



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 16, 2026 – 10:24 AM EDT

PDB ID : 10TV / pdb\_000010tv  
Title : Tissue Non-specific Alkaline Phosphatase -S110A bound to phosphocreatine  
Authors : Krishnan, S.S.; Carroll, B.L.; Guarne, A.  
Deposited on : 2026-02-09  
Resolution : 2.26 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

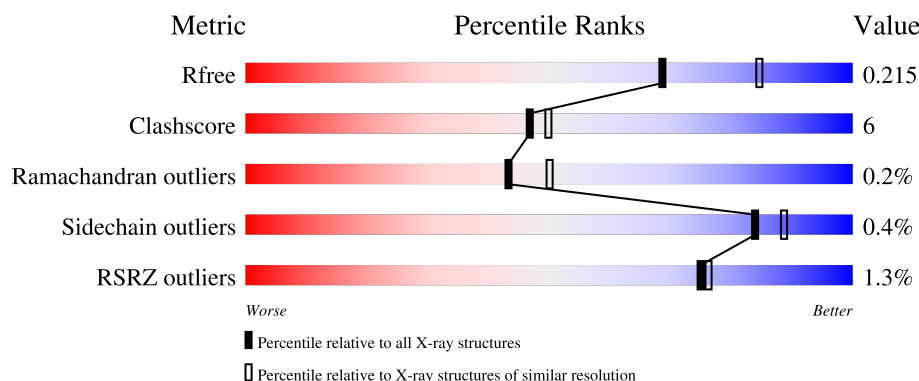
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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.




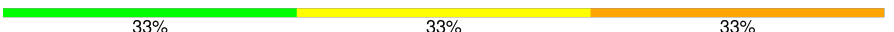

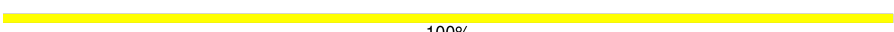


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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  $\geq 3$ , 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>88%</div> <div>10%</div> <div>.</div> </div> </div>
1	B	493	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	493	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>
1	D	493	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
2	E	4	<div> <div>25%</div> <div>75%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	FLC	C	608	-	X	-	-

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 16800 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	482	Total	C	N	O	S	0	2	0
			3755	2349	670	716	20			
1	B	481	Total	C	N	O	S	0	2	0
			3751	2346	669	716	20			
1	C	482	Total	C	N	O	S	0	2	0
			3756	2349	670	717	20			
1	D	482	Total	C	N	O	S	0	1	0
			3748	2344	668	716	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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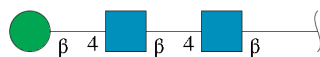
Chain	Residue	Modelled	Actual	Comment	Reference
C	502	HIS	-	expression tag	UNP P09242
C	503	HIS	-	expression tag	UNP P09242
C	504	HIS	-	expression tag	UNP P09242
C	505	HIS	-	expression tag	UNP P09242
C	506	HIS	-	expression tag	UNP P09242
C	507	HIS	-	expression tag	UNP P09242
D	15	ASP	-	expression tag	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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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.



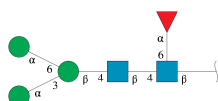
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



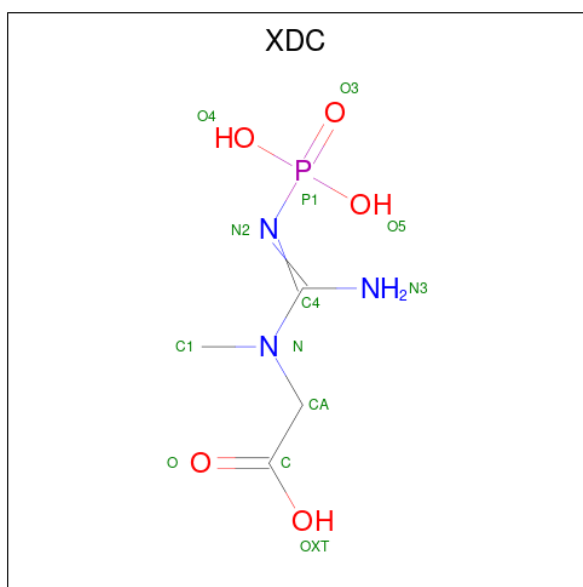
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is Phosphocreatine (CCD ID: XDC) (formula: C<sub>4</sub>H<sub>10</sub>N<sub>3</sub>O<sub>5</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	1
			26	8	6	10	2		
6	B	1	Total	C	N	O	P	0	0
			13	4	3	5	1		
6	C	1	Total	C	N	O	P	0	1
			26	8	6	10	2		
6	D	1	Total	C	N	O	P	0	0
			13	4	3	5	1		

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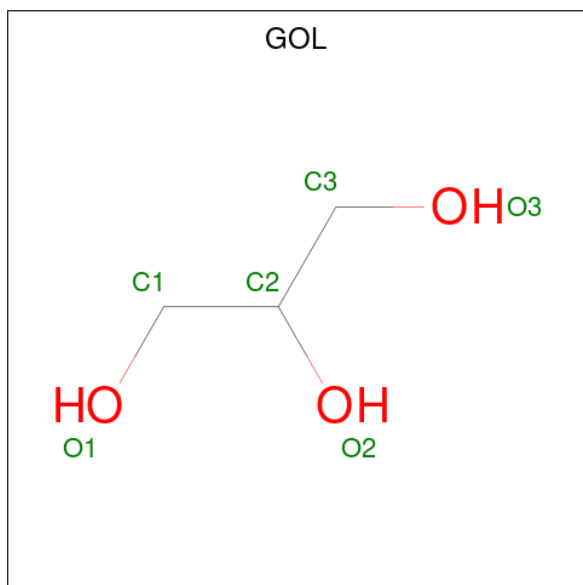
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		

- 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: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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	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		
10	D	1	Total	C	O	0	0
			6	3	3		

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

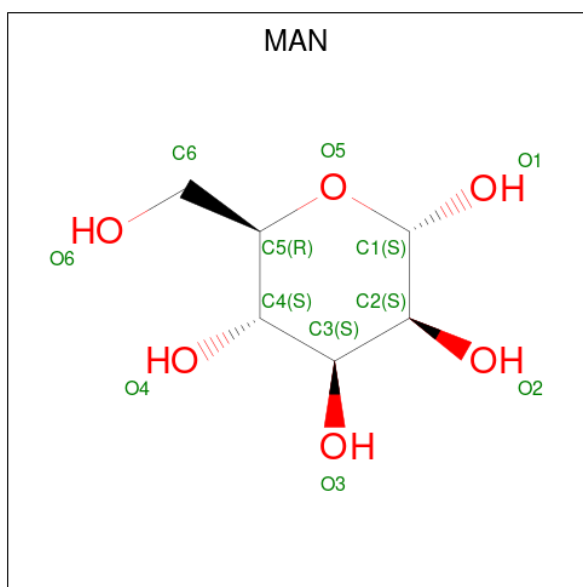
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Na	0	0
			1	1		
11	B	1	Total	Na	0	0
			1	1		
11	C	1	Total	Na	0	0
			1	1		
11	D	1	Total	Na	0	0
			1	1		

- 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>).



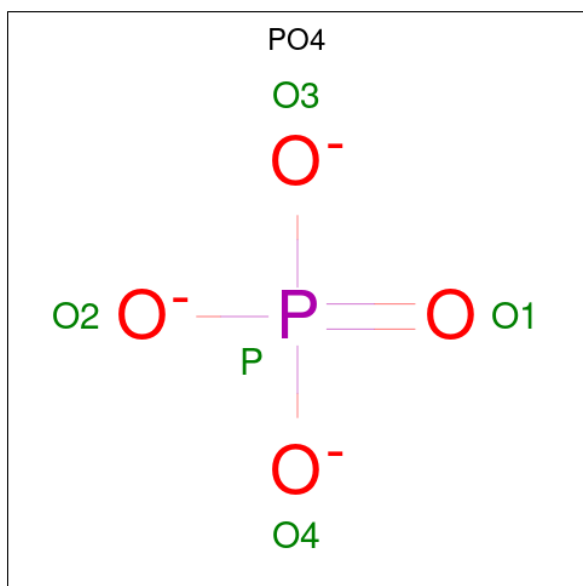
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	A	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	B	1	Total	C	N	O	0	0
			14	8	1	5		
12	C	1	Total	C	N	O	0	0
			14	8	1	5		
12	C	1	Total	C	N	O	0	0
			14	8	1	5		
12	C	1	Total	C	N	O	0	0
			14	8	1	5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



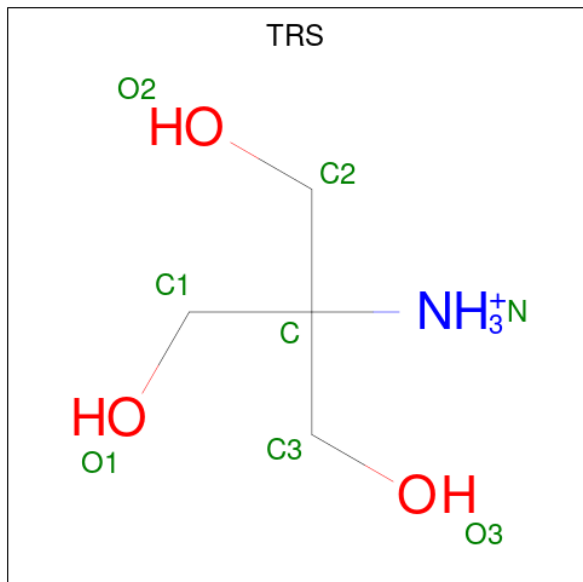
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			11	6	5		

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



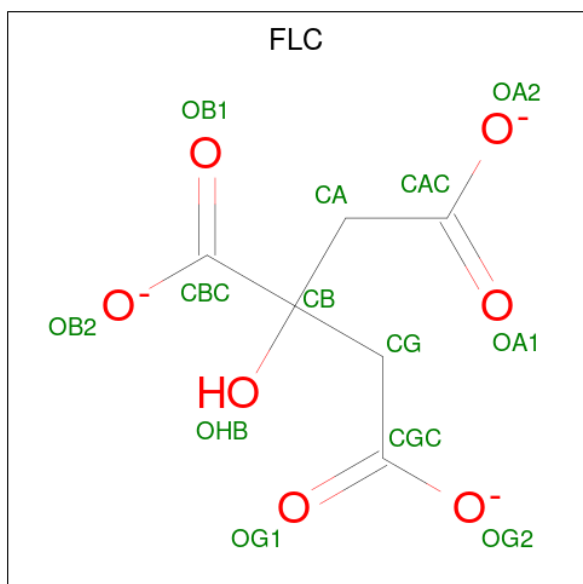
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	B	1	Total	O	P	0	0
			5	4	1		
14	C	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 15 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 16 is CITRATE ANION (CCD ID: FLC) (formula:  $C_6H_5O_7$ ).



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

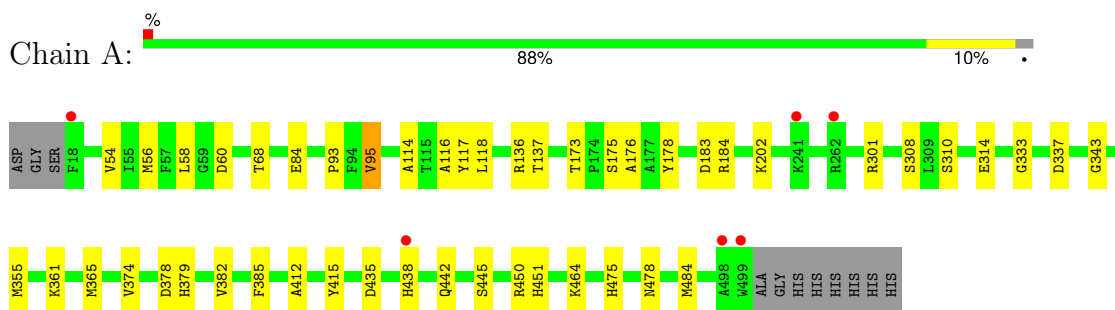
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	316	Total 316	O 316	0	0
17	B	250	Total 250	O 250	0	0
17	C	289	Total 289	O 289	0	0
17	D	272	Total 272	O 272	0	0

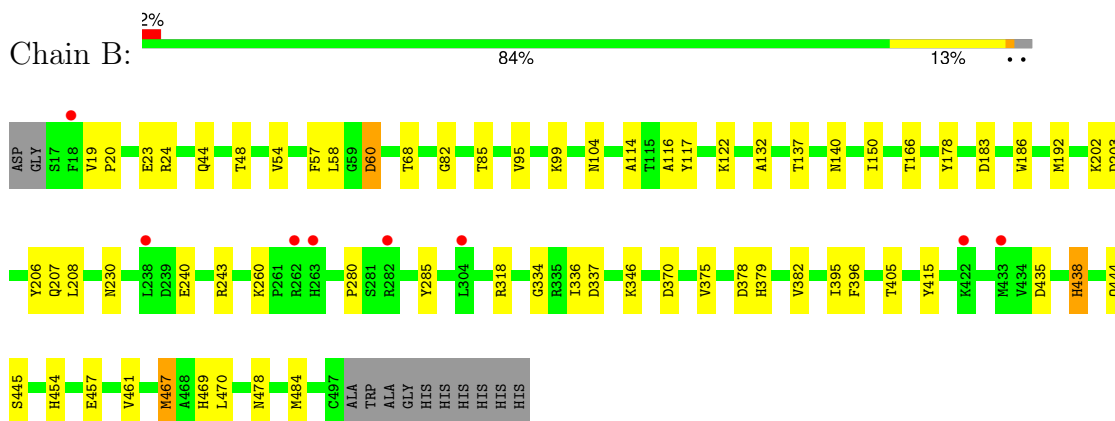
### 3 Residue-property plots [i](#)

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

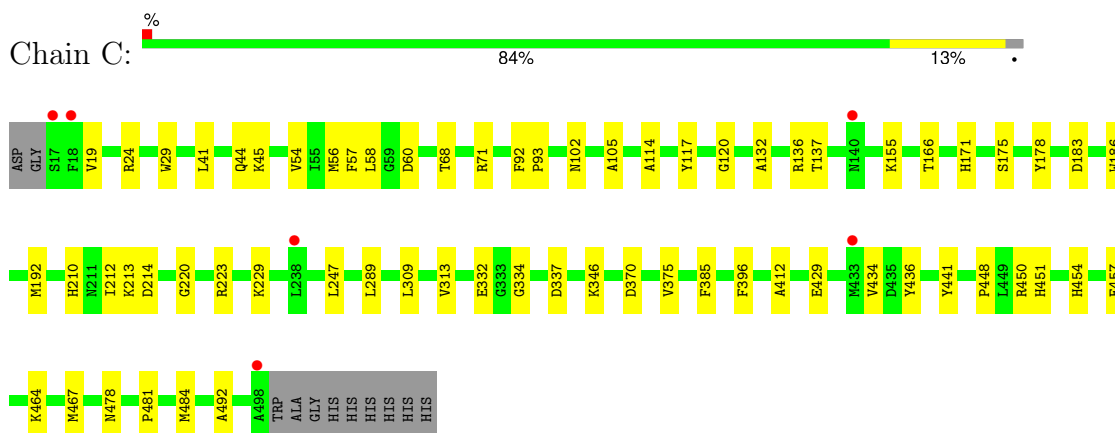
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



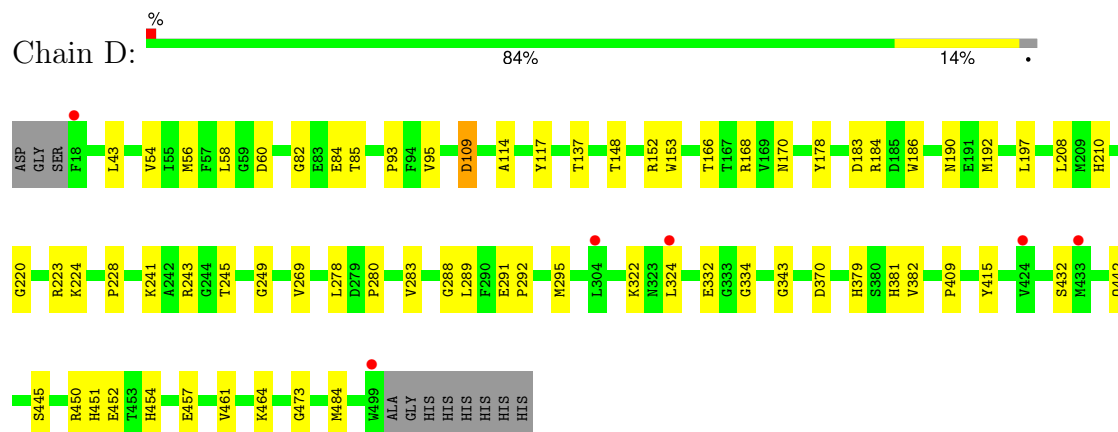
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



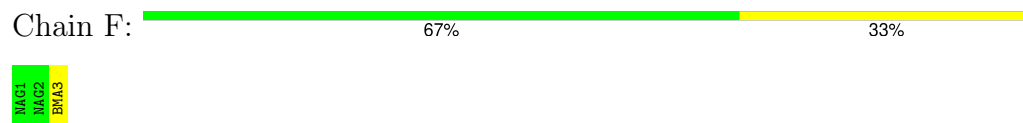
- Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



- Molecule 2: 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



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



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



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



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



NAG1  
NAG2

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

Chain I:  50% 50%

NAG1  
NAG2

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

Chain L:  100%

NAG1  
NAG2

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

Chain H:  50% 50%

NAG1  
NAG2  
MAN3  
MAN4  
MAN5  
FUC6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.33Å 119.12Å 346.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.64 – 2.26 39.64 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.64-2.26) 86.3 (39.64-2.26)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.36 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.179 , 0.216 0.179 , 0.215	Depositor DCC
$R_{free}$ test set	2011 reflections (1.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16800	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.95% 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: CA, GOL, MAN, NAG, MG, NA, XDC, FLC, ZN, BMA, PO4, TRS, FUC

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	0.35	0/3844	0.55	0/5209
1	B	0.35	0/3840	0.55	0/5203
1	C	0.33	0/3845	0.53	0/5210
1	D	0.35	0/3833	0.55	0/5194
All	All	0.34	0/15362	0.55	0/20816

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	3755	0	3649	37	0
1	B	3751	0	3648	50	0
1	C	3756	0	3653	48	0
1	D	3748	0	3643	46	1
2	E	50	0	43	0	0
3	F	39	0	34	0	0
3	J	39	0	34	1	0
3	K	39	0	34	0	0
4	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	28	0	25	0	0
4	L	28	0	25	0	0
5	H	71	0	61	0	0
6	A	26	0	0	3	0
6	B	13	0	0	0	0
6	C	26	0	0	5	0
6	D	13	0	0	5	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	12	0	16	0	0
10	B	12	0	16	1	0
10	C	18	0	24	1	0
10	D	18	0	24	2	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	28	0	26	0	0
12	C	42	0	39	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
14	D	5	0	0	0	0
15	B	8	0	12	1	0
16	C	13	0	5	0	1
17	A	316	0	0	2	0
17	B	250	0	0	2	0
17	C	289	0	0	2	0
17	D	272	0	0	0	0
All	All	16800	0	15111	174	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 6.

All (174) 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:D:184:ARG:NH1	6:D:602:XDC:O3	2.00	0.95
1:B:48:THR:HA	1:B:467:MET:HE3	1.51	0.92
1:D:184:ARG:HH12	6:D:602:XDC:P1	1.97	0.88
6:D:602:XDC:O3	6:D:602:XDC:N3	2.06	0.85
1:A:137:THR:HG22	1:A:183:ASP:OD2	1.95	0.67
1:C:56:MET:HB2	1:C:484:MET:HE1	1.78	0.66
1:C:137:THR:HG22	1:C:183:ASP:OD2	1.96	0.64
1:D:450:ARG:NH1	1:D:451:HIS:HE1	1.95	0.63
1:B:137:THR:HG22	1:B:183:ASP:OD2	2.00	0.62
1:B:467:MET:HE2	1:B:469:HIS:CE1	2.34	0.61
1:B:150:ILE:HD13	1:B:484:MET:HE2	1.83	0.60
1:C:54:VAL:CG1	1:C:484:MET:HE2	2.32	0.60
1:D:409:PRO:HG2	1:D:432:SER:HB3	1.84	0.60
1:C:166:THR:OG1	1:C:334:GLY:HA2	2.01	0.60
1:A:56:MET:HB2	1:A:484:MET:HE1	1.85	0.59
1:B:24:ARG:HA	1:C:132:ALA:HB3	1.84	0.59
1:B:467:MET:HE2	1:B:467:MET:HA	1.83	0.59
1:D:148:THR:HG22	1:D:153:TRP:NE1	2.17	0.59
1:D:370:ASP:OD1	10:D:606:GOL:O1	2.21	0.58
1:B:202:LYS:HA	1:B:202:LYS:HE2	1.84	0.58
1:B:48:THR:HG22	1:B:467:MET:HE1	1.86	0.58
1:B:457:GLU:HA	1:C:68:THR:HG21	1.86	0.58
1:B:240:GLU:O	1:B:243:ARG:HG2	2.05	0.57
1:B:243:ARG:NH2	17:B:704:HOH:O	2.34	0.57
1:D:283:VAL:O	1:D:322:LYS:NZ	2.37	0.56
6:C:602[B]:XDC:C1	6:C:602[B]:XDC:P1	2.93	0.56
1:C:175:SER:HA	1:C:178:TYR:CE2	2.42	0.55
1:C:370:ASP:OD1	10:C:606:GOL:O1	2.23	0.55
1:D:93:PRO:HD2	1:D:464:LYS:HB3	1.89	0.55
1:B:82:GLY:O	1:B:85:THR:HB	2.06	0.55
1:A:450:ARG:NH1	1:A:451:HIS:HE1	2.05	0.55
1:D:450:ARG:NH1	1:D:451:HIS:CE1	2.73	0.54
1:C:454:HIS:CE1	6:C:602[B]:XDC:C1	2.91	0.54
1:A:58:LEU:HD12	1:A:60:ASP:OD1	2.06	0.54
1:B:114:ALA:HA	1:B:117:TYR:CZ	2.43	0.54
6:A:601[B]:XDC:OXT	6:A:601[B]:XDC:N3	2.40	0.53
1:A:54:VAL:HG13	1:A:484:MET:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:HB3	1:B:318:ARG:HB3	1.91	0.53
1:A:314:GLU:CD	1:A:361:LYS:HE3	2.34	0.52
1:D:166:THR:OG1	1:D:334:GLY:HA2	2.08	0.52
1:D:291:GLU:HG3	1:D:295:MET:HA	1.91	0.52
1:B:230:ASN:HA	1:B:243:ARG:HD3	1.91	0.52
1:A:450:ARG:NH1	1:A:451:HIS:CE1	2.78	0.52
1:D:148:THR:HG23	1:D:152:ARG:HG2	1.92	0.52
1:A:118:LEU:HD12	1:A:176:ALA:HB3	1.92	0.51
1:D:278:LEU:O	1:D:280:PRO:HD3	2.09	0.51
1:B:467:MET:HE1	1:C:44:GLN:HE22	1.76	0.50
1:A:60:ASP:HB3	1:A:337:ASP:HB2	1.92	0.50
1:A:374:VAL:HB	1:A:484:MET:HE3	1.92	0.50
1:D:415:TYR:O	1:D:445:SER:HA	2.10	0.50
1:C:114:ALA:HA	1:C:117:TYR:CE2	2.46	0.50
1:D:54:VAL:CG1	1:D:484:MET:HE2	2.41	0.50
1:B:57:PHE:HB2	1:B:375:VAL:HG22	1.93	0.50
1:B:467:MET:HE1	1:C:44:GLN:NE2	2.27	0.50
1:C:60:ASP:HB2	1:C:332[B]:GLU:OE2	2.11	0.50
1:D:228:PRO:HB3	1:D:249:GLY:HA2	1.94	0.49
1:A:314:GLU:HG2	1:A:361:LYS:HG2	1.95	0.49
1:B:132:ALA:HB3	1:C:24:ARG:HA	1.95	0.49
1:C:136:ARG:HG2	1:C:137:THR:HG23	1.95	0.49
1:A:95:VAL:HB	1:D:473:GLY:HA2	1.94	0.48
15:B:609:TRS:H12	1:C:492:ALA:HB2	1.94	0.48
1:C:93:PRO:HD2	1:C:464:LYS:HB3	1.95	0.48
1:A:116:ALA:O	1:A:478:ASN:HA	2.14	0.48
1:D:82:GLY:O	1:D:85:THR:HB	2.13	0.48
1:A:93:PRO:HD2	1:A:464:LYS:HB3	1.96	0.48
1:B:116:ALA:O	1:B:478:ASN:HA	2.13	0.48
1:D:190:ASN:HB2	1:D:245:THR:O	2.14	0.48
1:C:102:ASN:HB2	1:C:105:ALA:HB3	1.96	0.48
1:D:56:MET:HB2	1:D:484:MET:HE1	1.95	0.48
1:D:224:LYS:HG2	1:D:292:PRO:O	2.14	0.48
1:B:68:THR:HG21	1:C:457:GLU:HA	1.95	0.47
1:A:475:HIS:ND1	17:A:703:HOH:O	2.32	0.47
1:B:435:ASP:OD2	1:B:438:HIS:ND1	2.47	0.47
1:B:203:ASP:O	1:B:207:GLN:HG3	2.14	0.47
1:B:95:VAL:HA	1:B:461:VAL:O	2.14	0.47
1:C:212:ILE:C	1:C:214:ASP:H	2.23	0.47
1:D:114:ALA:HA	1:D:117:TYR:CZ	2.50	0.47
1:B:202:LYS:HD3	1:B:206:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:CG1	1:A:484:MET:HE2	2.45	0.47
1:A:202:LYS:NZ	17:A:717:HOH:O	2.47	0.47
1:B:166:THR:OG1	1:B:334:GLY:HA2	2.14	0.47
1:B:346:LYS:HD2	1:B:396:PHE:CE2	2.50	0.47
1:D:148:THR:HG22	1:D:153:TRP:CD1	2.50	0.47
1:A:184:ARG:NH1	6:A:601[A]:XDC:O3	2.30	0.47
1:A:450:ARG:CZ	1:A:451:HIS:CE1	2.98	0.47
1:A:136:ARG:HG2	1:A:137:THR:HG23	1.97	0.46
1:B:444:GLN:HG3	17:B:762:HOH:O	2.14	0.46
1:B:60:ASP:HB3	1:B:337:ASP:HB2	1.96	0.46
1:A:415:TYR:O	1:A:445:SER:HA	2.15	0.46
1:B:122:LYS:HB2	1:C:29:TRP:CE2	2.51	0.46
1:B:370:ASP:OD1	10:B:606:GOL:O1	2.32	0.46
1:B:20:PRO:HB2	1:B:23:GLU:HG3	1.99	0.45
1:D:60:ASP:HB2	1:D:332[B]:GLU:OE2	2.17	0.45
1:D:109:ASP:HB2	6:D:602:XDC:N3	2.30	0.45
1:A:310:SER:O	1:A:314:GLU:HG3	2.17	0.45
1:D:223:ARG:HD3	1:D:289:LEU:O	2.16	0.45
1:B:260:LYS:HD2	1:B:285:TYR:CG	2.52	0.45
1:C:429:GLU:OE2	1:C:434:VAL:HG21	2.17	0.45
6:C:602[A]:XDC:O4	6:C:602[A]:XDC:N3	2.48	0.45
1:C:450:ARG:NH2	1:C:451:HIS:CE1	2.85	0.45
1:C:171[B]:HIS:NE2	17:C:702:HOH:O	2.36	0.44
1:D:137:THR:HG22	1:D:183:ASP:OD2	2.16	0.44
1:A:114:ALA:HA	1:A:117:TYR:CZ	2.52	0.44
1:C:60:ASP:HB3	1:C:337:ASP:HB2	2.00	0.43
1:C:309:LEU:O	1:C:313:VAL:HG23	2.18	0.43
1:D:241:LYS:HA	1:D:241:LYS:HD2	1.87	0.43
1:D:197:LEU:HD22	10:D:607:GOL:H11	2.00	0.43
1:C:451:HIS:CG	6:C:602[A]:XDC:O	2.72	0.43
1:D:148:THR:HG22	1:D:153:TRP:HE1	1.81	0.43
1:B:58:LEU:HD12	1:B:60:ASP:OD1	2.19	0.43
1:C:478:ASN:O	1:C:481:PRO:HD2	2.18	0.43
1:B:60:ASP:O	1:B:336:ILE:HB	2.19	0.43
1:B:405:THR:HG21	1:C:448:PRO:HB2	2.00	0.43
1:C:346:LYS:HA	1:C:396:PHE:CE1	2.54	0.43
1:B:19:VAL:HB	1:B:24:ARG:NH1	2.33	0.43
1:C:120:GLY:C	1:C:478:ASN:HB2	2.44	0.43
1:D:184:ARG:NH2	6:D:602:XDC:O5	2.45	0.43
1:B:99:LYS:HD2	1:C:71:ARG:NH1	2.33	0.43
1:A:450:ARG:CZ	1:A:451:HIS:HE1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:HB3	1:C:19:VAL:HG22	2.00	0.43
1:B:415:TYR:O	1:B:445:SER:HA	2.19	0.43
1:D:95:VAL:HA	1:D:461:VAL:O	2.18	0.43
1:D:220:GLY:O	1:D:289:LEU:HA	2.19	0.43
1:A:365:MET:HE2	1:A:365:MET:HB3	1.84	0.43
1:C:229:LYS:HG3	1:C:247:LEU:HD23	2.01	0.42
1:C:436:TYR:HA	1:C:441:TYR:CG	2.55	0.42
1:D:381:HIS:HB3	1:D:452:GLU:OE2	2.19	0.42
1:B:379:HIS:CE1	1:B:454:HIS:CD2	3.08	0.42
1:C:220:GLY:O	1:C:289:LEU:HA	2.19	0.42
1:D:54:VAL:HG13	1:D:484:MET:HE2	2.02	0.42
1:D:324:LEU:HD22	1:D:324:LEU:H	1.84	0.42
1:C:114:ALA:HA	1:C:117:TYR:CZ	2.54	0.42
1:C:223:ARG:HD3	1:C:289:LEU:O	2.19	0.42
1:A:385:PHE:HA	1:A:412:ALA:O	2.20	0.42
1:B:114:ALA:HA	1:B:117:TYR:CE2	2.55	0.42
1:D:186:TRP:HB3	1:D:192:MET:HG2	2.00	0.42
1:D:269:VAL:O	1:D:288:GLY:HA2	2.19	0.42
1:A:84:GLU:H	1:A:84:GLU:CD	2.27	0.41
1:A:175:SER:HA	1:A:178:TYR:CE2	2.55	0.41
1:B:260:LYS:HD2	1:B:285:TYR:CD2	2.56	0.41
1:B:54:VAL:HG11	1:B:484:MET:HE3	2.02	0.41
1:B:470:LEU:HD21	1:C:41:LEU:HD23	2.02	0.41
1:A:301:ARG:CZ	1:A:308:SER:HB3	2.50	0.41
1:A:343:GLY:O	1:A:442:GLN:HA	2.19	0.41
1:D:84:GLU:H	1:D:84:GLU:CD	2.28	0.41
1:A:117:TYR:OH	1:A:173:THR:HG23	2.20	0.41
1:C:186:TRP:CE3	1:C:192:MET:HE3	2.54	0.41
1:C:385:PHE:HA	1:C:412:ALA:O	2.20	0.41
1:C:210:HIS:O	1:C:213:LYS:HE3	2.21	0.41
1:A:114:ALA:HA	1:A:117:TYR:CE2	2.55	0.41
1:B:178:TYR:CE1	1:B:208:LEU:HB2	2.56	0.41
1:C:92:PHE:CZ	1:C:464:LYS:HE2	2.55	0.41
1:C:450:ARG:HH21	1:C:451:HIS:HE1	1.69	0.41
3:J:2:NAG:O3	3:J:3:BMA:H2	2.19	0.41
1:C:45:LYS:NZ	17:C:718:HOH:O	2.53	0.41
1:D:343:GLY:O	1:D:442:GLN:HA	2.20	0.41
1:A:68:THR:HG21	1:D:457:GLU:HA	2.03	0.41
1:A:314:GLU:CG	1:A:361:LYS:HG2	2.50	0.41
6:A:601[A]:XDC:O3	6:A:601[A]:XDC:C1	2.69	0.41
1:B:44:GLN:OE1	1:C:467:MET:HE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ILE:HD12	1:B:395:ILE:HA	1.91	0.41
1:D:168:ARG:HB3	1:D:170:ASN:OD1	2.21	0.41
1:D:379:HIS:CE1	1:D:454:HIS:CD2	3.09	0.41
6:C:602[A]:XDC:OXT	6:C:602[A]:XDC:C1	2.69	0.41
1:A:378:ASP:CG	1:A:379:HIS:CD2	2.99	0.40
1:C:155:LYS:HE3	1:C:214:ASP:HB3	2.02	0.40
1:D:43:LEU:HA	1:D:43:LEU:HD23	1.88	0.40
1:D:178:TYR:CE2	1:D:208:LEU:HD13	2.56	0.40
1:B:378:ASP:CG	1:B:379:HIS:CD2	2.99	0.40
1:A:435:ASP:HB3	1:A:438:HIS:ND1	2.37	0.40
1:B:186:TRP:CG	1:B:192:MET:HG2	2.56	0.40
1:A:333:GLY:HA3	1:A:355:MET:SD	2.61	0.40
1:C:57:PHE:HB2	1:C:375:VAL:HG22	2.04	0.40
1:D:243:ARG:HH12	12:D:611:NAG:H82	1.87	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:210:HIS:CD2	16:C:608:FLC:OB1[2_454]	1.39	0.81

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/493 (98%)	471 (98%)	10 (2%)	1 (0%)	43	50
1	B	481/493 (98%)	469 (98%)	10 (2%)	2 (0%)	30	31
1	C	482/493 (98%)	467 (97%)	15 (3%)	0	100	100
1	D	481/493 (98%)	469 (98%)	11 (2%)	1 (0%)	43	50
All	All	1926/1972 (98%)	1876 (97%)	46 (2%)	4 (0%)	43	50



All (4) 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

### 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	398/405 (98%)	397 (100%)	1 (0%)	86	90
1	B	399/405 (98%)	396 (99%)	3 (1%)	73	80
1	C	399/405 (98%)	398 (100%)	1 (0%)	86	90
1	D	397/405 (98%)	395 (100%)	2 (0%)	81	87
All	All	1593/1620 (98%)	1586 (100%)	7 (0%)	84	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	B	60	ASP
1	B	438	HIS
1	B	467	MET
1	C	58	LEU
1	D	58	LEU
1	D	109	ASP

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

Mol	Chain	Res	Type
1	A	32	GLN
1	A	53	ASN
1	A	440	ASN
1	A	451	HIS

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Mol	Chain	Res	Type
1	B	190	ASN
1	C	53	ASN
1	C	440	ASN
1	C	451	HIS
1	D	32	GLN
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 ⓘ

25 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	1.06	1 (7%)	17,19,21	1.10	1 (5%)
2	NAG	E	2	2	14,14,15	0.55	0	17,19,21	0.71	0
2	BMA	E	3	2	11,11,12	0.76	1 (9%)	15,15,17	0.89	0
2	MAN	E	4	2	11,11,12	0.93	0	15,15,17	1.12	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.45	0	17,19,21	0.69	0
3	NAG	F	2	3	14,14,15	0.27	0	17,19,21	0.40	0
3	BMA	F	3	3	11,11,12	1.17	1 (9%)	15,15,17	1.28	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.24	0	17,19,21	1.10	2 (11%)
4	NAG	G	2	4	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
5	NAG	H	1	1,5	14,14,15	1.61	1 (7%)	17,19,21	1.17	1 (5%)
5	NAG	H	2	5	14,14,15	0.45	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	H	3	5	11,11,12	0.85	0	15,15,17	0.66	0
5	MAN	H	4	5	11,11,12	0.76	0	15,15,17	1.28	2 (13%)
5	MAN	H	5	5	11,11,12	1.30	2 (18%)	15,15,17	1.09	1 (6%)
5	FUC	H	6	5	10,10,11	1.17	0	14,14,16	0.74	0
4	NAG	I	1	1,4	14,14,15	0.30	0	17,19,21	0.43	0
4	NAG	I	2	4	14,14,15	0.32	0	17,19,21	0.65	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.67	0	17,19,21	0.61	0
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	0.73	0
3	BMA	J	3	3	11,11,12	1.64	3 (27%)	15,15,17	1.01	0
3	NAG	K	1	1,3	14,14,15	0.34	0	17,19,21	0.54	0
3	NAG	K	2	3	14,14,15	0.31	0	17,19,21	0.68	1 (5%)
3	BMA	K	3	3	11,11,12	1.32	1 (9%)	15,15,17	0.92	0
4	NAG	L	1	1,4	14,14,15	0.45	0	17,19,21	0.56	0
4	NAG	L	2	4	14,14,15	0.63	0	17,19,21	0.57	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	BMA	K	3	3	-	2/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1	NAG	O5-C1	-5.80	1.33	1.43
3	J	3	BMA	C1-C2	3.33	1.60	1.52
3	F	3	BMA	C1-C2	3.32	1.60	1.52
2	E	1	NAG	O5-C1	-3.32	1.38	1.43
3	J	3	BMA	O5-C1	2.63	1.48	1.43
5	H	5	MAN	O5-C5	2.43	1.48	1.43
3	J	3	BMA	C4-C5	2.37	1.58	1.53
5	H	5	MAN	C4-C5	2.22	1.57	1.53
3	K	3	BMA	C4-C5	2.10	1.57	1.53
2	E	3	BMA	O5-C1	-2.04	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	4	MAN	C1-O5-C5	3.96	117.49	112.19
5	H	1	NAG	C1-O5-C5	-3.82	107.07	112.19
2	E	1	NAG	C1-O5-C5	-3.45	107.57	112.19
5	H	5	MAN	C1-O5-C5	2.90	116.07	112.19
2	E	4	MAN	C1-O5-C5	2.79	115.93	112.19
4	G	1	NAG	C1-O5-C5	2.70	115.80	112.19
4	G	2	NAG	C1-O5-C5	2.43	115.44	112.19
4	I	2	NAG	C1-O5-C5	2.12	115.03	112.19
4	G	1	NAG	C3-C4-C5	2.11	114.06	110.23
3	K	2	NAG	C1-O5-C5	2.11	115.01	112.19
3	F	3	BMA	C1-O5-C5	2.08	114.97	112.19
3	F	3	BMA	O5-C5-C4	-2.01	105.95	110.83
5	H	4	MAN	O2-C2-C3	-2.00	106.00	110.15

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	K	3	BMA	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
3	K	3	BMA	O5-C5-C6-O6
5	H	1	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6

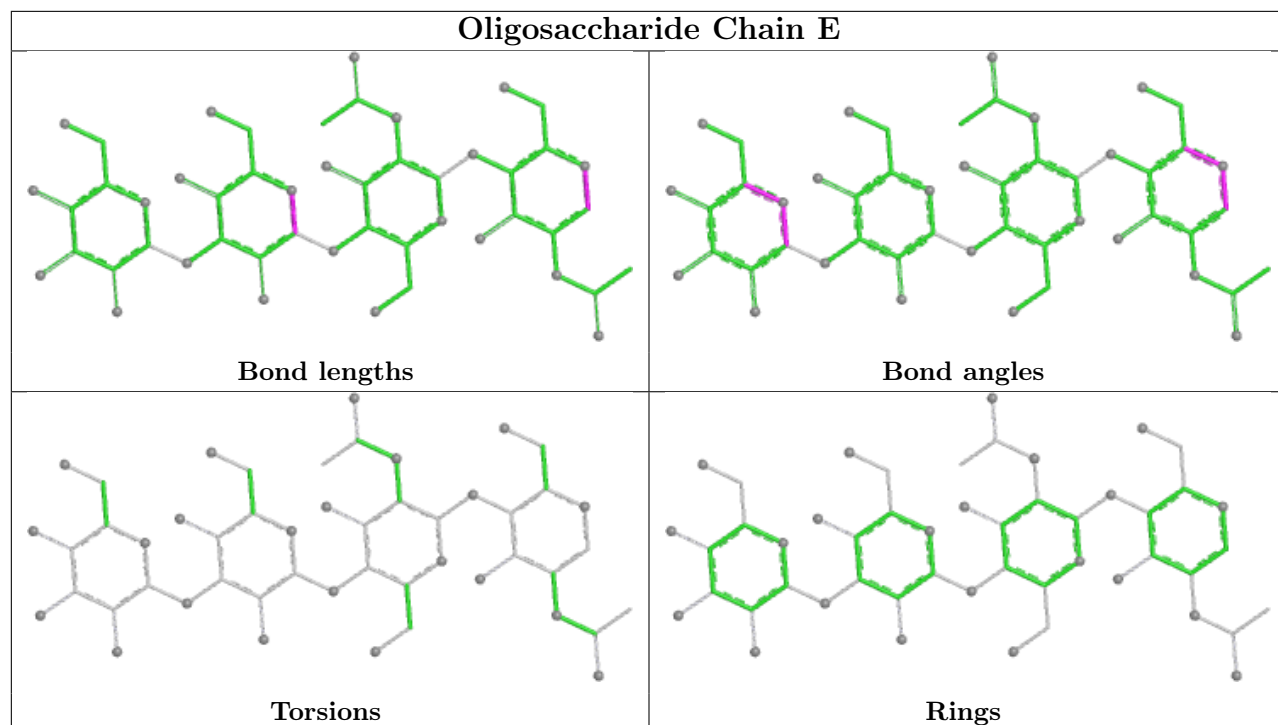
There are no ring outliers.

2 monomers are involved in 1 short contact:

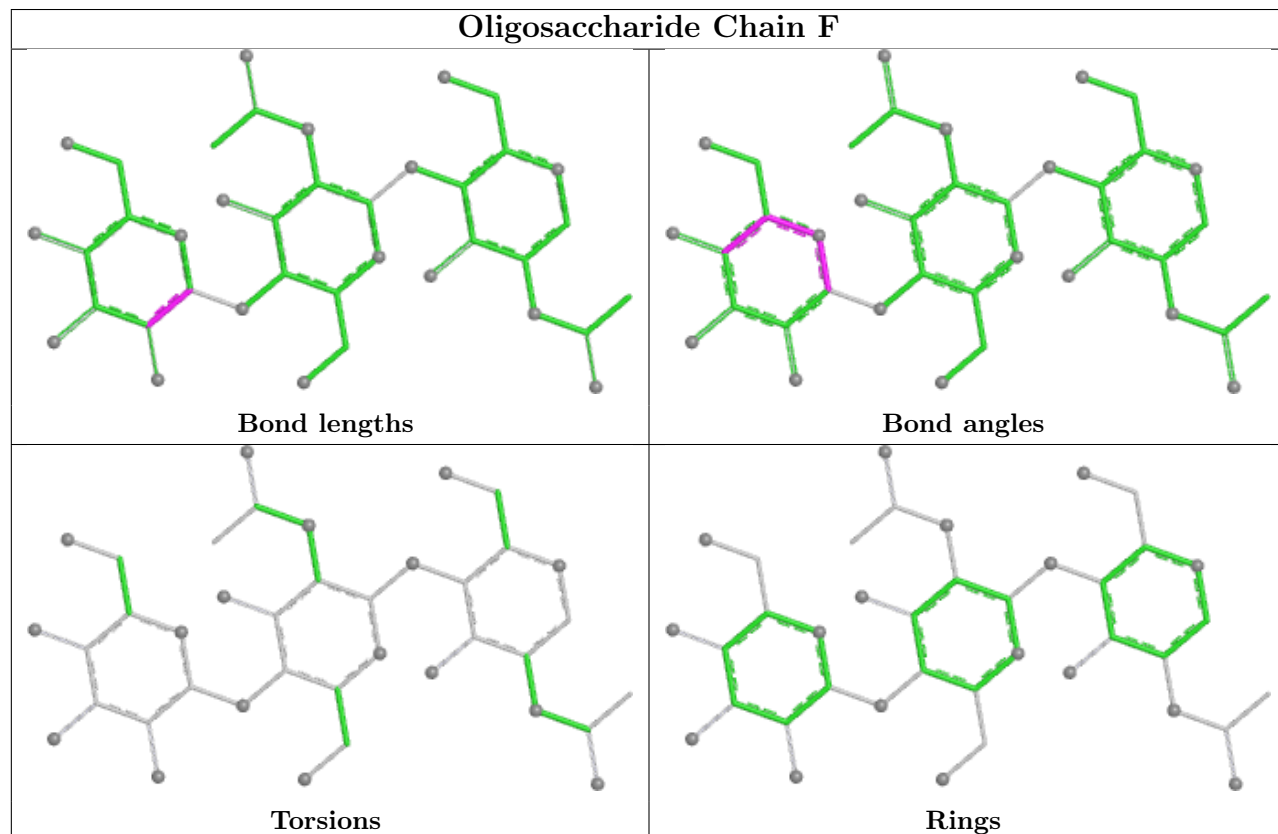
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	1	0
3	J	3	BMA	1	0

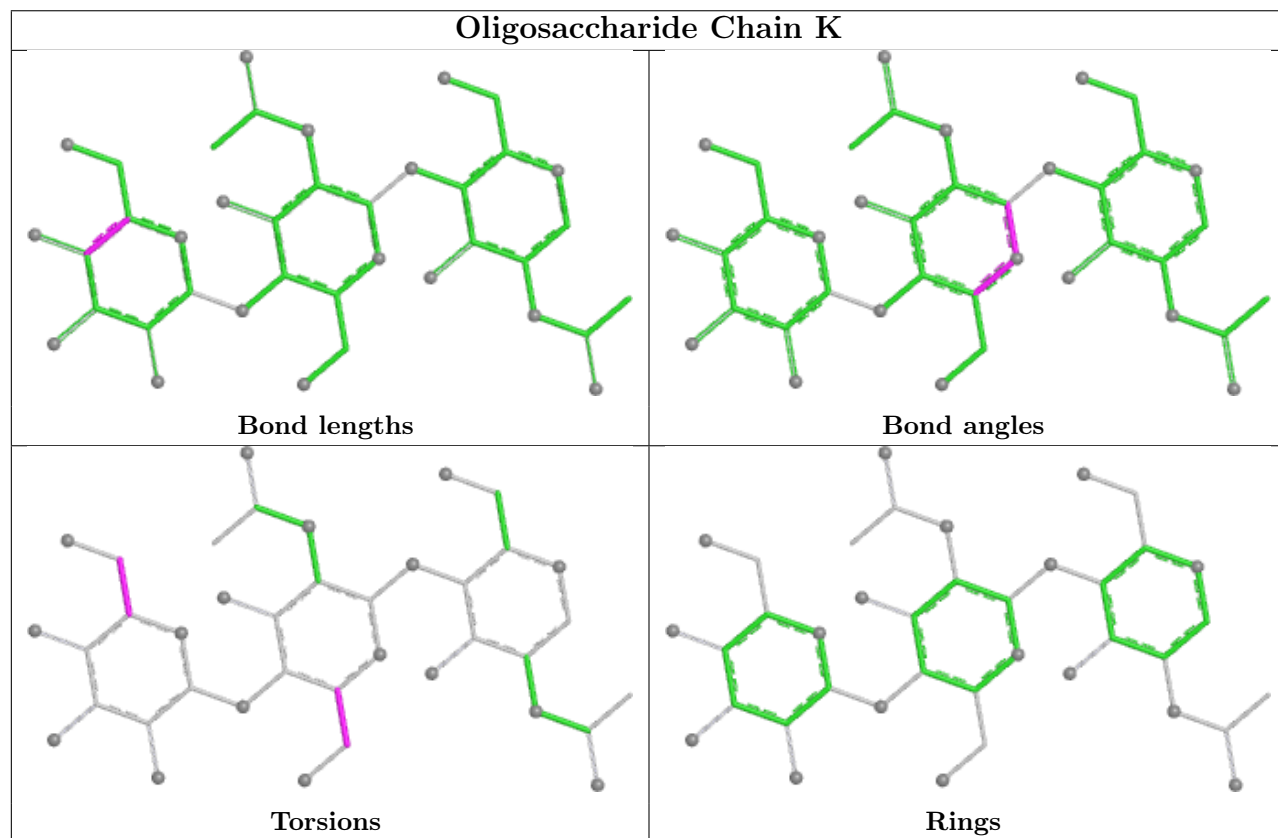
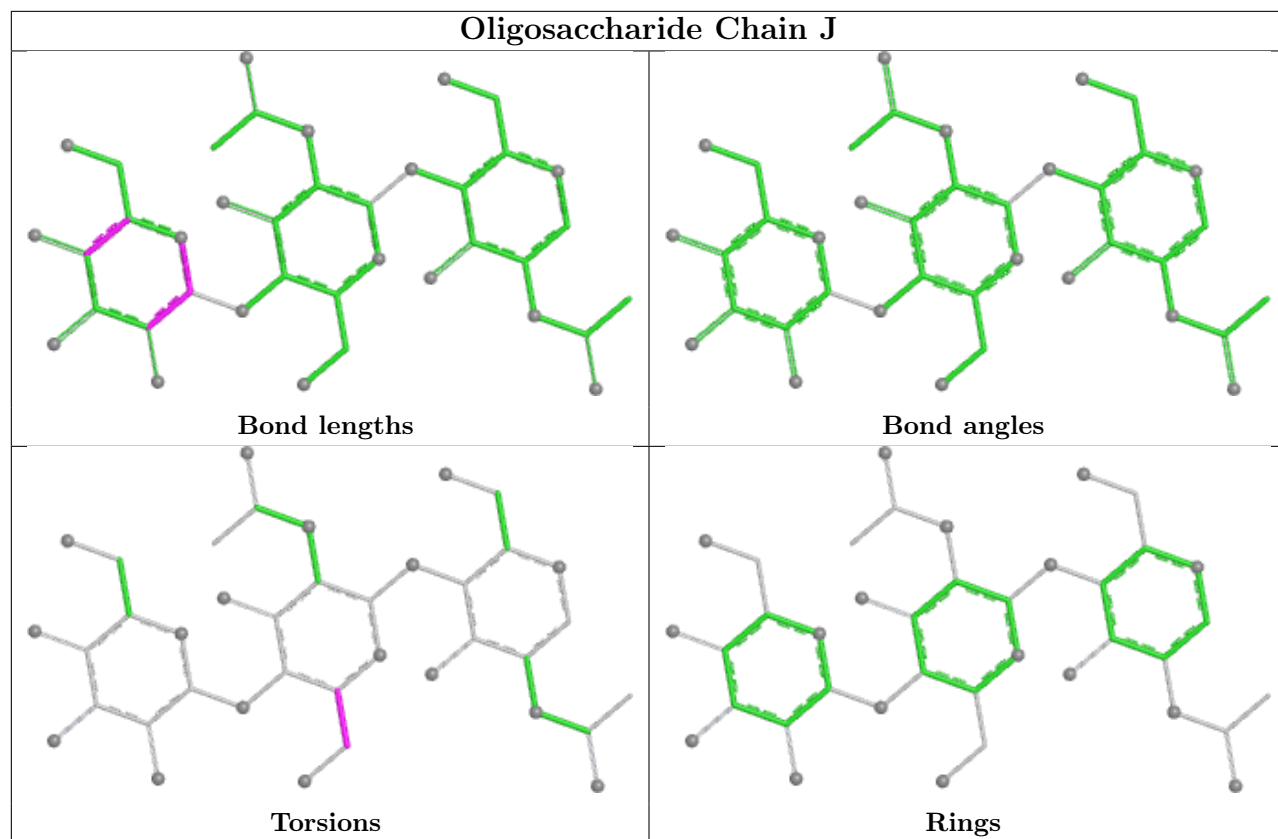
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

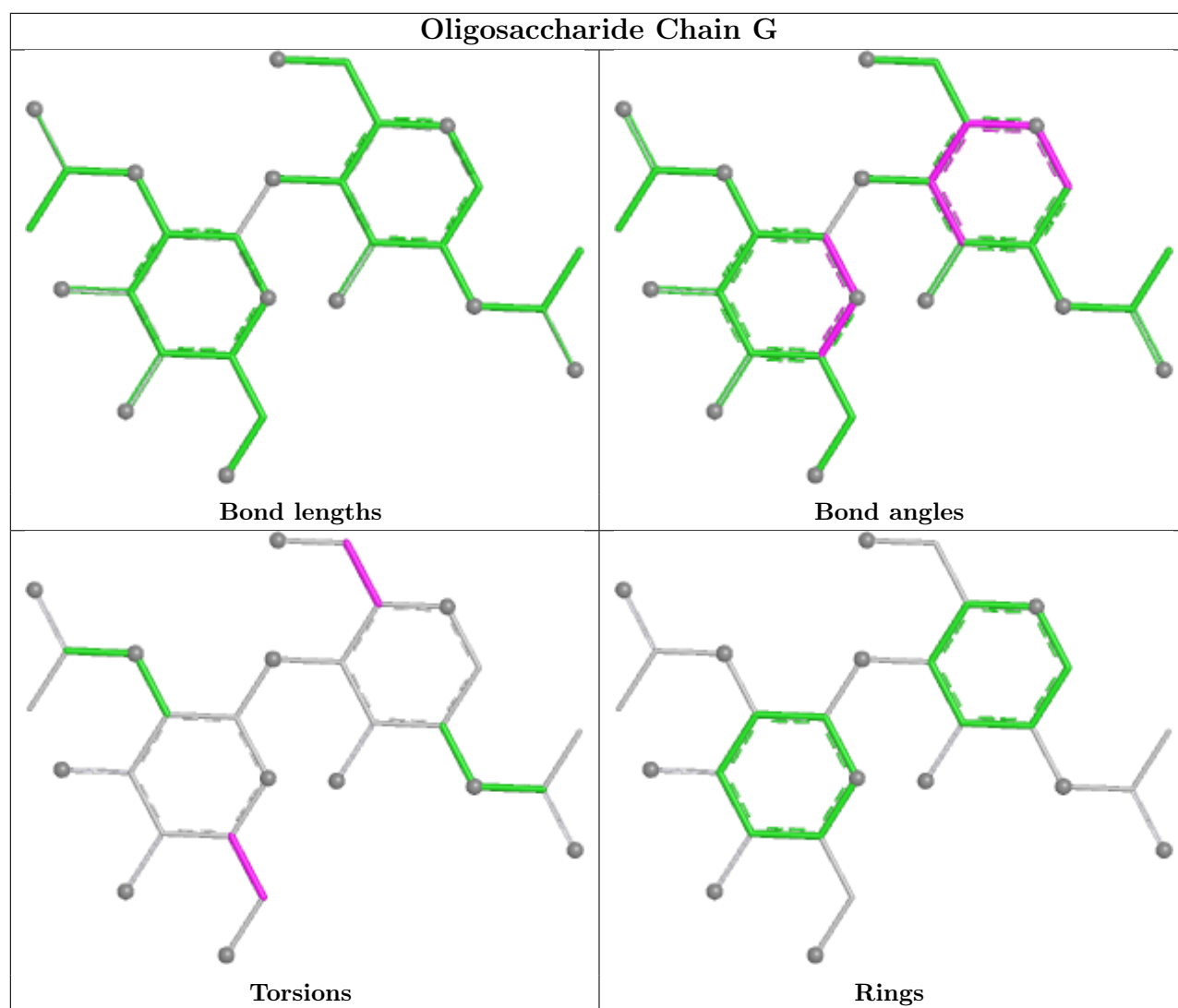
## Oligosaccharide Chain E



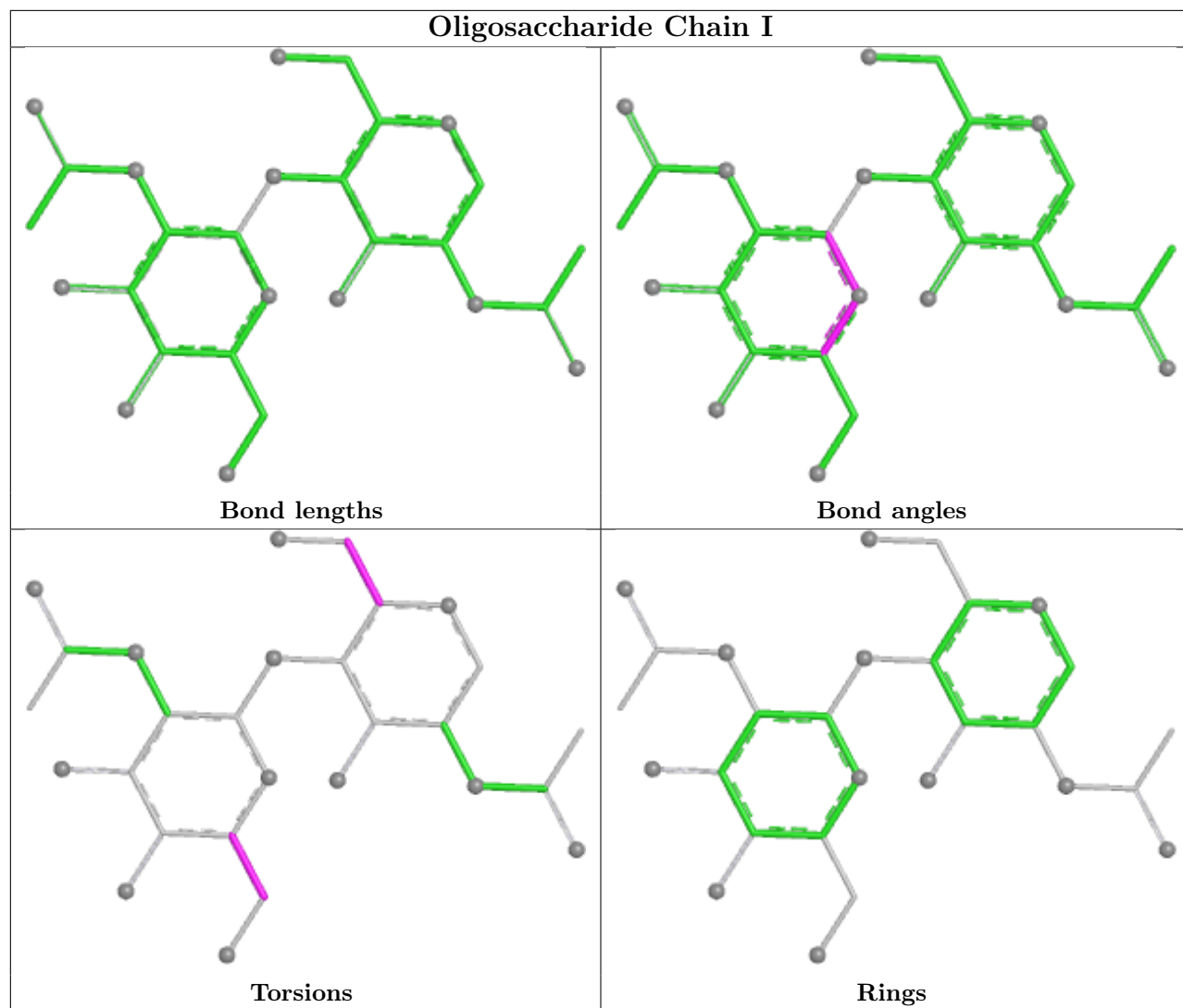
## Oligosaccharide Chain F

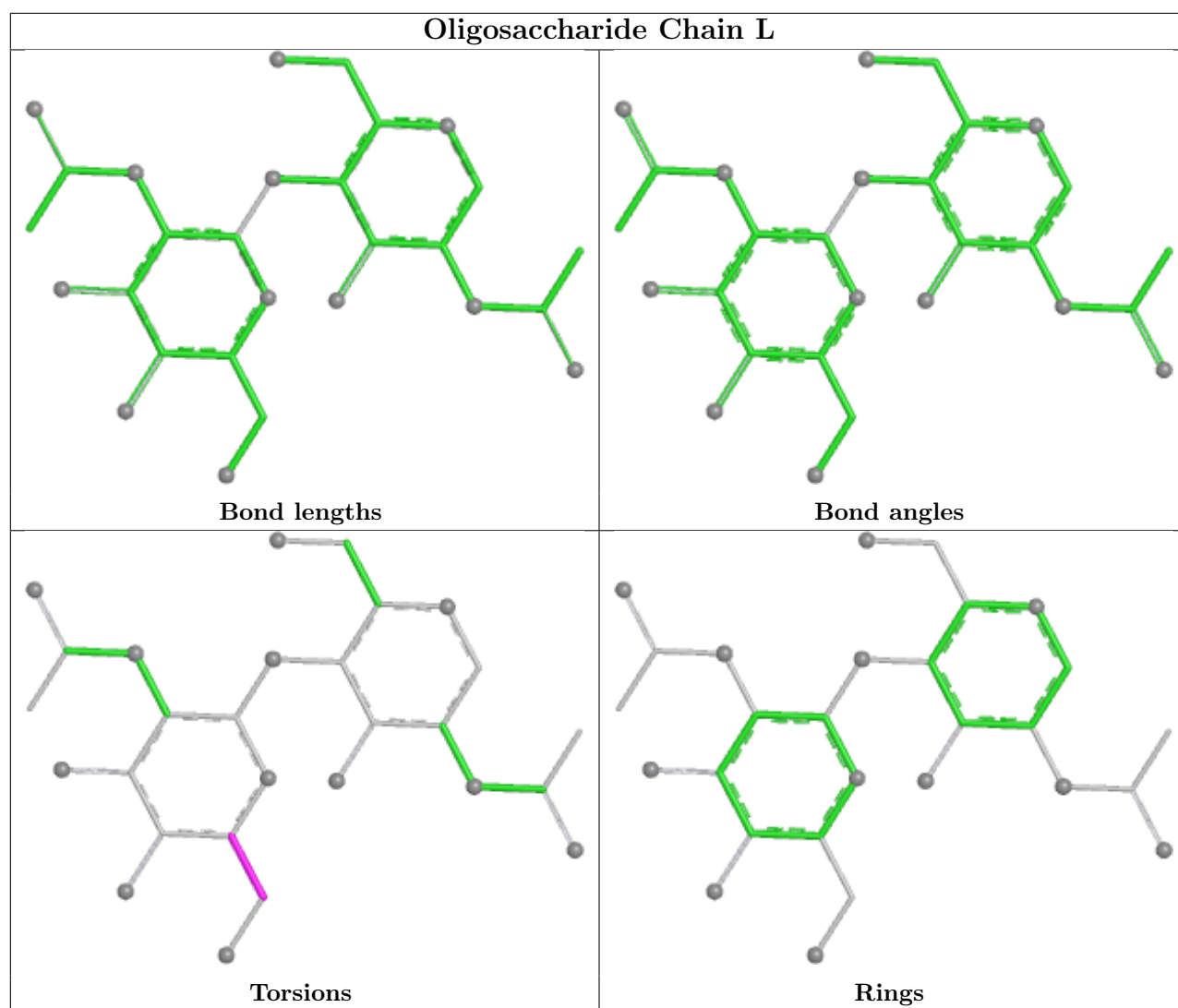


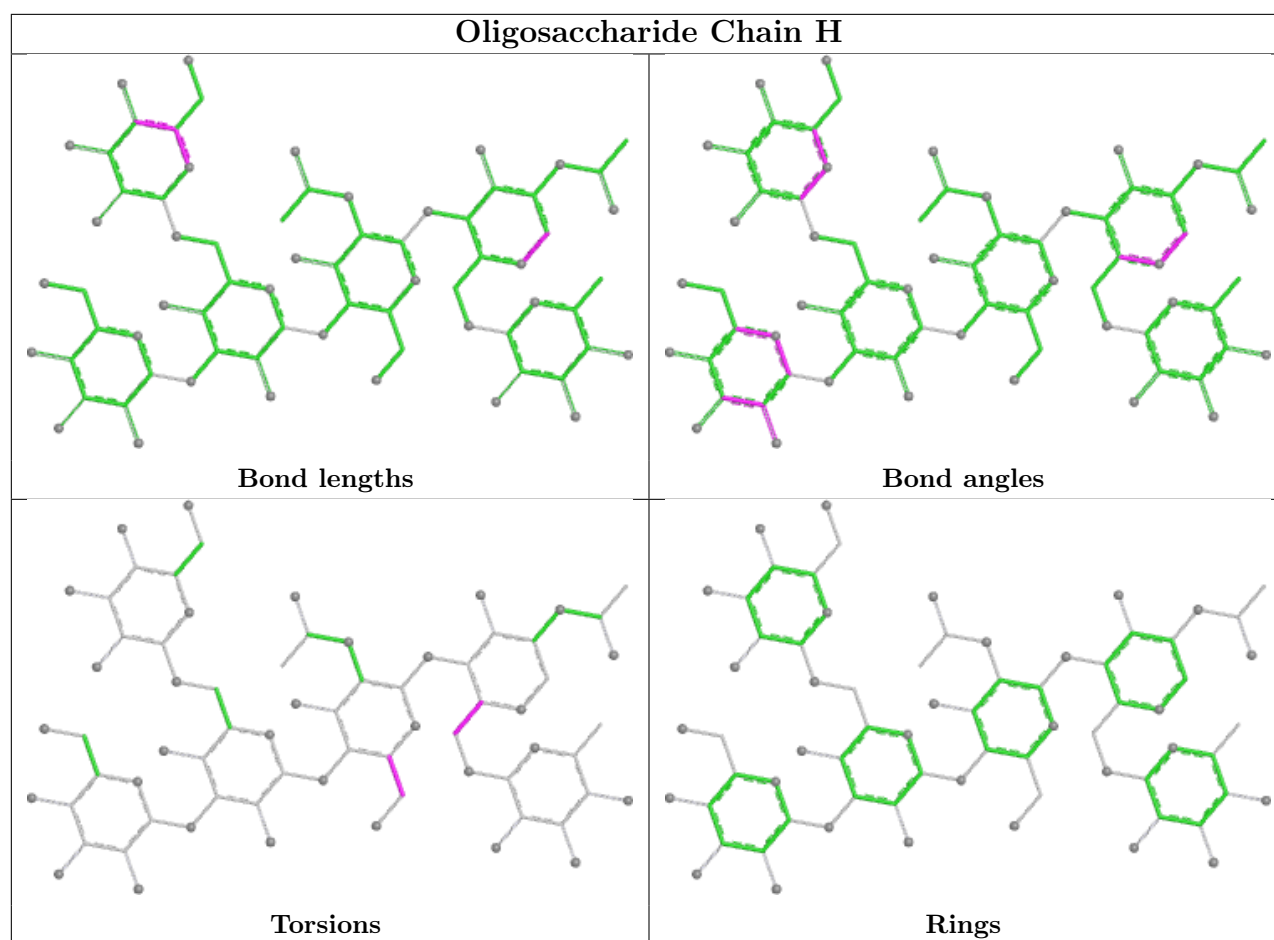












## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 16 are monoatomic - leaving 32 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	B	612	-	5,5,5	0.79	0	5,5,5	1.12	0
12	NAG	B	611	1	14,14,15	0.92	2 (14%)	17,19,21	0.66	0
12	NAG	C	612	-	14,14,15	0.73	1 (7%)	17,19,21	0.58	0
10	GOL	B	606	-	5,5,5	1.02	0	5,5,5	1.37	1 (20%)
14	PO4	B	607	-	4,4,4	0.77	0	6,6,6	0.92	0
14	PO4	C	609	-	4,4,4	1.04	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	NAG	D	611	1	14,14,15	0.95	1 (7%)	17,19,21	0.71	0
10	GOL	D	601	-	5,5,5	0.75	0	5,5,5	1.08	0
6	XDC	B	602	8,7	10,12,12	1.68	2 (20%)	11,17,17	1.38	1 (9%)
12	NAG	D	610	1	14,14,15	0.94	1 (7%)	17,19,21	0.55	0
16	FLC	C	608	-	12,12,12	2.00	6 (50%)	17,17,17	2.01	6 (35%)
12	NAG	D	612	1	14,14,15	1.09	2 (14%)	17,19,21	0.79	0
12	NAG	C	613	1	14,14,15	0.78	1 (7%)	17,19,21	0.86	1 (5%)
6	XDC	A	601[A]	8,7	10,12,12	3.00	3 (30%)	11,17,17	2.13	2 (18%)
12	NAG	A	607	1	14,14,15	0.71	1 (7%)	17,19,21	0.49	0
12	NAG	B	610	1	14,14,15	0.99	1 (7%)	17,19,21	0.60	0
10	GOL	D	607	-	5,5,5	0.96	0	5,5,5	1.08	0
12	NAG	A	608	1	14,14,15	0.84	2 (14%)	17,19,21	0.59	0
14	PO4	D	608	-	4,4,4	0.78	0	6,6,6	0.54	0
6	XDC	A	601[B]	8,7	10,12,12	2.71	3 (30%)	11,17,17	2.84	3 (27%)
13	MAN	B	601	-	11,11,12	1.12	1 (9%)	15,15,17	1.38	1 (6%)
6	XDC	C	602[A]	7	10,12,12	3.10	3 (30%)	11,17,17	1.18	1 (9%)
10	GOL	A	605	-	5,5,5	0.94	0	5,5,5	1.42	1 (20%)
10	GOL	D	606	-	5,5,5	1.14	1 (20%)	5,5,5	1.27	0
15	TRS	B	609	-	7,7,7	0.26	0	9,9,9	0.57	0
10	GOL	C	607	-	5,5,5	0.88	0	5,5,5	1.08	0
12	NAG	C	611	1	14,14,15	0.72	1 (7%)	17,19,21	0.52	0
6	XDC	C	602[B]	7	10,12,12	2.23	3 (30%)	11,17,17	1.99	2 (18%)
10	GOL	C	601	-	5,5,5	0.16	0	5,5,5	0.20	0
6	XDC	D	602	7	10,12,12	1.93	2 (20%)	11,17,17	2.52	5 (45%)
10	GOL	A	609	-	5,5,5	0.68	0	5,5,5	1.35	1 (20%)
10	GOL	C	606	-	5,5,5	0.82	0	5,5,5	1.32	1 (20%)

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	B	612	-	-	1/4/4/4	-
12	NAG	B	611	1	-	0/6/23/26	0/1/1/1
12	NAG	C	612	-	-	3/6/23/26	0/1/1/1
10	GOL	B	606	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	D	611	1	-	3/6/23/26	0/1/1/1
10	GOL	D	601	-	-	0/4/4/4	-
6	XDC	B	602	8,7	-	4/8/13/13	-
12	NAG	D	610	1	-	1/6/23/26	0/1/1/1
16	FLC	C	608	-	-	9/16/16/16	-
12	NAG	D	612	1	-	0/6/23/26	0/1/1/1
12	NAG	C	613	1	-	1/6/23/26	0/1/1/1
6	XDC	A	601[A]	8,7	-	5/8/13/13	-
12	NAG	A	607	1	-	2/6/23/26	0/1/1/1
12	NAG	B	610	1	-	2/6/23/26	0/1/1/1
10	GOL	D	607	-	-	4/4/4/4	-
12	NAG	A	608	1	-	1/6/23/26	0/1/1/1
6	XDC	A	601[B]	8,7	-	7/8/13/13	-
13	MAN	B	601	-	-	1/2/19/22	0/1/1/1
6	XDC	C	602[A]	7	-	4/8/13/13	-
10	GOL	A	605	-	-	4/4/4/4	-
10	GOL	D	606	-	-	3/4/4/4	-
15	TRS	B	609	-	-	5/9/9/9	-
10	GOL	C	607	-	-	0/4/4/4	-
12	NAG	C	611	1	-	2/6/23/26	0/1/1/1
6	XDC	C	602[B]	7	-	7/8/13/13	-
10	GOL	C	601	-	-	1/4/4/4	-
6	XDC	D	602	7	-	2/8/13/13	-
10	GOL	A	609	-	-	2/4/4/4	-
10	GOL	C	606	-	-	4/4/4/4	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601[A]	XDC	P1-O3	7.00	1.57	1.46
6	A	601[B]	XDC	P1-N2	-6.11	1.52	1.61
6	C	602[A]	XDC	P1-N2	-5.73	1.52	1.61
6	C	602[A]	XDC	P1-O5	-5.68	1.42	1.54
6	C	602[A]	XDC	P1-O4	-4.92	1.44	1.54
6	C	602[B]	XDC	P1-O5	-4.38	1.45	1.54
6	A	601[A]	XDC	P1-N2	-4.33	1.54	1.61
6	D	602	XDC	P1-O4	-4.10	1.46	1.54
6	C	602[B]	XDC	P1-O4	-4.07	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601[B]	XDC	P1-O4	-4.05	1.46	1.54
6	A	601[A]	XDC	P1-O4	-3.97	1.46	1.54
6	B	602	XDC	P1-O3	3.75	1.52	1.46
16	C	608	FLC	OG1-CGC	3.30	1.32	1.22
16	C	608	FLC	OB1-CBC	3.27	1.32	1.22
6	C	602[B]	XDC	P1-N2	-3.19	1.56	1.61
6	D	602	XDC	P1-O3	3.11	1.51	1.46
12	B	610	NAG	O5-C1	3.08	1.48	1.43
12	D	610	NAG	O5-C1	3.02	1.48	1.43
6	A	601[B]	XDC	P1-O5	-3.02	1.48	1.54
12	D	612	NAG	C1-C2	2.97	1.56	1.52
16	C	608	FLC	OA1-CAC	2.87	1.31	1.22
16	C	608	FLC	OG2-CGC	-2.71	1.21	1.30
12	D	611	NAG	O5-C1	-2.69	1.39	1.43
12	D	612	NAG	O5-C1	2.65	1.48	1.43
12	B	611	NAG	O5-C1	2.56	1.48	1.43
13	B	601	MAN	C2-C3	2.40	1.56	1.52
12	C	612	NAG	C1-C2	2.34	1.55	1.52
6	B	602	XDC	P1-O4	-2.32	1.49	1.54
12	C	613	NAG	C1-C2	2.32	1.55	1.52
16	C	608	FLC	OA2-CAC	-2.32	1.23	1.30
16	C	608	FLC	OB2-CBC	-2.28	1.22	1.30
12	A	607	NAG	O5-C1	2.22	1.47	1.43
12	A	608	NAG	C1-C2	2.17	1.55	1.52
12	C	611	NAG	O5-C1	2.15	1.47	1.43
12	A	608	NAG	O5-C1	2.15	1.47	1.43
12	B	611	NAG	C1-C2	2.12	1.55	1.52
10	D	606	GOL	C1-C2	2.05	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601[B]	XDC	O4-P1-O3	-6.81	99.56	113.77
6	A	601[A]	XDC	O4-P1-O3	-5.98	101.28	113.77
6	D	602	XDC	N3-C4-N	-5.09	114.18	118.74
6	C	602[B]	XDC	O5-P1-O3	-4.99	103.36	113.77
6	A	601[B]	XDC	N3-C4-N	4.54	122.81	118.74
16	C	608	FLC	OB2-CBC-CB	4.50	121.78	113.14
16	C	608	FLC	OB1-CBC-CB	-4.40	113.56	122.09
6	D	602	XDC	N3-C4-N2	-4.39	112.84	124.28
6	A	601[B]	XDC	N3-C4-N2	-4.11	113.56	124.28
13	B	601	MAN	C1-O5-C5	4.10	117.67	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	XDC	O4-P1-O3	-3.47	106.52	113.77
16	C	608	FLC	OA1-CAC-CA	-3.17	113.98	122.95
12	C	613	NAG	C1-O5-C5	2.87	116.03	112.19
6	D	602	XDC	O4-P1-O3	-2.73	108.06	113.77
6	D	602	XDC	O5-P1-O3	-2.72	108.10	113.77
16	C	608	FLC	OA2-CAC-CA	2.65	122.76	114.35
6	D	602	XDC	N-C4-N2	2.55	132.86	122.30
6	C	602[A]	XDC	O5-P1-O3	-2.51	108.53	113.77
16	C	608	FLC	OG1-CGC-CG	-2.51	115.85	122.95
6	C	602[B]	XDC	N3-C4-N2	-2.36	118.14	124.28
6	A	601[A]	XDC	O5-P1-O3	2.35	118.67	113.77
10	A	609	GOL	C3-C2-C1	-2.31	103.32	111.80
10	B	606	GOL	C3-C2-C1	-2.24	103.60	111.80
10	A	605	GOL	C3-C2-C1	-2.19	103.77	111.80
10	C	606	GOL	C3-C2-C1	-2.19	103.78	111.80
16	C	608	FLC	OG2-CGC-CG	2.15	121.17	114.35

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601[A]	XDC	O-C-CA-N
6	A	601[A]	XDC	OXT-C-CA-N
6	A	601[A]	XDC	C-CA-N-C1
6	A	601[A]	XDC	C-CA-N-C4
6	A	601[B]	XDC	O-C-CA-N
6	A	601[B]	XDC	OXT-C-CA-N
6	A	601[B]	XDC	C-CA-N-C1
6	A	601[B]	XDC	C-CA-N-C4
6	A	601[B]	XDC	N2-C4-N-C1
6	A	601[B]	XDC	N3-C4-N-C1
6	A	601[B]	XDC	N3-C4-N-CA
6	B	602	XDC	OXT-C-CA-N
6	B	602	XDC	C-CA-N-C1
6	B	602	XDC	C-CA-N-C4
6	C	602[A]	XDC	C-CA-N-C1
6	C	602[A]	XDC	C-CA-N-C4
6	C	602[B]	XDC	C-CA-N-C1
6	C	602[B]	XDC	C-CA-N-C4
6	C	602[B]	XDC	N2-C4-N-C1
6	C	602[B]	XDC	N3-C4-N-C1
6	C	602[B]	XDC	N3-C4-N-CA

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Mol	Chain	Res	Type	Atoms
10	A	605	GOL	C1-C2-C3-O3
10	A	609	GOL	O1-C1-C2-C3
10	B	606	GOL	O1-C1-C2-C3
10	B	606	GOL	C1-C2-C3-O3
10	C	606	GOL	O1-C1-C2-C3
10	C	606	GOL	C1-C2-C3-O3
10	D	606	GOL	O1-C1-C2-C3
10	D	607	GOL	O1-C1-C2-C3
15	B	609	TRS	C3-C-C1-O1
16	C	608	FLC	CAC-CA-CB-OHB
16	C	608	FLC	OHB-CB-CBC-OB1
12	C	611	NAG	O5-C5-C6-O6
6	B	602	XDC	O-C-CA-N
6	C	602[A]	XDC	O-C-CA-N
6	C	602[A]	XDC	OXT-C-CA-N
6	D	602	XDC	O-C-CA-N
6	D	602	XDC	OXT-C-CA-N
12	C	612	NAG	O5-C5-C6-O6
12	C	612	NAG	C4-C5-C6-O6
12	C	611	NAG	C4-C5-C6-O6
10	C	606	GOL	O1-C1-C2-O2
12	D	611	NAG	O5-C5-C6-O6
12	B	610	NAG	O5-C5-C6-O6
12	B	610	NAG	C4-C5-C6-O6
16	C	608	FLC	CAC-CA-CB-CBC
10	A	605	GOL	O1-C1-C2-C3
16	C	608	FLC	CG-CB-CBC-OB1
10	A	605	GOL	O2-C2-C3-O3
10	A	609	GOL	O1-C1-C2-O2
10	B	606	GOL	O1-C1-C2-O2
10	D	606	GOL	O1-C1-C2-O2
10	D	607	GOL	O1-C1-C2-O2
15	B	609	TRS	C2-C-C1-O1
16	C	608	FLC	CAC-CA-CB-CG
10	B	606	GOL	O2-C2-C3-O3
10	C	606	GOL	O2-C2-C3-O3
10	D	606	GOL	O2-C2-C3-O3
12	D	611	NAG	C4-C5-C6-O6
16	C	608	FLC	CA-CB-CBC-OB2
10	A	605	GOL	O1-C1-C2-O2
6	C	602[B]	XDC	OXT-C-CA-N
15	B	609	TRS	N-C-C2-O2

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Mol	Chain	Res	Type	Atoms
16	C	608	FLC	CG-CB-CBC-OB2
12	A	607	NAG	C4-C5-C6-O6
12	D	611	NAG	C3-C2-N2-C7
13	B	601	MAN	C4-C5-C6-O6
6	C	602[B]	XDC	O-C-CA-N
16	C	608	FLC	OHB-CB-CBC-OB2
15	B	609	TRS	N-C-C1-O1
10	C	601	GOL	O1-C1-C2-C3
10	D	607	GOL	C1-C2-C3-O3
12	A	607	NAG	O5-C5-C6-O6
12	A	608	NAG	C1-C2-N2-C7
12	C	612	NAG	C1-C2-N2-C7
12	C	613	NAG	C1-C2-N2-C7
12	D	610	NAG	C1-C2-N2-C7
16	C	608	FLC	CA-CB-CBC-OB1
15	B	609	TRS	C1-C-C2-O2
10	B	612	GOL	O2-C2-C3-O3
6	A	601[A]	XDC	N2-C4-N-CA
10	D	607	GOL	O2-C2-C3-O3

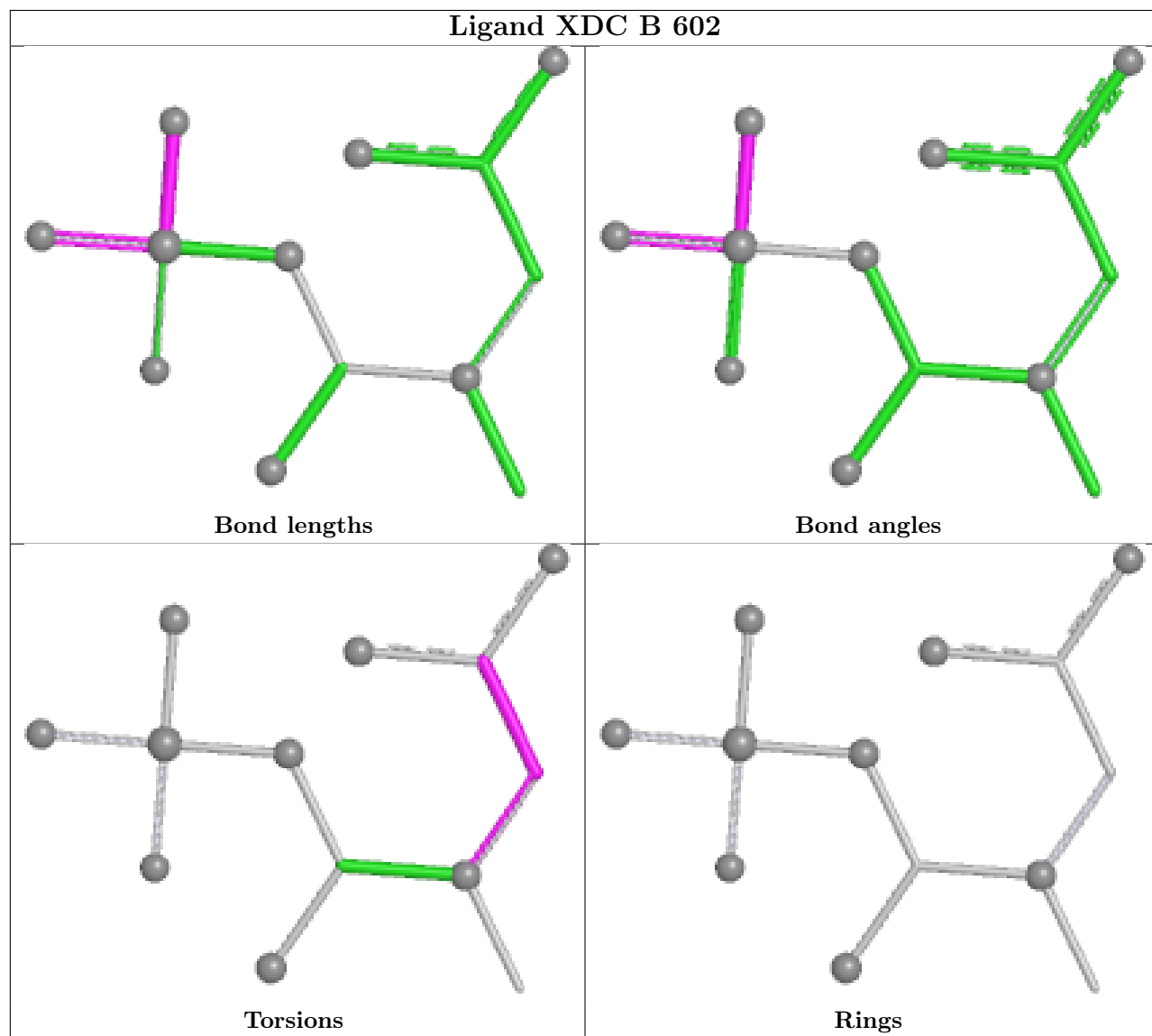
There are no ring outliers.

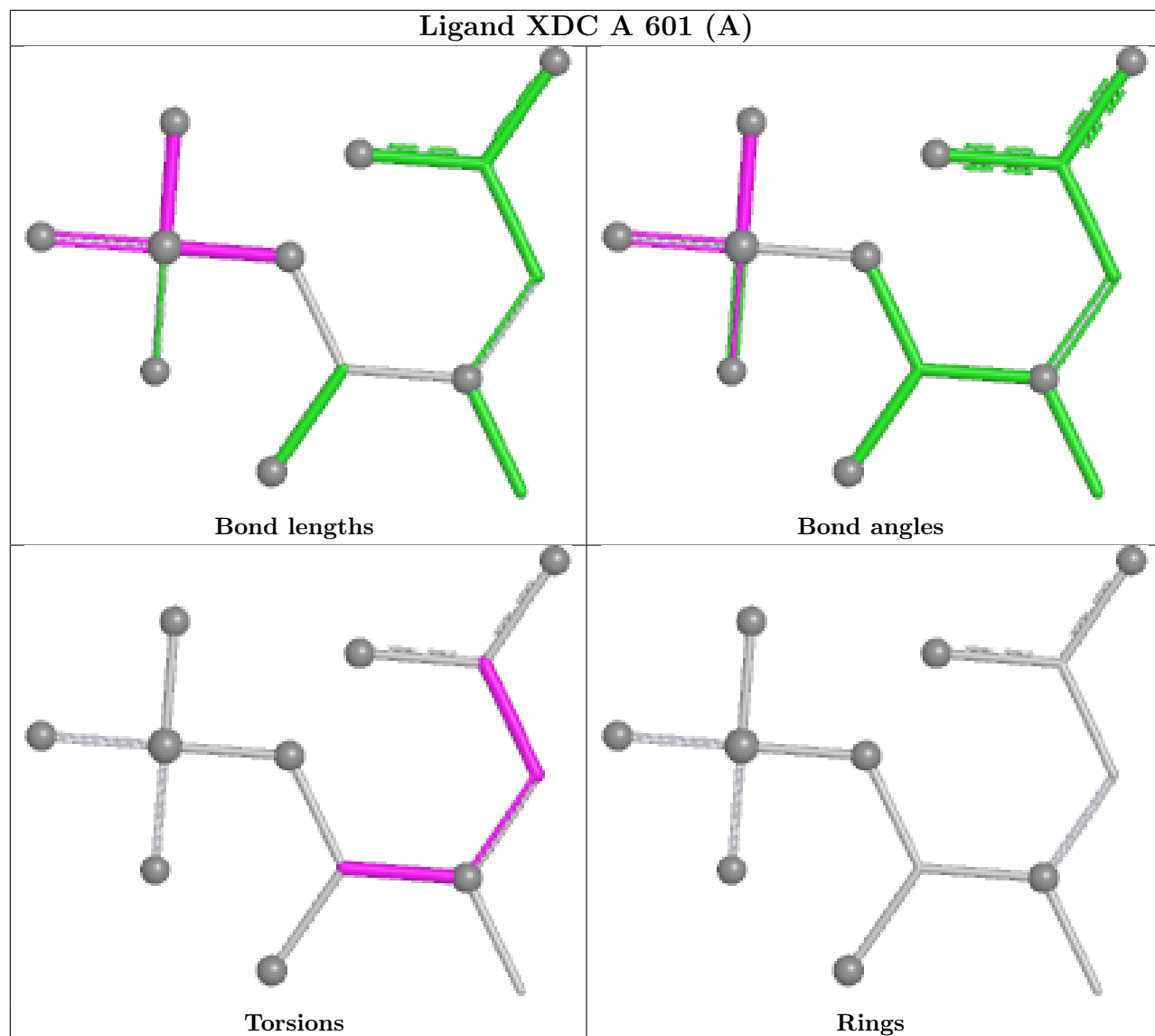
12 monomers are involved in 20 short contacts:

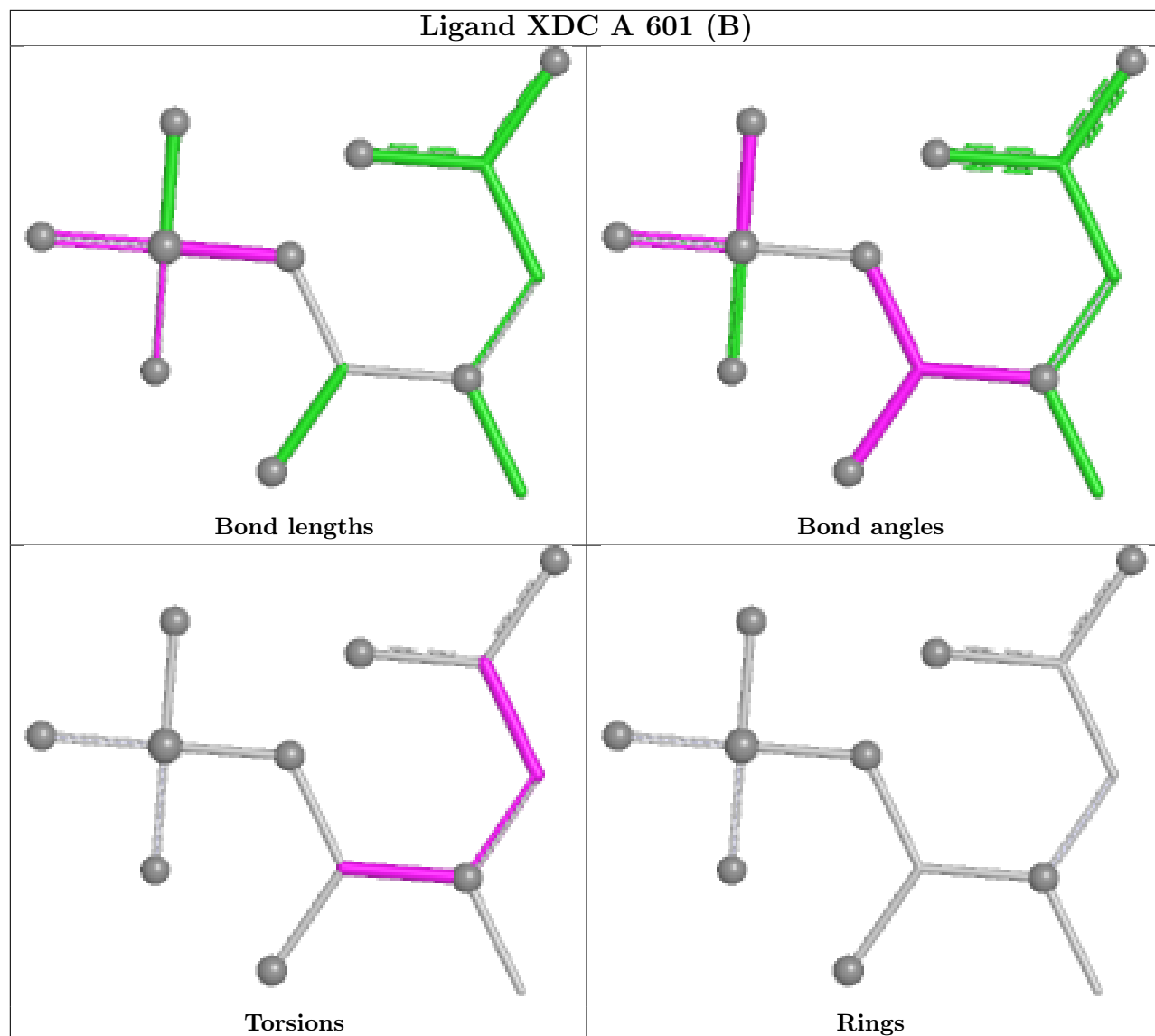
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	606	GOL	1	0
12	D	611	NAG	1	0
16	C	608	FLC	0	1
6	A	601[A]	XDC	2	0
10	D	607	GOL	1	0
6	A	601[B]	XDC	1	0
6	C	602[A]	XDC	3	0
10	D	606	GOL	1	0
15	B	609	TRS	1	0
6	C	602[B]	XDC	2	0
6	D	602	XDC	5	0
10	C	606	GOL	1	0

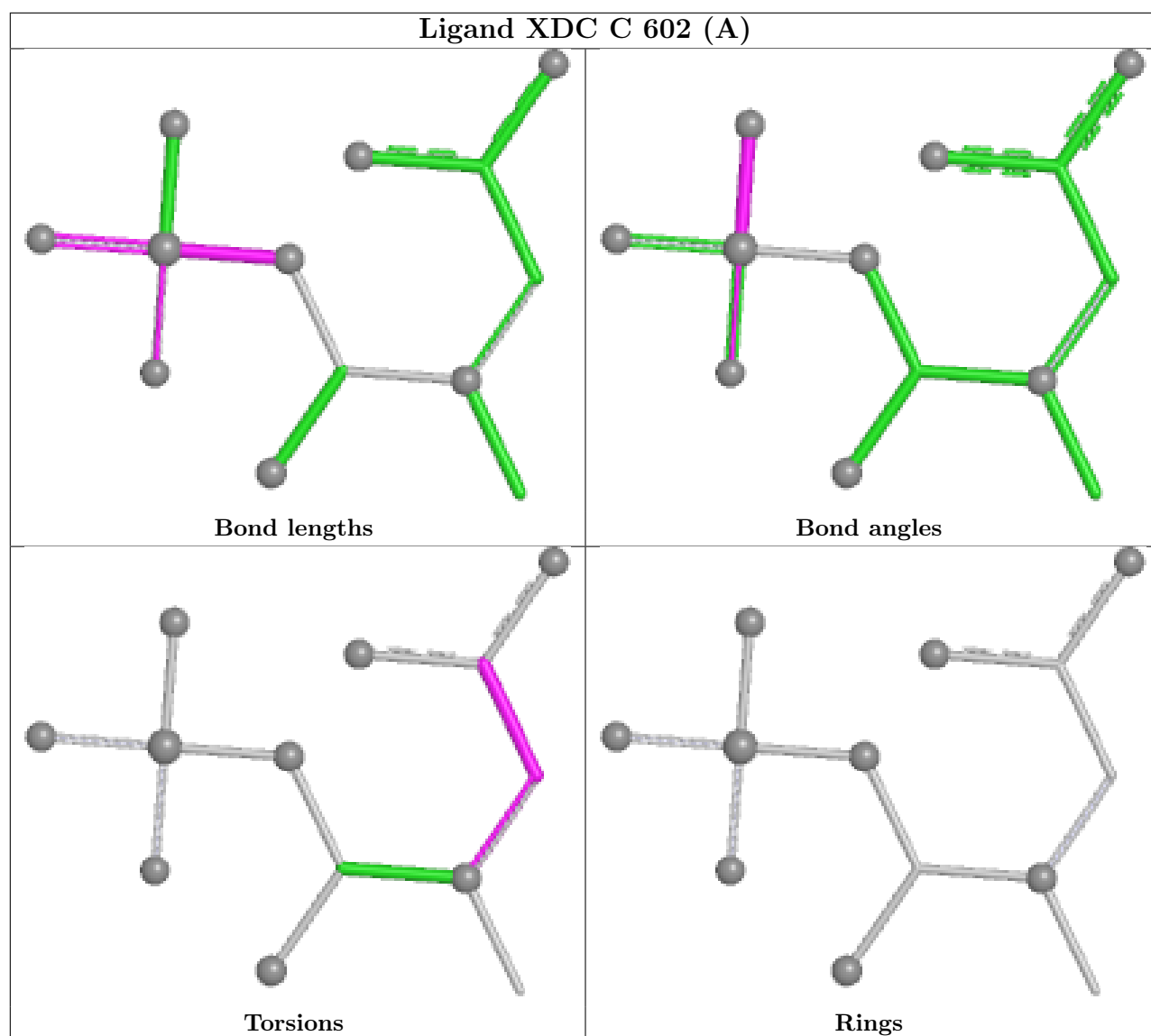
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

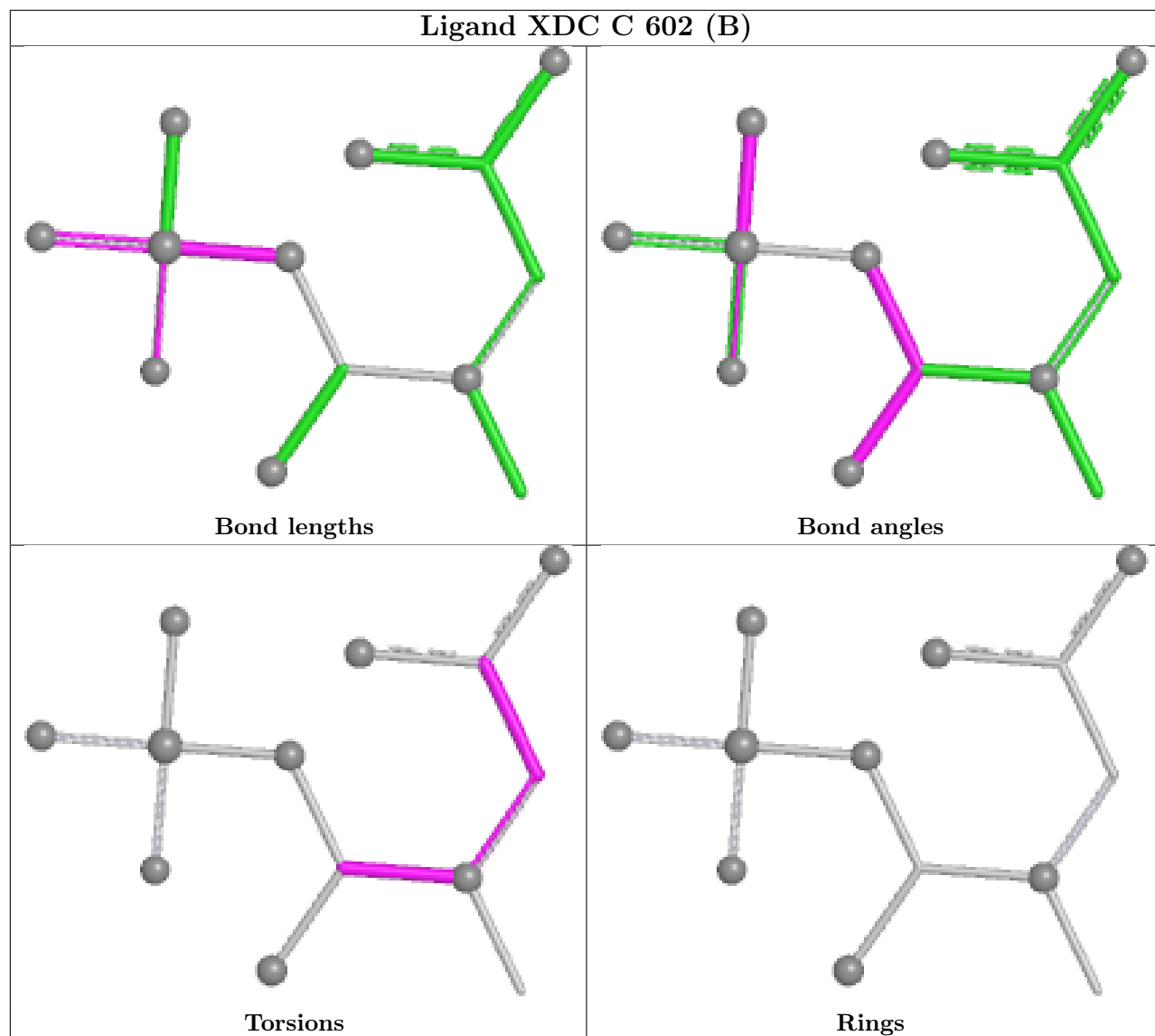
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

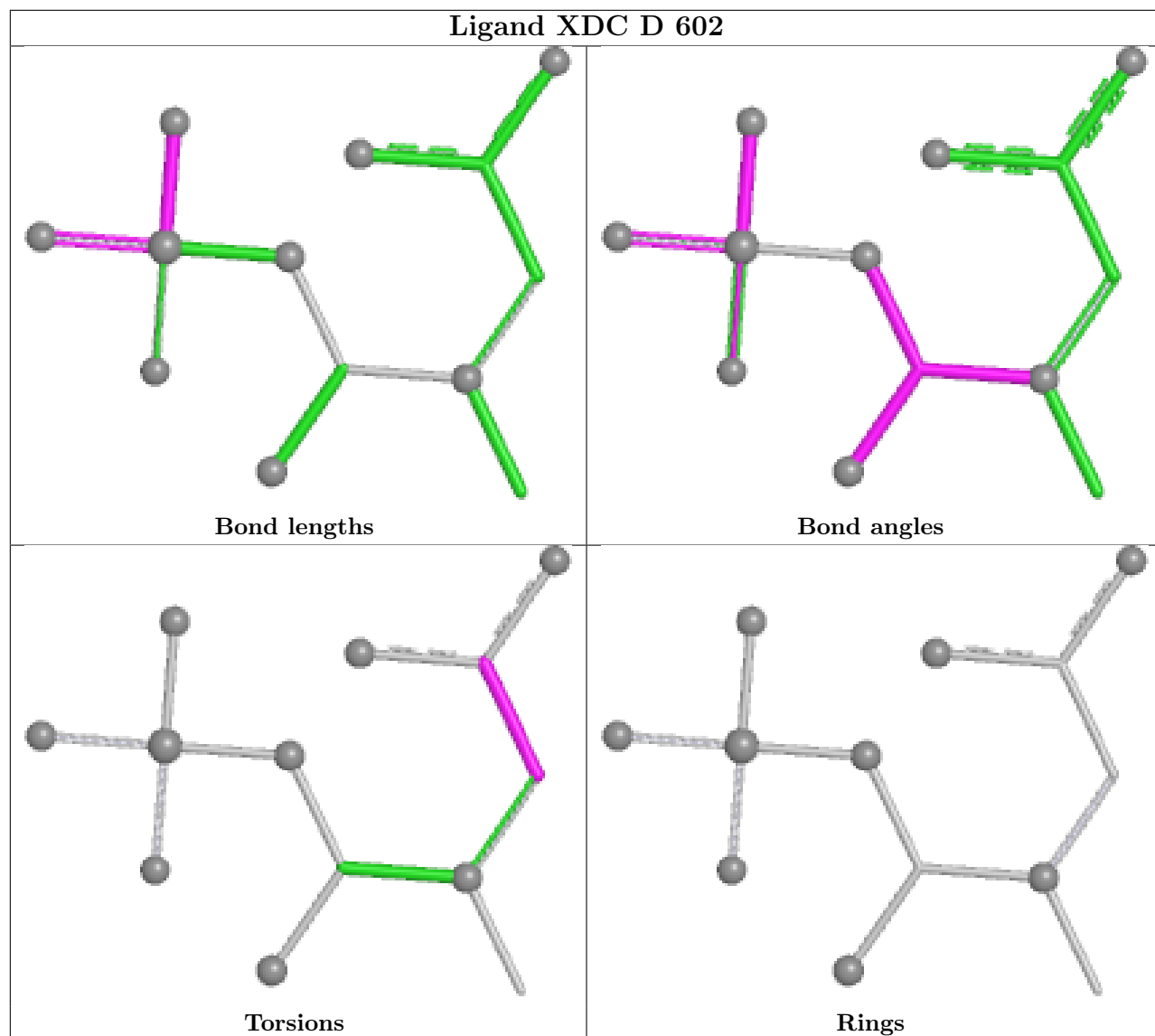












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	482/493 (97%)	-0.03	6 (1%) 76 77	20, 37, 53, 76	4 (0%)
1	B	481/493 (97%)	0.09	8 (1%) 69 70	21, 38, 59, 93	3 (0%)
1	C	482/493 (97%)	0.06	6 (1%) 76 77	22, 38, 56, 76	3 (0%)
1	D	482/493 (97%)	0.01	6 (1%) 76 77	21, 37, 55, 77	1 (0%)
All	All	1927/1972 (97%)	0.03	26 (1%) 75 76	20, 37, 56, 93	11 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	499	TRP	4.9
1	B	304	LEU	3.6
1	C	498	ALA	3.2
1	B	433	MET	3.2
1	B	263	HIS	3.1
1	A	499	TRP	3.0
1	C	433	MET	3.0
1	C	18	PHE	2.9
1	A	498	ALA	2.7
1	A	241	LYS	2.6
1	B	422	LYS	2.4
1	C	238	LEU	2.3
1	C	17	SER	2.3
1	D	324	LEU	2.2
1	D	424	VAL	2.3
1	B	262	ARG	2.2
1	D	433	MET	2.2
1	D	18	PHE	2.2
1	A	438	HIS	2.2
1	A	18	PHE	2.1
1	B	18	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	ARG	2.1
1	D	304	LEU	2.1
1	C	140	ASN	2.1
1	B	238	LEU	2.0
1	B	282	ARG	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

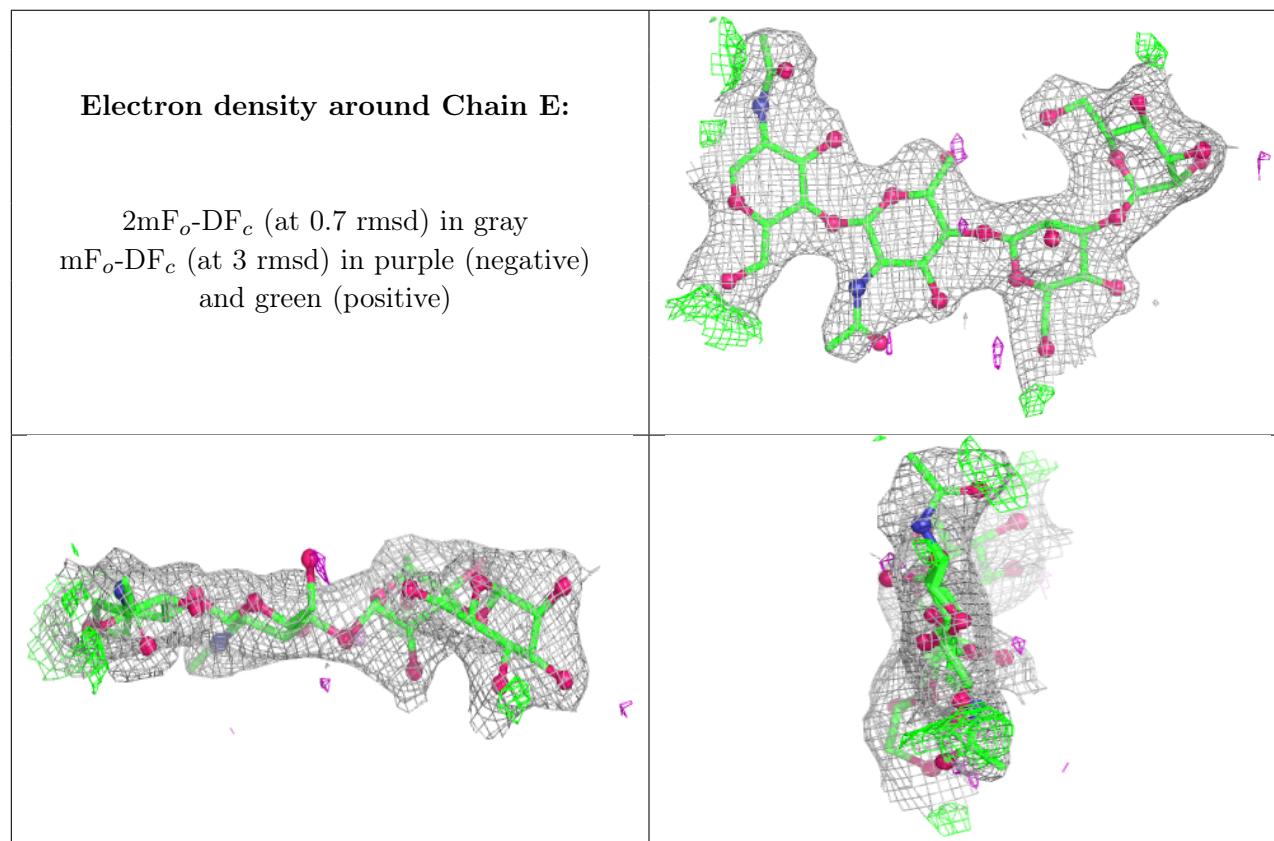
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BMA	J	3	11/12	0.35	0.19	90,98,102,103	0
3	BMA	K	3	11/12	0.41	0.23	86,96,101,107	0
4	NAG	G	2	14/15	0.47	0.20	87,91,101,108	0
4	NAG	L	2	14/15	0.50	0.20	83,89,93,96	0
3	BMA	F	3	11/12	0.61	0.17	76,83,91,93	0
3	NAG	K	2	14/15	0.63	0.19	60,84,94,97	0
4	NAG	I	2	14/15	0.72	0.15	68,83,90,91	0
3	NAG	J	2	14/15	0.72	0.18	72,83,95,103	0
4	NAG	L	1	14/15	0.73	0.14	45,73,84,90	0
5	MAN	H	5	11/12	0.74	0.16	66,73,81,83	0
4	NAG	G	1	14/15	0.76	0.16	50,69,81,83	0
3	NAG	F	2	14/15	0.78	0.16	65,69,80,84	0
5	MAN	H	4	11/12	0.82	0.13	57,62,66,73	0
5	FUC	H	6	10/11	0.82	0.17	64,71,74,81	0
3	NAG	J	1	14/15	0.84	0.14	59,63,77,81	0
4	NAG	I	1	14/15	0.84	0.14	57,62,75,76	0
5	NAG	H	2	14/15	0.86	0.14	54,59,67,71	0
2	NAG	E	1	14/15	0.87	0.11	41,46,52,53	0
3	NAG	K	1	14/15	0.88	0.12	48,57,67,74	0
2	MAN	E	4	11/12	0.88	0.10	46,53,56,61	0
5	BMA	H	3	11/12	0.88	0.11	60,63,67,73	0
5	NAG	H	1	14/15	0.89	0.11	48,53,62,65	0
2	NAG	E	2	14/15	0.89	0.15	48,55,65,73	0

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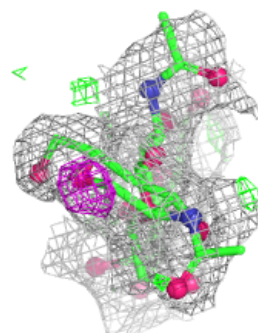
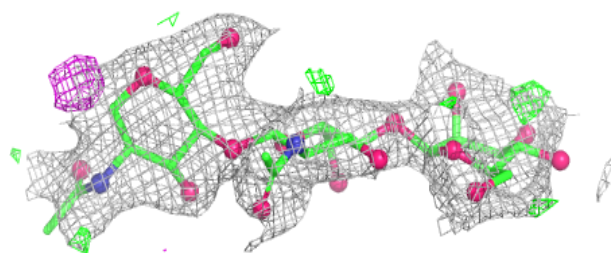
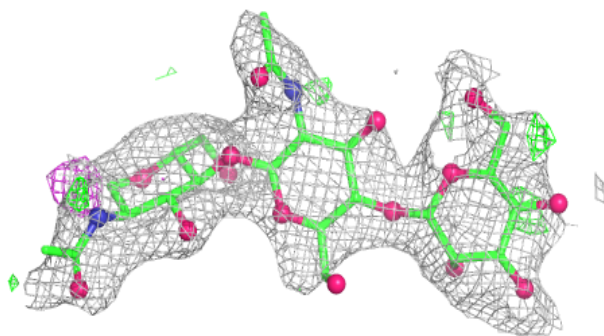
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BMA	E	3	11/12	0.90	0.11	52,53,55,58	0
3	NAG	F	1	14/15	0.90	0.12	49,54,63,63	0

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.

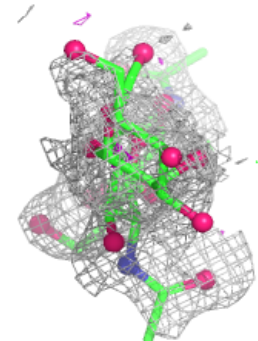
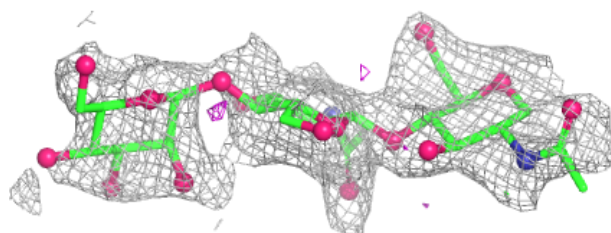
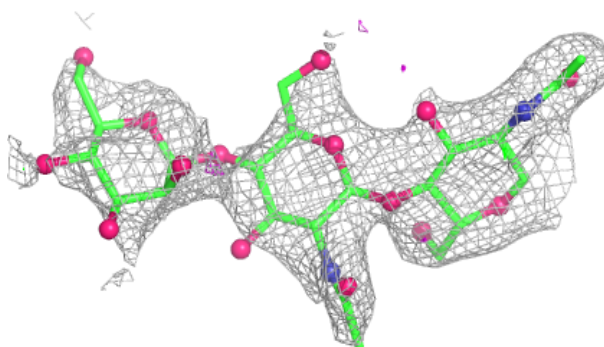


**Electron density around Chain F:**

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

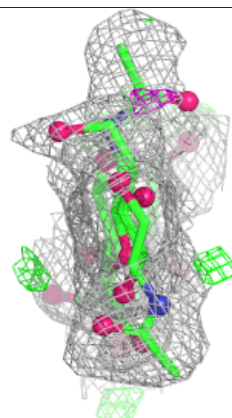
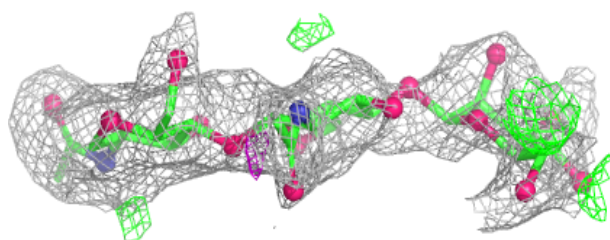
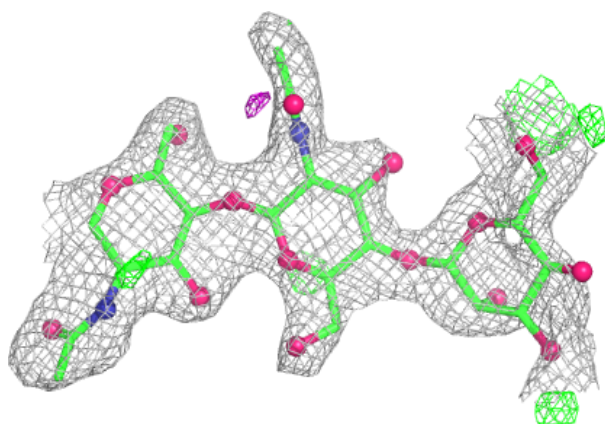
**Electron density around Chain J:**

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



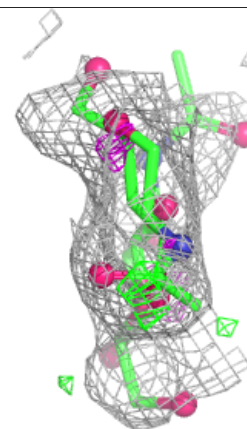
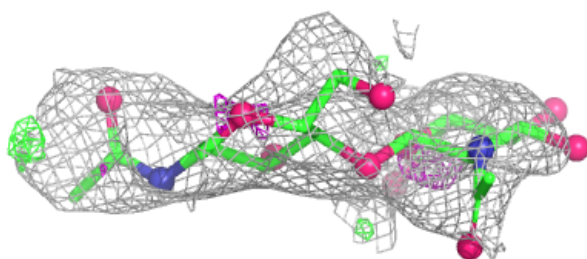
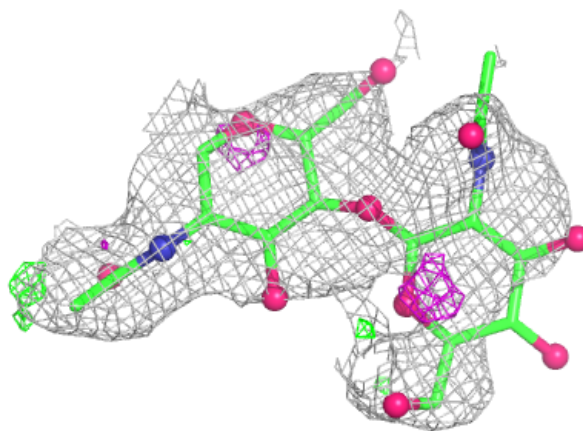
**Electron density around Chain K:**

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

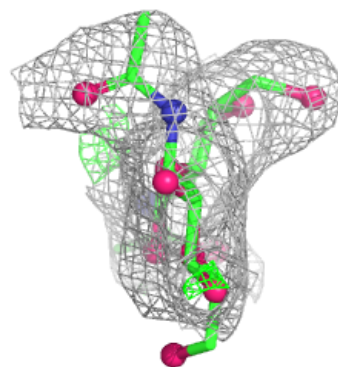
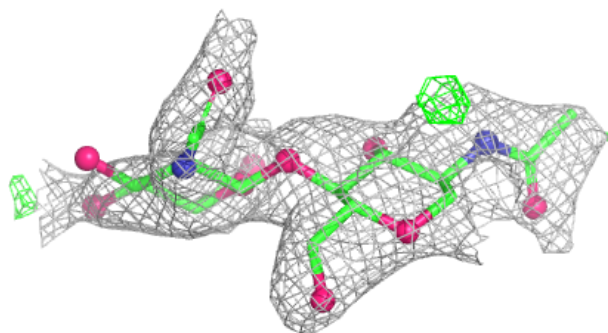
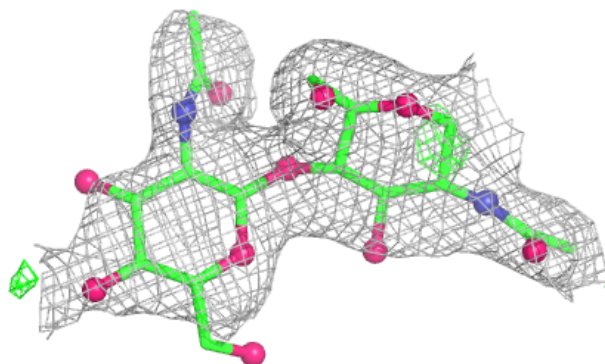


**Electron density around Chain G:**

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

**Electron density around Chain I:**

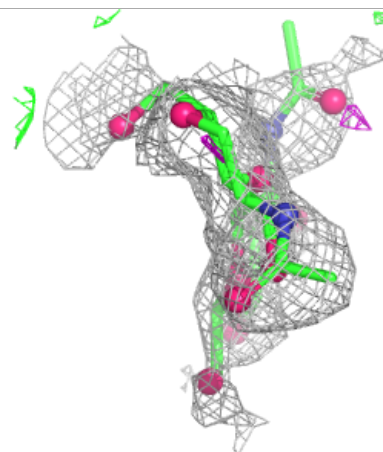
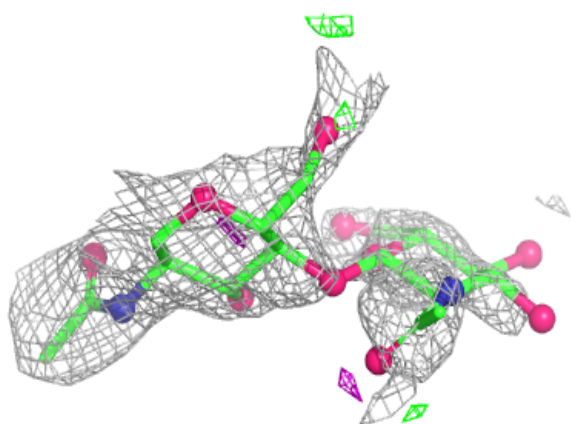
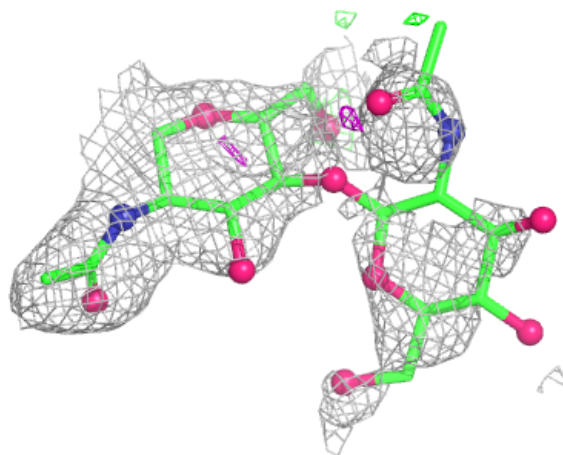
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

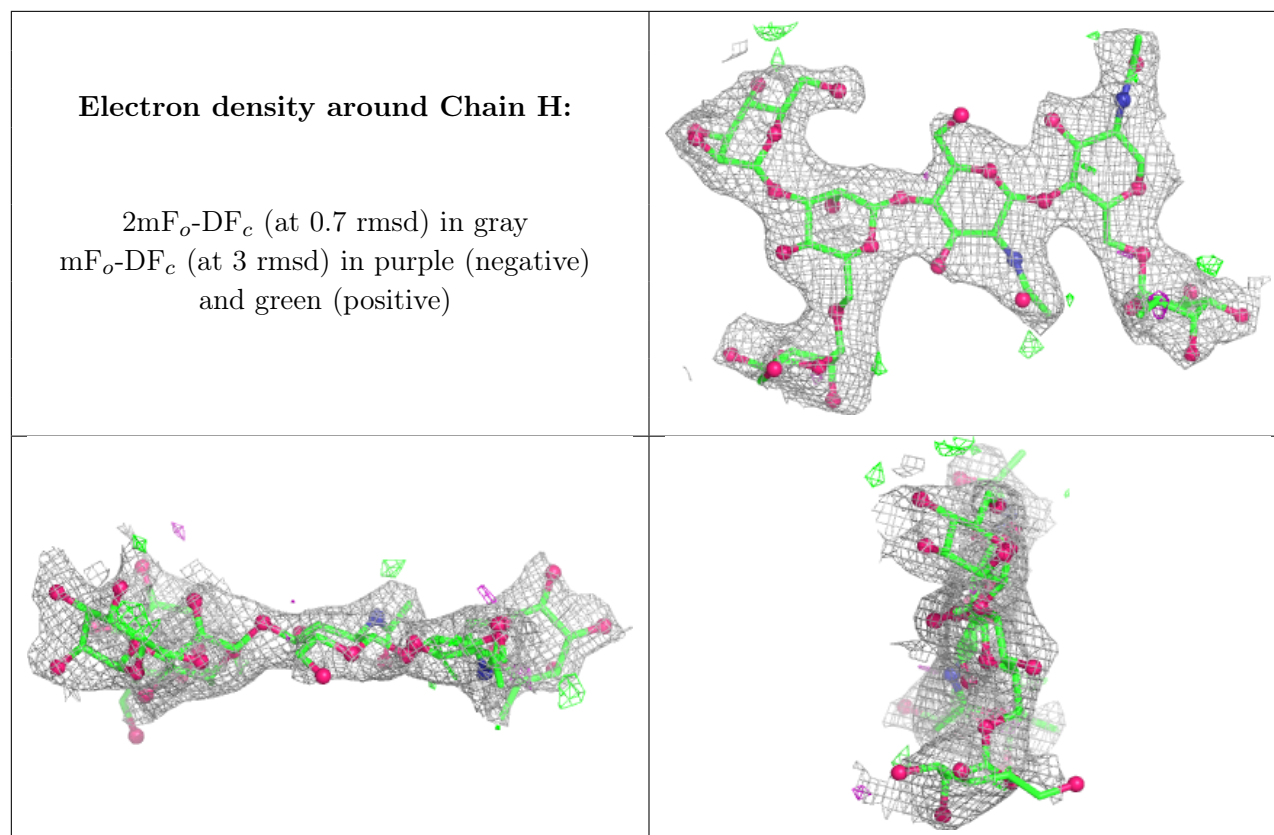




**Electron density around Chain L:**

$2mF_o-DF_c$  (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, 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	B	610	14/15	0.48	0.20	60,88,93,95	0
12	NAG	D	611	14/15	0.48	0.21	77,93,98,99	0
12	NAG	A	608	14/15	0.51	0.23	77,83,91,92	0
12	NAG	C	611	14/15	0.52	0.20	71,83,90,91	0
12	NAG	A	607	14/15	0.53	0.21	64,78,89,93	0
12	NAG	C	612	14/15	0.64	0.19	59,71,81,81	0
12	NAG	D	610	14/15	0.65	0.18	74,87,96,97	0
12	NAG	D	612	14/15	0.66	0.17	66,75,80,81	0
12	NAG	B	611	14/15	0.68	0.18	54,73,80,81	0
6	XDC	C	602[B]	13/13	0.68	0.31	38,43,48,54	13
6	XDC	C	602[A]	13/13	0.68	0.31	42,46,48,51	13
6	XDC	A	601[B]	13/13	0.75	0.24	42,48,54,58	13
6	XDC	A	601[A]	13/13	0.75	0.24	42,47,52,58	13
8	MG	D	604	1/1	0.78	0.17	38,38,38,38	1

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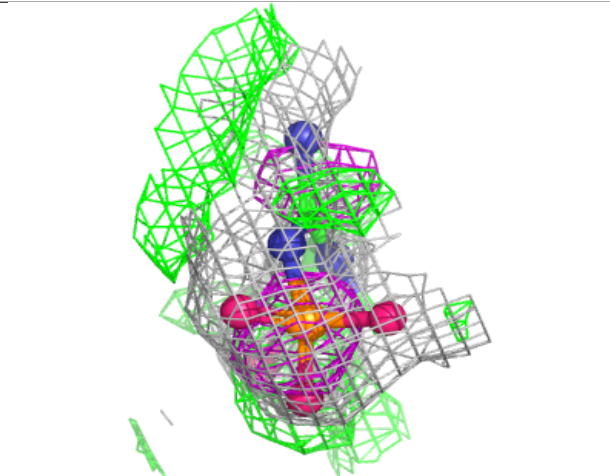
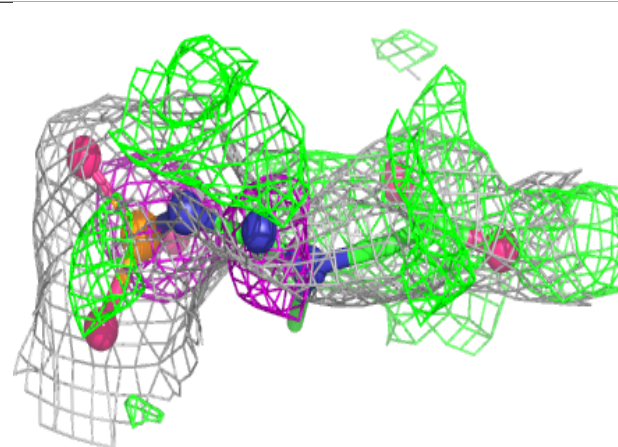
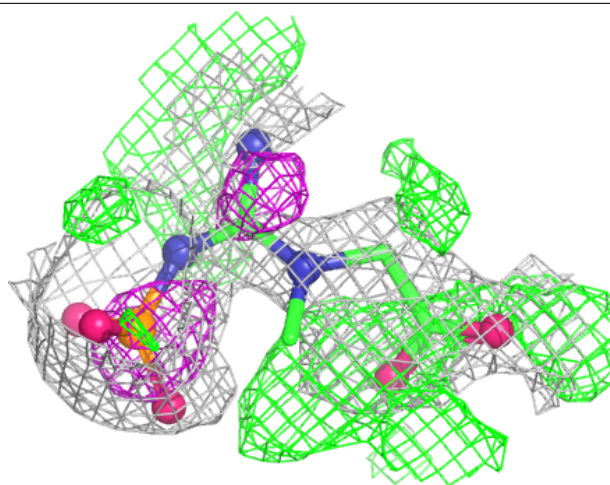
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
16	FLC	C	608	13/13	0.80	0.14	50,56,67,68	0
13	MAN	B	601	11/12	0.81	0.15	59,62,67,68	0
6	XDC	D	602	13/13	0.81	0.20	37,49,53,56	13
12	NAG	C	613	14/15	0.82	0.12	47,61,68,69	0
6	XDC	B	602	13/13	0.83	0.18	36,46,53,58	13
10	GOL	A	609	6/6	0.83	0.17	38,45,52,55	6
8	MG	C	604	1/1	0.84	0.16	42,42,42,42	0
10	GOL	C	601	6/6	0.84	0.16	39,44,46,48	6
15	TRS	B	609	8/8	0.84	0.16	45,56,64,67	0
10	GOL	D	607	6/6	0.84	0.15	39,51,52,52	0
10	GOL	B	612	6/6	0.85	0.17	35,42,43,44	6
14	PO4	C	609	5/5	0.85	0.17	39,48,54,58	5
14	PO4	D	608	5/5	0.87	0.17	41,44,56,56	5
10	GOL	D	601	6/6	0.88	0.17	41,45,51,52	0
8	MG	B	604	1/1	0.89	0.12	31,31,31,31	1
10	GOL	C	607	6/6	0.92	0.11	47,51,52,53	0
9	CA	B	605	1/1	0.92	0.20	70,70,70,70	0
10	GOL	A	605	6/6	0.93	0.10	38,39,41,45	0
14	PO4	B	607	5/5	0.93	0.11	36,41,45,49	5
9	CA	A	604	1/1	0.93	0.15	69,69,69,69	0
10	GOL	B	606	6/6	0.93	0.11	45,51,53,53	0
10	GOL	D	606	6/6	0.93	0.09	38,42,45,45	0
8	MG	A	603	1/1	0.93	0.10	34,34,34,34	1
9	CA	C	605	1/1	0.95	0.17	70,70,70,70	0
9	CA	D	605	1/1	0.96	0.10	61,61,61,61	0
10	GOL	C	606	6/6	0.96	0.09	38,42,43,43	0
11	NA	B	608	1/1	0.98	0.04	19,19,19,19	0
11	NA	D	609	1/1	0.98	0.05	21,21,21,21	0
7	ZN	D	603	1/1	0.98	0.03	38,38,38,38	0
11	NA	A	606	1/1	0.99	0.07	22,22,22,22	0
7	ZN	C	603	1/1	0.99	0.03	37,37,37,37	0
11	NA	C	610	1/1	0.99	0.03	22,22,22,22	0
7	ZN	B	603	1/1	0.99	0.03	35,35,35,35	0
7	ZN	A	602	1/1	1.00	0.02	35,35,35,35	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.



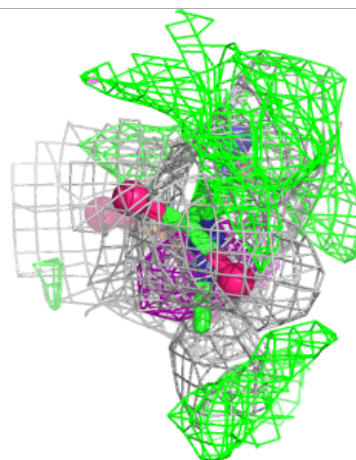
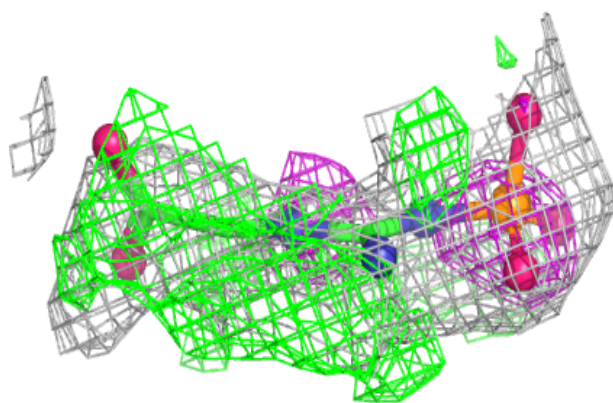
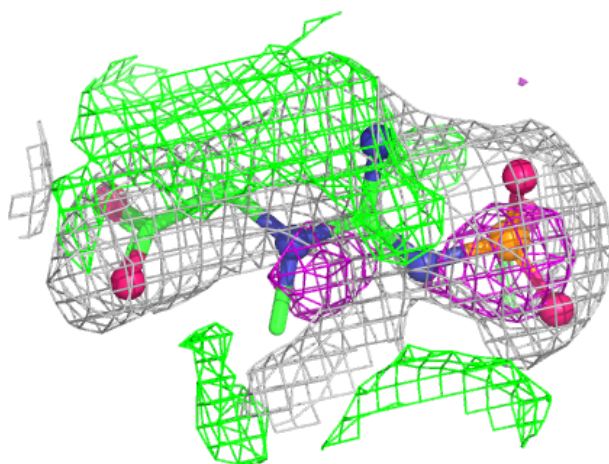
**Electron density around XDC C 602 (B):**

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



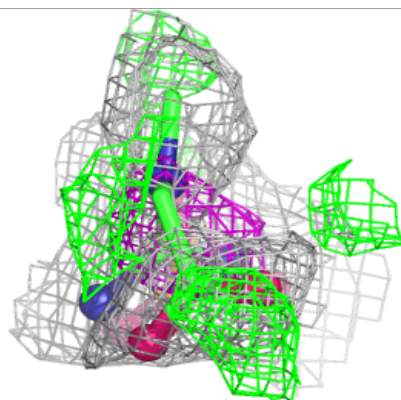
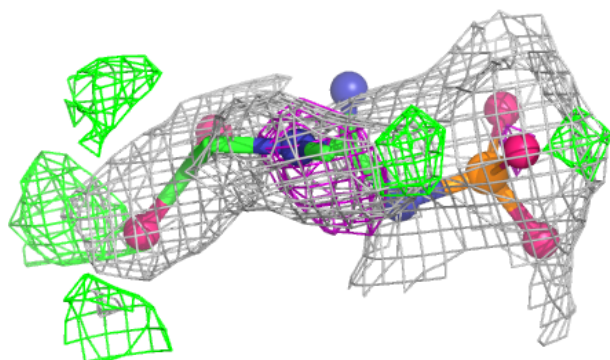
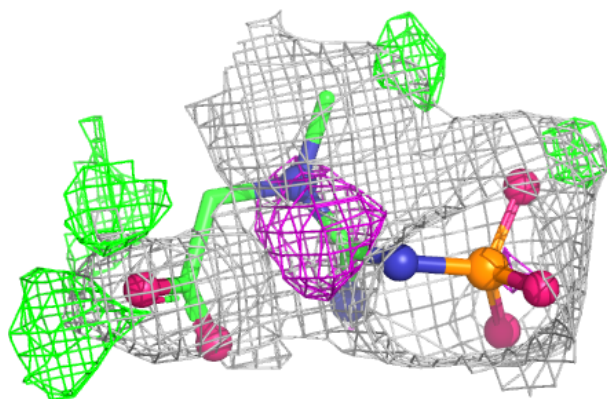
**Electron density around XDC C 602 (A):**

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

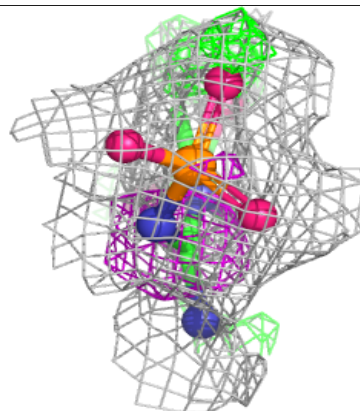
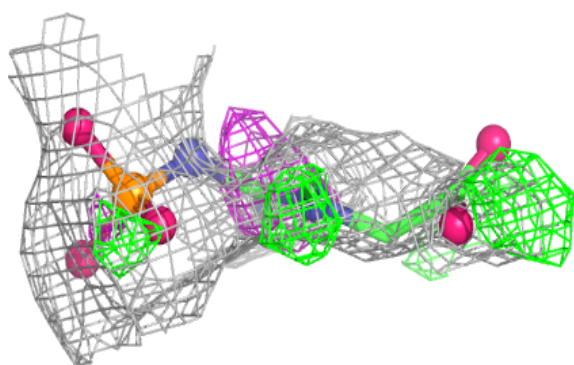
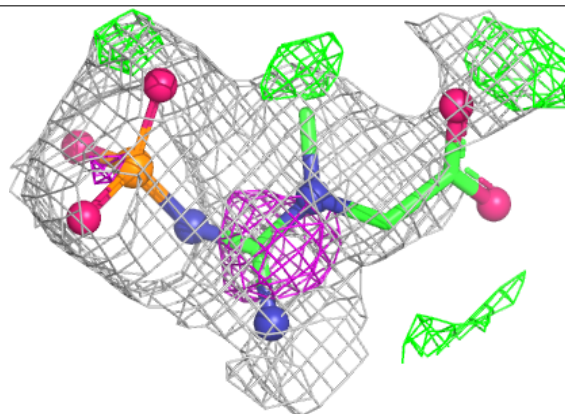


**Electron density around XDC A 601 (B):**

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

**Electron density around XDC A 601 (A):**

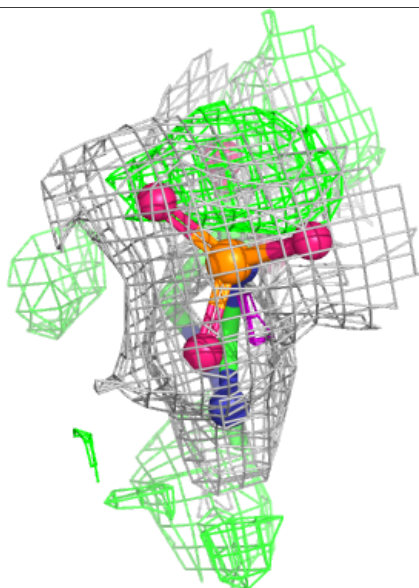
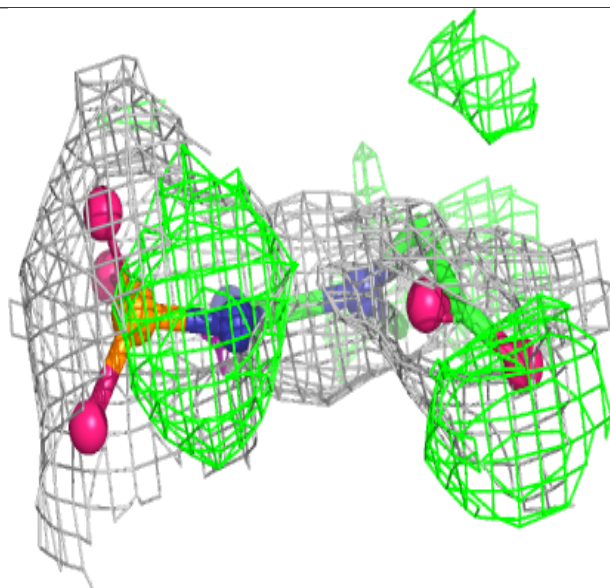
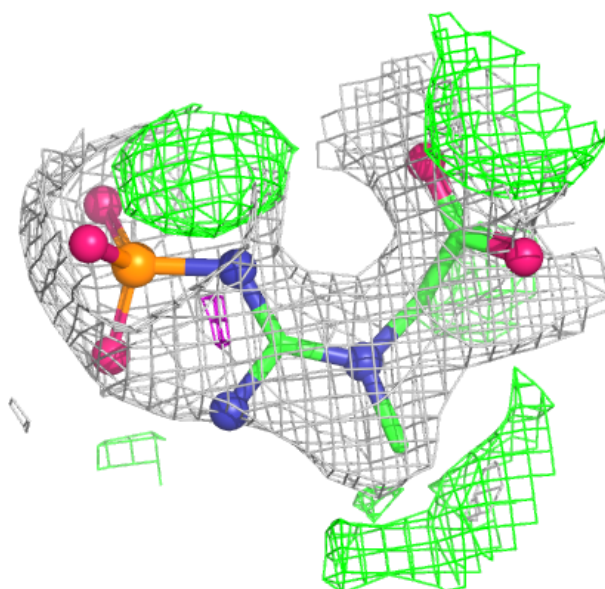
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





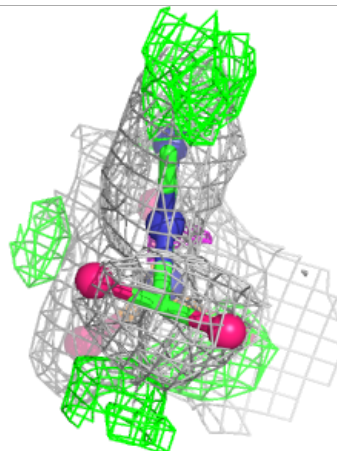
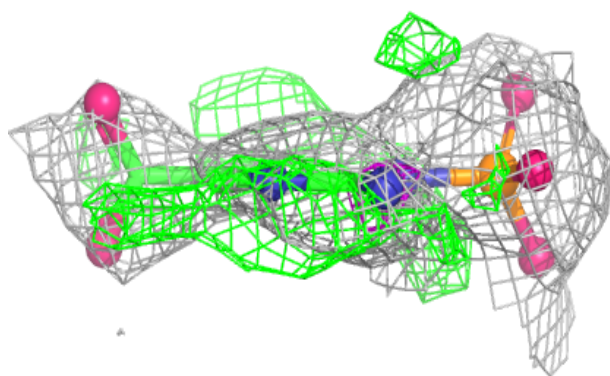
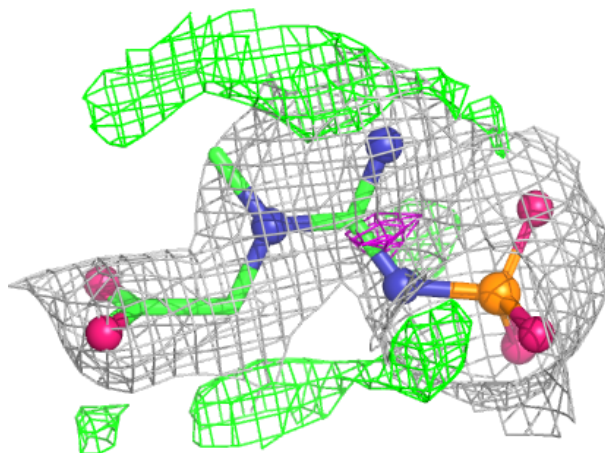
**Electron density around XDC D 602:**

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



**Electron density around XDC 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.