



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2026 – 10:23 AM EDT

PDB ID : 10TX / pdb_000010tx
Title : Tissue Non-specific Alkaline Phosphatase -S110A bound to PPI
Authors : Krishnan, S.S.; Carroll, B.L.; Guarne, A.
Deposited on : 2026-02-09
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

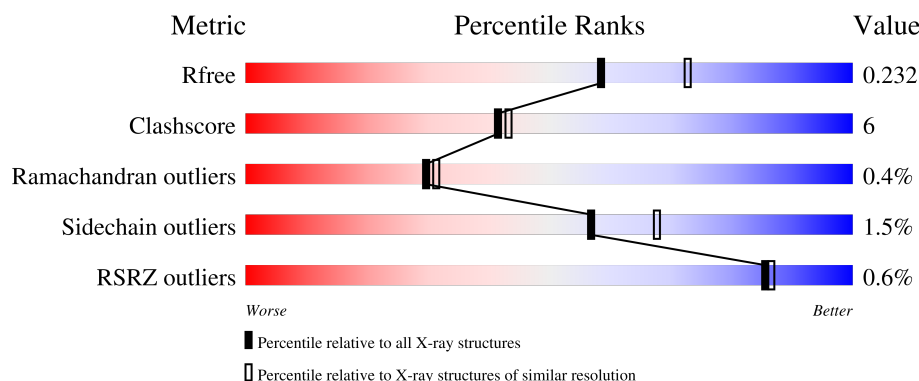
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



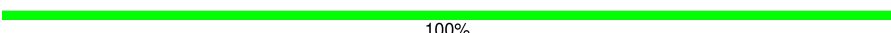

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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 ≥ 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>84%</div> <div>14%</div> <div>.</div> </div>
1	B	493	<div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	C	493	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	D	493	<div> <div>79%</div> <div>18%</div> <div>.</div> </div>
2	E	6	<div> <div>17%</div> <div>83%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	6	 17%50%33%
3	F	3	 67%33%
4	G	2	 100%
4	I	2	 100%
4	J	2	 100%
4	K	2	 100%
4	L	2	 50%50%
4	M	2	 100%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 16274 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	480	Total	C	N	O	S	0	3	0
			3729	2331	662	716	20			
1	B	479	Total	C	N	O	S	0	2	0
			3728	2329	664	715	20			
1	C	480	Total	C	N	O	S	0	1	0
			3723	2326	665	712	20			
1	D	480	Total	C	N	O	S	0	2	0
			3729	2330	665	714	20			

There are 36 discrepancies between the modelled and reference sequences:

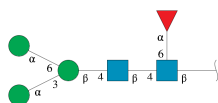
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ASP	-	expression tag	UNP P09242
A	16	GLY	-	expression tag	UNP P09242
A	110	ALA	SER	engineered mutation	UNP P09242
A	502	HIS	-	expression tag	UNP P09242
A	503	HIS	-	expression tag	UNP P09242
A	504	HIS	-	expression tag	UNP P09242
A	505	HIS	-	expression 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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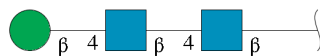
Chain	Residue	Modelled	Actual	Comment	Reference
C	502	HIS	-	expression tag	UNP P09242
C	503	HIS	-	expression tag	UNP P09242
C	504	HIS	-	expression tag	UNP P09242
C	505	HIS	-	expression tag	UNP P09242
C	506	HIS	-	expression tag	UNP P09242
C	507	HIS	-	expression tag	UNP P09242
D	15	ASP	-	expression tag	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)-[alpha-D-mannopyranose-(1-6)]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	6	Total	C	N	O	0	0	0
			71	40	2	29			
2	H	6	Total	C	N	O	0	0	0
			71	40	2	29			

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

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

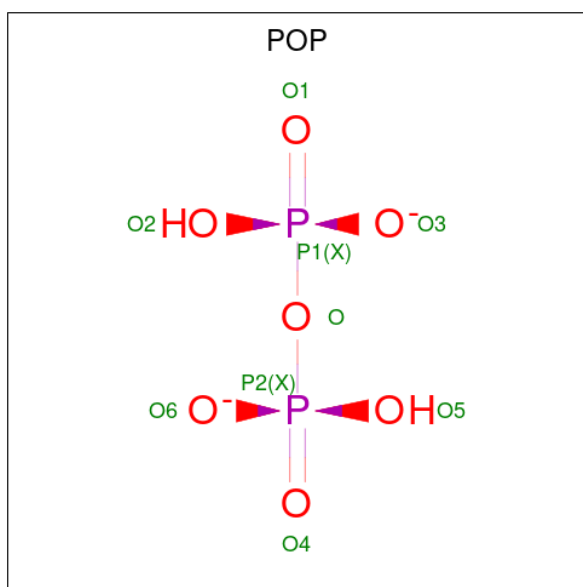


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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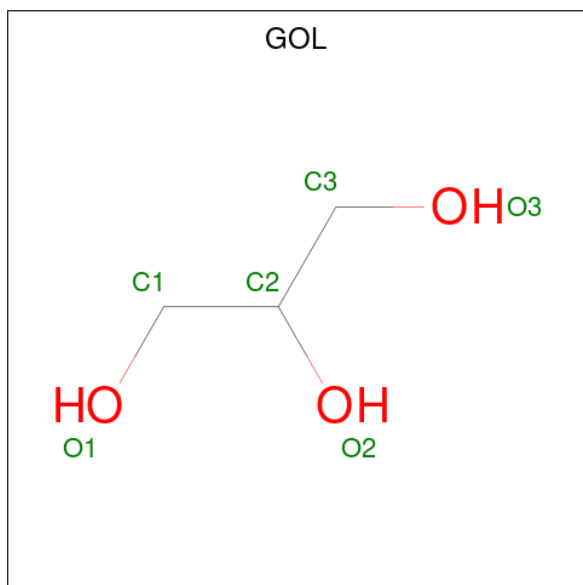
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



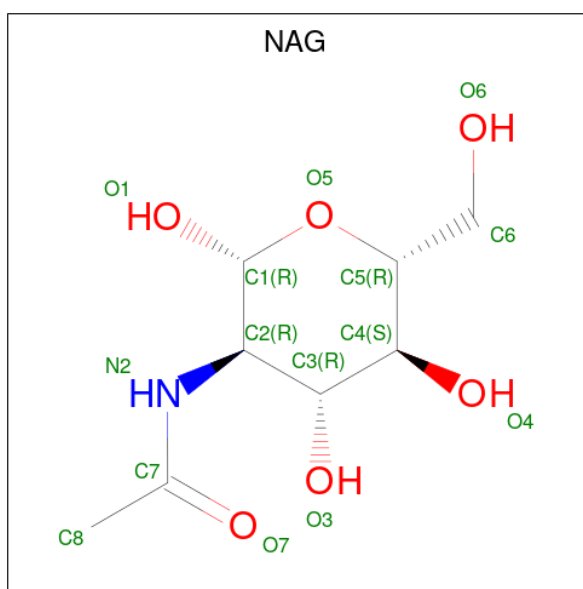
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



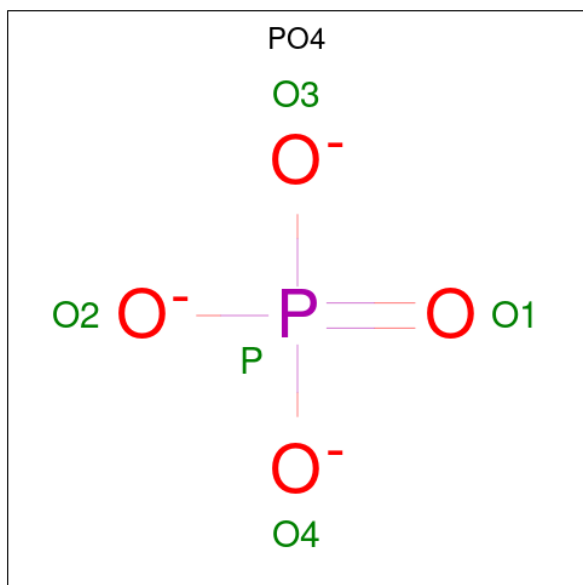
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		

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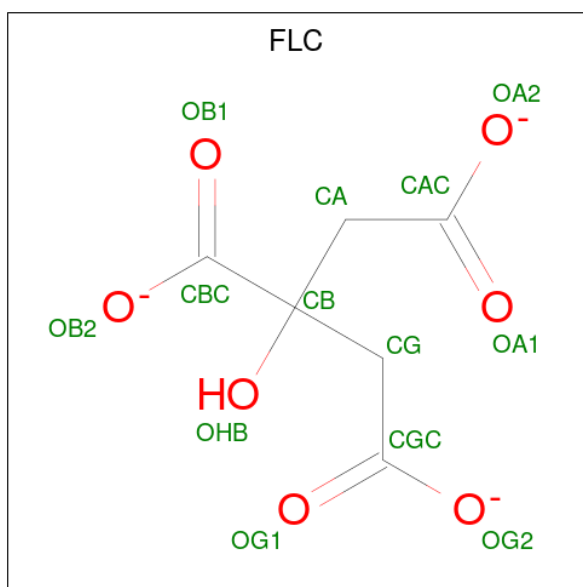
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	C	1	Total	C	N	O	0	0
			14	8	1	5		
11	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

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



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

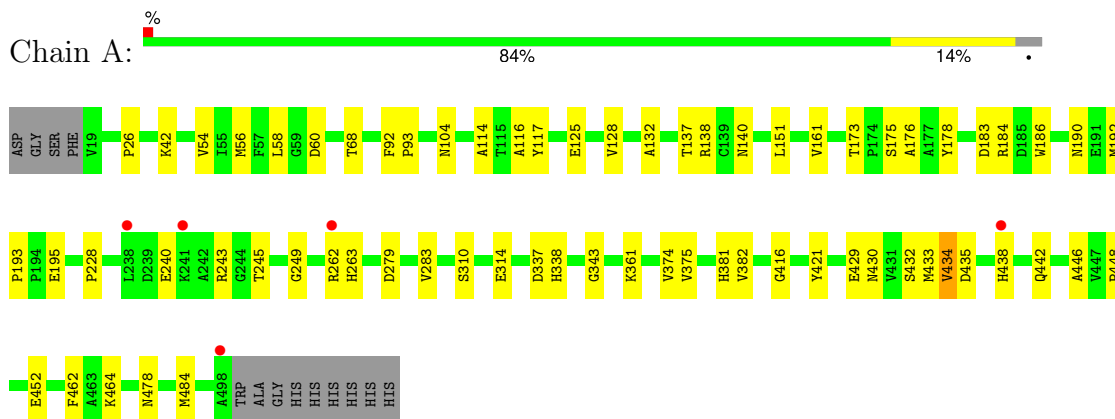
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	222	Total	O	0	0
			222	222		
14	B	183	Total	O	0	0
			183	183		
14	C	203	Total	O	0	0
			203	203		
14	D	189	Total	O	0	0
			189	189		

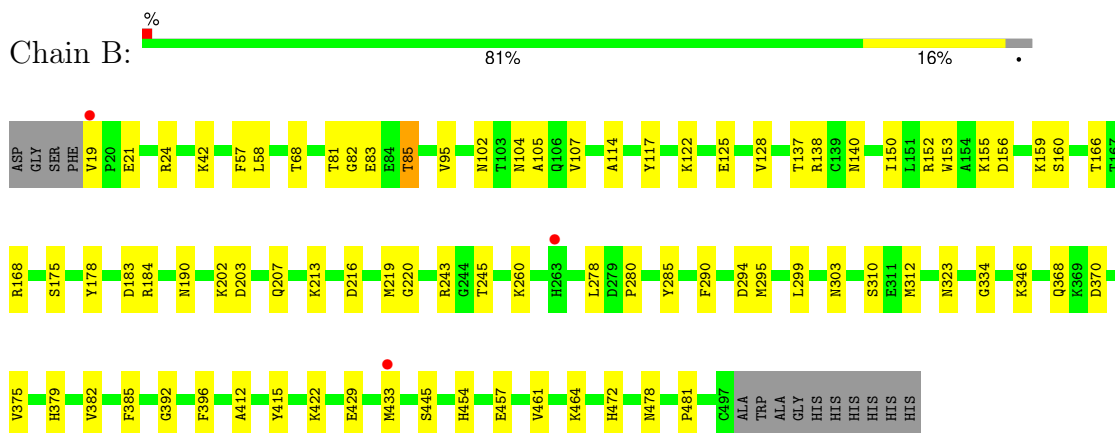
3 Residue-property plots

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

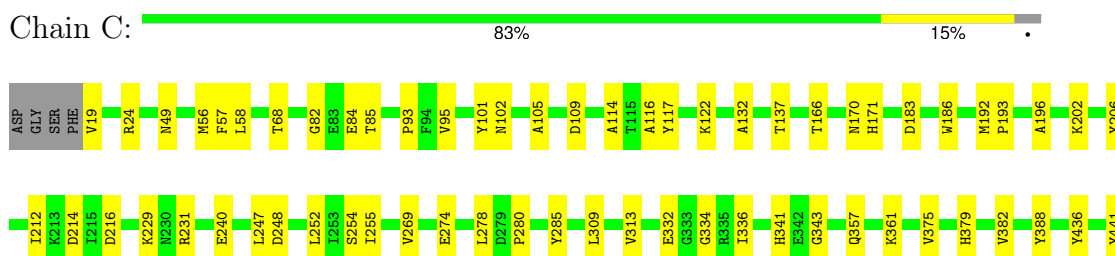
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



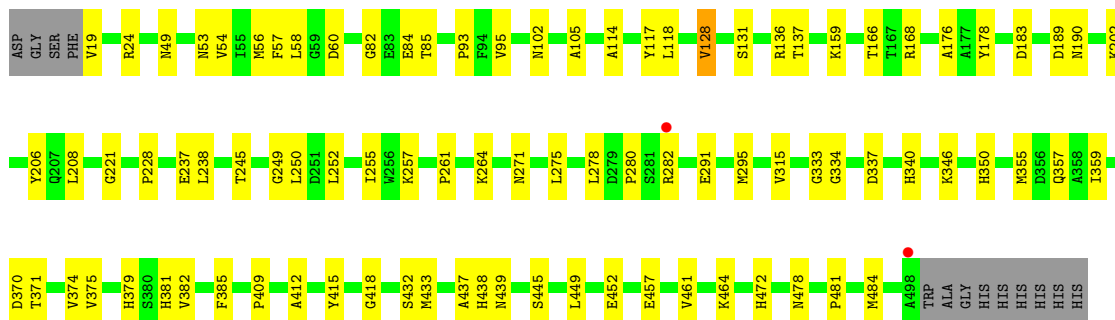
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme





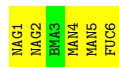
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain D: 79% 18%



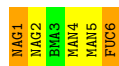
- Molecule 2: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 17% 83%



- Molecule 2: 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-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 17% 50% 33%



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

Chain F: 67% 33%



- 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 I:  100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  50%  50%



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

Chain M:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.31Å 118.89Å 346.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.66 – 2.25 39.66 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.66-2.25) 99.9 (39.66-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.190 , 0.232 0.190 , 0.232	Depositor DCC
R_{free} test set	1949 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16274	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POP, FUC, GOL, CA, BMA, NAG, NA, ZN, PO4, MAN, MG, FLC

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	0.33	0/3819	0.54	0/5178
1	B	0.34	0/3815	0.54	0/5171
1	C	0.34	0/3807	0.54	0/5161
1	D	0.33	0/3816	0.52	0/5173
All	All	0.34	0/15257	0.53	0/20683

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	3729	0	3616	47	0
1	B	3728	0	3620	54	0
1	C	3723	0	3617	43	0
1	D	3729	0	3623	57	0
2	E	71	0	61	3	0
2	H	71	0	61	3	0
3	F	39	0	34	0	0
4	G	28	0	25	1	0
4	I	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	1	0
4	M	28	0	25	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	9	0	0	2	0
6	B	9	0	0	0	0
6	C	9	0	0	0	0
6	D	9	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	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	18	0	24	1	0
10	B	12	0	16	2	0
10	C	18	0	24	1	0
10	D	12	0	16	2	0
11	A	28	0	26	0	0
11	B	28	0	26	0	0
11	C	14	0	13	0	0
11	D	14	0	13	0	0
12	B	5	0	0	0	0
12	C	5	0	0	0	0
13	D	13	0	5	0	0
14	A	222	0	0	3	0
14	B	183	0	0	8	0
14	C	203	0	0	5	0
14	D	189	0	0	6	0
All	All	16274	0	14945	196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (196) 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:B:166:THR:HA	1:B:295:MET:HE3	1.45	0.98
1:B:219:MET:HB3	1:B:312:MET:HE2	1.55	0.89
1:A:240:GLU:HA	1:A:243:ARG:HD3	1.73	0.71
1:C:56:MET:HB2	1:C:484:MET:HE1	1.74	0.69
1:A:184:ARG:NH2	6:A:602:POP:O3	2.26	0.68
1:A:314:GLU:HG2	1:A:361:LYS:HG2	1.75	0.68
1:C:171:HIS:ND1	14:C:705:HOH:O	2.29	0.65
1:D:56:MET:HB2	1:D:484:MET:HE1	1.79	0.64
1:D:409:PRO:HG2	1:D:432:SER:HB3	1.80	0.63
1:B:24:ARG:HA	1:C:132:ALA:HB3	1.80	0.63
1:B:220:GLY:HA2	1:B:295:MET:HE2	1.80	0.63
1:A:137:THR:HG22	1:A:183:ASP:OD2	2.00	0.62
1:D:252:LEU:HD23	1:D:255:ILE:HD12	1.80	0.61
1:B:137:THR:HG22	1:B:183:ASP:OD2	2.01	0.60
1:B:138:ARG:HG2	2:H:6:FUC:H4	1.84	0.60
1:D:189:ASP:HB3	10:D:607:GOL:H32	1.83	0.60
1:D:137:THR:HG22	1:D:183:ASP:OD2	2.02	0.60
1:B:82:GLY:O	1:B:85:THR:HB	2.03	0.59
1:C:269:VAL:HG12	1:C:274:GLU:HG3	1.85	0.59
1:B:422:LYS:HD3	1:B:429:GLU:OE1	2.03	0.58
1:C:137:THR:HG22	1:C:183:ASP:OD2	2.03	0.58
1:B:290:PHE:CE2	1:B:312:MET:HE3	2.38	0.58
1:B:57:PHE:HB2	1:B:375:VAL:HG22	1.87	0.57
1:B:422:LYS:NZ	14:B:706:HOH:O	2.39	0.56
1:C:252:LEU:HD23	1:C:255:ILE:HD12	1.88	0.56
1:D:136:ARG:HG2	1:D:137:THR:HG23	1.88	0.55
1:A:184:ARG:NH1	6:A:602:POP:O2	2.37	0.54
1:B:295:MET:HE1	1:B:312:MET:HE1	1.89	0.54
1:B:168:ARG:HD3	1:B:294:ASP:OD1	2.08	0.54
1:A:138:ARG:HH11	2:E:6:FUC:H5	1.73	0.54
1:A:262:ARG:HH21	1:A:263:HIS:CE1	2.25	0.54
1:D:291:GLU:HG3	1:D:295:MET:HA	1.91	0.54
1:A:132:ALA:HB3	1:D:24:ARG:HA	1.88	0.53
1:D:228:PRO:HB3	1:D:249:GLY:HA2	1.90	0.53
1:D:118:LEU:HD12	1:D:176:ALA:HB3	1.89	0.53
1:A:279:ASP:O	1:A:283:VAL:HG23	2.08	0.53
1:A:421:TYR:HB3	1:A:448:PRO:HB3	1.90	0.53
1:B:202:LYS:HA	1:B:202:LYS:HE2	1.91	0.53
1:B:290:PHE:HE2	1:B:312:MET:HE3	1.73	0.53
1:D:93:PRO:HD2	1:D:464:LYS:HB3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PHE:CZ	1:A:464:LYS:HE2	2.44	0.52
1:D:264:LYS:NZ	14:D:703:HOH:O	2.34	0.52
1:A:310:SER:O	1:A:314:GLU:HG3	2.10	0.52
1:C:102:ASN:HB2	1:C:105:ALA:HB3	1.91	0.52
1:C:212:ILE:C	1:C:214:ASP:H	2.17	0.52
1:D:202:LYS:HG2	1:D:206:TYR:CE1	2.44	0.51
1:A:375:VAL:HB	1:A:462:PHE:HB2	1.92	0.51
1:B:203:ASP:O	1:B:207:GLN:HG3	2.11	0.51
1:D:278:LEU:O	1:D:280:PRO:HD3	2.11	0.51
1:A:138:ARG:NH1	2:E:6:FUC:H5	2.25	0.51
1:C:122:LYS:HE2	14:C:777:HOH:O	2.11	0.51
1:B:175:SER:HA	1:B:178:TYR:CE2	2.46	0.51
1:B:202:LYS:NZ	14:B:708:HOH:O	2.43	0.50
1:A:228:PRO:HB3	1:A:249:GLY:HA2	1.93	0.50
1:A:56:MET:HB2	1:A:484:MET:HE1	1.94	0.49
1:A:104:ASN:HB3	1:D:19:VAL:HG22	1.95	0.49
1:B:213:LYS:NZ	14:B:711:HOH:O	2.46	0.49
1:B:260:LYS:HD2	1:B:285:TYR:CD2	2.48	0.49
1:D:337:ASP:OD1	1:D:381:HIS:NE2	2.45	0.49
1:B:95:VAL:HA	1:B:461:VAL:O	2.13	0.49
1:D:53:ASN:HB2	1:D:371:THR:HG23	1.93	0.49
1:D:350:HIS:HE1	14:D:869:HOH:O	1.95	0.49
1:B:114:ALA:HA	1:B:117:TYR:CZ	2.48	0.49
1:C:166:THR:OG1	1:C:334:GLY:HA2	2.13	0.49
1:D:166:THR:OG1	1:D:334:GLY:HA2	2.13	0.48
1:A:314:GLU:CG	1:A:361:LYS:HG2	2.41	0.48
1:D:57:PHE:HB2	1:D:375:VAL:HG22	1.96	0.48
1:A:93:PRO:HD2	1:A:464:LYS:HB3	1.96	0.48
1:A:175:SER:HA	1:A:178:TYR:CE2	2.49	0.48
1:A:430:ASN:ND2	1:A:433:MET:HE3	2.28	0.48
1:B:68:THR:HG21	1:C:457:GLU:HA	1.94	0.48
1:B:278:LEU:O	1:B:280:PRO:HD3	2.13	0.48
1:B:368:GLN:NE2	1:B:464:LYS:HD2	2.29	0.48
1:C:57:PHE:HB2	1:C:375:VAL:HG22	1.96	0.48
10:B:607:GOL:O1	14:B:701:HOH:O	2.20	0.47
1:B:457:GLU:HA	1:C:68:THR:HG21	1.96	0.47
1:D:54:VAL:CG1	1:D:484:MET:HE2	2.44	0.47
2:H:1:NAG:H83	2:H:1:NAG:H3	1.97	0.47
1:A:374:VAL:HB	1:A:484:MET:HE3	1.95	0.47
1:D:275:LEU:HD11	1:D:315:VAL:HG21	1.96	0.47
1:B:81:THR:HG22	1:B:392:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:LYS:HD3	1:C:247:LEU:HD23	1.96	0.47
1:C:361:LYS:NZ	14:C:706:HOH:O	2.48	0.47
1:D:168:ARG:HA	1:D:221:GLY:C	2.40	0.47
1:D:54:VAL:HG13	1:D:484:MET:HE2	1.98	0.46
1:C:193:PRO:HD2	1:C:196:ALA:HB3	1.97	0.46
1:B:21:GLU:O	1:B:24:ARG:HG3	2.15	0.46
1:C:248:ASP:OD2	10:C:609:GOL:O3	2.33	0.46
1:D:261:PRO:HB2	1:D:264:LYS:HG2	1.95	0.46
1:B:260:LYS:HD2	1:B:285:TYR:CG	2.51	0.46
1:D:337:ASP:OD1	1:D:379:HIS:HE1	1.99	0.46
1:D:359:ILE:HD13	1:D:375:VAL:HG21	1.98	0.46
1:D:19:VAL:N	14:D:711:HOH:O	2.49	0.46
1:A:125[B]:GLU:OE1	14:A:701:HOH:O	2.20	0.46
1:A:26:PRO:HG3	1:D:131:SER:HB3	1.98	0.46
1:A:54:VAL:HG13	1:A:484:MET:HE2	1.98	0.46
1:B:138:ARG:HE	2:H:6:FUC:H62	1.81	0.45
1:C:114:ALA:HA	1:C:117:TYR:CZ	2.51	0.45
1:A:42:LYS:HE2	1:A:42:LYS:HB3	1.73	0.45
1:A:54:VAL:CG1	1:A:484:MET:HE2	2.46	0.45
1:B:42:LYS:HB2	1:B:42:LYS:HE3	1.56	0.45
1:D:84:GLU:H	1:D:84:GLU:CD	2.24	0.45
1:D:159:LYS:NZ	14:D:709:HOH:O	2.48	0.45
1:D:114:ALA:HA	1:D:117:TYR:CZ	2.52	0.45
1:D:478:ASN:O	1:D:481:PRO:HD2	2.16	0.45
1:A:138:ARG:HG2	2:E:6:FUC:H4	1.99	0.45
1:C:278:LEU:O	1:C:280:PRO:HD3	2.17	0.45
1:D:370:ASP:OD1	10:D:606:GOL:O3	2.33	0.45
1:A:190:ASN:HB2	1:A:245:THR:O	2.17	0.45
1:C:467:MET:HE3	1:C:470:LEU:HD11	1.99	0.45
1:B:83:GLU:HB3	1:C:101:TYR:CD1	2.52	0.45
1:D:472:HIS:HA	14:D:725:HOH:O	2.17	0.44
1:B:370:ASP:OD1	10:B:607:GOL:O3	2.35	0.44
1:C:93:PRO:HD2	1:C:464:LYS:HB3	1.99	0.44
1:C:343:GLY:O	1:C:442:GLN:HA	2.17	0.44
1:D:346:LYS:HD3	1:D:439:ASN:HA	1.98	0.44
1:C:436:TYR:HA	1:C:441:TYR:CG	2.52	0.44
1:A:114:ALA:HA	1:A:117:TYR:CZ	2.53	0.44
10:A:606:GOL:O1	14:A:702:HOH:O	2.21	0.44
1:B:346:LYS:HA	1:B:396:PHE:CE1	2.52	0.44
1:B:415:TYR:O	1:B:445:SER:HA	2.18	0.44
1:B:150:ILE:HA	1:B:153:TRP:CE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:PHE:HA	1:D:412:ALA:O	2.18	0.43
1:A:337:ASP:OD1	1:A:381:HIS:NE2	2.51	0.43
1:D:271:ASN:HA	14:D:744:HOH:O	2.19	0.43
1:B:122:LYS:HE2	14:B:787:HOH:O	2.17	0.43
1:C:82:GLY:O	1:C:85:THR:HB	2.19	0.43
1:C:231:ARG:NH2	14:C:721:HOH:O	2.51	0.43
1:A:128:VAL:HG13	1:A:176:ALA:HA	2.01	0.43
1:B:472:HIS:NE2	14:B:704:HOH:O	2.37	0.43
1:D:128:VAL:HG23	1:D:176:ALA:HA	2.01	0.43
1:B:379:HIS:CE1	1:B:454:HIS:CD2	3.07	0.43
1:C:309:LEU:O	1:C:313:VAL:HG23	2.18	0.43
1:B:107:VAL:HB	1:C:388:TYR:HA	2.00	0.42
1:C:341:HIS:ND1	1:C:452:GLU:O	2.46	0.42
1:C:84:GLU:H	1:C:84:GLU:CD	2.27	0.42
1:A:429:GLU:OE2	1:A:434:VAL:HG21	2.19	0.42
1:C:170:ASN:OD1	1:C:170:ASN:N	2.52	0.42
1:A:435:ASP:HB3	1:A:438:HIS:ND1	2.35	0.42
1:B:166:THR:OG1	1:B:334:GLY:HA2	2.20	0.42
1:C:202:LYS:HD2	1:C:206:TYR:CE1	2.55	0.42
1:C:216:ASP:HA	1:C:285:TYR:CD1	2.54	0.42
1:B:102:ASN:HB2	1:B:105:ALA:HB3	2.02	0.42
1:C:19:VAL:HB	1:C:24:ARG:NH2	2.34	0.42
1:D:95:VAL:HA	1:D:461:VAL:O	2.19	0.42
1:D:190:ASN:HB2	1:D:245:THR:O	2.20	0.42
1:B:114:ALA:HA	1:B:117:TYR:CE2	2.54	0.42
1:B:160:SER:OG	1:B:323:ASN:HB2	2.19	0.42
1:D:102:ASN:HB2	1:D:105:ALA:HB3	2.01	0.42
1:D:250:LEU:HD23	1:D:250:LEU:HA	1.83	0.42
1:A:186:TRP:CG	1:A:192:MET:HG2	2.54	0.42
1:A:381:HIS:HB3	1:A:452:GLU:OE2	2.19	0.42
1:B:104:ASN:HB3	1:C:19:VAL:HG22	2.02	0.42
1:D:257:LYS:HE2	1:D:257:LYS:HB2	1.74	0.42
1:A:416:GLY:O	1:A:446:ALA:HB3	2.20	0.41
1:A:338:HIS:HE1	14:A:826:HOH:O	2.03	0.41
1:B:155:LYS:NZ	1:B:216:ASP:OD2	2.46	0.41
4:G:1:NAG:H61	4:G:2:NAG:C7	2.51	0.41
1:A:116:ALA:O	1:A:478:ASN:HA	2.20	0.41
1:B:385:PHE:HA	1:B:412:ALA:O	2.19	0.41
1:B:478:ASN:O	1:B:481:PRO:HD2	2.19	0.41
1:A:193:PRO:HB2	1:A:195:GLU:OE1	2.20	0.41
1:B:190:ASN:HB2	1:B:245:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:HIS:O	1:D:452:GLU:HB3	2.21	0.41
1:B:159:LYS:NZ	14:B:716:HOH:O	2.51	0.41
1:D:178:TYR:CE2	1:D:208:LEU:HD13	2.55	0.41
1:D:346:LYS:NZ	1:D:437:ALA:O	2.43	0.41
1:D:374:VAL:HB	1:D:484:MET:HE3	2.02	0.41
1:D:381:HIS:HB3	1:D:452:GLU:OE2	2.19	0.41
1:B:152:ARG:HD2	1:B:156:ASP:OD2	2.21	0.41
1:C:186:TRP:CE3	1:C:192:MET:HE3	2.55	0.41
4:L:1:NAG:H61	4:L:2:NAG:C7	2.51	0.41
1:A:314:GLU:HG2	1:A:361:LYS:CG	2.47	0.41
1:A:343:GLY:O	1:A:442:GLN:HA	2.20	0.41
1:A:151:LEU:HG	1:A:161:VAL:HB	2.02	0.41
1:B:303:ASN:ND2	14:B:720:HOH:O	2.53	0.41
1:A:68:THR:HG21	1:D:457:GLU:HA	2.03	0.41
1:C:216:ASP:HA	1:C:285:TYR:HD1	1.86	0.41
1:D:82:GLY:O	1:D:85:THR:HB	2.20	0.41
1:D:418:GLY:HA2	1:D:449:LEU:HB2	2.01	0.41
1:C:95:VAL:HA	1:C:461:VAL:O	2.20	0.40
1:D:333:GLY:HA3	1:D:355:MET:SD	2.61	0.40
1:D:202:LYS:HG2	1:D:206:TYR:CD1	2.55	0.40
1:D:237:GLU:HG3	1:D:238:LEU:HG	2.02	0.40
1:A:60[A]:ASP:OD2	1:A:173:THR:OG1	2.36	0.40
1:B:117:TYR:HA	1:B:481:PRO:HD3	2.03	0.40
1:B:299:LEU:HA	1:B:299:LEU:HD23	1.90	0.40
1:C:357:GLN:NE2	14:C:726:HOH:O	2.54	0.40
1:C:379:HIS:CE1	1:C:454:HIS:CD2	3.09	0.40
1:C:116:ALA:O	1:C:478:ASN:HA	2.22	0.40
1:A:435:ASP:HB3	1:A:438:HIS:CE1	2.57	0.40
1:C:114:ALA:HA	1:C:117:TYR:CE2	2.57	0.40
1:D:415:TYR:O	1:D:445:SER:HA	2.21	0.40

There are no symmetry-related clashes.

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	481/493 (98%)	470 (98%)	9 (2%)	2 (0%)	30	31
1	B	479/493 (97%)	461 (96%)	16 (3%)	2 (0%)	30	31
1	C	479/493 (97%)	461 (96%)	16 (3%)	2 (0%)	30	31
1	D	480/493 (97%)	467 (97%)	11 (2%)	2 (0%)	30	31
All	All	1919/1972 (97%)	1859 (97%)	52 (3%)	8 (0%)	30	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	49	ASN
1	A	140	ASN
1	C	49	ASN
1	B	140	ASN
1	A	382	VAL
1	D	382	VAL
1	B	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	395/405 (98%)	392 (99%)	3 (1%)	73	80
1	B	396/405 (98%)	387 (98%)	9 (2%)	44	55
1	C	394/405 (97%)	389 (99%)	5 (1%)	61	72
1	D	395/405 (98%)	389 (98%)	6 (2%)	57	68
All	All	1580/1620 (98%)	1557 (98%)	23 (2%)	57	68

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	432	SER
1	A	434	VAL
1	B	19	VAL
1	B	58	LEU
1	B	85	THR
1	B	125	GLU
1	B	128	VAL
1	B	184	ARG
1	B	243	ARG
1	B	310	SER
1	B	433	MET
1	C	58	LEU
1	C	109	ASP
1	C	240	GLU
1	C	254	SER
1	C	332	GLU
1	D	58	LEU
1	D	128	VAL
1	D	282	ARG
1	D	357	GLN
1	D	433	MET
1	D	438	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	263	HIS
1	A	267	HIS
1	A	451	HIS
1	B	53	ASN
1	B	368	GLN
1	C	323	ASN
1	C	338	HIS
1	D	39	ASN
1	D	267	HIS
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 ⓘ

27 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	1.23	1 (7%)	17,19,21	1.22	1 (5%)
2	NAG	E	2	2	14,14,15	0.60	1 (7%)	17,19,21	0.60	0
2	BMA	E	3	2	11,11,12	0.69	0	15,15,17	0.48	0
2	MAN	E	4	2	11,11,12	0.98	0	15,15,17	1.23	1 (6%)
2	MAN	E	5	2	11,11,12	0.93	1 (9%)	15,15,17	1.01	2 (13%)
2	FUC	E	6	2	10,10,11	0.91	0	14,14,16	0.68	0
3	NAG	F	1	1,3	14,14,15	0.51	0	17,19,21	0.65	0
3	NAG	F	2	3	14,14,15	0.28	0	17,19,21	0.35	0
3	BMA	F	3	3	11,11,12	0.95	1 (9%)	15,15,17	0.83	0
4	NAG	G	1	4,1	14,14,15	0.23	0	17,19,21	0.75	0
4	NAG	G	2	4	14,14,15	0.29	0	17,19,21	0.56	0
2	NAG	H	1	1,2	14,14,15	1.46	1 (7%)	17,19,21	1.93	3 (17%)
2	NAG	H	2	2	14,14,15	0.82	1 (7%)	17,19,21	0.71	1 (5%)
2	BMA	H	3	2	11,11,12	0.72	0	15,15,17	0.61	0
2	MAN	H	4	2	11,11,12	0.81	0	15,15,17	1.21	2 (13%)
2	MAN	H	5	2	11,11,12	1.12	1 (9%)	15,15,17	1.24	2 (13%)
2	FUC	H	6	2	10,10,11	1.26	1 (10%)	14,14,16	0.89	1 (7%)
4	NAG	I	1	4,1	14,14,15	0.35	0	17,19,21	0.43	0
4	NAG	I	2	4	14,14,15	0.62	0	17,19,21	0.60	0
4	NAG	J	1	4,1	14,14,15	0.57	0	17,19,21	0.63	0
4	NAG	J	2	4	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	K	1	4,1	14,14,15	0.45	0	17,19,21	0.60	0
4	NAG	K	2	4	14,14,15	0.57	0	17,19,21	0.45	0
4	NAG	L	1	4,1	14,14,15	0.52	0	17,19,21	0.51	0
4	NAG	L	2	4	14,14,15	0.36	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	M	1	4,1	14,14,15	0.64	0	17,19,21	0.65	0
4	NAG	M	2	4	14,14,15	0.59	0	17,19,21	0.58	0

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

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NAG	O5-C1	-5.18	1.35	1.43
2	E	1	NAG	O5-C1	-4.10	1.36	1.43
2	H	2	NAG	O5-C1	-3.03	1.38	1.43
2	H	6	FUC	C1-C2	2.48	1.58	1.52
3	F	3	BMA	C1-C2	2.32	1.57	1.52
2	H	5	MAN	C2-C3	2.20	1.55	1.52
2	E	2	NAG	O5-C1	-2.16	1.40	1.43
2	E	5	MAN	O5-C5	2.00	1.47	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	NAG	C2-N2-C7	5.11	129.75	122.90
2	H	1	NAG	C1-C2-N2	3.76	116.36	110.43
2	E	1	NAG	C1-O5-C5	-3.59	107.37	112.19
2	E	4	MAN	C1-O5-C5	3.42	116.77	112.19
2	H	4	MAN	C1-O5-C5	3.25	116.54	112.19
2	H	1	NAG	C1-O5-C5	-3.07	108.07	112.19
2	H	5	MAN	C1-O5-C5	3.01	116.21	112.19
2	E	5	MAN	O2-C2-C3	-2.48	105.02	110.15
2	H	6	FUC	O2-C2-C1	2.47	114.87	109.22
2	E	5	MAN	C1-O5-C5	2.40	115.40	112.19
4	L	2	NAG	C1-O5-C5	2.36	115.34	112.19
2	H	2	NAG	C1-O5-C5	2.23	115.18	112.19
2	H	5	MAN	O2-C2-C3	-2.06	105.88	110.15
2	H	4	MAN	O2-C2-C3	-2.05	105.90	110.15

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

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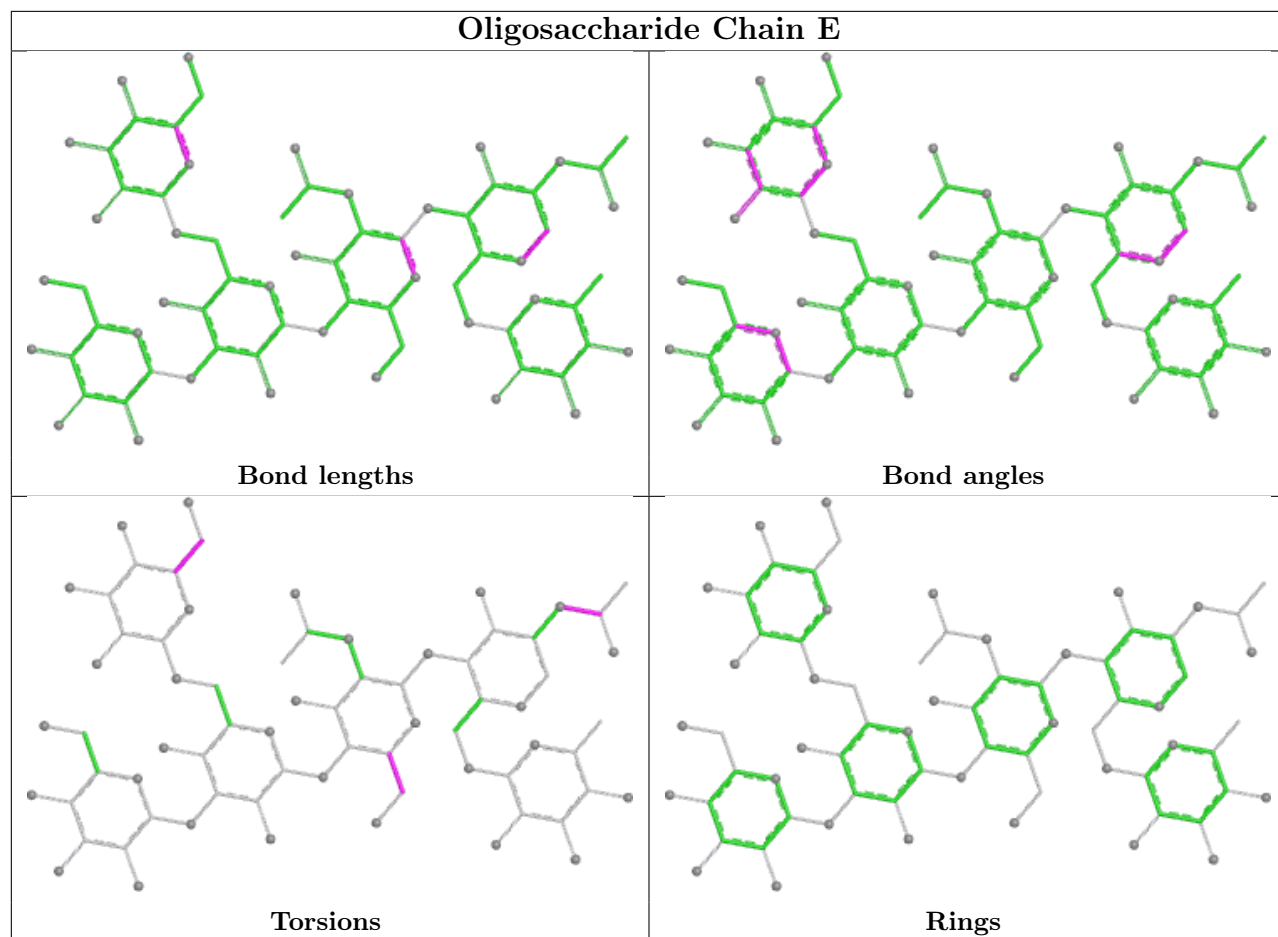
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	E	2	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
2	E	5	MAN	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
4	J	2	NAG	C1-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7
4	J	1	NAG	C4-C5-C6-O6
2	E	5	MAN	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6

There are no ring outliers.

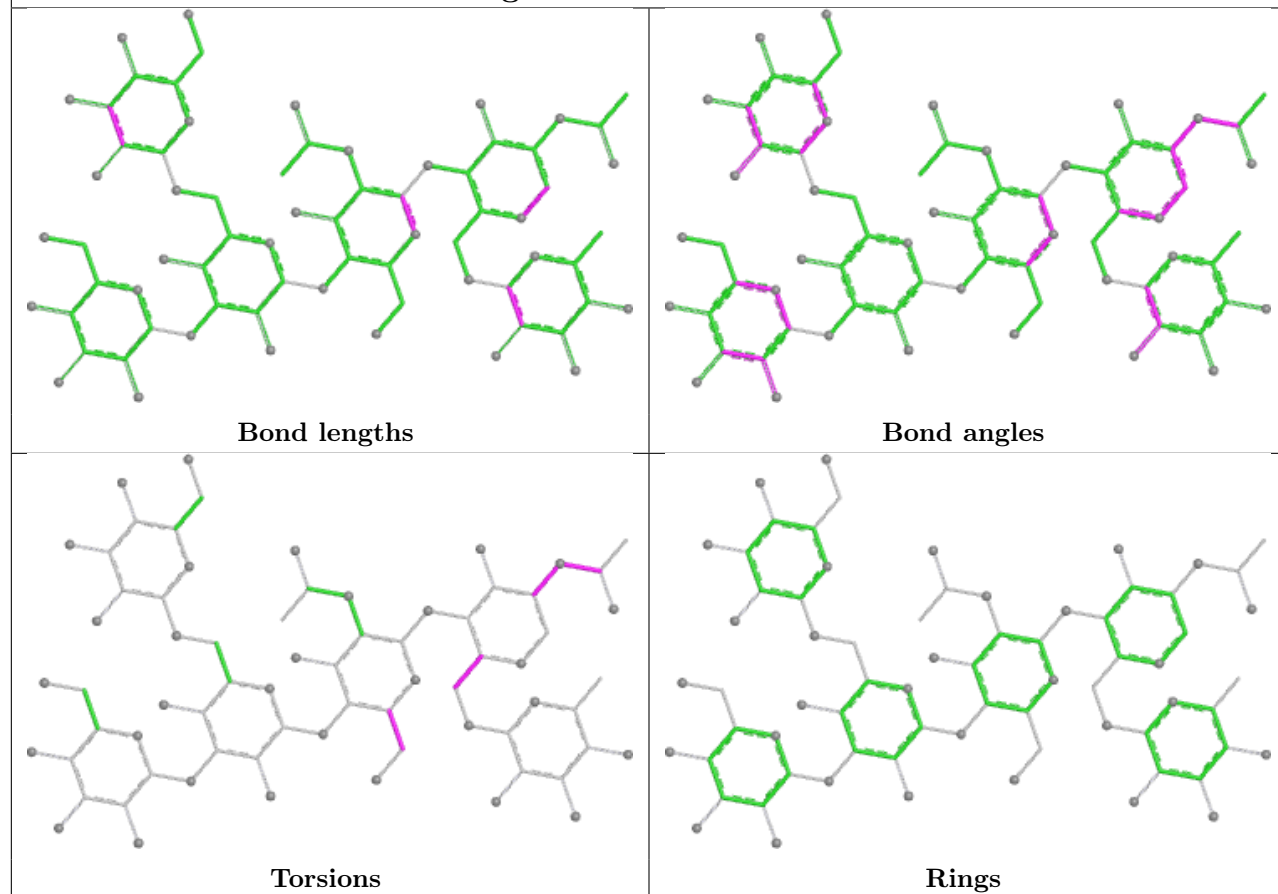
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
4	L	2	NAG	1	0
4	G	1	NAG	1	0
4	G	2	NAG	1	0
2	E	6	FUC	3	0
2	H	6	FUC	2	0
4	L	1	NAG	1	0

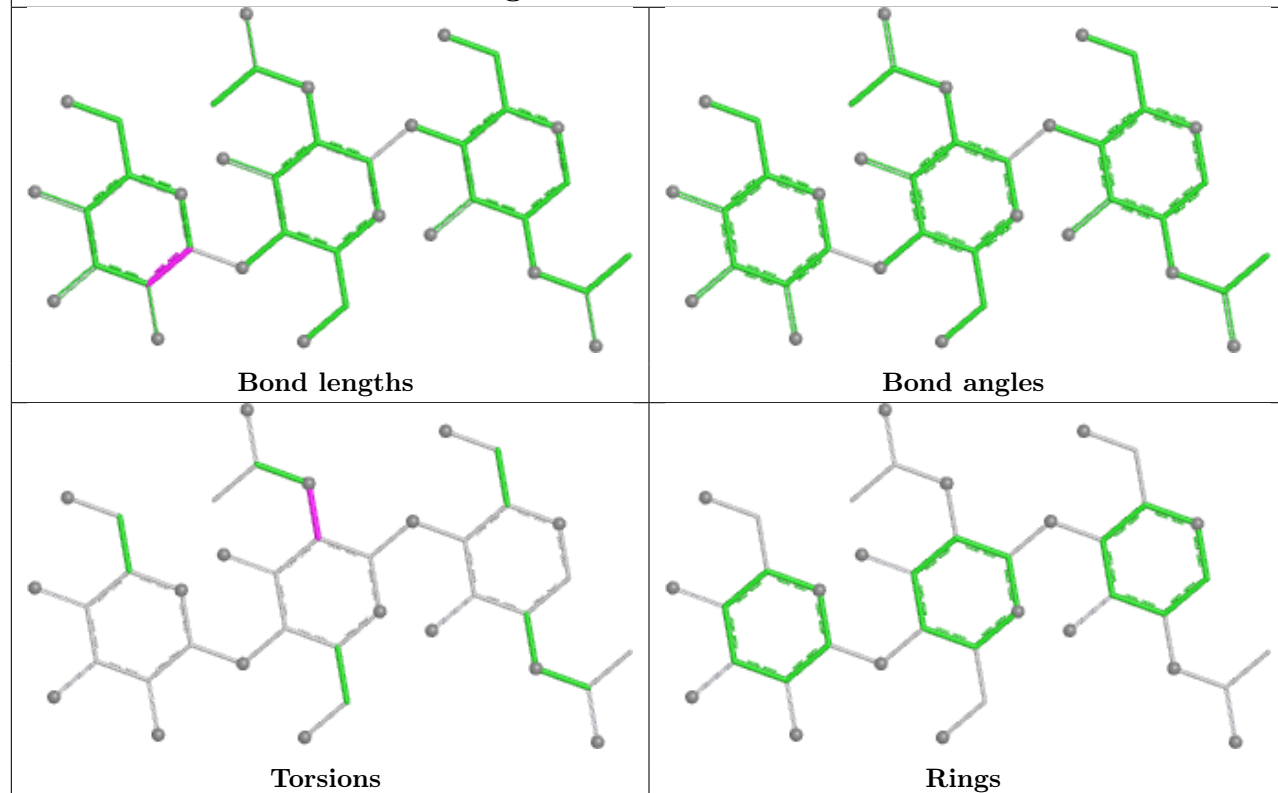
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

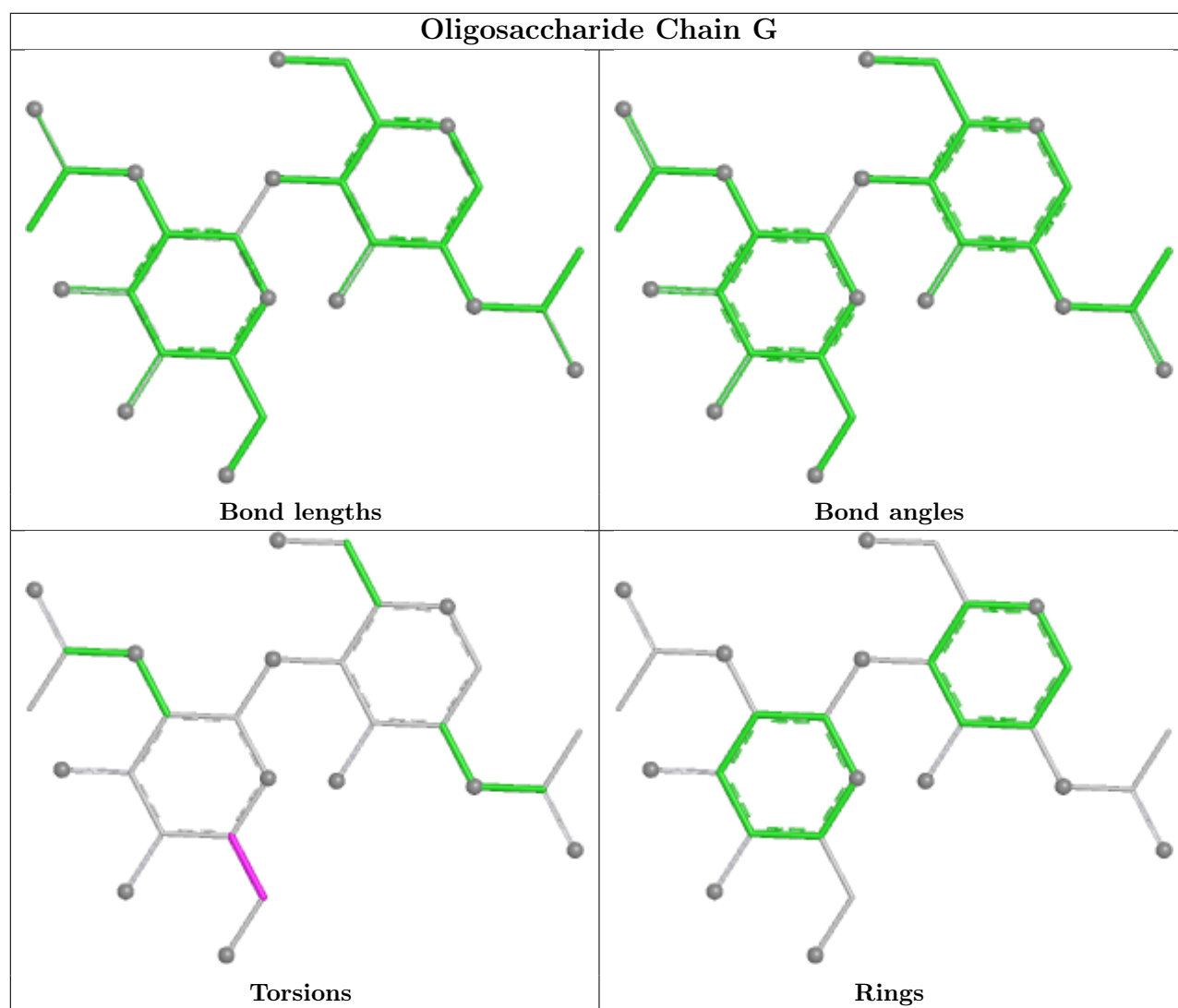


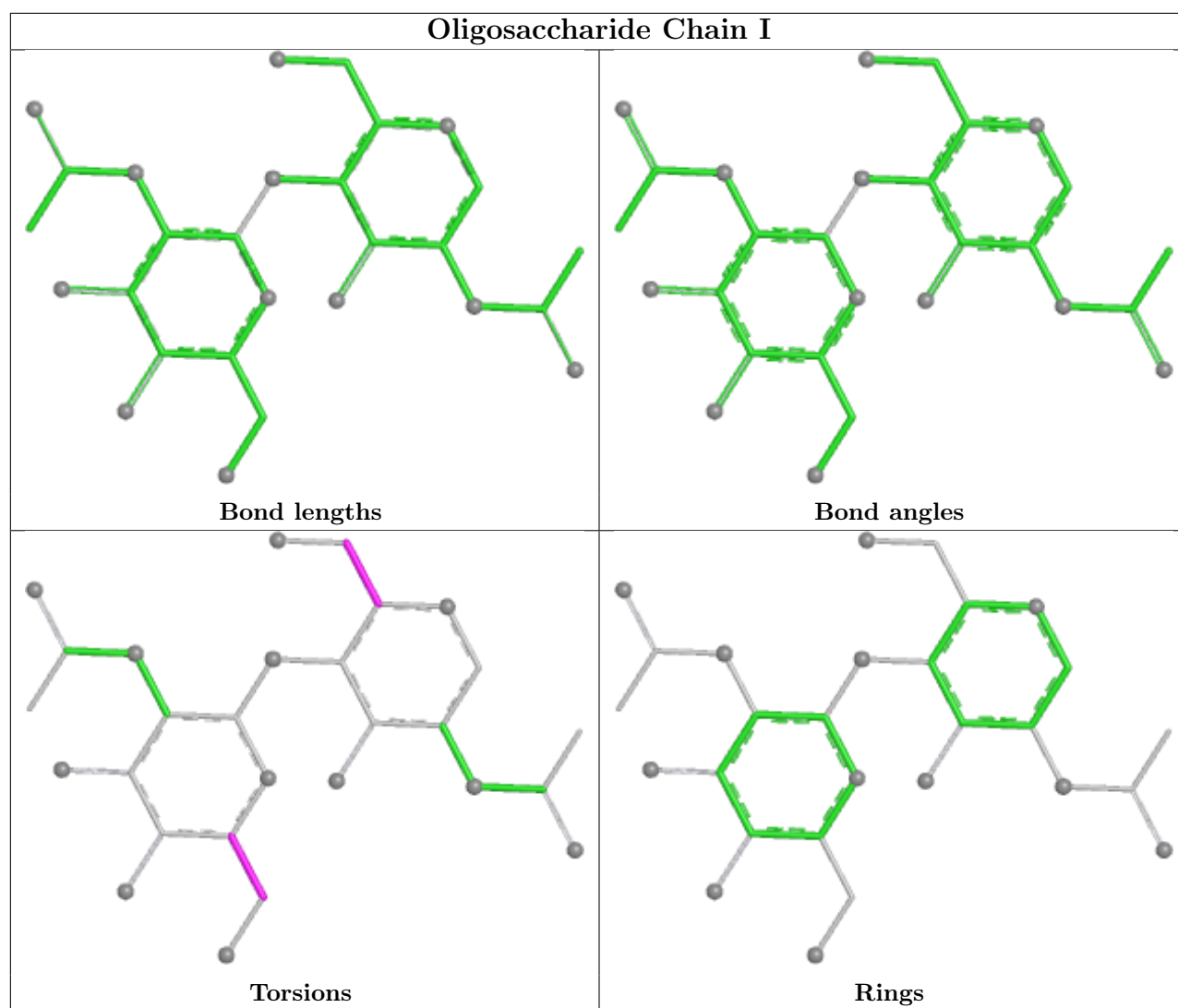
Oligosaccharide Chain H

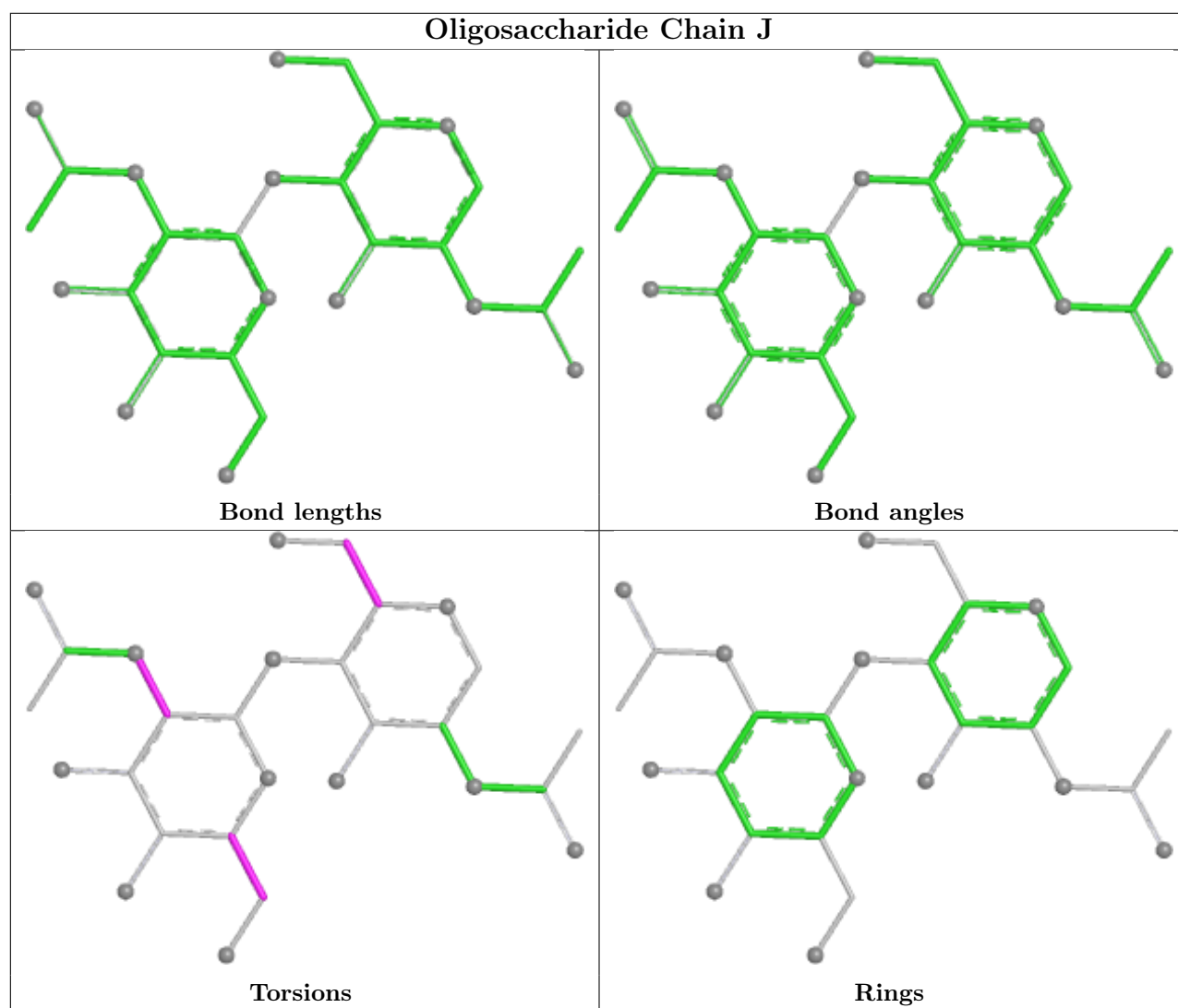


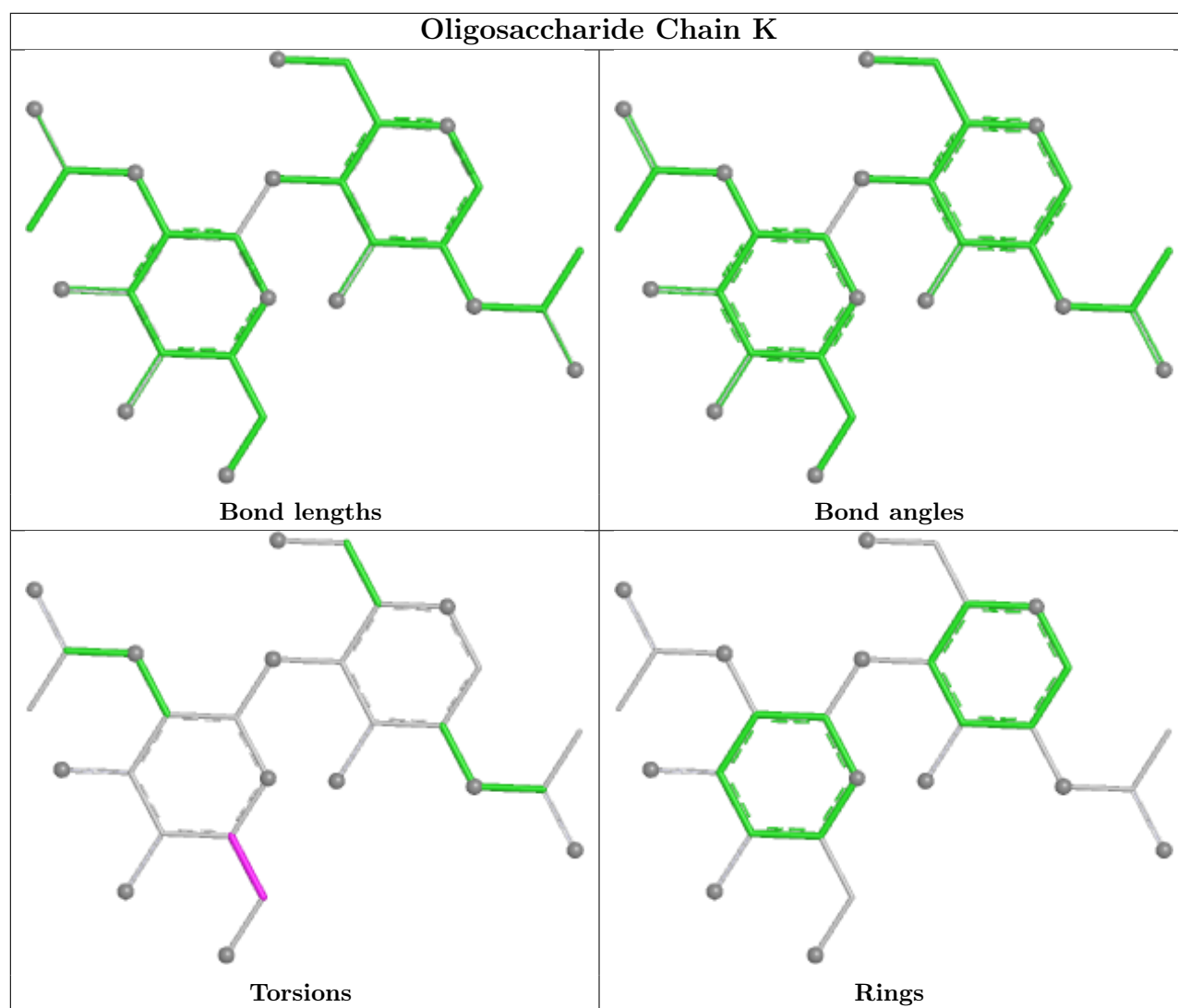
Oligosaccharide Chain F

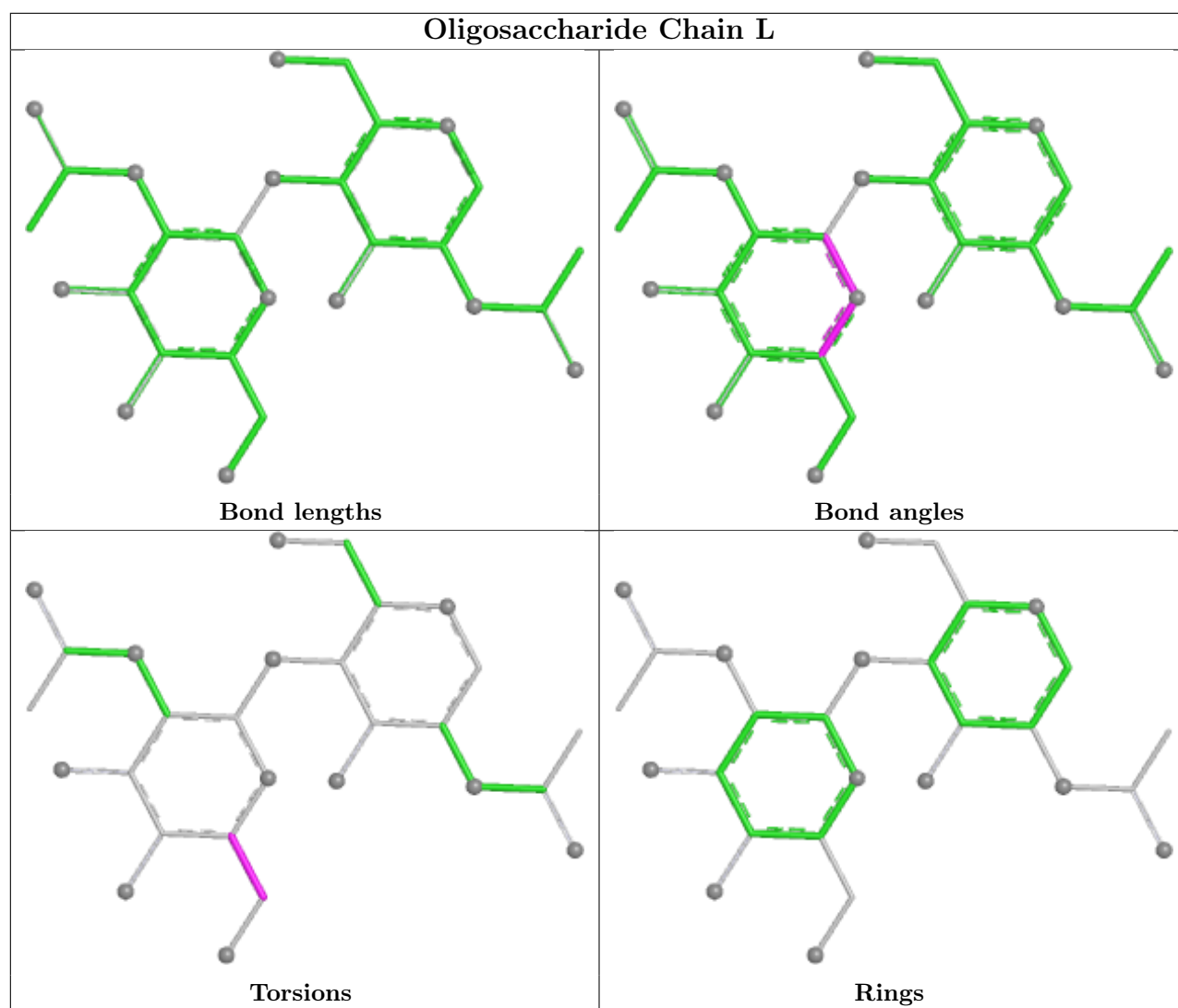


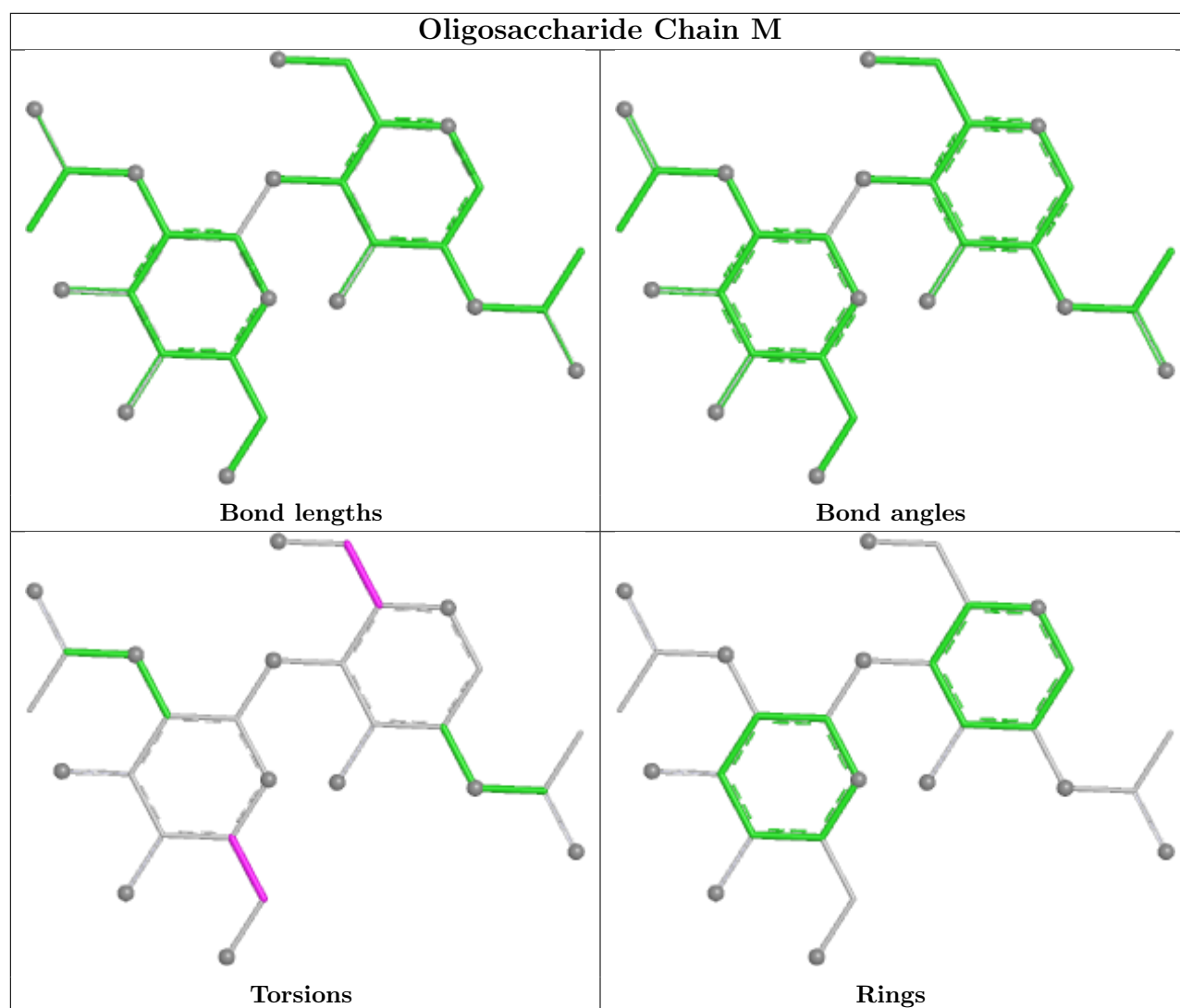












5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 16 are monoatomic - leaving 23 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	$\# Z > 2$
10	GOL	A	606	-	5,5,5	0.84	0	5,5,5	1.54	2 (40%)
11	NAG	A	608	1	14,14,15	0.85	1 (7%)	17,19,21	0.40	0
11	NAG	B	609	1	14,14,15	0.86	1 (7%)	17,19,21	0.86	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	NAG	D	609	1	14,14,15	0.68	0	17,19,21	0.45	0
10	GOL	A	610	-	5,5,5	1.02	0	5,5,5	1.04	0
10	GOL	C	609	-	5,5,5	1.01	0	5,5,5	1.11	0
11	NAG	A	609	1	14,14,15	0.87	1 (7%)	17,19,21	0.54	0
10	GOL	D	606	-	5,5,5	0.99	0	5,5,5	1.11	0
12	PO4	C	602	-	4,4,4	0.70	0	6,6,6	0.65	0
10	GOL	D	607	-	5,5,5	0.85	0	5,5,5	1.06	0
6	POP	D	602	7,8	6,8,8	0.74	0	12,13,13	1.19	1 (8%)
6	POP	C	604	7,8	6,8,8	0.68	0	12,13,13	0.89	1 (8%)
10	GOL	C	608	-	5,5,5	1.11	0	5,5,5	0.95	0
13	FLC	D	608	-	12,12,12	1.95	6 (50%)	17,17,17	2.31	6 (35%)
11	NAG	B	608	1	14,14,15	0.78	1 (7%)	17,19,21	0.61	1 (5%)
10	GOL	A	607	-	5,5,5	0.85	0	5,5,5	1.10	0
12	PO4	B	601	-	4,4,4	0.93	0	6,6,6	0.69	0
6	POP	A	602	7,8	6,8,8	0.61	0	12,13,13	0.95	0
10	GOL	B	610	-	5,5,5	1.00	0	5,5,5	1.07	0
10	GOL	C	601	-	5,5,5	0.70	0	5,5,5	1.18	0
10	GOL	B	607	-	5,5,5	1.01	0	5,5,5	1.05	0
11	NAG	C	610	1	14,14,15	1.07	2 (14%)	17,19,21	0.56	0
6	POP	B	603	7,8	6,8,8	0.64	0	12,13,13	1.11	1 (8%)

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
10	GOL	A	606	-	-	3/4/4/4	-
11	NAG	A	608	1	-	2/6/23/26	0/1/1/1
11	NAG	B	609	1	-	2/6/23/26	0/1/1/1
11	NAG	D	609	1	-	1/6/23/26	0/1/1/1
10	GOL	A	610	-	-	2/4/4/4	-
10	GOL	C	609	-	-	2/4/4/4	-
11	NAG	A	609	1	-	2/6/23/26	0/1/1/1
10	GOL	D	606	-	-	2/4/4/4	-
10	GOL	D	607	-	-	2/4/4/4	-
6	POP	D	602	7,8	-	1/6/6/6	-
6	POP	C	604	7,8	-	1/6/6/6	-
10	GOL	C	608	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FLC	D	608	-	-	3/16/16/16	-
11	NAG	B	608	1	-	2/6/23/26	0/1/1/1
10	GOL	A	607	-	-	0/4/4/4	-
6	POP	A	602	7,8	-	2/6/6/6	-
10	GOL	B	610	-	-	2/4/4/4	-
10	GOL	C	601	-	-	4/4/4/4	-
10	GOL	B	607	-	-	2/4/4/4	-
11	NAG	C	610	1	-	0/6/23/26	0/1/1/1
6	POP	B	603	7,8	-	0/6/6/6	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	608	FLC	OA1-CAC	3.02	1.32	1.22
13	D	608	FLC	OG1-CGC	2.97	1.31	1.22
13	D	608	FLC	OB2-CBC	-2.89	1.20	1.30
11	C	610	NAG	O5-C1	2.79	1.48	1.43
13	D	608	FLC	OB1-CBC	2.73	1.30	1.22
11	C	610	NAG	C1-C2	2.70	1.56	1.52
11	A	608	NAG	O5-C1	2.67	1.48	1.43
13	D	608	FLC	OG2-CGC	-2.60	1.22	1.30
11	A	609	NAG	C1-C2	2.56	1.55	1.52
11	B	609	NAG	O5-C1	2.38	1.47	1.43
11	B	608	NAG	O5-C1	2.37	1.47	1.43
13	D	608	FLC	OA2-CAC	-2.06	1.24	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	608	FLC	OB2-CBC-CB	4.93	122.59	113.14
13	D	608	FLC	OB1-CBC-CB	-4.60	113.18	122.09
13	D	608	FLC	OA1-CAC-CA	-3.78	112.24	122.95
13	D	608	FLC	OG1-CGC-CG	-3.11	114.14	122.95
13	D	608	FLC	OA2-CAC-CA	3.09	124.13	114.35
13	D	608	FLC	OG2-CGC-CG	2.57	122.49	114.35
11	B	609	NAG	C1-O5-C5	2.50	115.53	112.19
6	D	602	POP	O5-P2-O	2.37	112.58	104.64
10	A	606	GOL	C3-C2-C1	-2.21	103.69	111.80
11	B	608	NAG	C1-O5-C5	2.11	115.02	112.19
6	B	603	POP	O3-P1-O	2.08	111.60	104.64
6	C	604	POP	O5-P2-O	2.05	111.50	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	606	GOL	O2-C2-C3	2.04	117.65	109.18

There are no chirality outliers.

All (35) torsion outliers are listed below:

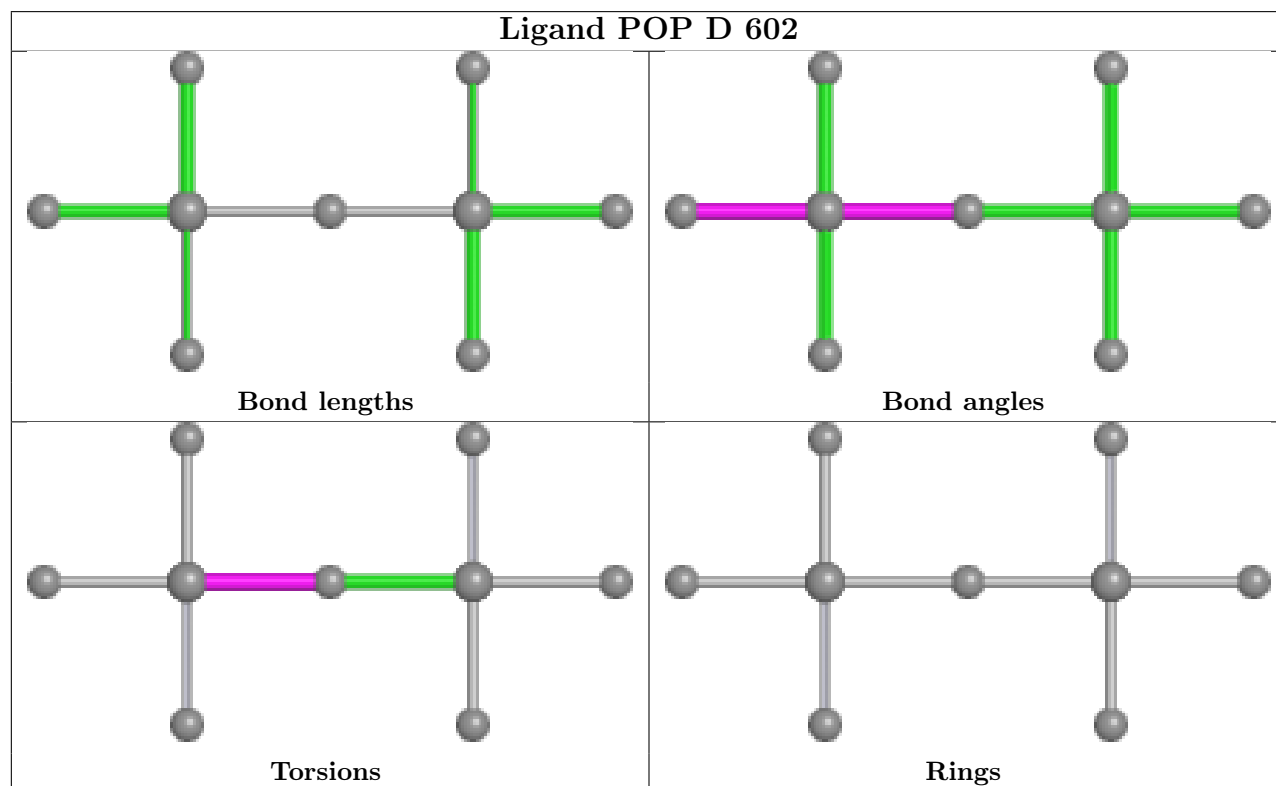
Mol	Chain	Res	Type	Atoms
6	A	602	POP	P2-O-P1-O2
10	A	606	GOL	C1-C2-C3-O3
10	A	610	GOL	C1-C2-C3-O3
10	B	610	GOL	C1-C2-C3-O3
10	C	601	GOL	O1-C1-C2-C3
10	C	601	GOL	C1-C2-C3-O3
13	D	608	FLC	CAC-CA-CB-CBC
13	D	608	FLC	CAC-CA-CB-OHB
11	B	609	NAG	O5-C5-C6-O6
11	A	608	NAG	O5-C5-C6-O6
13	D	608	FLC	CAC-CA-CB-CG
11	A	608	NAG	C4-C5-C6-O6
11	B	609	NAG	C4-C5-C6-O6
11	A	609	NAG	C4-C5-C6-O6
10	B	607	GOL	O1-C1-C2-C3
10	D	606	GOL	C1-C2-C3-O3
10	D	607	GOL	C1-C2-C3-O3
10	A	606	GOL	O2-C2-C3-O3
10	A	610	GOL	O2-C2-C3-O3
10	D	607	GOL	O2-C2-C3-O3
11	B	608	NAG	C4-C5-C6-O6
11	A	609	NAG	O5-C5-C6-O6
11	B	608	NAG	O5-C5-C6-O6
10	B	610	GOL	O2-C2-C3-O3
10	D	606	GOL	O2-C2-C3-O3
6	C	604	POP	P1-O-P2-O4
10	A	606	GOL	O1-C1-C2-O2
10	B	607	GOL	O1-C1-C2-O2
10	C	609	GOL	O1-C1-C2-C3
10	C	601	GOL	O2-C2-C3-O3
11	D	609	NAG	C1-C2-N2-C7
10	C	601	GOL	O1-C1-C2-O2
10	C	609	GOL	O1-C1-C2-O2
6	D	602	POP	P1-O-P2-O5
6	A	602	POP	P2-O-P1-O1

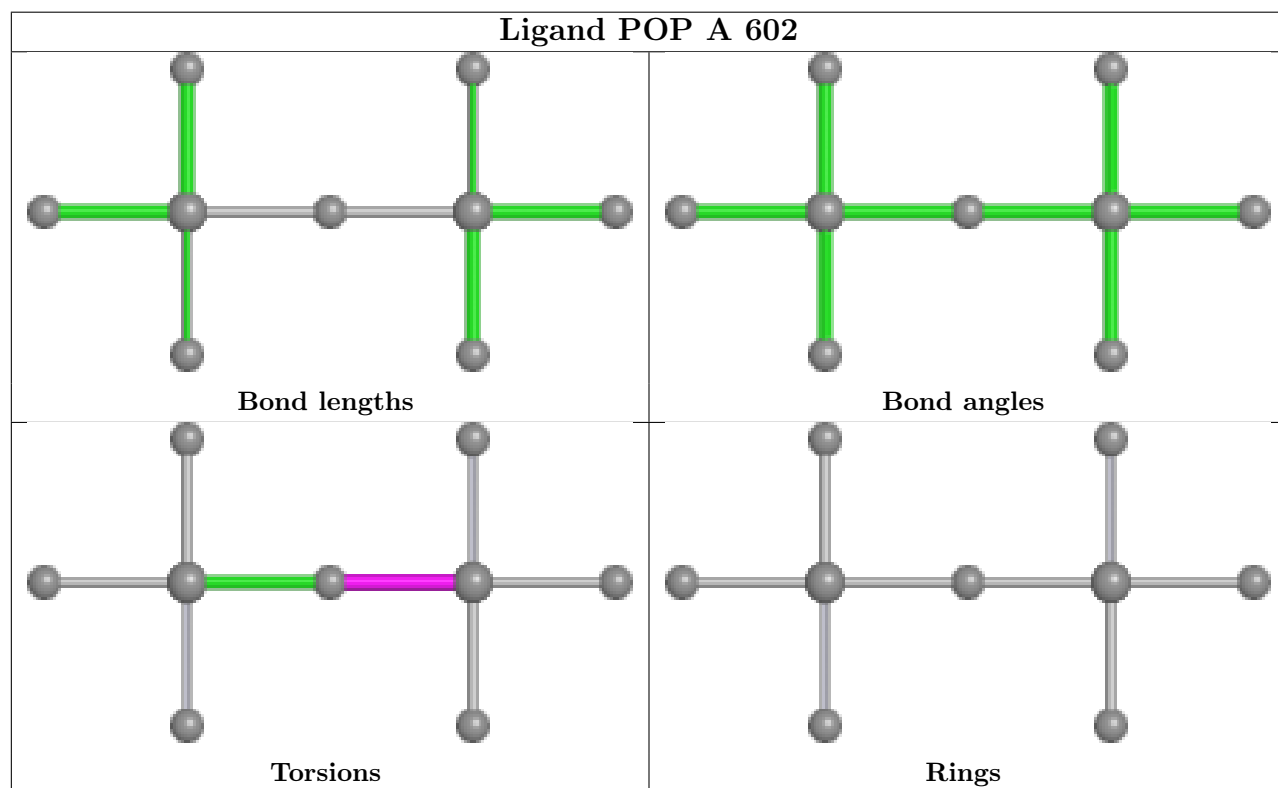
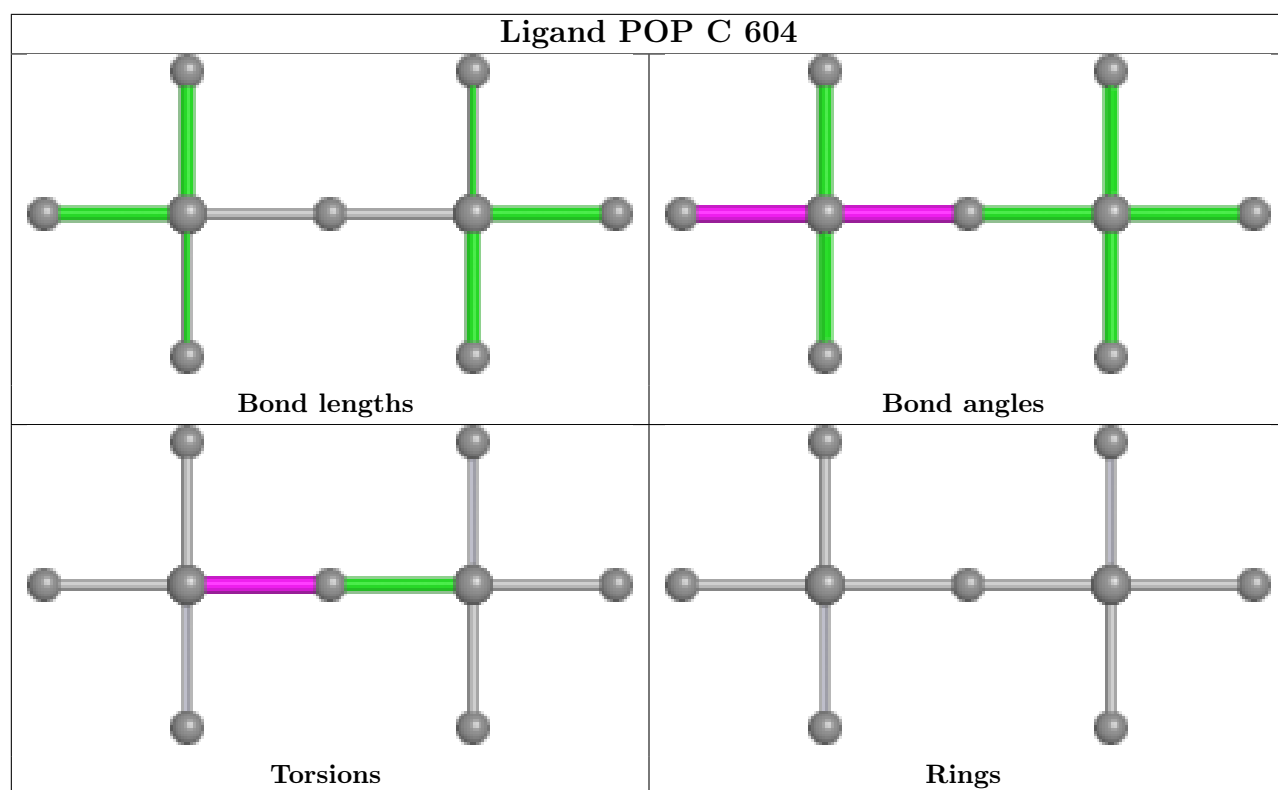
There are no ring outliers.

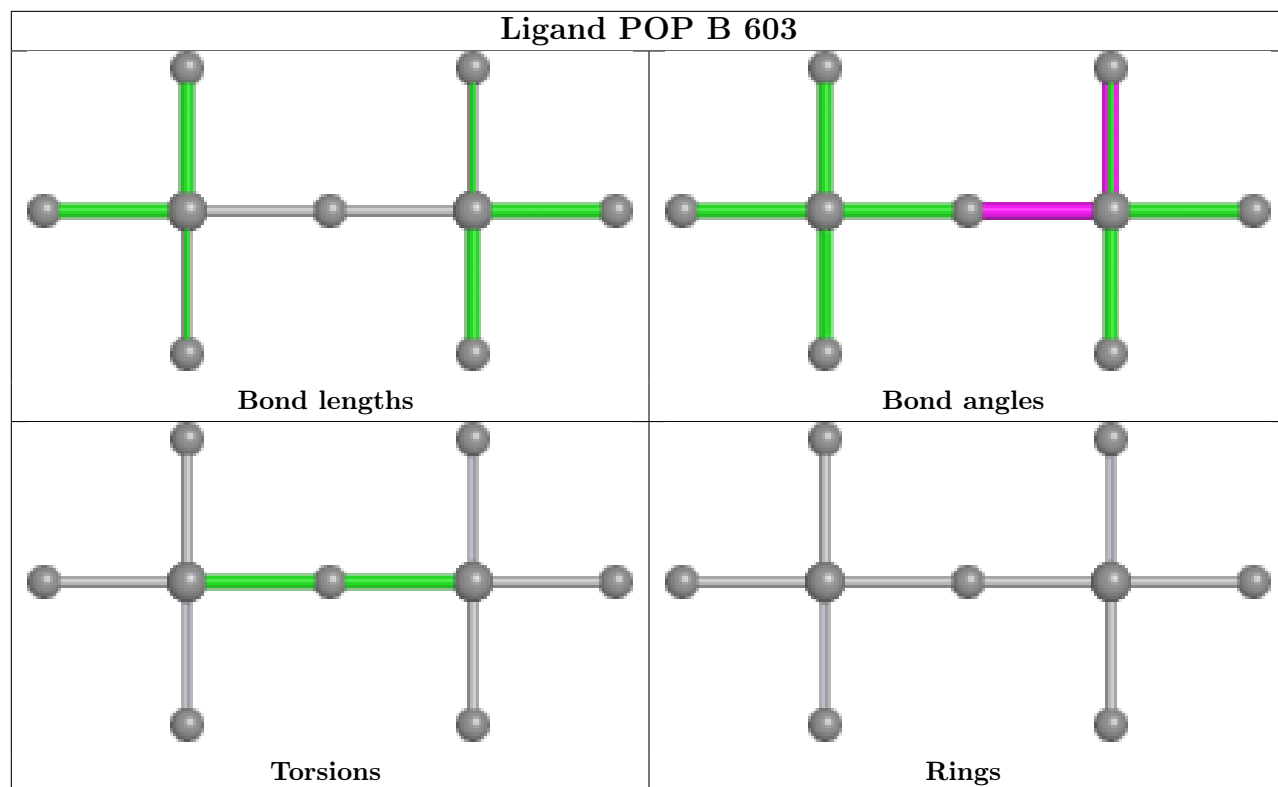
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	606	GOL	1	0
10	C	609	GOL	1	0
10	D	606	GOL	1	0
10	D	607	GOL	1	0
6	A	602	POP	2	0
10	B	607	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	480/493 (97%)	-0.28	5 (1%) 79 81	24, 44, 60, 84	3 (0%)
1	B	479/493 (97%)	-0.20	3 (0%) 85 86	23, 45, 64, 100	2 (0%)
1	C	480/493 (97%)	-0.23	1 (0%) 91 92	25, 45, 63, 78	2 (0%)
1	D	480/493 (97%)	-0.27	2 (0%) 88 89	25, 44, 60, 82	2 (0%)
All	All	1919/1972 (97%)	-0.24	11 (0%) 85 86	23, 45, 63, 100	9 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	498	ALA	4.7
1	B	263	HIS	3.5
1	B	433	MET	3.2
1	A	262	ARG	2.6
1	C	498	ALA	2.5
1	D	282	ARG	2.4
1	A	498	ALA	2.4
1	A	438	HIS	2.4
1	B	19	VAL	2.3
1	A	241	LYS	2.1
1	A	238	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

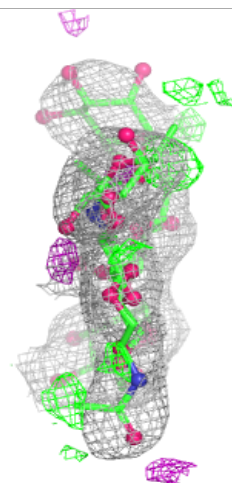
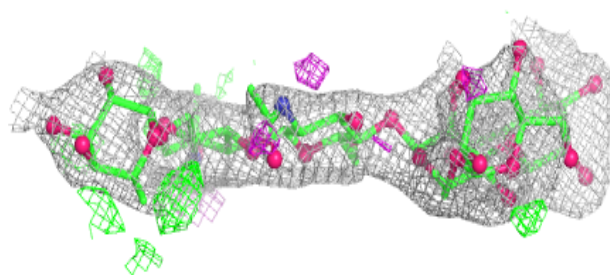
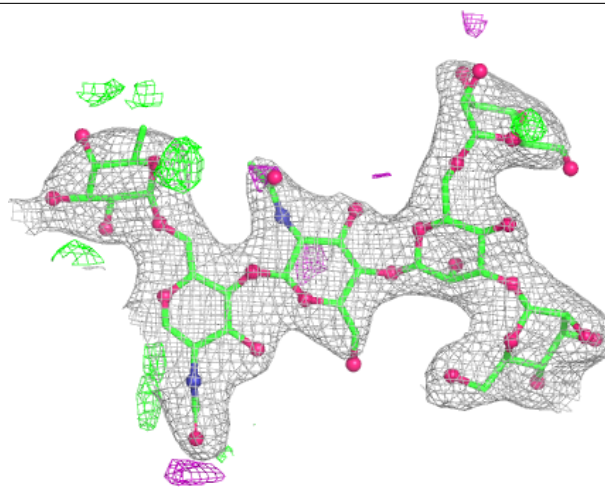
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	G	2	14/15	0.64	0.16	81,89,99,100	0
4	NAG	J	2	14/15	0.66	0.16	84,94,105,106	0
4	NAG	K	2	14/15	0.68	0.15	83,92,100,100	0
4	NAG	L	2	14/15	0.68	0.14	81,87,90,91	0
2	MAN	H	5	11/12	0.71	0.15	77,83,90,92	0
4	NAG	M	2	14/15	0.71	0.15	82,92,98,99	0
3	BMA	F	3	11/12	0.74	0.13	75,83,87,89	0
2	MAN	H	4	11/12	0.79	0.13	68,72,76,76	0
2	NAG	H	1	14/15	0.79	0.13	56,62,70,80	0
2	FUC	H	6	10/11	0.80	0.15	69,77,80,82	0
4	NAG	I	2	14/15	0.80	0.13	82,87,98,99	0
2	MAN	E	5	11/12	0.82	0.14	67,71,77,81	0
2	FUC	E	6	10/11	0.84	0.15	68,70,77,83	0
4	NAG	M	1	14/15	0.85	0.11	58,76,84,90	0
3	NAG	F	1	14/15	0.85	0.12	61,66,74,74	0
2	NAG	H	2	14/15	0.87	0.13	61,68,79,82	0
4	NAG	K	1	14/15	0.87	0.12	56,74,86,88	0
4	NAG	I	1	14/15	0.88	0.10	58,71,75,83	0
4	NAG	J	1	14/15	0.88	0.11	65,74,82,91	0
2	BMA	H	3	11/12	0.89	0.09	70,72,74,79	0
3	NAG	F	2	14/15	0.89	0.11	71,75,79,81	0
4	NAG	L	1	14/15	0.89	0.10	61,69,77,82	0
2	NAG	E	1	14/15	0.90	0.10	55,59,63,64	0
2	NAG	E	2	14/15	0.90	0.13	56,60,74,76	0
4	NAG	G	1	14/15	0.91	0.08	54,70,77,85	0
2	MAN	E	4	11/12	0.91	0.09	58,60,63,64	0
2	BMA	E	3	11/12	0.94	0.07	57,61,65,67	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.

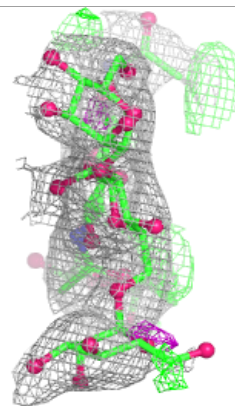
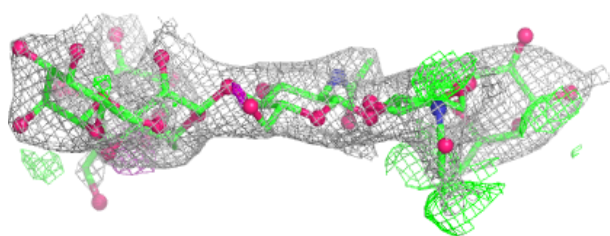
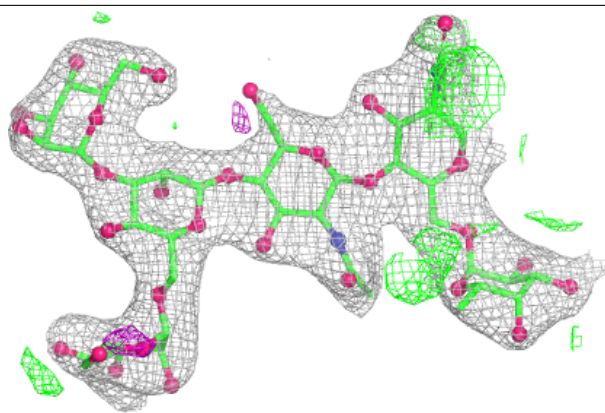
Electron density around Chain E:

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

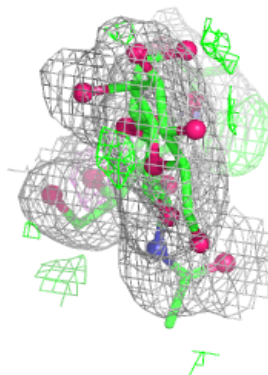
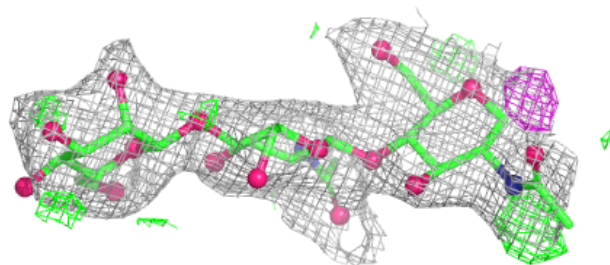
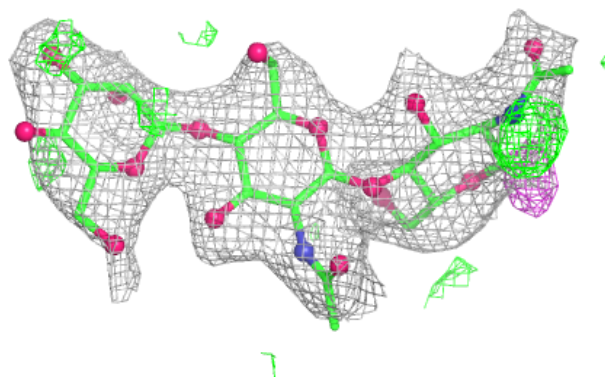


Electron density around Chain H:

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

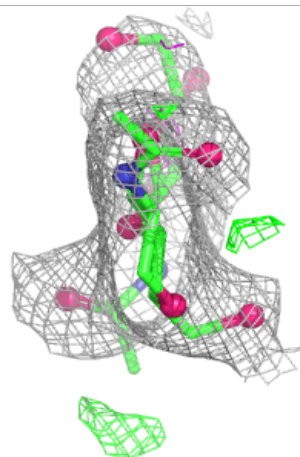
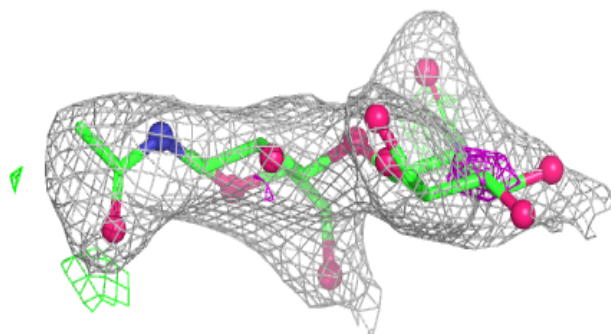
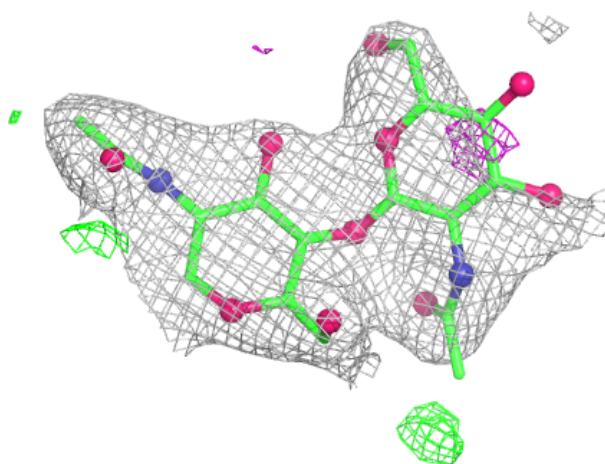
**Electron density around Chain F:**

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



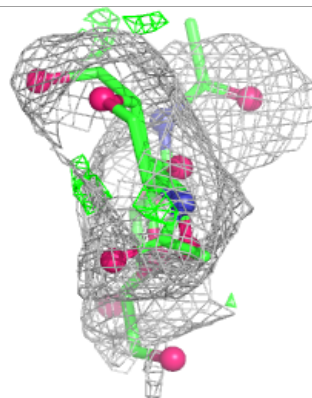
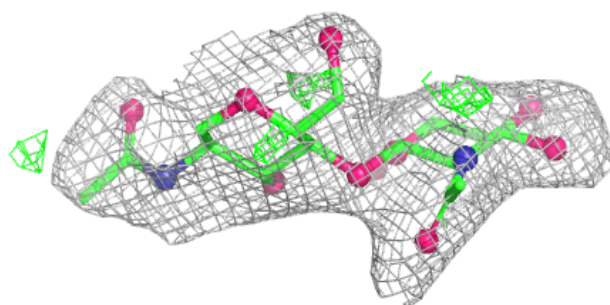
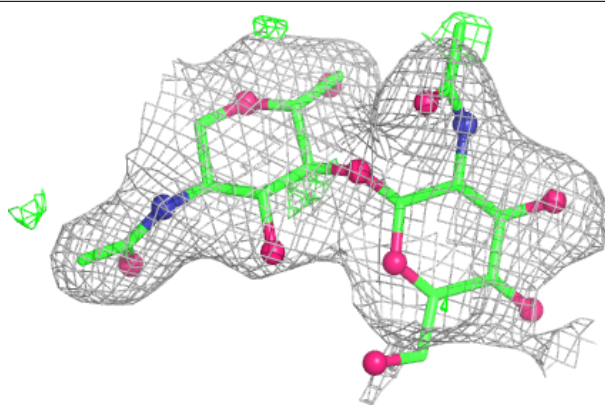
Electron density around Chain G:

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

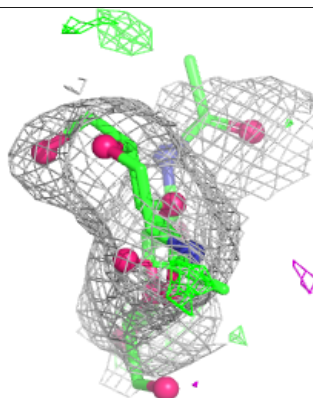
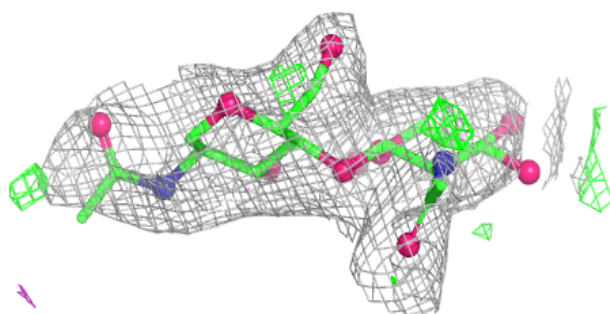
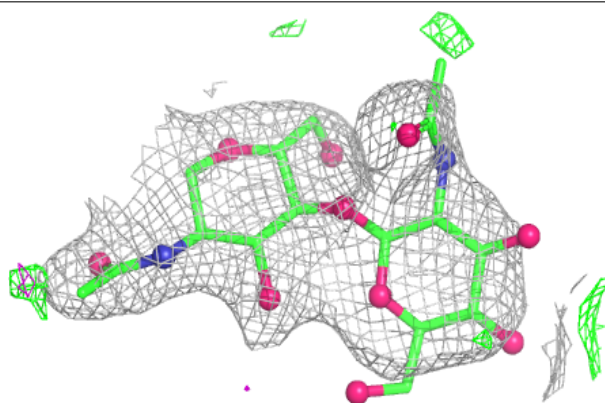


Electron density around Chain I:

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

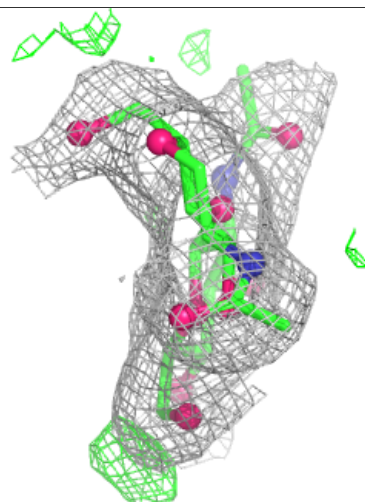
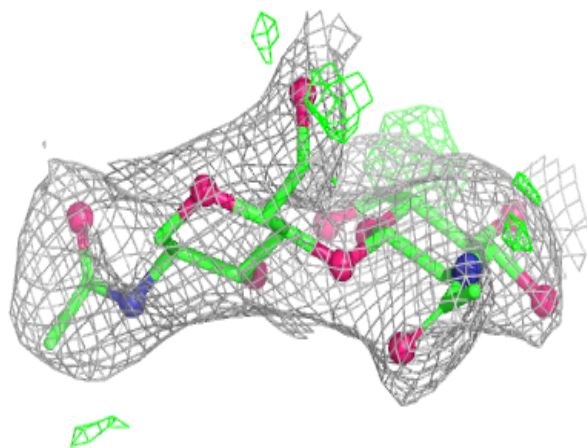
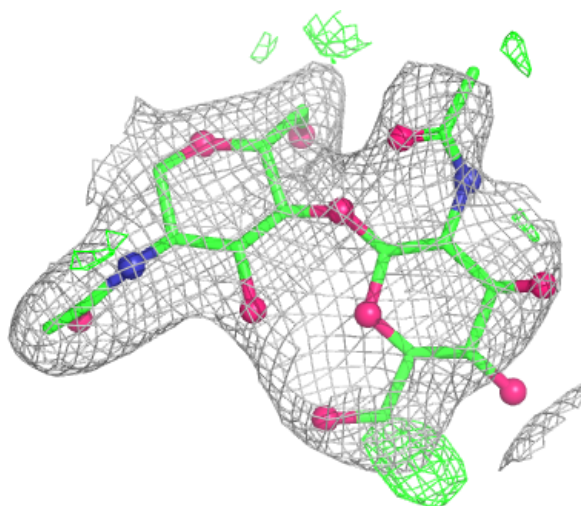
**Electron density around Chain J:**

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



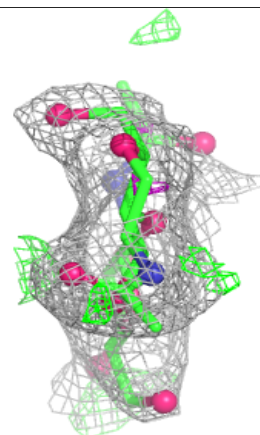
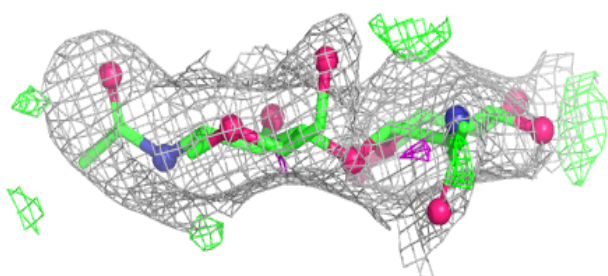
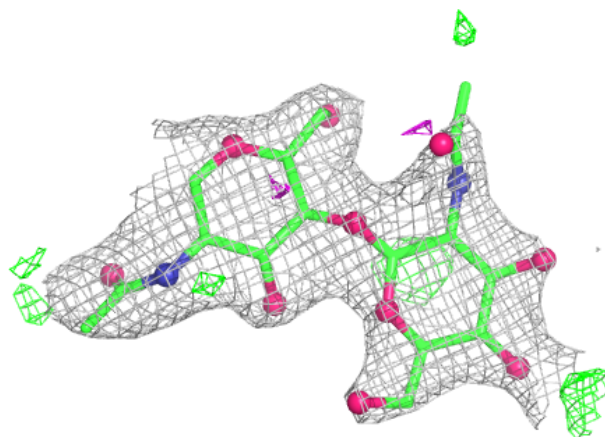
Electron density around Chain K:

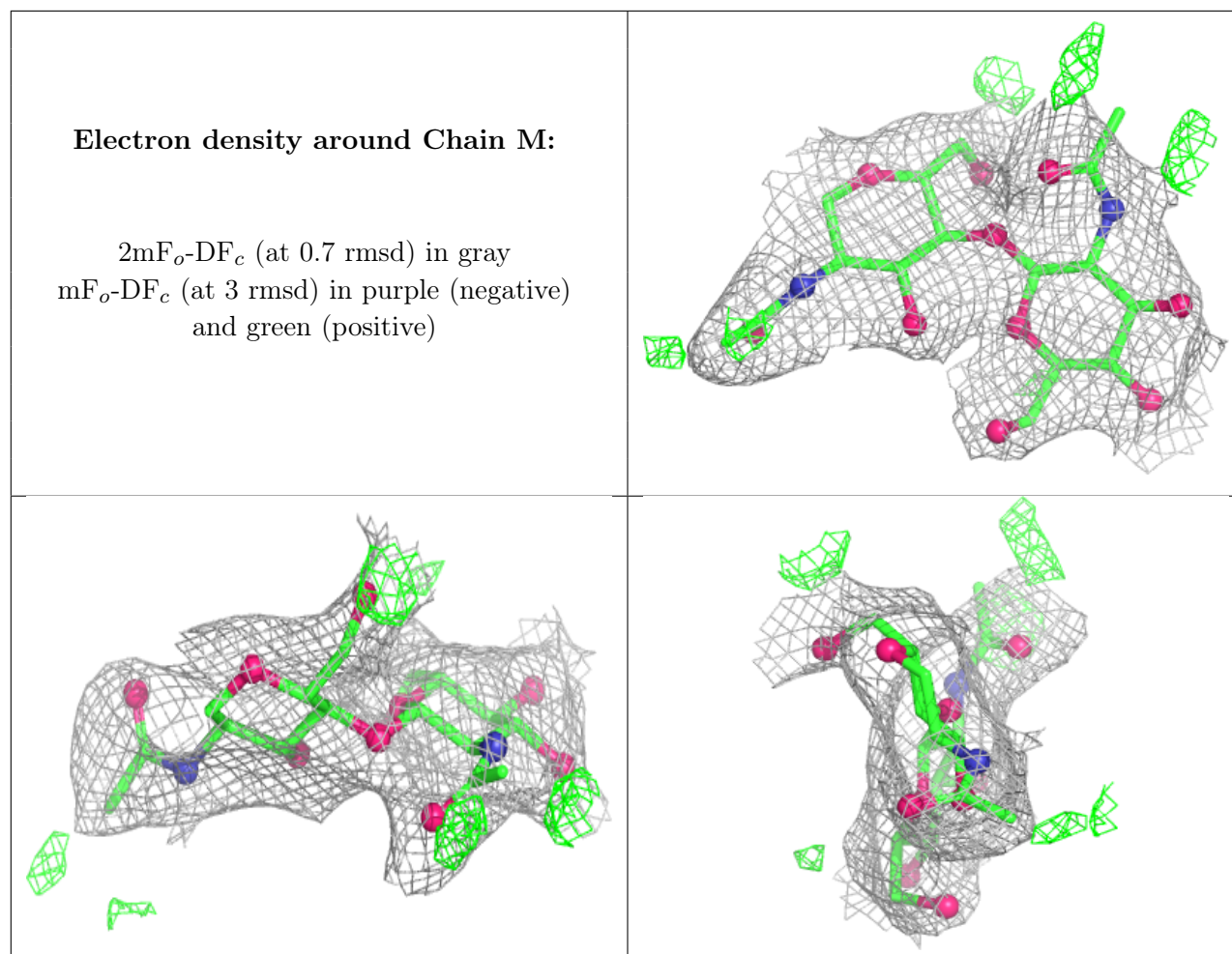
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain L:

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	NAG	B	608	14/15	0.53	0.19	83,97,100,101	0
11	NAG	A	608	14/15	0.54	0.18	68,87,97,100	0
11	NAG	D	609	14/15	0.55	0.17	75,88,92,94	0
11	NAG	C	610	14/15	0.60	0.16	73,79,81,84	0
11	NAG	A	609	14/15	0.67	0.17	77,83,89,92	0
11	NAG	B	609	14/15	0.81	0.13	55,73,83,86	0
6	POP	D	602	9/9	0.82	0.18	49,58,70,80	9
13	FLC	D	608	13/13	0.85	0.13	60,64,73,76	0
6	POP	B	603	9/9	0.86	0.16	40,50,64,67	9
10	GOL	D	607	6/6	0.89	0.14	52,58,62,62	0

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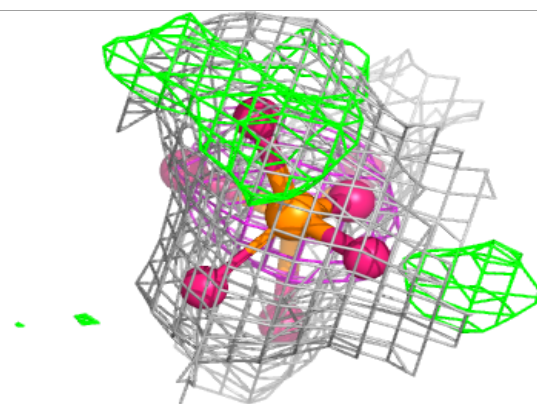
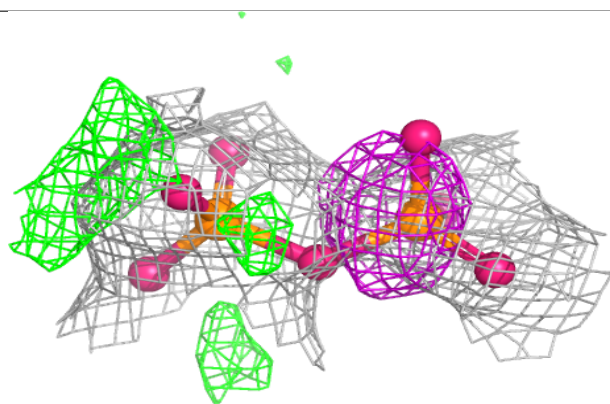
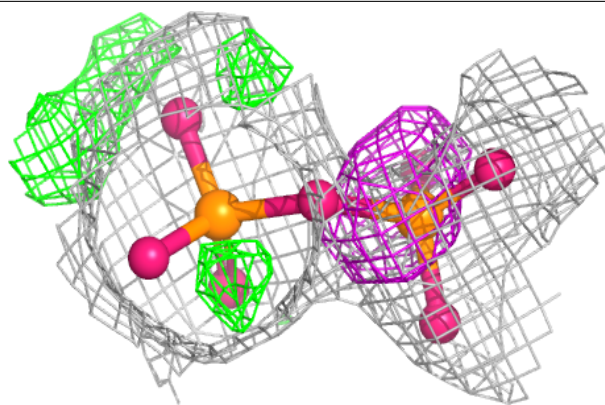
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	GOL	B	610	6/6	0.89	0.14	47,53,55,58	0
6	POP	C	604	9/9	0.90	0.13	48,54,70,80	9
6	POP	A	602	9/9	0.90	0.14	43,52,63,71	9
10	GOL	A	607	6/6	0.90	0.13	52,54,60,60	0
10	GOL	A	610	6/6	0.91	0.14	47,54,59,66	0
12	PO4	C	602	5/5	0.91	0.14	50,53,58,63	5
10	GOL	C	601	6/6	0.91	0.14	44,51,54,56	0
10	GOL	A	606	6/6	0.93	0.09	45,52,53,54	0
12	PO4	B	601	5/5	0.93	0.11	46,48,53,55	5
10	GOL	C	608	6/6	0.95	0.09	47,48,49,50	0
10	GOL	C	609	6/6	0.95	0.09	52,56,58,61	0
10	GOL	B	607	6/6	0.95	0.10	54,61,65,67	0
8	MG	A	604	1/1	0.97	0.26	48,48,48,48	0
8	MG	C	606	1/1	0.97	0.12	45,45,45,45	0
8	MG	D	604	1/1	0.97	0.07	51,51,51,51	0
9	CA	D	605	1/1	0.97	0.10	77,77,77,77	0
10	GOL	D	606	6/6	0.97	0.07	43,47,49,52	0
5	NA	C	603	1/1	0.98	0.06	33,33,33,33	0
9	CA	A	605	1/1	0.98	0.11	65,65,65,65	0
9	CA	B	606	1/1	0.98	0.10	76,76,76,76	0
9	CA	C	607	1/1	0.98	0.11	75,75,75,75	0
8	MG	B	605	1/1	0.98	0.23	43,43,43,43	0
5	NA	D	601	1/1	0.98	0.07	33,33,33,33	0
5	NA	A	601	1/1	0.99	0.09	28,28,28,28	0
5	NA	B	602	1/1	0.99	0.06	27,27,27,27	0
7	ZN	A	603	1/1	0.99	0.04	46,46,46,46	0
7	ZN	B	604	1/1	1.00	0.05	41,41,41,41	0
7	ZN	C	605	1/1	1.00	0.05	43,43,43,43	0
7	ZN	D	603	1/1	1.00	0.04	46,46,46,46	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.

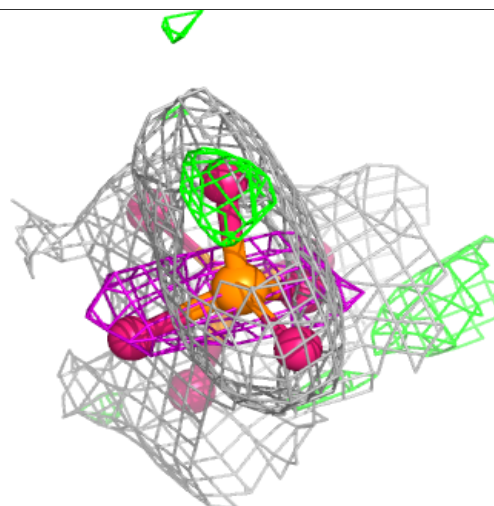
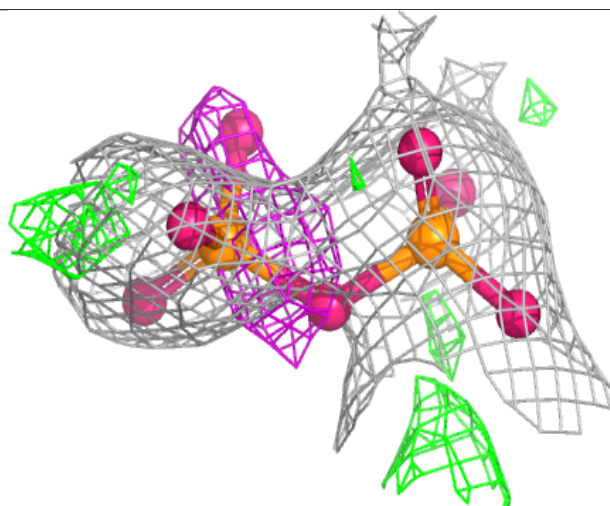
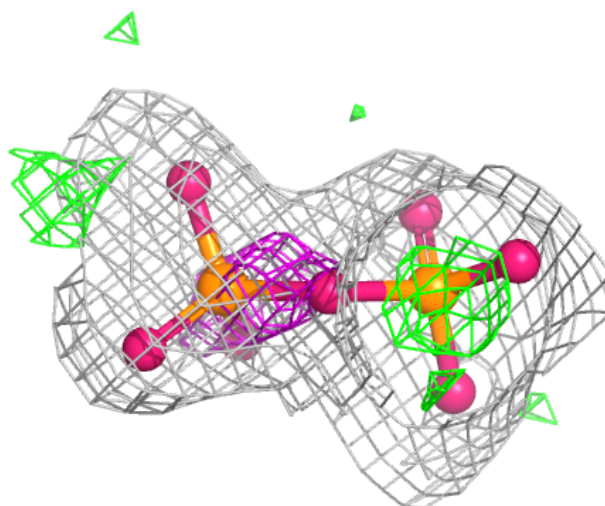
Electron density around POP D 602:

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



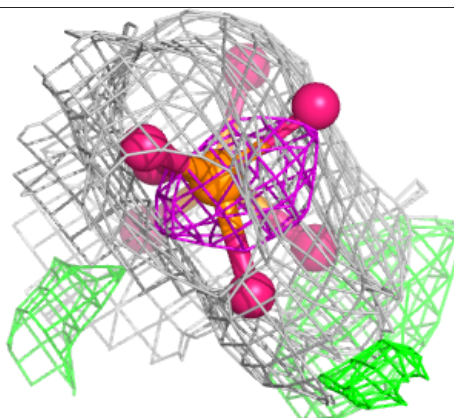
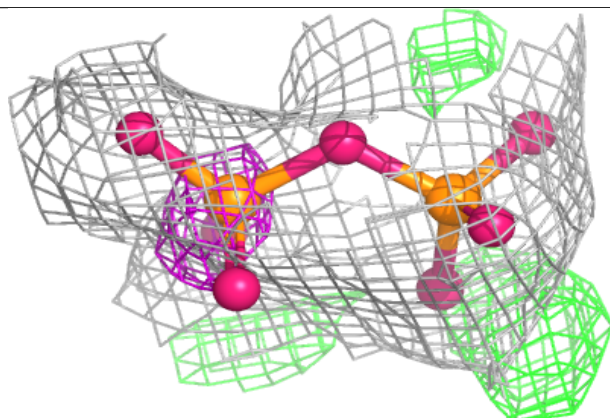
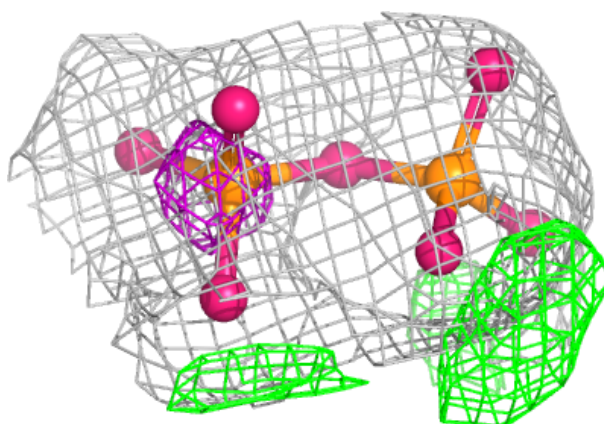
Electron density around POP B 603:

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

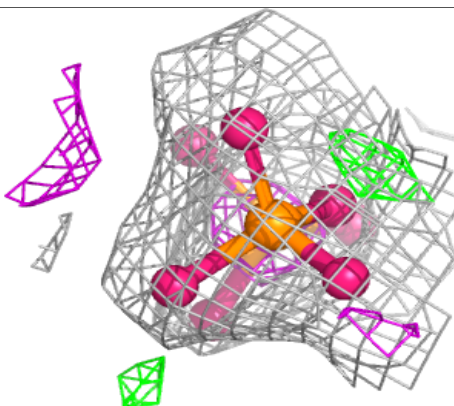
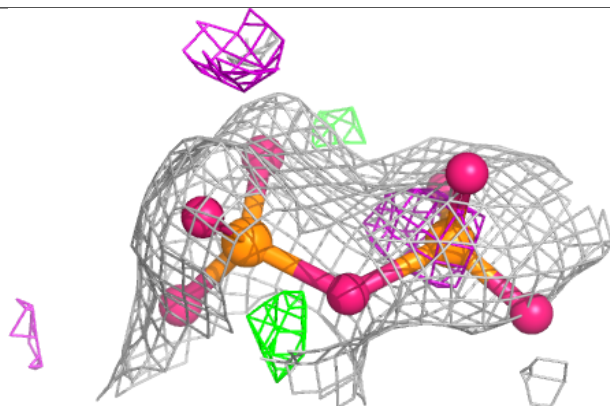
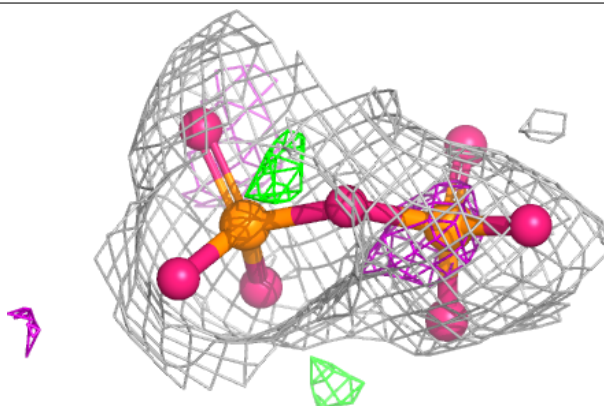


Electron density around POP C 604:

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

**Electron density around POP A 602:**

$2mF_o-DF_c$ (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.