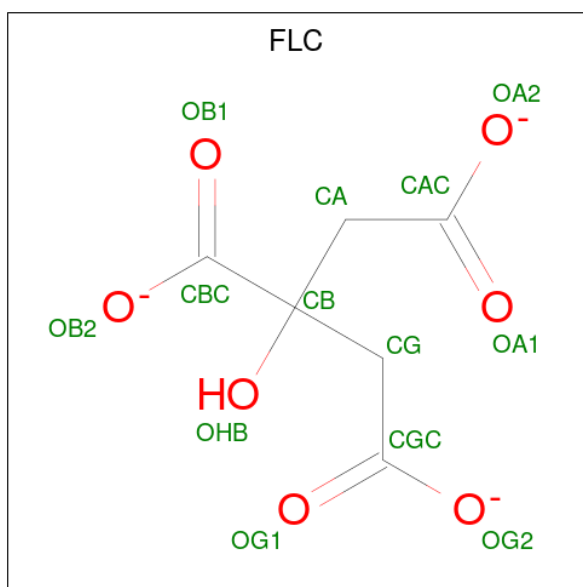
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 14 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	O	P	0	0
			5	4	1		
14	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 15 is CITRATE ANION (CCD ID: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			13	6	7		

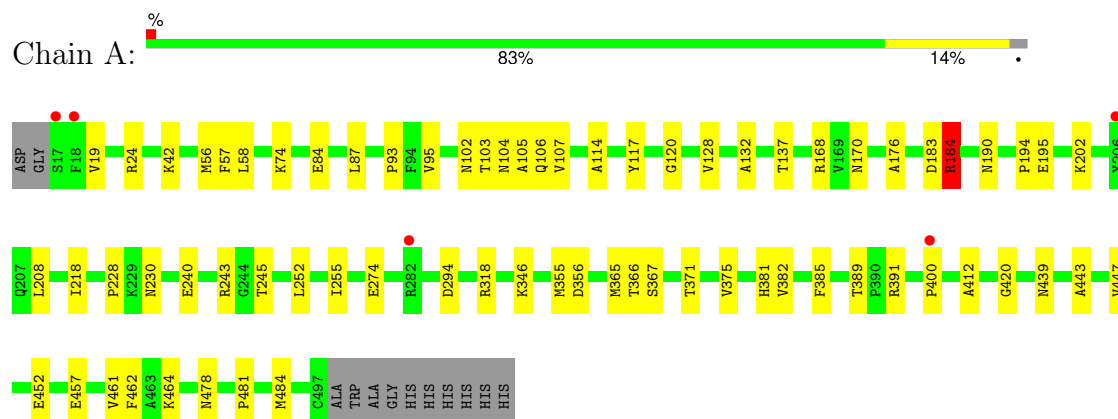
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	186	Total	O	0	0
			186	186		
16	B	177	Total	O	0	0
			177	177		
16	C	186	Total	O	0	0
			186	186		
16	D	196	Total	O	0	0
			196	196		

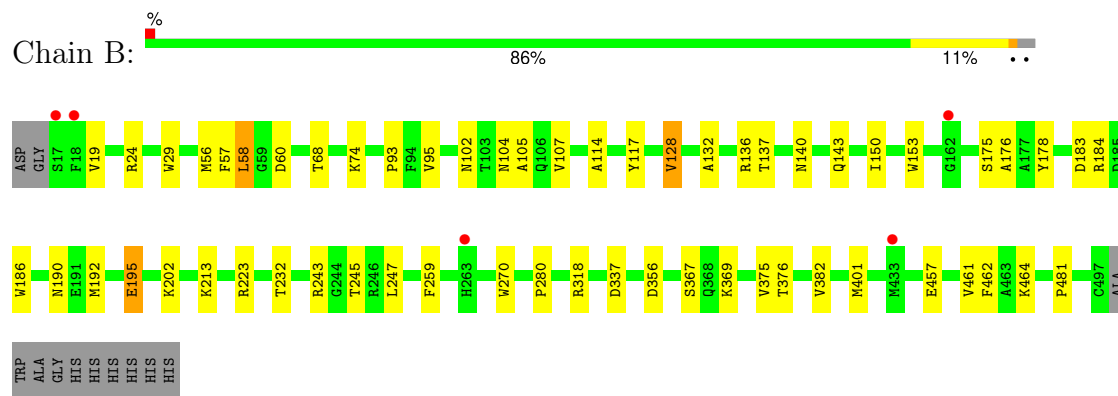
### 3 Residue-property plots [i](#)

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.

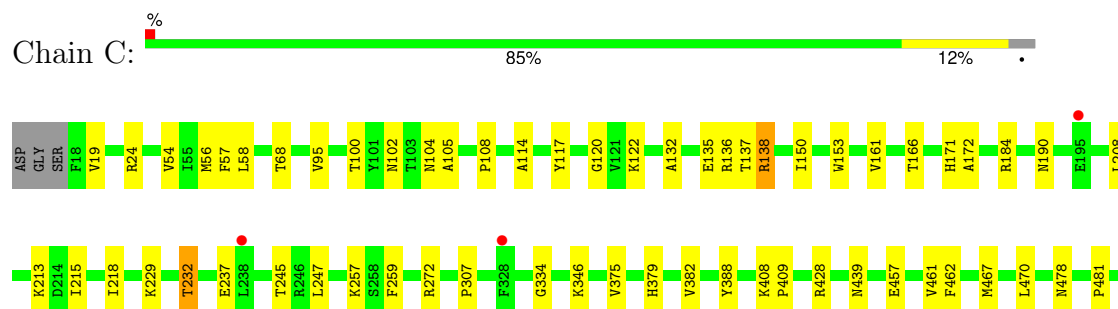
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

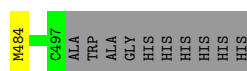


- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



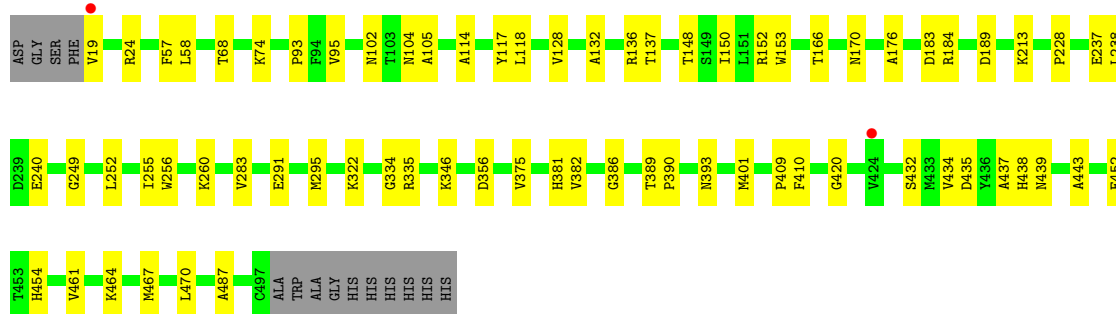
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme





- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain D: 83% 14%



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

Chain E: 80% 20%



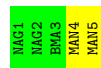
- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 100%



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

Chain F: 60% 40%



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

Chain G: 100%



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

Chain J:  100%

NAG1  
NAG2

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

Chain K:  50% 50%

NAG1  
NAG2

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

Chain M:  100%

NAG1  
NAG2

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

NAG1  
NAG2  
BMA3

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

Chain L:  75% 25%

NAG1  
NAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.27Å 118.68Å 346.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.69 – 2.28 39.69 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.69-2.28) 98.8 (39.69-2.28)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.211 , 0.249 0.216 , 0.252	Depositor DCC
$R_{free}$ test set	1995 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.70% 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: ZN, PO4, BMA, NA, FLC, MG, FUC, NAG, POP, CA, MAN

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	0.13	0/3814	0.30	0/5169
1	B	0.13	0/3812	0.32	0/5168
1	C	0.13	0/3810	0.30	0/5164
1	D	0.14	0/3796	0.31	0/5145
All	All	0.13	0/15232	0.31	0/20646

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	ARG	Sidechain

### 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	3732	0	3623	47	0
1	B	3731	0	3612	39	0
1	C	3729	0	3618	37	0
1	D	3715	0	3610	42	1
2	E	60	0	52	0	0
2	H	60	0	52	1	0
3	F	61	0	52	0	0
4	G	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	1	0
4	M	28	0	25	0	0
5	I	39	0	34	0	0
6	L	50	0	43	0	0
7	A	9	0	0	1	0
7	B	9	0	0	1	0
7	C	9	0	0	0	0
7	D	9	0	0	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	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	28	0	26	0	0
12	B	42	0	39	0	0
12	C	14	0	13	0	0
12	D	42	0	39	1	0
13	B	11	0	10	0	0
14	B	5	0	0	0	0
14	C	5	0	0	0	0
15	C	13	0	5	0	1
16	A	186	0	0	0	0
16	B	177	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C	186	0	0	0	0
16	D	196	0	0	1	0
All	All	16246	0	14928	147	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.

All (147) 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:184:ARG:NH2	7:A:601:POP:O2	1.92	1.01
1:D:166:THR:HA	1:D:295:MET:HE3	1.63	0.78
1:A:228:PRO:HG3	2:H:2:NAG:H61	1.71	0.73
1:D:237:GLU:HG3	1:D:238:LEU:HD12	1.72	0.72
1:A:57:PHE:HB3	1:A:355:MET:HE2	1.72	0.72
1:B:24:ARG:HA	1:C:132:ALA:HB3	1.72	0.71
1:A:366:THR:HB	1:A:371:THR:HG21	1.73	0.71
1:A:106:GLN:HB3	1:D:389:THR:HG23	1.74	0.70
1:A:114:ALA:HA	1:A:117:TYR:CZ	2.30	0.65
1:B:60[B]:ASP:OD1	1:B:60[B]:ASP:N	2.26	0.64
1:A:103:THR:HB	1:D:19:VAL:HG13	1.80	0.63
1:D:454:HIS:CE1	7:D:601:POP:O5	2.52	0.63
1:C:114:ALA:HA	1:C:117:TYR:CZ	2.35	0.61
1:B:132:ALA:HB3	1:C:24:ARG:HA	1.83	0.61
1:C:56:MET:HB2	1:C:484:MET:HE1	1.84	0.60
1:A:367:SER:O	1:A:371:THR:HG22	2.03	0.59
1:D:114:ALA:HA	1:D:117:TYR:CZ	2.38	0.58
1:B:60[B]:ASP:HB2	1:B:337:ASP:HB2	1.85	0.58
1:B:114:ALA:HA	1:B:117:TYR:CZ	2.38	0.58
1:B:57:PHE:HB2	1:B:375:VAL:HG22	1.84	0.58
1:B:19:VAL:HG22	1:C:104:ASN:HB3	1.85	0.58
1:B:60[A]:ASP:HB3	1:B:337:ASP:HB2	1.87	0.56
1:C:409:PRO:O	1:C:428:ARG:NH2	2.37	0.56
1:D:409:PRO:HG2	1:D:432:SER:HB3	1.87	0.56
1:D:148:THR:HB	1:D:153:TRP:HE1	1.70	0.56
1:C:57:PHE:HB2	1:C:375:VAL:HG22	1.87	0.56
1:A:102:ASN:HB2	1:A:105:ALA:HB3	1.88	0.55
1:A:194:PRO:HB2	1:B:247:LEU:HD13	1.88	0.55
1:B:74:LYS:NZ	1:B:356:ASP:OD2	2.37	0.55
1:C:375:VAL:HB	1:C:462:PHE:HB2	1.87	0.55
1:A:230:ASN:HA	1:A:243:ARG:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ALA:HB3	1:D:24:ARG:HA	1.89	0.54
1:A:19:VAL:HG22	1:D:104:ASN:HB3	1.89	0.54
1:B:68:THR:HG21	1:C:457:GLU:HA	1.89	0.54
1:C:135:GLU:HB2	1:C:138:ARG:HG3	1.89	0.54
1:A:107:VAL:HG21	1:D:386:GLY:HA2	1.88	0.54
1:D:228:PRO:HB3	1:D:249:GLY:HA2	1.90	0.54
1:C:102:ASN:HB2	1:C:105:ALA:HB3	1.90	0.54
1:B:102:ASN:HB2	1:B:105:ALA:HB3	1.89	0.54
1:C:136:ARG:HG2	1:C:137:THR:HG23	1.89	0.54
1:D:252:LEU:HD23	1:D:255:ILE:HD12	1.90	0.53
1:B:457:GLU:HA	1:C:68:THR:HG21	1.91	0.53
1:B:93:PRO:HD2	1:B:464:LYS:HB3	1.92	0.52
1:D:74:LYS:NZ	1:D:356:ASP:OD2	2.40	0.52
1:B:104:ASN:HB3	1:C:19:VAL:HG22	1.92	0.52
1:A:57:PHE:HB2	1:A:375:VAL:HG22	1.92	0.52
1:A:117:TYR:HA	1:A:481:PRO:HD3	1.92	0.52
1:A:104:ASN:HB3	1:D:19:VAL:HG22	1.92	0.51
1:D:93:PRO:HD2	1:D:464:LYS:HB3	1.91	0.51
1:A:56:MET:HE1	1:A:117:TYR:HB2	1.93	0.51
1:D:184:ARG:NH1	7:D:601:POP:O1	2.43	0.51
1:A:74:LYS:NZ	1:A:356:ASP:OD2	2.41	0.50
1:C:232:THR:HG23	1:C:237:GLU:HA	1.94	0.50
1:A:420:GLY:HA3	1:A:443:ALA:O	2.12	0.49
1:D:118:LEU:HD12	1:D:176:ALA:HB3	1.94	0.49
1:A:202:LYS:HA	1:A:202:LYS:HE2	1.94	0.49
1:D:346:LYS:NZ	1:D:437:ALA:O	2.31	0.49
1:C:100:THR:HG22	1:C:108:PRO:HG3	1.95	0.49
1:A:137:THR:HG22	1:A:183:ASP:OD2	2.13	0.48
1:B:137:THR:HG22	1:B:183:ASP:OD2	2.13	0.48
1:A:24:ARG:HA	1:D:132:ALA:HB3	1.95	0.48
1:B:195:GLU:H	1:B:195:GLU:CD	2.22	0.48
1:D:390:PRO:HG2	1:D:393:ASN:HB2	1.96	0.48
1:A:128:VAL:HG13	1:A:176:ALA:HA	1.96	0.48
1:B:223:ARG:HH11	1:B:270:TRP:HB2	1.79	0.48
1:C:467:MET:HE3	1:C:470:LEU:HD11	1.96	0.47
1:A:381:HIS:HB3	1:A:452:GLU:OE2	2.13	0.47
1:C:346:LYS:HD3	1:C:439:ASN:HA	1.95	0.47
1:D:346:LYS:HD3	1:D:439:ASN:HA	1.95	0.47
1:C:208:LEU:HD11	1:C:218:ILE:HD13	1.97	0.46
1:A:240:GLU:O	1:A:243:ARG:HG2	2.15	0.46
1:B:190:ASN:HB2	1:B:245:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:HB	1:A:462:PHE:HB2	1.97	0.46
1:B:213:LYS:HB3	1:B:259:PHE:HB3	1.98	0.46
1:C:272:ARG:HD2	1:C:307:PRO:HA	1.97	0.46
1:B:107:VAL:HB	1:C:388:TYR:HA	1.98	0.46
1:B:128:VAL:HG13	1:B:176:ALA:HA	1.96	0.46
1:D:381:HIS:HB3	1:D:452:GLU:OE2	2.16	0.46
1:D:170:ASN:OD1	1:D:170:ASN:N	2.43	0.46
1:A:74:LYS:HD3	1:A:87:LEU:HD23	1.98	0.46
1:B:136:ARG:HG2	1:B:137:THR:HG23	1.97	0.46
1:A:93:PRO:HD2	1:A:464:LYS:HB3	1.97	0.45
1:D:467:MET:HE3	1:D:470:LEU:HD11	1.98	0.45
1:C:408:LYS:HG3	4:K:1:NAG:H82	1.98	0.45
1:A:95:VAL:HA	1:A:461:VAL:O	2.16	0.45
1:B:232:THR:HG22	1:B:243:ARG:NH1	2.31	0.45
1:A:195:GLU:HG3	1:B:247:LEU:O	2.16	0.45
1:B:375:VAL:HB	1:B:462:PHE:HB2	1.99	0.45
1:D:137:THR:HG22	1:D:183:ASP:OD2	2.17	0.45
1:B:56:MET:HE1	1:B:117:TYR:HB2	1.99	0.44
1:D:435:ASP:OD2	1:D:438:HIS:NE2	2.51	0.44
1:B:29:TRP:CE2	1:C:122:LYS:HB2	2.52	0.44
1:D:95:VAL:HA	1:D:461:VAL:O	2.17	0.44
1:C:100:THR:HG21	1:C:379:HIS:HA	1.99	0.44
1:D:291:GLU:HG3	1:D:295:MET:HA	2.00	0.43
1:A:457:GLU:HA	1:D:68:THR:HG21	2.00	0.43
1:C:117:TYR:HA	1:C:481:PRO:HD3	2.00	0.43
1:A:318:ARG:HG3	1:A:365:MET:HE1	2.00	0.43
1:C:95:VAL:HA	1:C:461:VAL:O	2.19	0.43
12:D:608:NAG:O7	12:D:608:NAG:O3	2.32	0.43
1:A:42:LYS:HE2	1:A:42:LYS:HB3	1.80	0.43
1:A:447:VAL:HG21	1:D:410:PHE:HB2	2.00	0.43
1:B:202:LYS:HA	1:B:202:LYS:HE2	1.99	0.43
1:C:161:VAL:HG23	1:C:215:ILE:HG23	2.00	0.43
1:A:346:LYS:HD3	1:A:439:ASN:HA	2.00	0.43
1:A:56:MET:HB2	1:A:484:MET:HE1	2.01	0.43
1:C:120:GLY:C	1:C:478:ASN:HB2	2.43	0.43
1:D:150:ILE:HA	1:D:153:TRP:CD2	2.53	0.43
1:A:389:THR:HA	1:A:400:PRO:HD3	2.00	0.43
1:D:335:ARG:NH2	16:D:724:HOH:O	2.52	0.43
1:C:166:THR:OG1	1:C:334:GLY:HA2	2.18	0.43
1:A:240:GLU:HG2	1:A:243:ARG:HH21	1.84	0.42
1:A:170:ASN:OD1	1:A:170:ASN:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HH12	7:B:602:POP:P1	2.42	0.42
1:A:208:LEU:HD11	1:A:218:ILE:HD13	2.00	0.42
1:B:367:SER:OG	1:B:369:LYS:HG2	2.20	0.42
1:C:56:MET:HE1	1:C:117:TYR:HB2	2.02	0.42
1:A:84:GLU:OE1	1:A:391:ARG:NH1	2.53	0.42
1:B:280:PRO:HB2	1:B:318:ARG:HB3	2.02	0.42
1:B:117:TYR:HA	1:B:481:PRO:HD3	2.02	0.42
1:A:385:PHE:HA	1:A:412:ALA:O	2.20	0.42
1:C:54:VAL:CG1	1:C:484:MET:HE2	2.50	0.42
1:A:168:ARG:HG3	1:A:294:ASP:OD1	2.19	0.41
1:D:57:PHE:HB2	1:D:375:VAL:HG22	2.02	0.41
1:D:189:ASP:N	1:D:189:ASP:OD1	2.53	0.41
1:D:166:THR:OG1	1:D:334:GLY:HA2	2.20	0.41
1:A:190:ASN:HB2	1:A:245:THR:O	2.21	0.41
1:B:150:ILE:HA	1:B:153:TRP:CE3	2.56	0.41
1:D:420:GLY:HA3	1:D:443:ALA:O	2.20	0.41
1:B:175:SER:HA	1:B:178:TYR:CE2	2.55	0.41
1:A:120:GLY:C	1:A:478:ASN:HB2	2.46	0.41
1:D:467:MET:HB2	1:D:487:ALA:HB2	2.03	0.41
1:A:252:LEU:HD23	1:A:255:ILE:HD12	2.01	0.41
1:C:190:ASN:HB2	1:C:245:THR:O	2.21	0.41
1:C:257:LYS:HE3	1:C:257:LYS:HB2	1.81	0.41
1:B:95:VAL:HA	1:B:461:VAL:O	2.20	0.41
1:C:184:ARG:H	1:C:184:ARG:HG3	1.74	0.41
1:D:256:TRP:O	1:D:260:LYS:HD3	2.21	0.41
1:D:283:VAL:O	1:D:322:LYS:NZ	2.54	0.41
1:B:186:TRP:CG	1:B:192:MET:HG2	2.56	0.40
1:D:136:ARG:HG2	1:D:137:THR:HG23	2.03	0.40
1:C:229:LYS:HG3	1:C:247:LEU:HD23	2.03	0.40
1:B:223:ARG:NH1	1:B:270:TRP:HB2	2.36	0.40
1:C:150:ILE:HA	1:C:153:TRP:CD2	2.56	0.40
1:B:58:LEU:HD12	1:B:376:THR:HG23	2.04	0.40
1:C:171:HIS:CG	1:C:172:ALA:N	2.90	0.40
1:D:102:ASN:HB2	1:D:105:ALA:HB3	2.03	0.40

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)
1:D:213:LYS:NZ	15:C:605:FLC:OB2[2_454]	1.30	0.90

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	479/493 (97%)	464 (97%)	14 (3%)	1 (0%)	43	53
1	B	480/493 (97%)	465 (97%)	13 (3%)	2 (0%)	30	36
1	C	479/493 (97%)	465 (97%)	13 (3%)	1 (0%)	43	53
1	D	477/493 (97%)	465 (98%)	11 (2%)	1 (0%)	43	53
All	All	1915/1972 (97%)	1859 (97%)	51 (3%)	5 (0%)	36	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	ASN
1	A	382	VAL
1	B	382	VAL
1	D	382	VAL
1	C	382	VAL

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/405 (98%)	393 (99%)	3 (1%)	73	84
1	B	395/405 (98%)	390 (99%)	5 (1%)	61	76
1	C	395/405 (98%)	390 (99%)	5 (1%)	61	76
1	D	394/405 (97%)	388 (98%)	6 (2%)	57	72
All	All	1580/1620 (98%)	1561 (99%)	19 (1%)	63	77

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	184	ARG
1	A	274	GLU
1	B	58	LEU
1	B	128	VAL
1	B	143	GLN
1	B	195	GLU
1	B	401	MET
1	C	58	LEU
1	C	138	ARG
1	C	213	LYS
1	C	232	THR
1	C	259	PHE
1	D	58	LEU
1	D	128	VAL
1	D	152	ARG
1	D	240	GLU
1	D	401	MET
1	D	434	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	267	HIS
1	C	393	ASN
1	D	53	ASN
1	D	190	ASN
1	D	451	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

30 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	2,1	14,14,15	0.22	0	17,19,21	0.48	0
2	NAG	E	2	2	14,14,15	0.31	0	17,19,21	0.50	0
2	BMA	E	3	2	11,11,12	0.55	0	15,15,17	0.74	0
2	MAN	E	4	2	11,11,12	0.73	0	15,15,17	1.13	2 (13%)
2	FUC	E	5	2	10,10,11	0.70	0	14,14,16	0.62	0
3	NAG	F	1	3,1	14,14,15	0.36	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.20	0	17,19,21	0.51	0
3	BMA	F	3	3	11,11,12	0.67	0	15,15,17	0.86	0
3	MAN	F	4	3	11,11,12	0.80	0	15,15,17	1.33	2 (13%)
3	MAN	F	5	3	11,11,12	0.93	1 (9%)	15,15,17	1.21	1 (6%)
4	NAG	G	1	1,4	14,14,15	0.31	0	17,19,21	0.59	0
4	NAG	G	2	4	14,14,15	0.18	0	17,19,21	0.53	0
2	NAG	H	1	2,1	14,14,15	1.84	1 (7%)	17,19,21	1.51	4 (23%)
2	NAG	H	2	2	14,14,15	0.31	0	17,19,21	0.47	0
2	BMA	H	3	2	11,11,12	0.78	0	15,15,17	1.14	2 (13%)
2	MAN	H	4	2	11,11,12	0.69	0	15,15,17	1.07	1 (6%)
2	FUC	H	5	2	10,10,11	0.95	1 (10%)	14,14,16	0.97	1 (7%)
5	NAG	I	1	5,1	14,14,15	0.33	0	17,19,21	0.44	0
5	NAG	I	2	5	14,14,15	0.27	0	17,19,21	0.41	0
5	BMA	I	3	5	11,11,12	0.66	0	15,15,17	0.76	0
4	NAG	J	1	1,4	14,14,15	0.29	0	17,19,21	0.44	0
4	NAG	J	2	4	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	K	1	1,4	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	K	2	4	14,14,15	0.26	0	17,19,21	0.50	0
6	NAG	L	1	6,1	14,14,15	0.30	0	17,19,21	0.42	0
6	NAG	L	2	6	14,14,15	0.18	0	17,19,21	0.53	0
6	BMA	L	3	6	11,11,12	0.61	0	15,15,17	0.78	0
6	MAN	L	4	6	11,11,12	0.75	0	15,15,17	0.96	2 (13%)
4	NAG	M	1	1,4	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	M	2	4	14,14,15	0.32	0	17,19,21	0.42	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	2,1	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	FUC	E	5	2	-	-	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	2/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	1/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	MAN	H	4	2	-	0/2/19/22	0/1/1/1
2	FUC	H	5	2	-	-	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	BMA	I	3	5	-	1/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O5-C1	-6.48	1.32	1.43
2	H	5	FUC	C1-C2	2.53	1.58	1.52
3	F	5	MAN	O5-C5	2.11	1.47	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	C1-O5-C5	4.03	117.58	112.19
3	F	5	MAN	C1-O5-C5	3.70	117.15	112.19
2	H	1	NAG	C3-C4-C5	3.35	116.30	110.23
2	E	4	MAN	C1-O5-C5	3.25	116.54	112.19
2	H	1	NAG	C1-O5-C5	-3.11	108.02	112.19
2	H	4	MAN	C1-O5-C5	2.98	116.18	112.19
2	H	3	BMA	C1-O5-C5	2.79	115.92	112.19
6	L	4	MAN	C1-O5-C5	2.70	115.81	112.19
2	H	3	BMA	C1-C2-C3	2.50	113.29	109.64
2	H	1	NAG	C4-C3-C2	2.33	114.43	111.02
2	E	4	MAN	O2-C2-C3	-2.19	105.61	110.15
2	H	1	NAG	O4-C4-C5	-2.19	103.93	109.32
3	F	4	MAN	O2-C2-C3	-2.14	105.72	110.15
6	L	4	MAN	O2-C2-C3	-2.04	105.93	110.15
2	H	5	FUC	C1-C2-C3	2.03	112.60	109.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
4	M	2	NAG	C8-C7-N2-C2
4	M	2	NAG	O7-C7-N2-C2
4	G	2	NAG	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
3	F	3	BMA	C4-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C3-C2-N2-C7
5	I	2	NAG	C4-C5-C6-O6

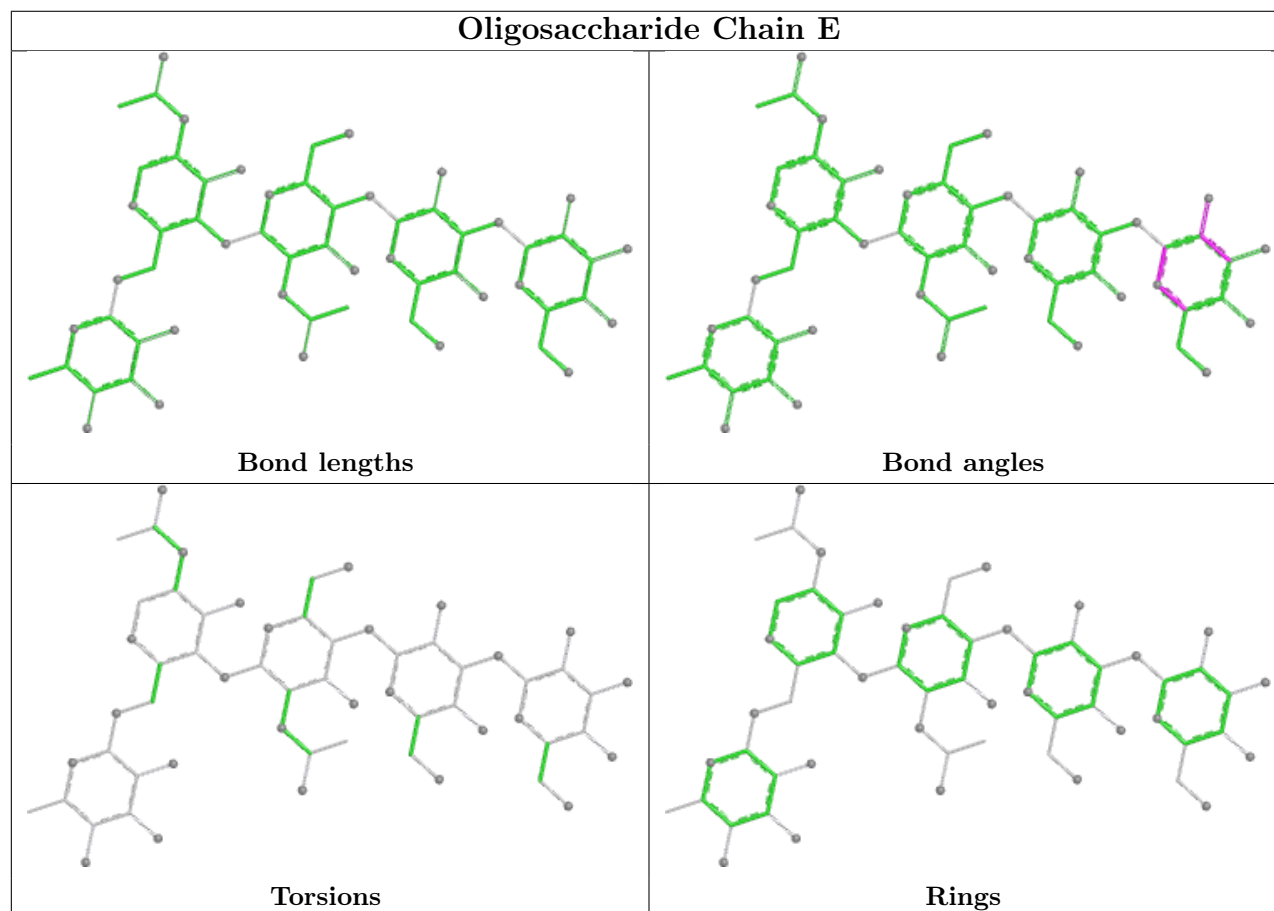
All (1) ring outliers are listed below:

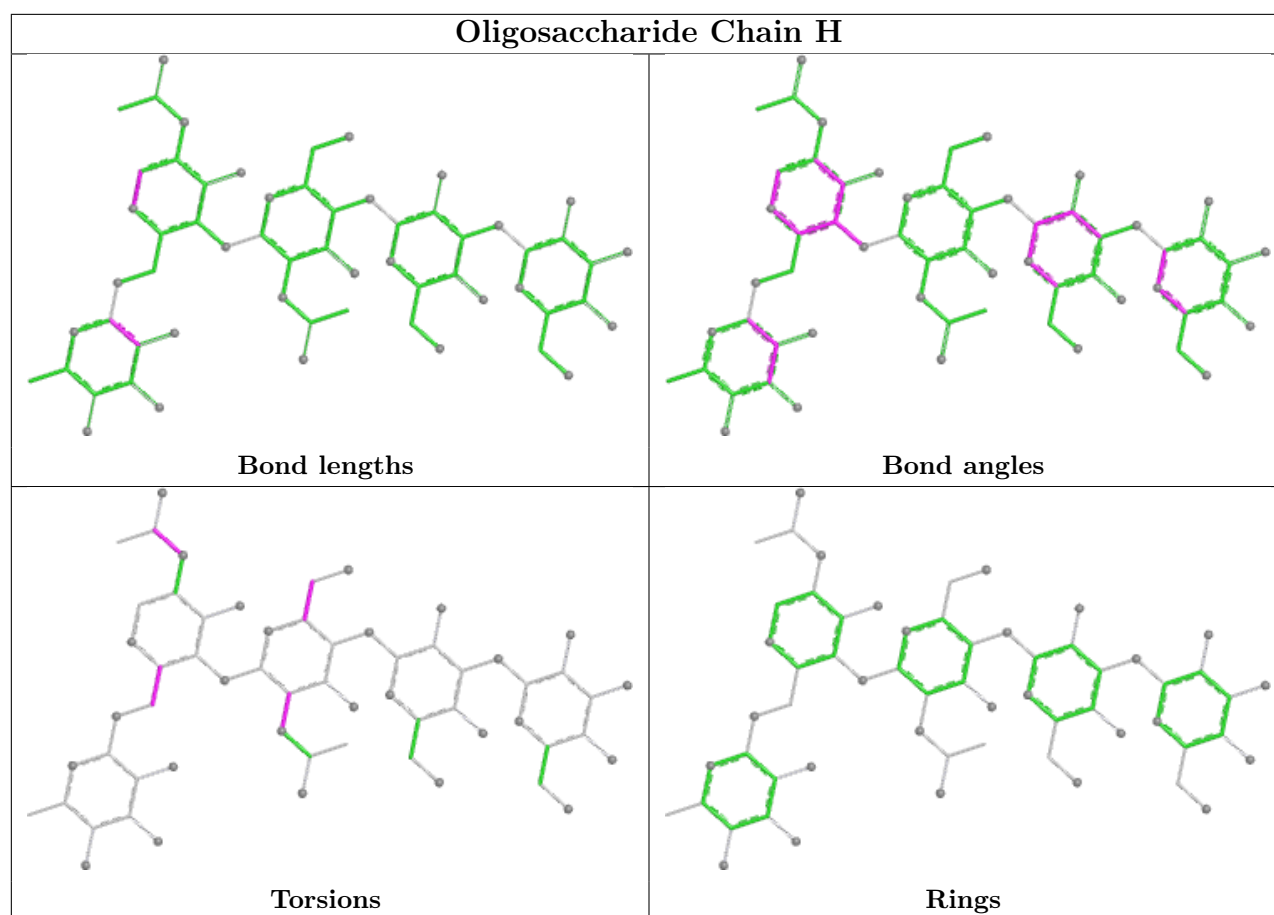
Mol	Chain	Res	Type	Atoms
3	F	5	MAN	C1-C2-C3-C4-C5-O5

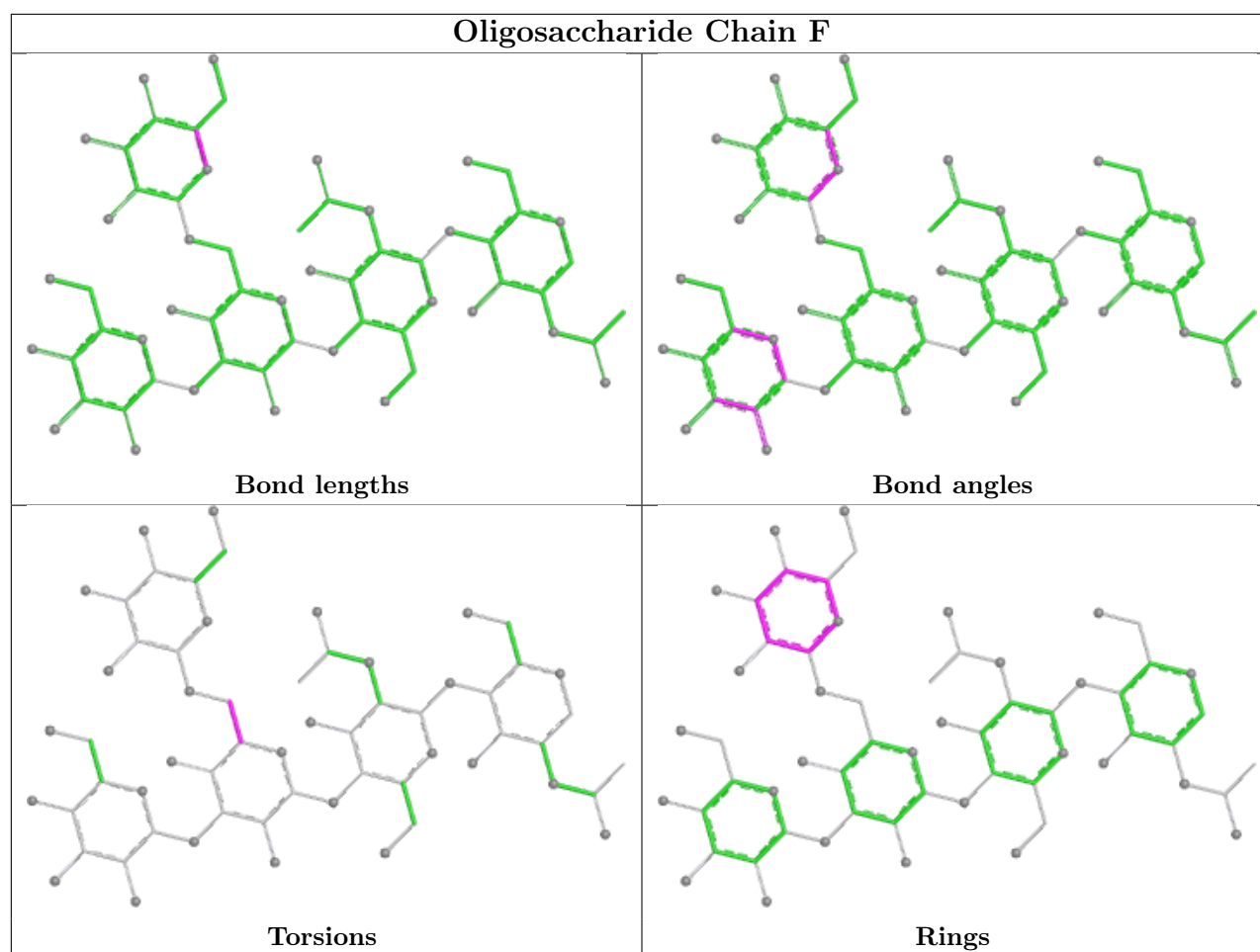
2 monomers are involved in 2 short contacts:

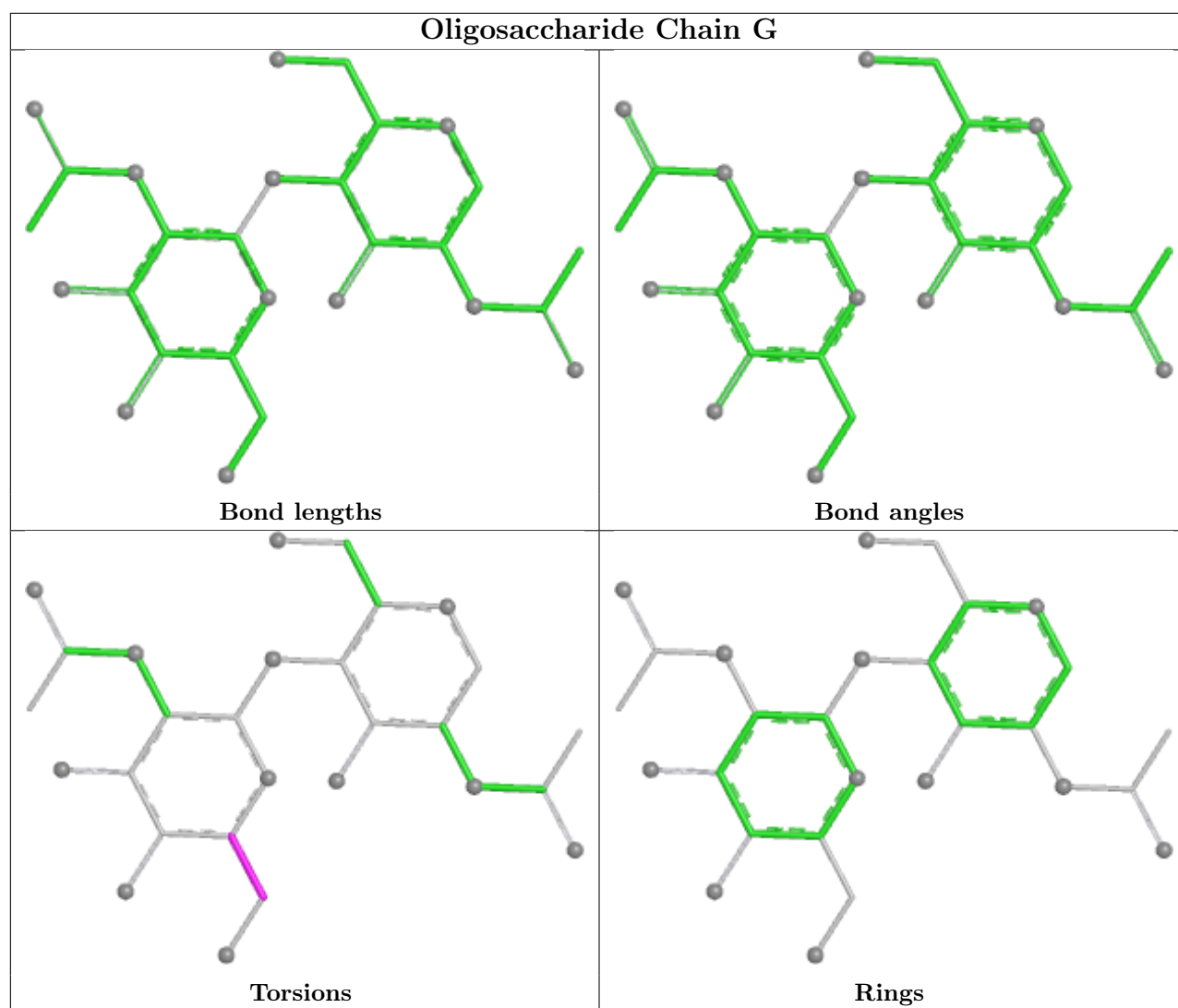
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	1	0
4	K	1	NAG	1	0

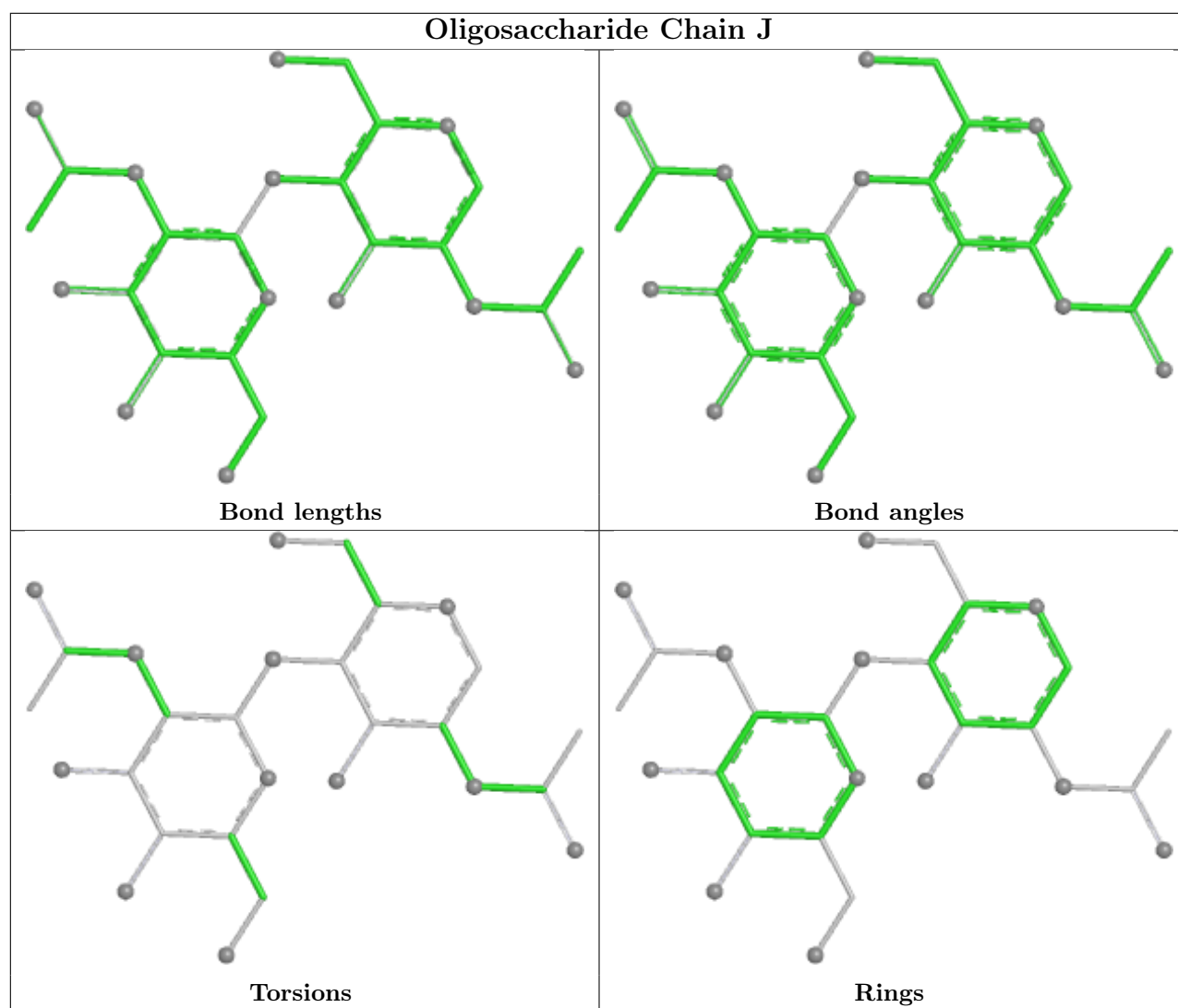
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

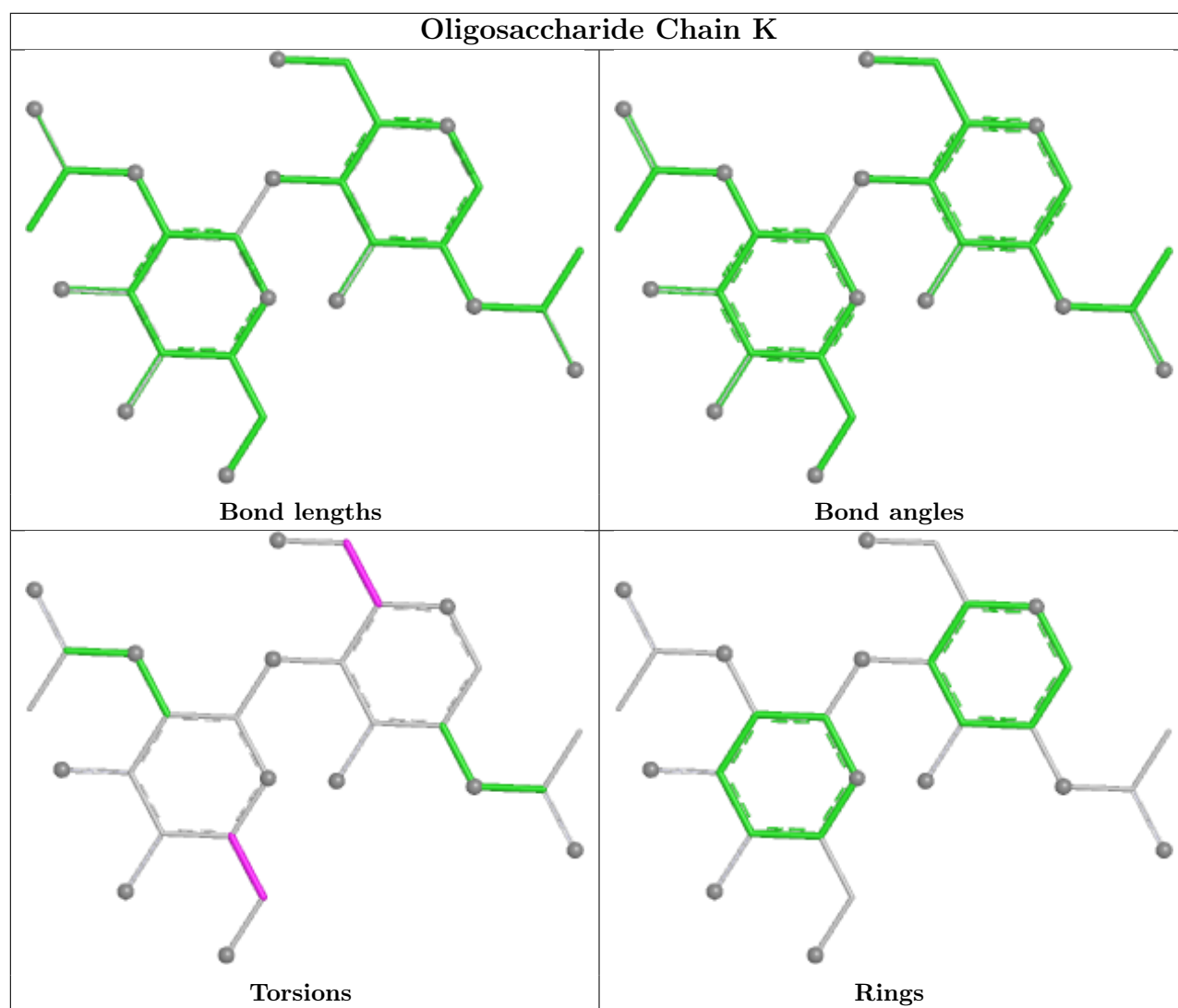




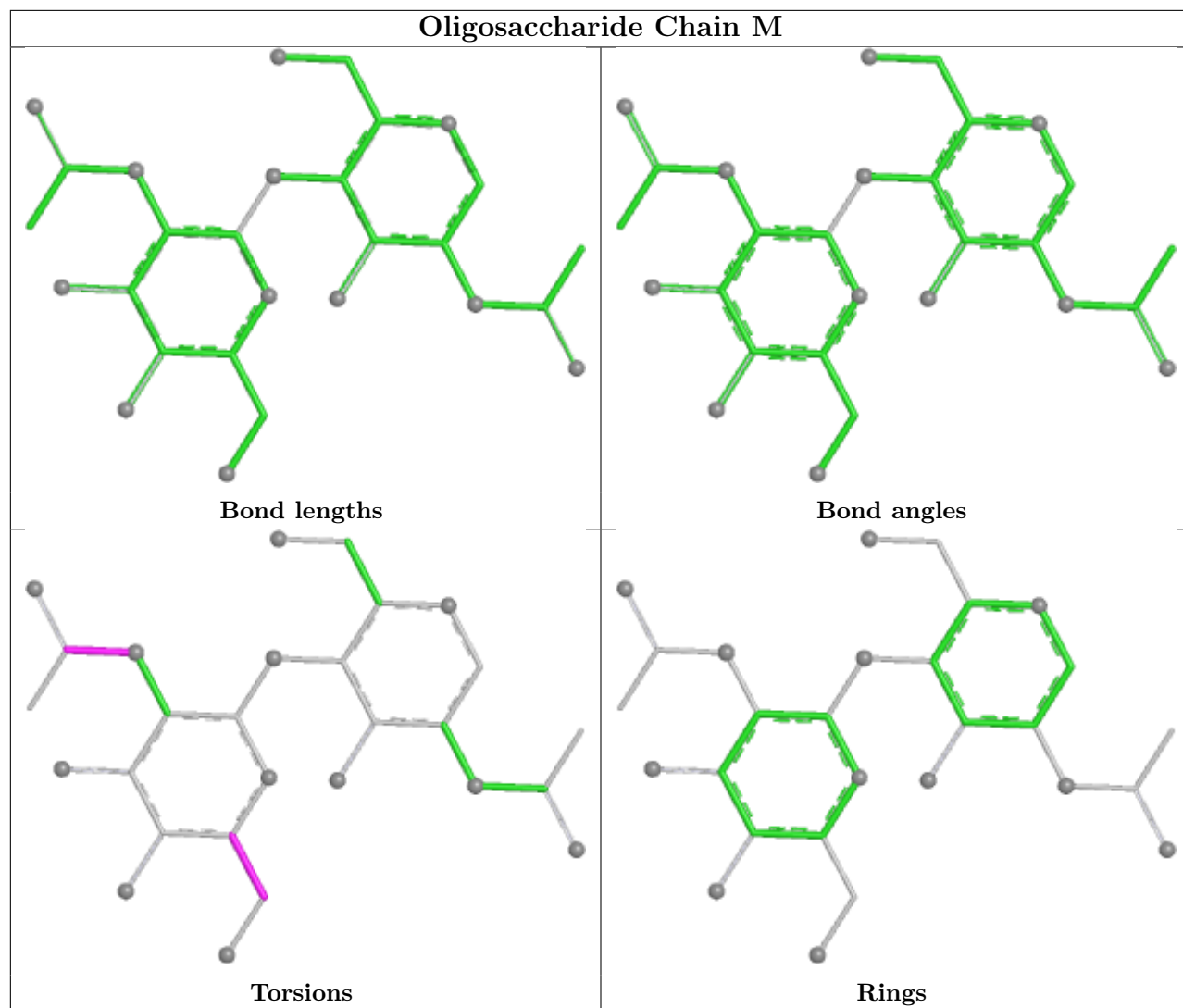


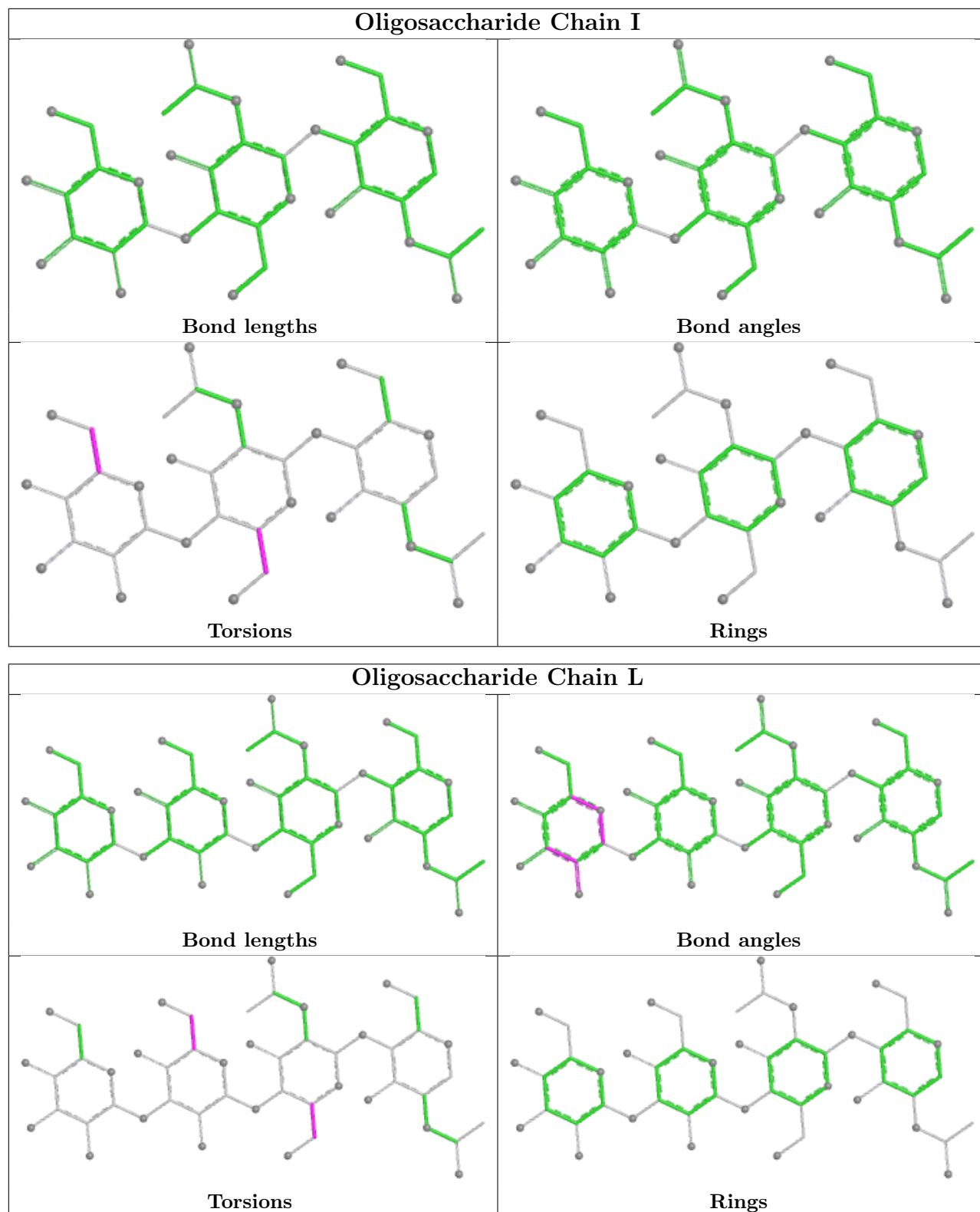












## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 16 are monoatomic - leaving 17 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	NAG	D	608	1	14,14,15	0.55	0	17,19,21	0.48	0
7	POP	A	601	8	6,8,8	0.73	0	12,13,13	0.84	0
12	NAG	A	607	1	14,14,15	0.44	0	17,19,21	0.54	0
7	POP	C	601	8	6,8,8	0.77	0	12,13,13	0.92	1 (8%)
12	NAG	D	606	1	14,14,15	0.40	0	17,19,21	0.61	1 (5%)
13	MAN	B	601	-	11,11,12	0.92	0	15,15,17	1.04	0
12	NAG	B	608	1	14,14,15	0.58	1 (7%)	17,19,21	0.46	0
12	NAG	B	610	1	14,14,15	0.36	0	17,19,21	0.50	0
12	NAG	A	606	1	14,14,15	0.24	0	17,19,21	0.46	0
12	NAG	B	609	1	14,14,15	0.36	0	17,19,21	0.54	0
12	NAG	D	607	1	14,14,15	0.37	0	17,19,21	0.55	0
15	FLC	C	605	-	12,12,12	1.89	6 (50%)	17,17,17	2.30	6 (35%)
14	PO4	B	606	-	4,4,4	0.94	0	6,6,6	0.58	0
7	POP	D	601	8	6,8,8	1.21	0	12,13,13	1.50	2 (16%)
7	POP	B	602	8	6,8,8	0.77	0	12,13,13	0.98	0
12	NAG	C	608	1	14,14,15	0.45	0	17,19,21	0.54	0
14	PO4	C	606	-	4,4,4	0.96	0	6,6,6	0.49	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	NAG	D	608	1	-	1/6/23/26	0/1/1/1
7	POP	A	601	8	-	1/6/6/6	-
12	NAG	A	607	1	-	2/6/23/26	0/1/1/1
7	POP	C	601	8	-	0/6/6/6	-
12	NAG	D	606	1	-	2/6/23/26	0/1/1/1
13	MAN	B	601	-	-	2/2/19/22	0/1/1/1
12	NAG	B	608	1	-	2/6/23/26	0/1/1/1
12	NAG	B	610	1	-	0/6/23/26	0/1/1/1
12	NAG	A	606	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	B	609	1	-	0/6/23/26	0/1/1/1
12	NAG	D	607	1	-	2/6/23/26	0/1/1/1
7	POP	D	601	8	-	0/6/6/6	-
7	POP	B	602	8	-	0/6/6/6	-
12	NAG	C	608	1	-	2/6/23/26	0/1/1/1
15	FLC	C	605	-	-	5/16/16/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	605	FLC	OB1-CBC	2.89	1.31	1.22
15	C	605	FLC	OA1-CAC	2.79	1.31	1.22
15	C	605	FLC	OG1-CGC	2.79	1.31	1.22
15	C	605	FLC	OG2-CGC	-2.66	1.22	1.30
15	C	605	FLC	OA2-CAC	-2.65	1.22	1.30
15	C	605	FLC	OB2-CBC	-2.03	1.23	1.30
12	B	608	NAG	C1-C2	2.01	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	605	FLC	OB2-CBC-CB	5.08	122.88	113.14
15	C	605	FLC	OB1-CBC-CB	-4.80	112.79	122.09
7	D	601	POP	O3-P1-O	3.61	116.75	104.64
15	C	605	FLC	OA1-CAC-CA	-3.49	113.08	122.95
15	C	605	FLC	OG1-CGC-CG	-3.17	113.98	122.95
15	C	605	FLC	OA2-CAC-CA	2.98	123.79	114.35
15	C	605	FLC	OG2-CGC-CG	2.68	122.84	114.35
7	D	601	POP	O6-P2-O5	2.26	116.28	107.80
7	C	601	POP	O3-P1-O	2.06	111.54	104.64
12	D	606	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	606	NAG	C4-C5-C6-O6
12	A	606	NAG	O5-C5-C6-O6
12	D	606	NAG	C4-C5-C6-O6
12	D	607	NAG	O5-C5-C6-O6

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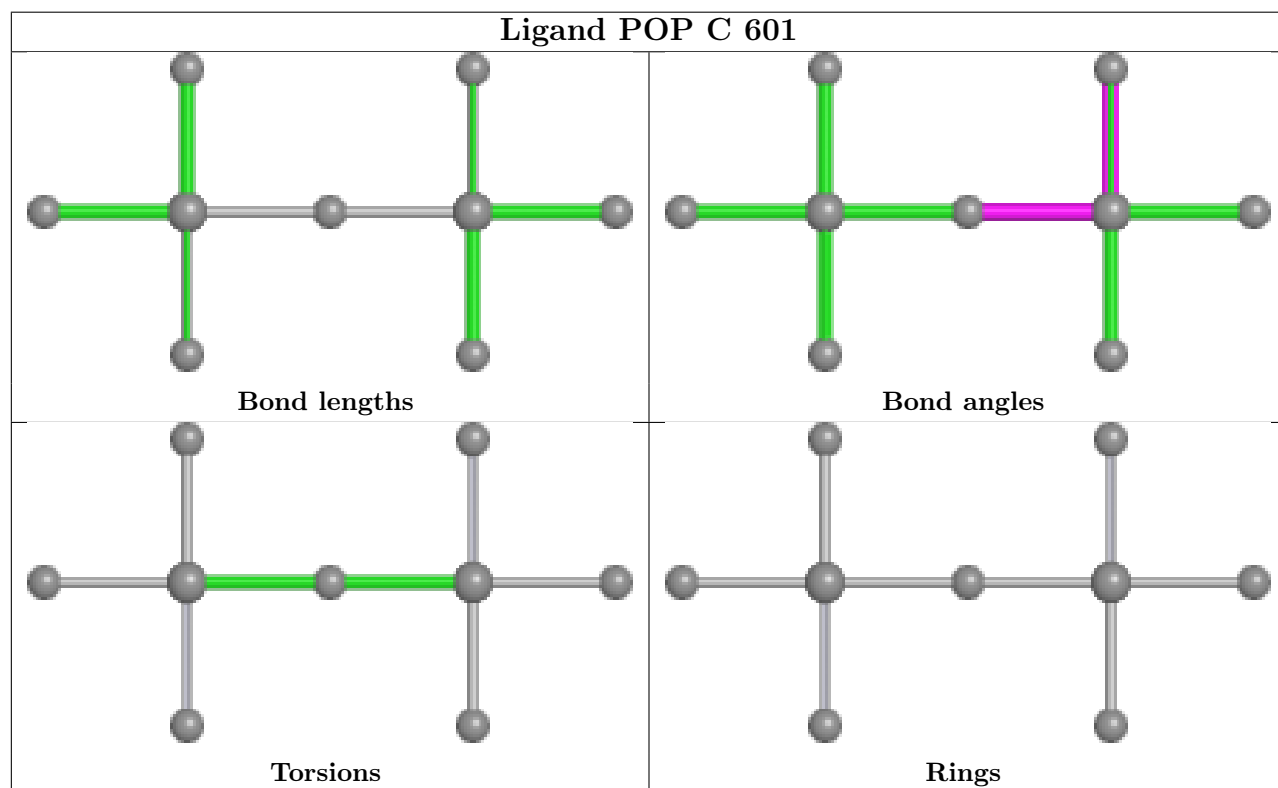
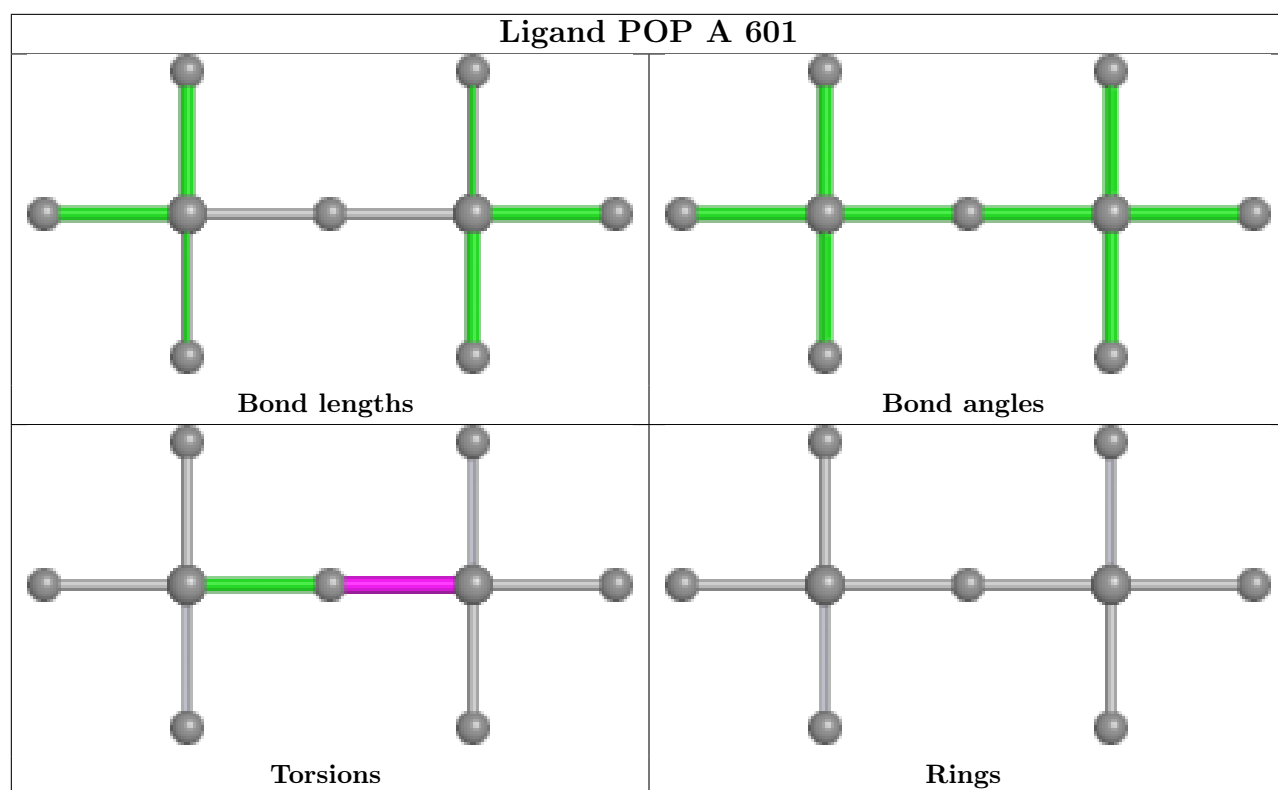
Mol	Chain	Res	Type	Atoms
12	A	607	NAG	O5-C5-C6-O6
12	D	607	NAG	C4-C5-C6-O6
12	D	606	NAG	O5-C5-C6-O6
12	B	608	NAG	C8-C7-N2-C2
12	B	608	NAG	O7-C7-N2-C2
13	B	601	MAN	C4-C5-C6-O6
13	B	601	MAN	O5-C5-C6-O6
15	C	605	FLC	CAC-CA-CB-CBC
15	C	605	FLC	CAC-CA-CB-OHB
15	C	605	FLC	CAC-CA-CB-CG
7	A	601	POP	P2-O-P1-O1
12	C	608	NAG	C4-C5-C6-O6
12	A	607	NAG	C4-C5-C6-O6
12	D	608	NAG	C3-C2-N2-C7
12	C	608	NAG	O5-C5-C6-O6
15	C	605	FLC	CB-CA-CAC-OA1
15	C	605	FLC	CB-CA-CAC-OA2

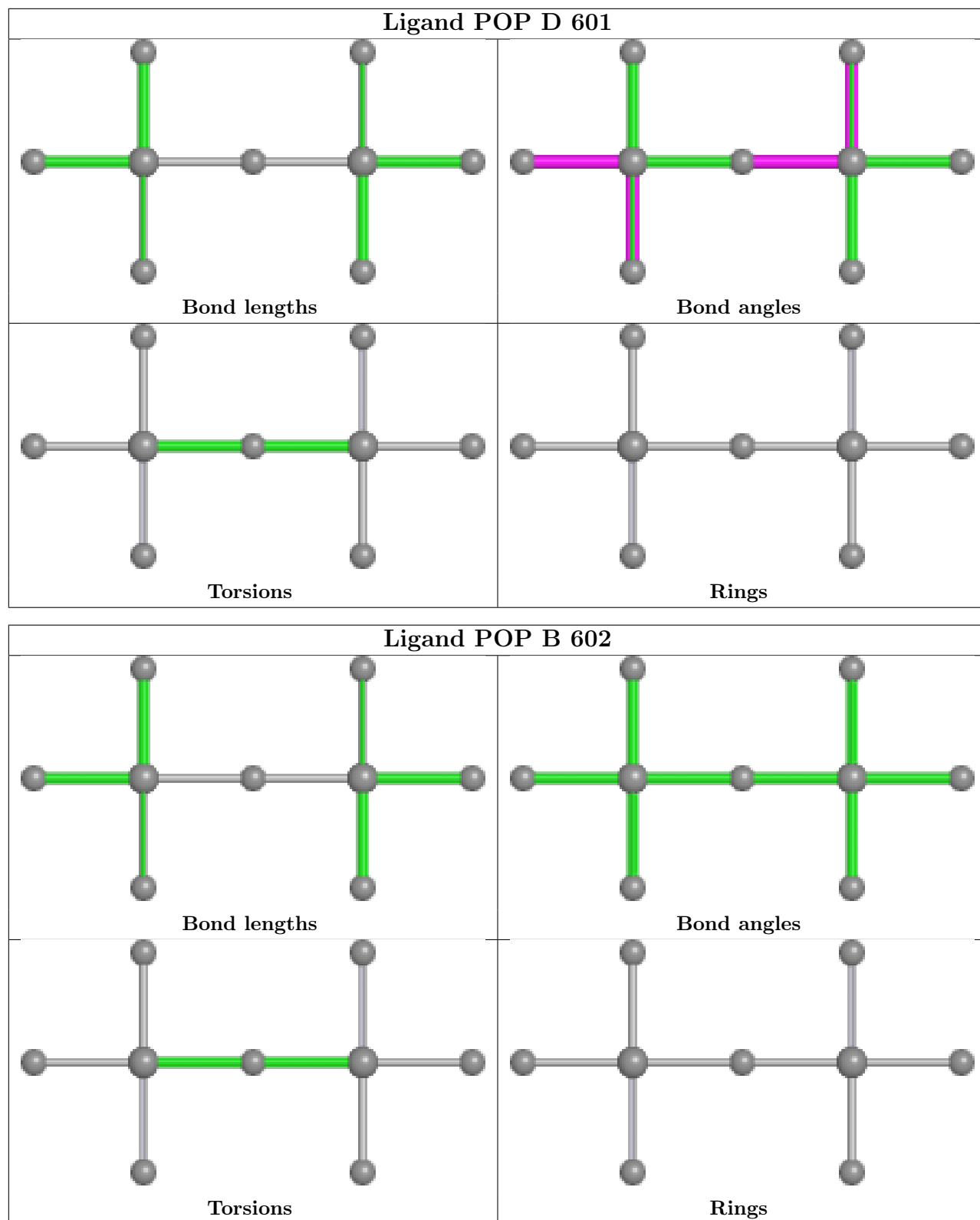
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	608	NAG	1	0
7	A	601	POP	1	0
15	C	605	FLC	0	1
7	D	601	POP	2	0
7	B	602	POP	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 ⓘ

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	481/493 (97%)	0.19	5 (1%) 79 81	33, 44, 62, 82	2 (0%)
1	B	481/493 (97%)	0.16	5 (1%) 79 81	20, 43, 62, 82	1 (0%)
1	C	480/493 (97%)	0.19	3 (0%) 85 86	22, 43, 59, 76	2 (0%)
1	D	479/493 (97%)	0.13	2 (0%) 88 89	33, 44, 59, 75	0
All	All	1921/1972 (97%)	0.17	15 (0%) 82 84	20, 43, 61, 82	5 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	PHE	3.0
1	D	19	VAL	2.8
1	B	433	MET	2.8
1	A	282	ARG	2.6
1	B	18	PHE	2.5
1	A	17	SER	2.5
1	A	400	PRO	2.4
1	C	328	PHE	2.4
1	B	17	SER	2.3
1	B	162	GLY	2.3
1	B	263	HIS	2.2
1	C	195	GLU	2.2
1	D	424	VAL	2.1
1	C	238	LEU	2.1
1	A	206	TYR	2.1

### 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 ⓘ

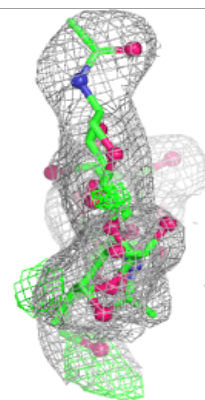
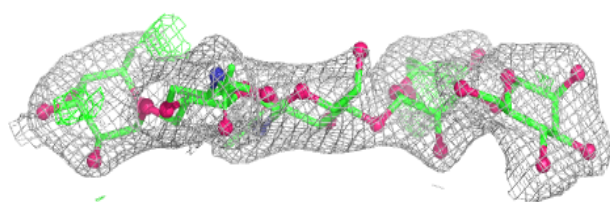
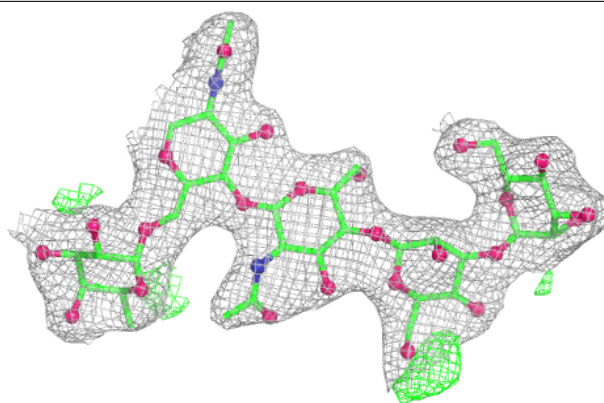
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
5	BMA	I	3	11/12	0.31	0.18	98,111,117,119	0
3	MAN	F	4	11/12	0.35	0.18	101,109,115,116	0
3	MAN	F	5	11/12	0.45	0.20	105,108,111,114	0
3	BMA	F	3	11/12	0.52	0.17	98,101,106,111	0
6	BMA	L	3	11/12	0.58	0.14	84,92,95,96	0
4	NAG	J	2	14/15	0.64	0.15	73,88,92,96	0
4	NAG	M	2	14/15	0.68	0.15	87,92,96,96	0
4	NAG	K	2	14/15	0.70	0.14	80,85,88,90	0
4	NAG	G	2	14/15	0.70	0.14	81,86,97,105	0
6	NAG	L	2	14/15	0.71	0.13	75,85,90,97	0
5	NAG	I	2	14/15	0.73	0.17	80,90,105,111	0
2	NAG	H	2	14/15	0.75	0.17	60,66,83,85	0
2	FUC	H	5	10/11	0.78	0.16	69,73,75,78	0
6	MAN	L	4	11/12	0.79	0.14	61,80,89,90	0
3	NAG	F	2	14/15	0.81	0.12	76,83,89,93	0
3	NAG	F	1	14/15	0.83	0.12	57,68,73,82	0
4	NAG	J	1	14/15	0.84	0.12	63,73,79,87	0
4	NAG	G	1	14/15	0.84	0.11	53,66,76,78	0
2	NAG	H	1	14/15	0.84	0.13	50,58,74,74	0
4	NAG	K	1	14/15	0.85	0.10	45,70,74,79	0
2	FUC	E	5	10/11	0.86	0.14	58,64,66,67	0
4	NAG	M	1	14/15	0.87	0.09	51,70,82,89	0
2	BMA	H	3	11/12	0.87	0.10	55,60,65,65	0
5	NAG	I	1	14/15	0.87	0.12	57,66,71,85	0
2	MAN	H	4	11/12	0.87	0.13	56,62,65,69	0
6	NAG	L	1	14/15	0.88	0.11	56,64,70,83	0
2	BMA	E	3	11/12	0.89	0.10	41,48,52,57	0
2	NAG	E	2	14/15	0.91	0.12	48,51,62,69	0
2	MAN	E	4	11/12	0.93	0.08	48,52,57,58	0
2	NAG	E	1	14/15	0.95	0.08	46,48,54,60	0

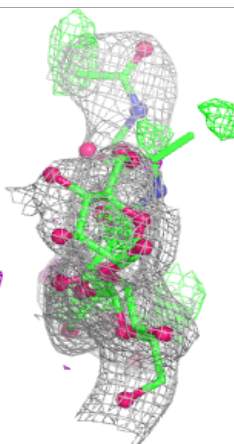
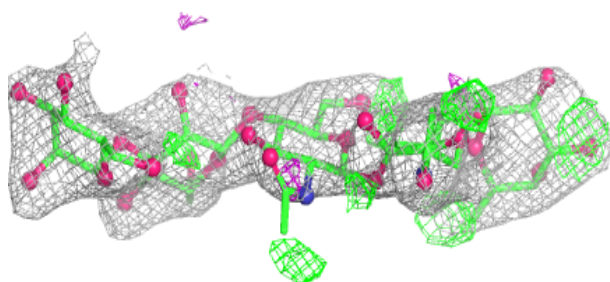
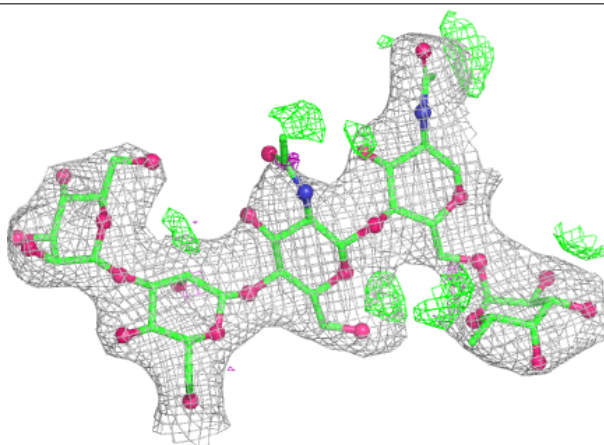
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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)

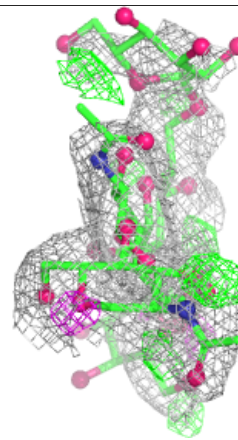
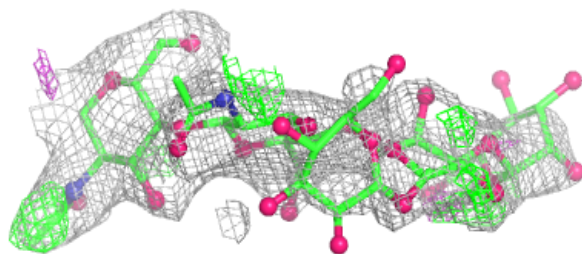
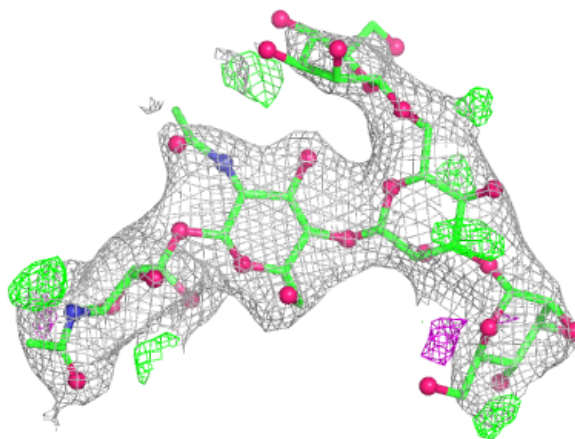
**Electron density around Chain H:**

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



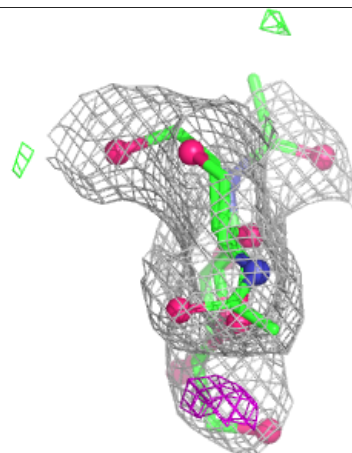
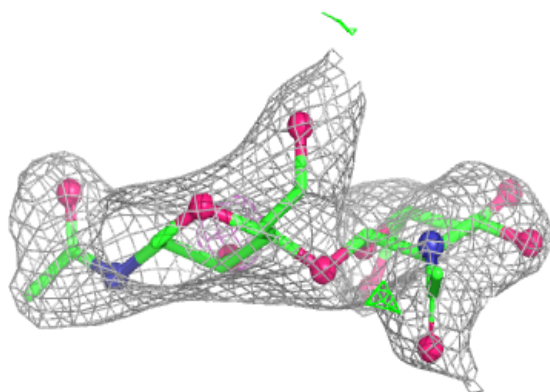
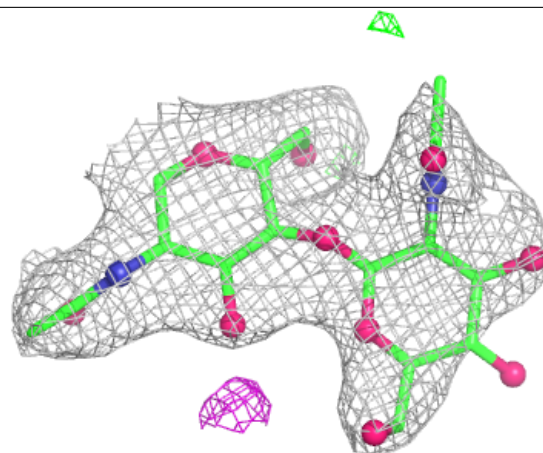
**Electron density around Chain F:**

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



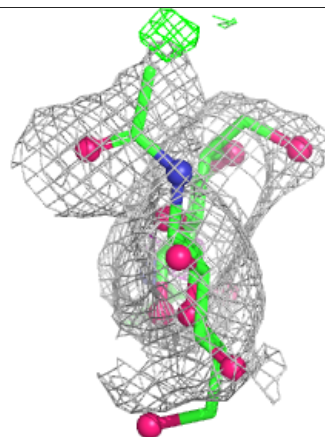
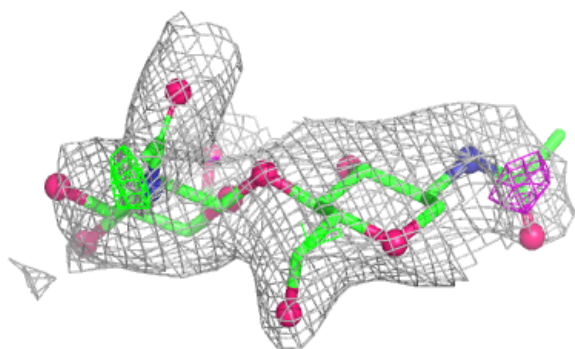
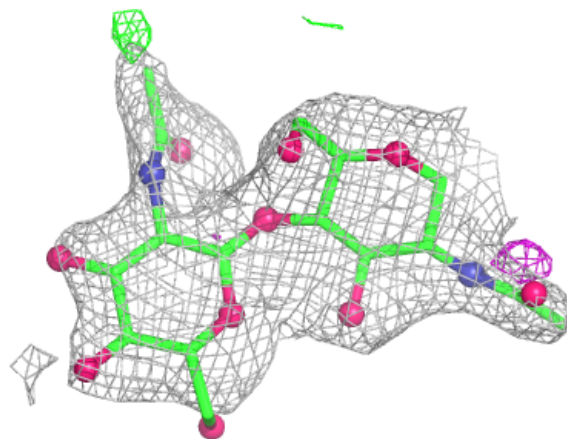
**Electron density around Chain G:**

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



**Electron density around Chain J:**

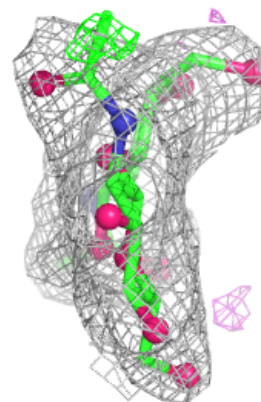
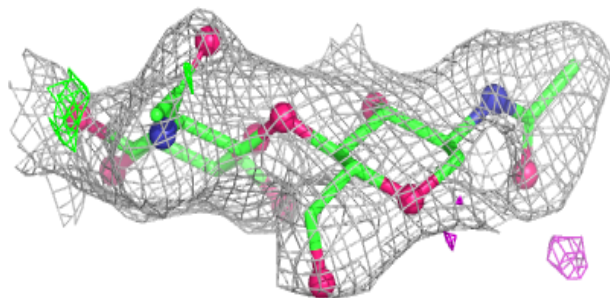
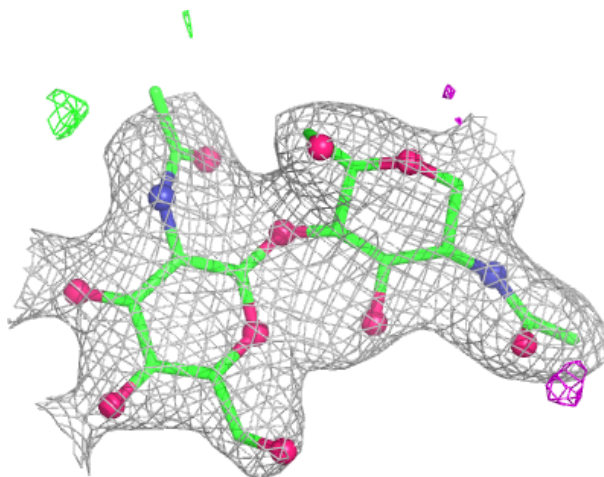
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





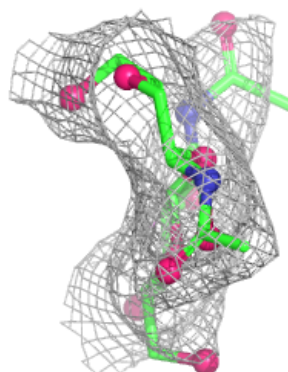
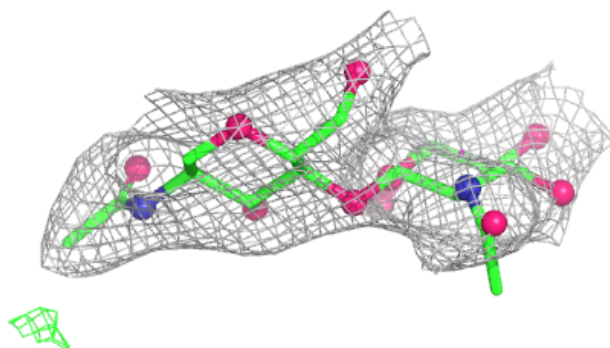
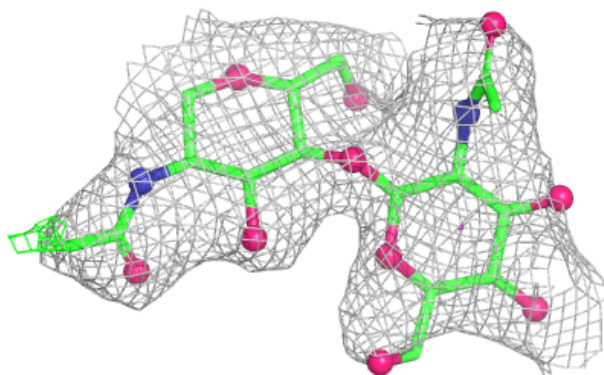
**Electron density around Chain K:**

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

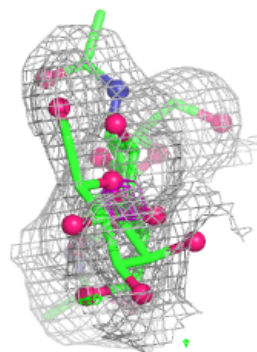
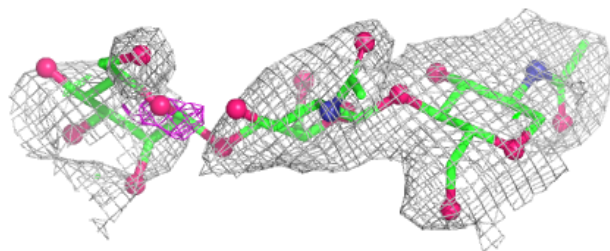
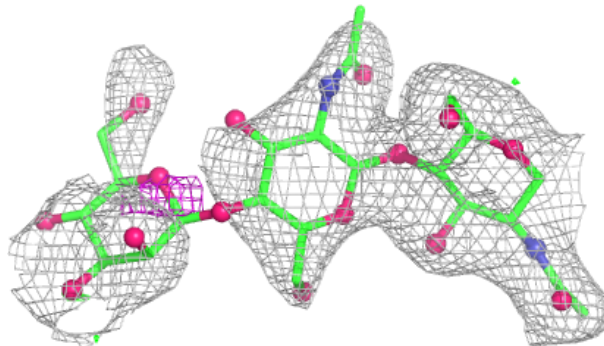


**Electron density around Chain M:**

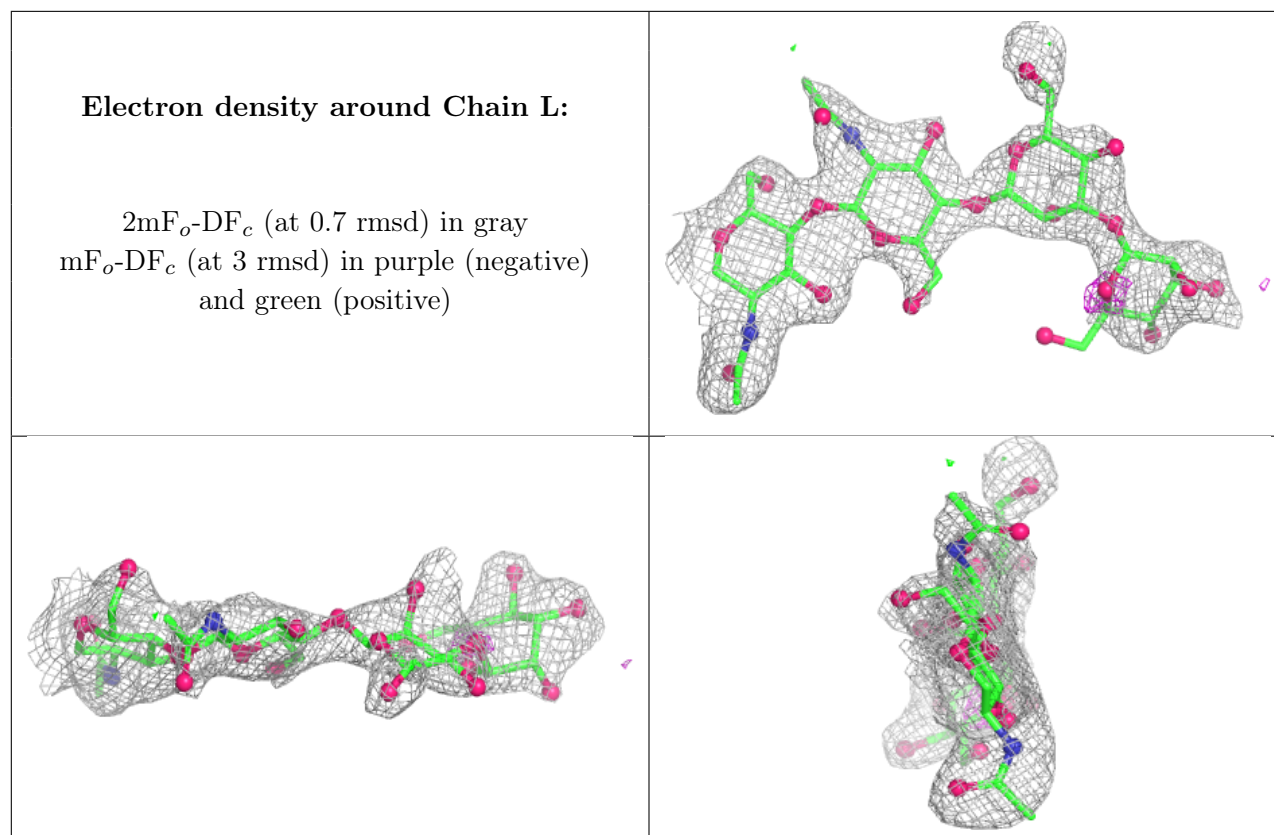
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain I:**

$2mF_o-DF_c$  (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
12	NAG	D	608	14/15	0.49	0.17	75,84,99,101	0
12	NAG	D	607	14/15	0.53	0.17	73,84,94,98	0
12	NAG	B	608	14/15	0.57	0.18	76,91,99,101	0
12	NAG	A	607	14/15	0.59	0.17	75,86,92,94	0
12	NAG	B	609	14/15	0.59	0.16	66,87,93,94	0
12	NAG	C	608	14/15	0.61	0.15	64,72,77,80	0
12	NAG	A	606	14/15	0.66	0.15	58,74,80,82	0
9	MG	D	603	1/1	0.67	0.24	52,52,52,52	0
12	NAG	D	606	14/15	0.67	0.15	76,95,101,101	0
9	MG	C	603	1/1	0.72	0.24	47,47,47,47	0
13	MAN	B	601	11/12	0.72	0.16	56,61,72,76	0
7	POP	D	601	9/9	0.77	0.20	45,58,67,72	9
12	NAG	B	610	14/15	0.78	0.13	51,73,80,90	0
9	MG	B	604	1/1	0.79	0.37	51,51,51,51	0

*Continued on next page...*

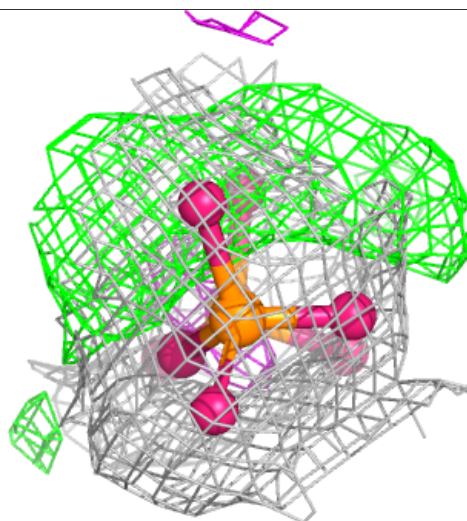
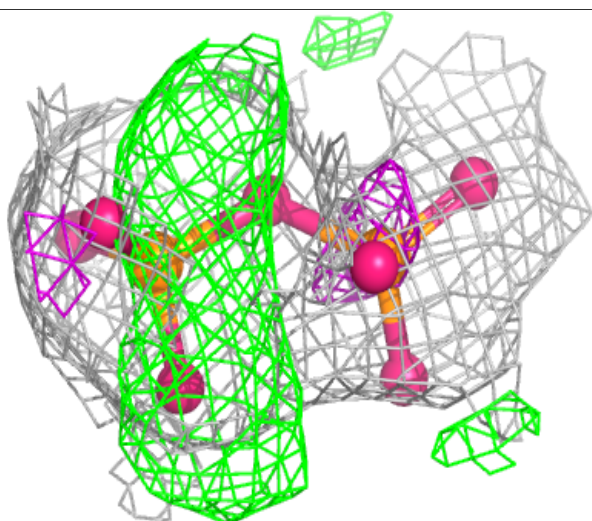
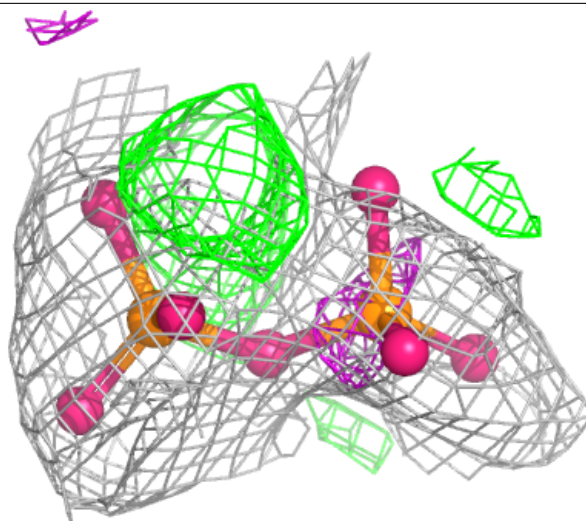
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	POP	B	602	9/9	0.83	0.20	40,50,60,62	9
7	POP	C	601	9/9	0.83	0.18	40,53,72,75	9
15	FLC	C	605	13/13	0.83	0.12	58,63,67,70	0
7	POP	A	601	9/9	0.85	0.16	46,54,59,69	9
14	PO4	C	606	5/5	0.87	0.15	41,45,52,52	5
9	MG	A	603	1/1	0.90	0.25	46,46,46,46	0
14	PO4	B	606	5/5	0.90	0.14	40,44,53,54	5
10	CA	D	604	1/1	0.93	0.13	77,77,77,77	0
11	NA	B	607	1/1	0.94	0.06	32,32,32,32	0
10	CA	C	604	1/1	0.96	0.10	75,75,75,75	0
8	ZN	D	602	1/1	0.96	0.06	49,49,49,49	0
10	CA	A	604	1/1	0.96	0.09	73,73,73,73	0
10	CA	B	605	1/1	0.96	0.07	67,67,67,67	0
11	NA	C	607	1/1	0.97	0.08	33,33,33,33	0
11	NA	A	605	1/1	0.97	0.07	28,28,28,28	0
8	ZN	C	602	1/1	0.98	0.04	44,44,44,44	0
8	ZN	A	602	1/1	0.98	0.04	43,43,43,43	0
11	NA	D	605	1/1	0.99	0.08	30,30,30,30	0
8	ZN	B	603	1/1	0.99	0.03	42,42,42,42	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.

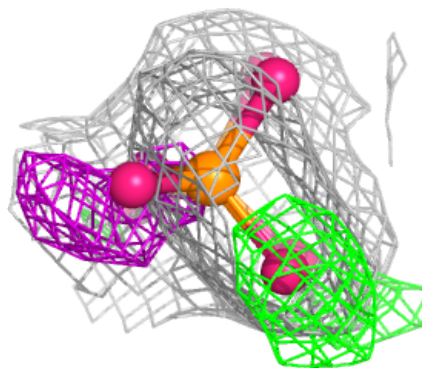
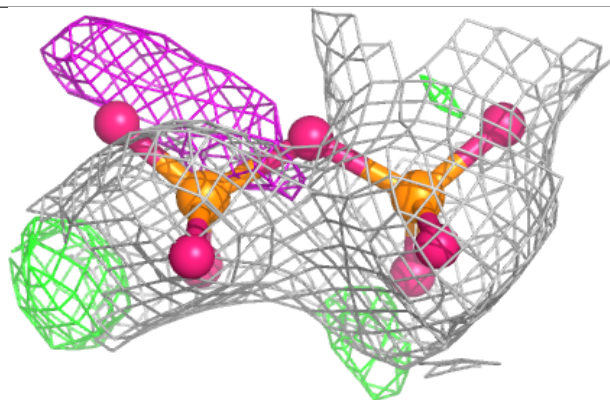
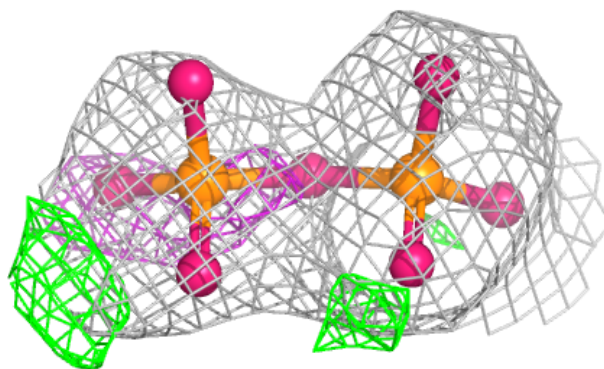
**Electron density around POP D 601:**

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



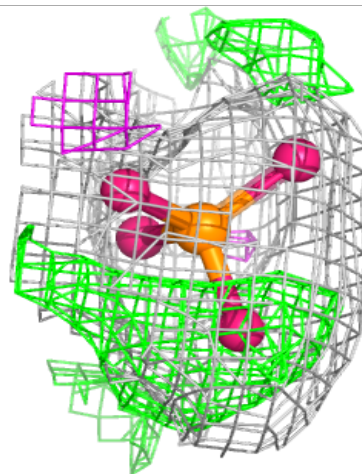
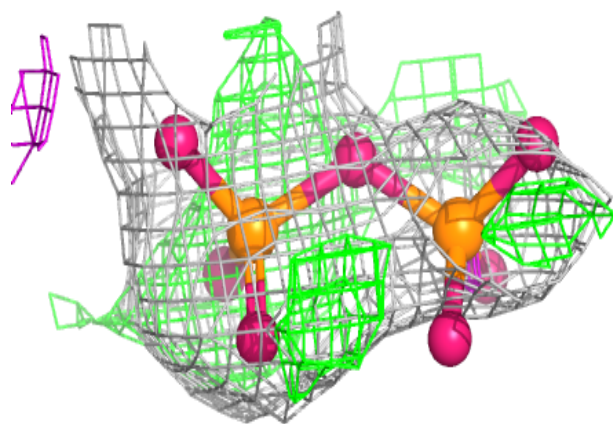
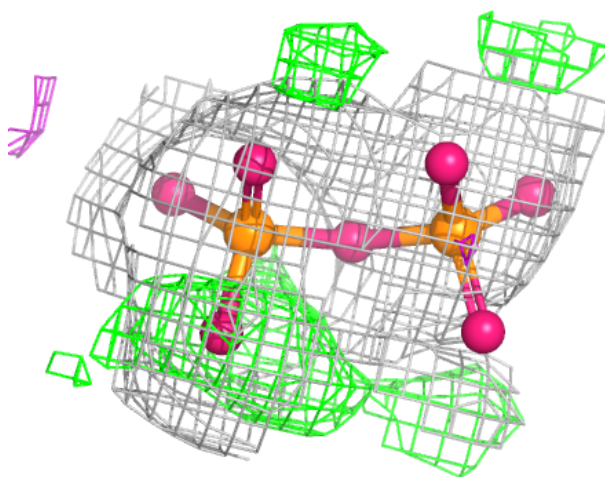
**Electron density around POP B 602:**

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

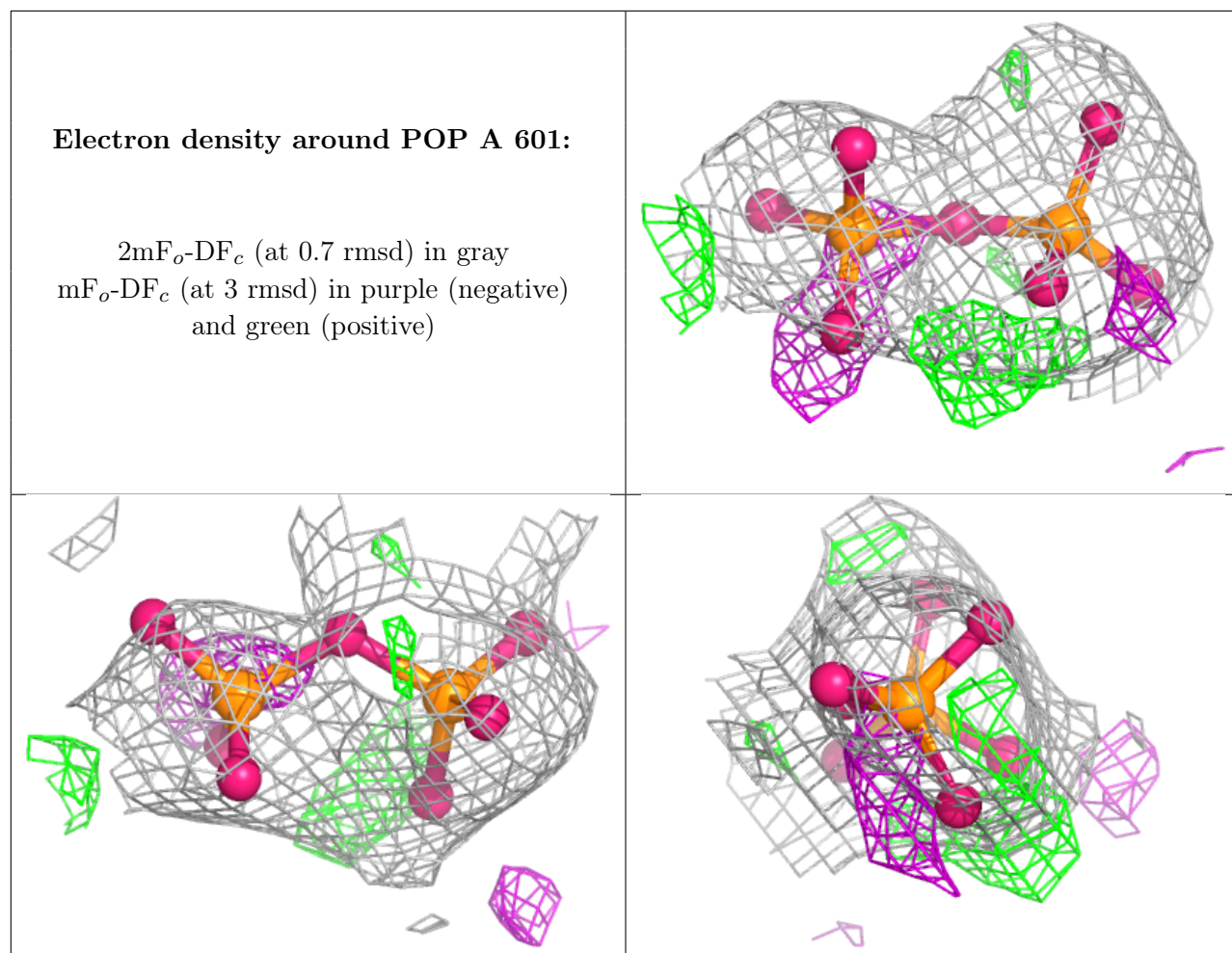


**Electron density around POP C 601:**

$2mF_o-DF_c$  (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.