



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:46 AM UTC

PDB ID : 8GYX / pdb_00008gyx
Title : Bifunctional xylosidase/glucosidase LXYL with intermediate substrate xylose,
120 seconds
Authors : Yang, L.Y.
Deposited on : 2022-09-24
Resolution : 2.07 Å(reported)

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

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

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

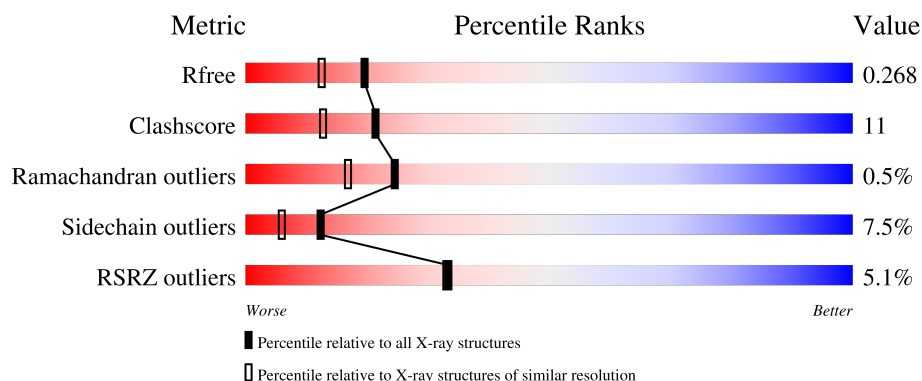
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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.



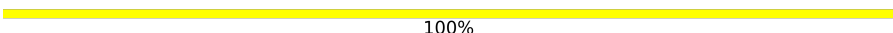
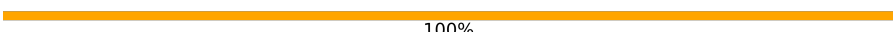
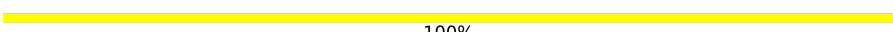
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	803	10% 78% 13% 6%
1	B	803	79% 11% 6%
1	C	803	10% 73% 18% 6%
1	D	803	8% 71% 20% 6%
2	E	2	100%

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

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
10	MAN	A	901	-	-	X	-
10	MAN	A	903	-	-	X	-
10	MAN	A	904	-	-	X	-
10	MAN	B	904	-	-	X	-
10	MAN	B	906	-	-	X	-
10	MAN	B	910	-	-	X	-
10	MAN	C	903	-	-	X	-
10	MAN	C	904	-	-	X	-
11	NAG	C	901	-	-	X	-
12	BMA	D	901	-	-	X	-
2	NAG	H	2	-	-	X	-
2	NAG	P	1	-	-	X	-
4	MAN	G	1	-	-	X	-
4	BMA	G	2	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 25439 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 Beta-D-xylosidase/beta-D-glucosidase.

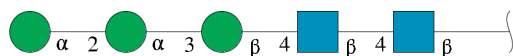
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	756	Total	C	N	O	S	0	3	0
			5738	3636	958	1127	17			
1	A	757	Total	C	N	O	S	0	1	0
			5721	3625	957	1122	17			
1	C	756	Total	C	N	O	S	0	2	0
			5717	3621	956	1123	17			
1	D	756	Total	C	N	O	S	0	2	0
			5720	3624	956	1123	17			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



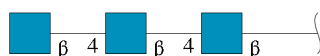
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose.



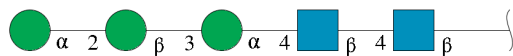
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



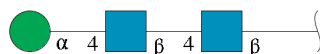
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			42	24	3	15			

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



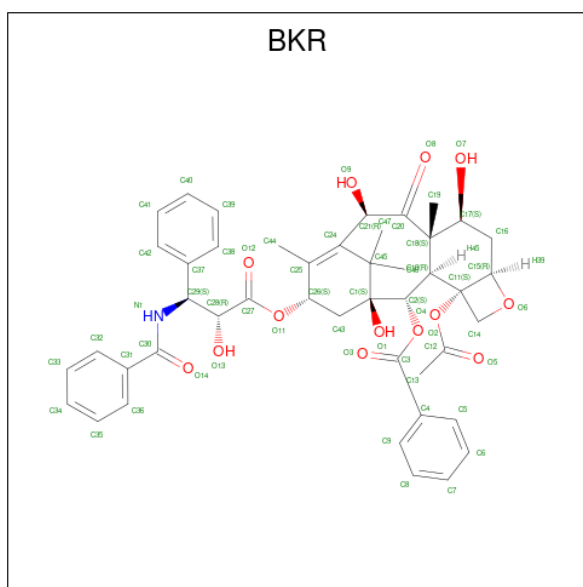
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

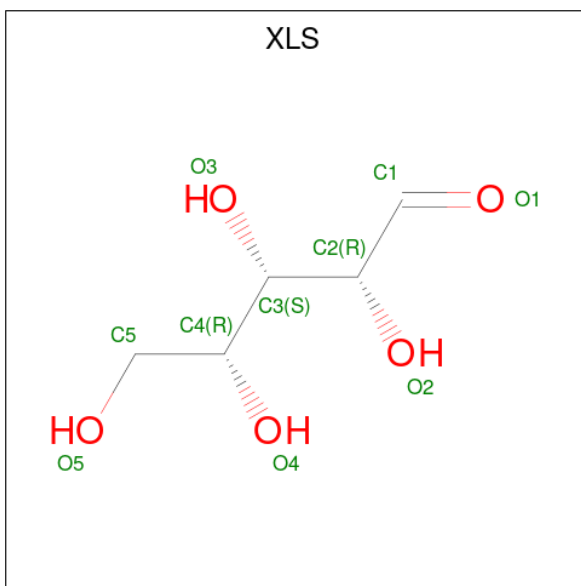
- Molecule 8 is Deacetyltaxol (CCD ID: BKR) (formula: $C_{45}H_{49}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			59	45	1	13		
8	A	1	Total	C	N	O	0	0
			59	45	1	13		
8	C	1	Total	C	N	O	0	0
			59	45	1	13		
8	D	1	Total	C	N	O	0	0
			59	45	1	13		

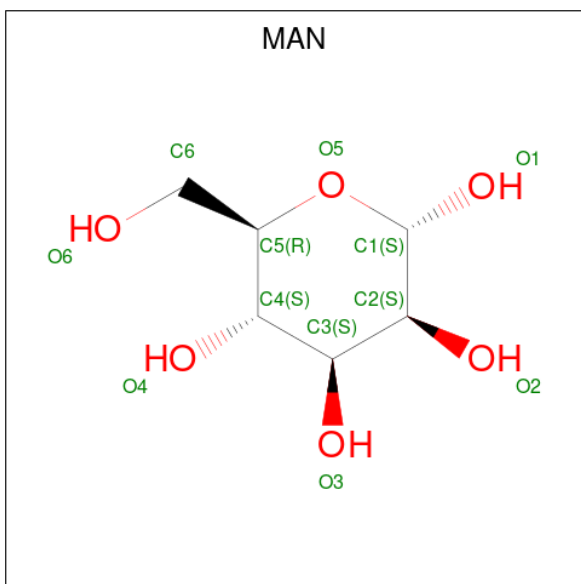
- Molecule 9 is D-xylose (CCD ID: XLS) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest")

by depositor).



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

- Molecule 10 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			11	6	5		
10	B	1	Total	C	O	0	0
			11	6	5		
10	B	1	Total	C	O	0	0
			11	6	5		
10	B	1	Total	C	O	0	0
			11	6	5		
10	B	1	Total	C	O	0	0
			12	6	6		
10	B	1	Total	C	O	0	0
			11	6	5		
10	A	1	Total	C	O	0	0
			11	6	5		
10	A	1	Total	C	O	0	0
			11	6	5		
10	A	1	Total	C	O	0	0
			11	6	5		
10	A	1	Total	C	O	0	0
			11	6	5		
10	A	1	Total	C	O	0	0
			12	6	6		
10	A	1	Total	C	O	0	0
			11	6	5		
10	C	1	Total	C	O	0	0
			11	6	5		
10	C	1	Total	C	O	0	0
			11	6	5		
10	C	1	Total	C	O	0	0
			11	6	5		
10	C	1	Total	C	O	0	0
			11	6	5		
10	D	1	Total	C	O	0	0
			11	6	5		
10	D	1	Total	C	O	0	0
			11	6	5		
10	D	1	Total	C	O	0	0
			11	6	5		
10	D	1	Total	C	O	0	0
			11	6	5		

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



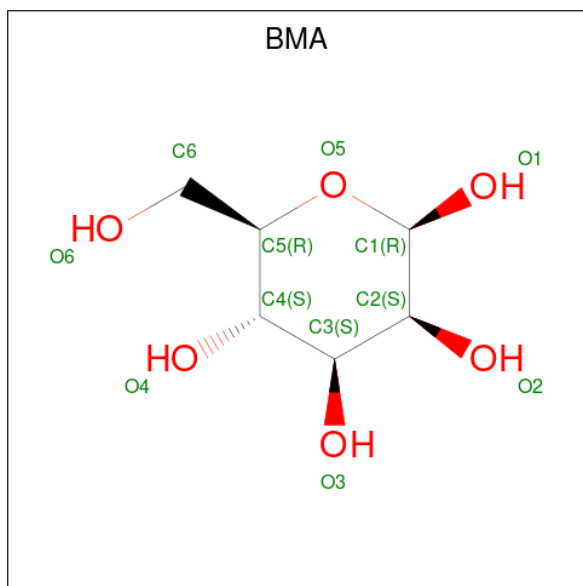
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			15	8	1	6		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	B	1	Total	C	N	O	0	0
			15	8	1	6		
11	B	1	Total	C	N	O	0	0
			14	8	1	5		
11	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	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	A	1	Total	C	N	O	0	0
			14	8	1	5		
11	C	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	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	C	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	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		
11	D	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 beta-D-mannopyranose (CCD ID: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	D	1	Total	C	O	0	0
			11	6	5		

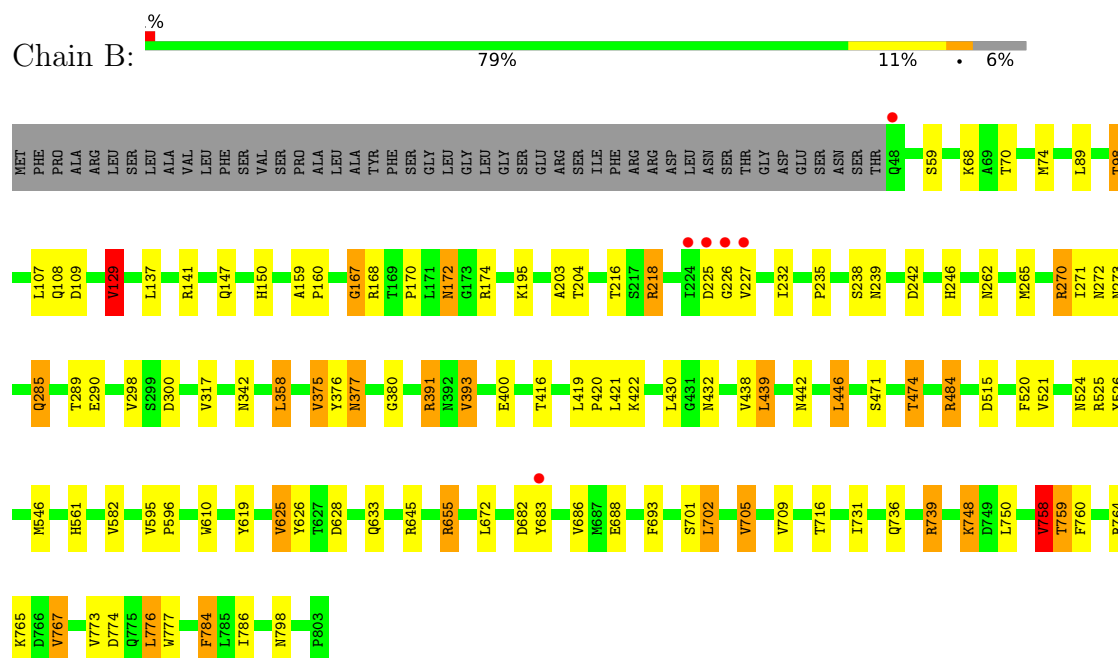
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	479	Total 479	O 479	0	0
13	A	436	Total 436	O 436	0	0
13	C	198	Total 198	O 198	0	0
13	D	181	Total 181	O 181	0	0

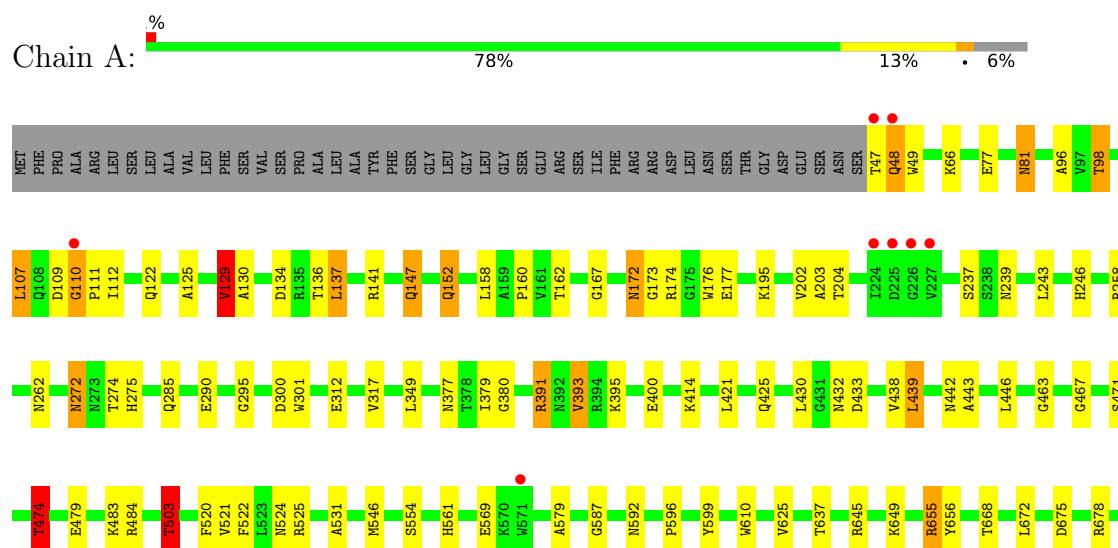
3 Residue-property plots [i](#)

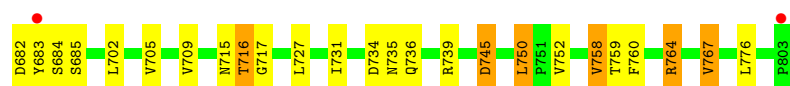
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-D-xylosidase/beta-D-glucosidase

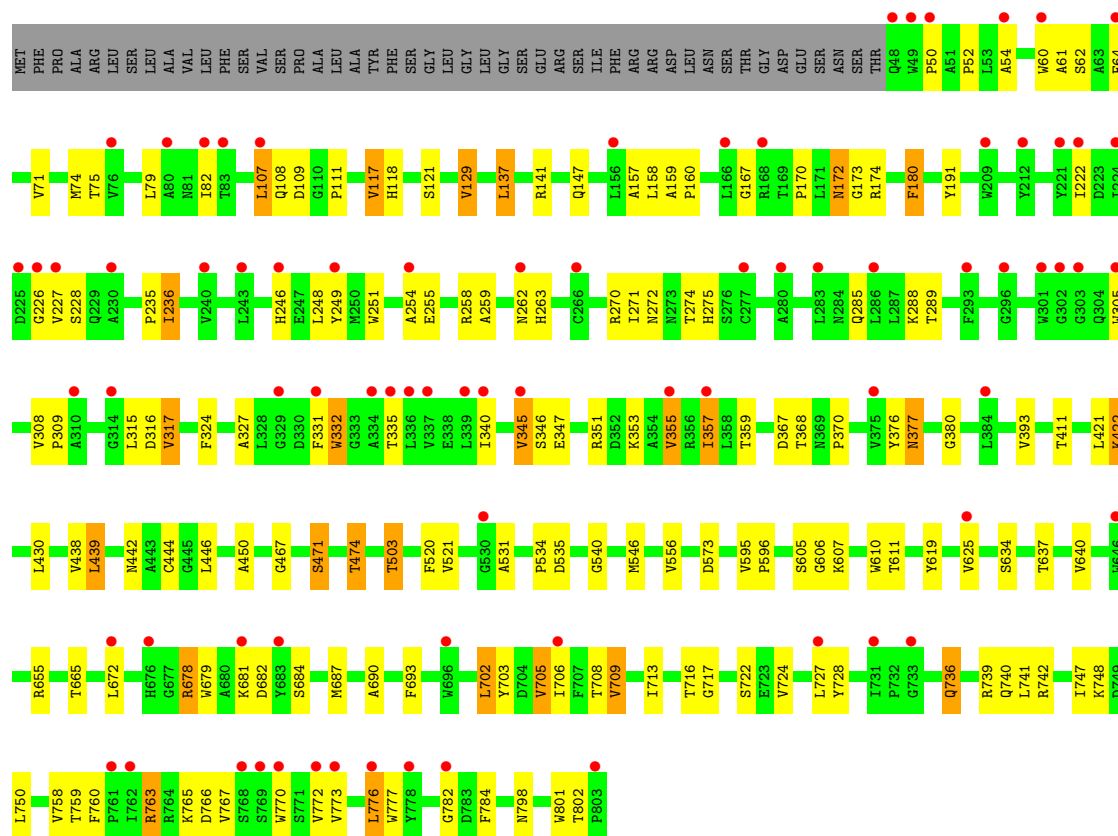
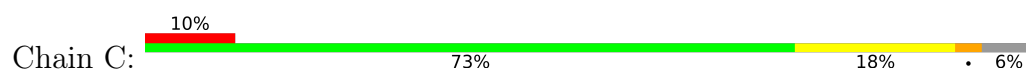


- Molecule 1: Beta-D-xylosidase/beta-D-glucosidase



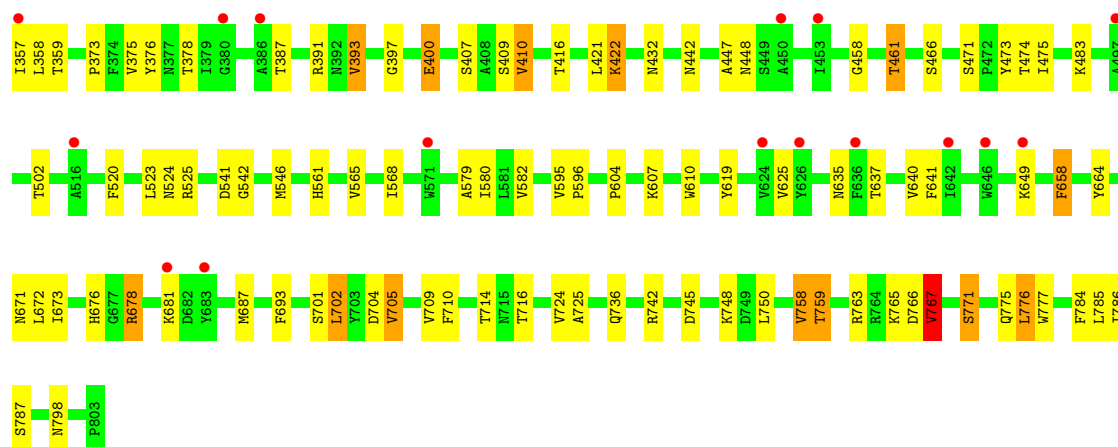


• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase



• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase





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

Chain E:  100%

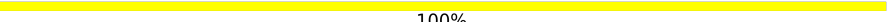


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50%



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

Chain L:  100%

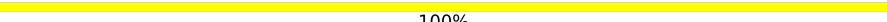


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



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

Chain P:  100%

NAG1
NAG2

- Molecule 3: alpha-D-mannopyranose-(1-2)-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

Chain F:  20% 80%

NAG1
NAG2
BMA3
MAN4
MAN5

- Molecule 4: beta-D-mannopyranose-(1-3)-alpha-D-mannopyranose

Chain G:  50% 50%

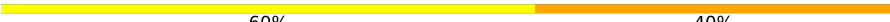
MAN1
BMA2

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

Chain I:  100%

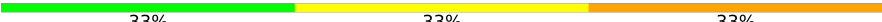
NAG1
NAG2
NAG3

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

Chain J:  60% 40%

NAG1
NAG2
AH23
BMA4
MAN5

- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  33% 33% 33%

NAG1
NAG2
MAN3

- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 67%

NAG1
NAG2
MAN3

- Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  100%

MAG1
MAG2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	228.43Å 89.23Å 218.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.97 – 2.07 35.97 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.97-2.07) 95.1 (35.97-2.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.219 , 0.259 0.231 , 0.268	Depositor DCC
R_{free} test set	12691 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25439	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: MAN, BMA, XLS, NAG, BKR, AH2

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	0.60	0/5865	1.04	10/8025 (0.1%)
1	B	0.62	0/5883	1.04	11/8049 (0.1%)
1	C	0.56	0/5864	1.02	4/8023 (0.0%)
1	D	0.58	0/5867	1.06	8/8027 (0.1%)
All	All	0.59	0/23479	1.04	33/32124 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	6
1	D	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	503	THR	CB-CA-C	8.94	123.67	110.26
1	A	48	GLN	N-CA-C	-7.96	103.57	113.20
1	B	218	ARG	N-CA-C	-7.51	103.17	111.36
1	A	675	ASP	CA-CB-CG	6.88	119.48	112.60
1	D	704	ASP	CA-CB-CG	6.87	119.47	112.60

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	168	ARG	Sidechain
1	B	218	ARG	Sidechain
1	B	270	ARG	Sidechain
1	B	391	ARG	Sidechain
1	B	484	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5721	0	5518	83	0
1	B	5738	0	5526	91	0
1	C	5717	0	5510	107	0
1	D	5720	0	5519	130	0
2	E	28	0	24	4	0
2	H	28	0	25	10	0
2	L	28	0	25	0	0
2	O	28	0	25	6	0
2	P	28	0	26	14	0
3	F	61	0	51	6	0
4	G	23	0	21	28	0
5	I	42	0	38	4	0
6	J	61	0	43	5	0
7	K	39	0	34	2	0
7	M	39	0	34	0	0
7	N	39	0	34	0	0
8	A	59	0	0	1	0
8	B	59	0	0	1	0
8	C	59	0	0	2	0
8	D	59	0	0	2	0
9	A	9	0	9	1	0
9	B	9	0	9	1	0
10	A	67	0	62	19	0
10	B	78	0	72	28	0
10	C	55	0	50	13	0
10	D	44	0	39	7	0
11	A	56	0	52	0	0
11	B	100	0	95	8	0
11	C	84	0	78	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	56	0	52	1	0
12	D	11	0	10	9	0
13	A	436	0	0	7	0
13	B	479	0	0	14	0
13	C	198	0	0	4	0
13	D	181	0	0	11	0
All	All	25439	0	22981	508	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 11.

The worst 5 of 508 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:C:272:ASN:HD21	11:C:901:NAG:C1	1.31	1.40
10:B:904:MAN:O6	10:B:906:MAN:C1	1.70	1.38
1:D:272:ASN:HD21	2:P:1:NAG:C1	1.39	1.33
10:B:906:MAN:O2	10:B:907:MAN:C1	1.76	1.32
10:B:904:MAN:O3	10:B:905:MAN:C1	1.76	1.30

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	756/803 (94%)	720 (95%)	34 (4%)	2 (0%)	36	30
1	B	757/803 (94%)	719 (95%)	37 (5%)	1 (0%)	48	44
1	C	756/803 (94%)	693 (92%)	56 (7%)	7 (1%)	14	7
1	D	756/803 (94%)	685 (91%)	67 (9%)	4 (0%)	24	17
All	All	3025/3212 (94%)	2817 (93%)	194 (6%)	14 (0%)	24	17

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	227	VAL
1	A	110	GLY
1	C	236	ILE
1	C	332	TRP
1	C	422	LYS

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	610/648 (94%)	563 (92%)	47 (8%)	12	5
1	B	612/648 (94%)	574 (94%)	38 (6%)	16	9
1	C	610/648 (94%)	564 (92%)	46 (8%)	12	6
1	D	611/648 (94%)	559 (92%)	52 (8%)	10	4
All	All	2443/2592 (94%)	2260 (92%)	183 (8%)	12	6

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	678	ARG
1	D	220	LEU
1	C	702	LEU
1	C	798	ASN
1	D	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	718	ASN
1	D	423	HIS
1	C	262	ASN
1	D	377	ASN
1	D	676	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 ⓘ

34 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	E	1	1,2	14,14,15	0.69	1 (7%)	17,19,21	3.23	4 (23%)
2	NAG	E	2	2	14,14,15	0.51	0	17,19,21	1.15	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.47	0	17,19,21	0.97	2 (11%)
3	NAG	F	2	3	14,14,15	0.41	0	17,19,21	1.22	1 (5%)
3	BMA	F	3	3	11,11,12	1.13	2 (18%)	15,15,17	1.29	2 (13%)
3	MAN	F	4	3	11,11,12	0.53	0	15,15,17	1.55	2 (13%)
3	MAN	F	5	3	11,11,12	0.65	0	15,15,17	1.49	2 (13%)
4	MAN	G	1	4	12,12,12	0.34	0	17,17,17	0.49	0
4	BMA	G	2	4	11,11,12	1.03	1 (9%)	15,15,17	1.78	4 (26%)
2	NAG	H	1	1,2	14,14,15	0.40	0	17,19,21	1.11	3 (17%)
2	NAG	H	2	2	14,14,15	0.44	0	17,19,21	1.19	2 (11%)
5	NAG	I	1	5,1	14,14,15	0.80	1 (7%)	17,19,21	1.63	3 (17%)
5	NAG	I	2	5	14,14,15	0.44	0	17,19,21	0.83	1 (5%)
5	NAG	I	3	5	14,14,15	0.34	0	17,19,21	1.78	3 (17%)
6	NAG	J	1	1,6	14,14,15	0.47	0	17,19,21	1.13	1 (5%)
6	NAG	J	2	6	14,14,15	0.43	0	17,19,21	1.16	3 (17%)
6	AH2	J	3	6	11,11,11	0.69	0	15,15,15	1.74	6 (40%)
6	BMA	J	4	6	11,11,12	0.47	0	15,15,17	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	J	5	6	11,11,12	0.82	0	15,15,17	1.08	1 (6%)
7	NAG	K	1	7,1	14,14,15	0.43	0	17,19,21	0.70	0
7	NAG	K	2	7	14,14,15	0.37	0	17,19,21	1.40	1 (5%)
7	MAN	K	3	7	11,11,12	0.86	1 (9%)	15,15,17	1.37	2 (13%)
2	NAG	L	1	1,2	14,14,15	0.75	1 (7%)	17,19,21	2.51	4 (23%)
2	NAG	L	2	2	14,14,15	0.53	0	17,19,21	1.39	3 (17%)
7	NAG	M	1	7,1	14,14,15	0.30	0	17,19,21	0.64	0
7	NAG	M	2	7	14,14,15	0.48	0	17,19,21	0.88	1 (5%)
7	MAN	M	3	7	11,11,12	1.04	1 (9%)	15,15,17	1.35	2 (13%)
7	NAG	N	1	7,1	14,14,15	0.29	0	17,19,21	0.94	1 (5%)
7	NAG	N	2	7	14,14,15	0.40	0	17,19,21	0.83	1 (5%)
7	MAN	N	3	7	11,11,12	0.95	0	15,15,17	1.19	3 (20%)
2	NAG	O	1	1,2	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
2	NAG	O	2	2	14,14,15	0.52	0	17,19,21	1.23	2 (11%)
2	NAG	P	1	2	14,14,15	0.40	0	17,19,21	1.08	0
2	NAG	P	2	2	14,14,15	0.42	0	17,19,21	1.00	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	-	0/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
4	MAN	G	1	4	-	0/2/22/22	0/1/1/1
4	BMA	G	2	4	-	2/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	NAG	I	3	5	-	4/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	AH2	J	3	6	-	0/2/19/19	0/1/1/1
6	BMA	J	4	6	-	0/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	MAN	K	3	7	-	2/2/19/22	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1
7	NAG	M	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	MAN	M	3	7	-	2/2/19/22	0/1/1/1
7	NAG	N	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	N	2	7	-	4/6/23/26	0/1/1/1
7	MAN	N	3	7	-	2/2/19/22	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
2	NAG	P	1	2	-	4/6/23/26	0/1/1/1
2	NAG	P	2	2	-	3/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1	NAG	C1-C2	2.54	1.55	1.52
4	G	2	BMA	C2-C3	-2.42	1.48	1.52
7	K	3	MAN	O5-C5	2.33	1.48	1.43
3	F	3	BMA	C4-C5	-2.28	1.48	1.53
2	L	1	NAG	O4-C4	2.23	1.48	1.43

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	O4-C4-C5	9.93	133.79	109.32
2	L	1	NAG	O4-C4-C3	7.77	128.70	110.38
2	E	1	NAG	O5-C1-C2	-5.88	102.20	111.29
7	K	2	NAG	C2-N2-C7	5.29	129.98	122.90
3	F	4	MAN	C1-O5-C5	4.97	118.85	112.19

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

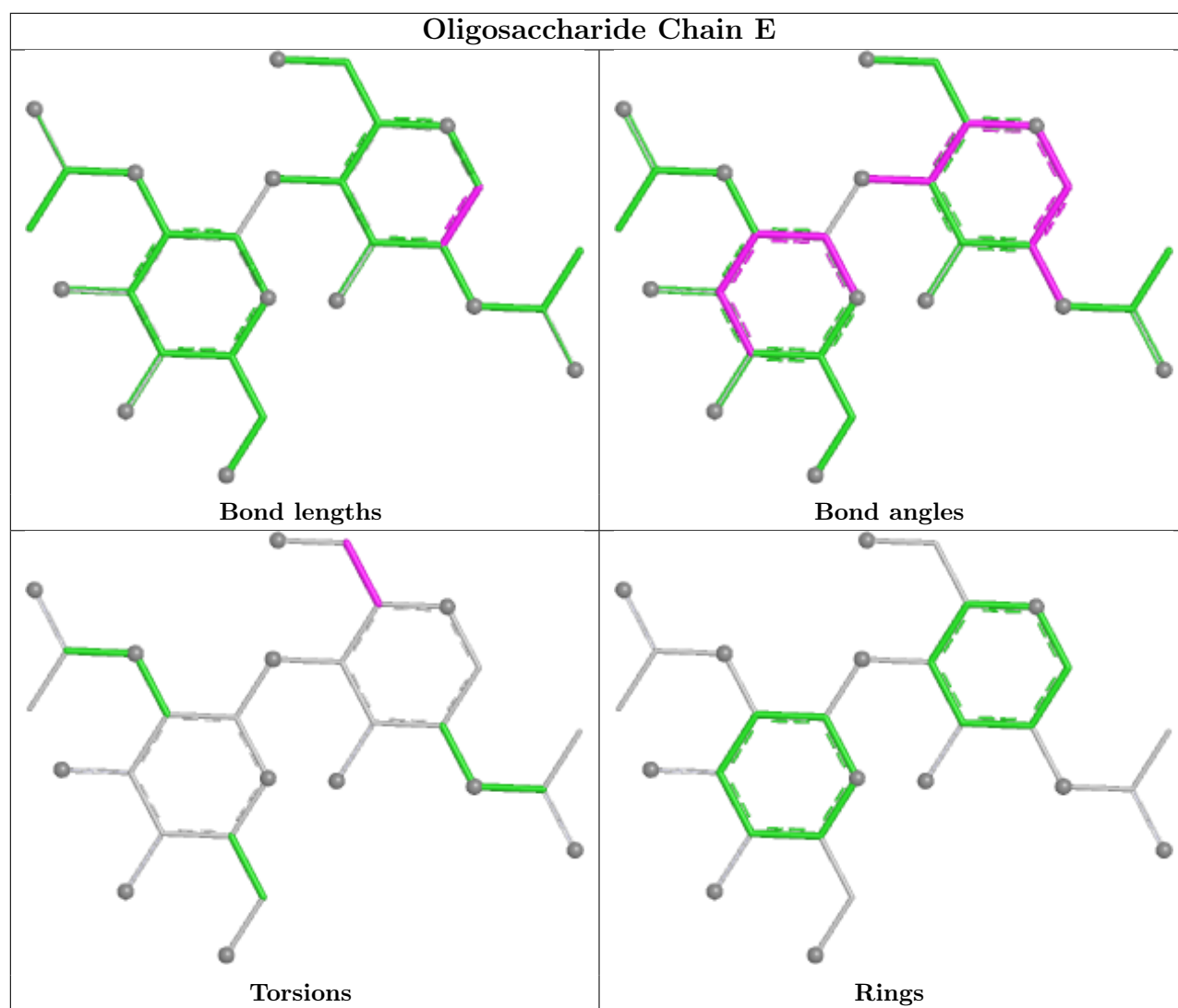
Mol	Chain	Res	Type	Atoms
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
5	I	3	NAG	C8-C7-N2-C2
5	I	3	NAG	O7-C7-N2-C2
4	G	2	BMA	C4-C5-C6-O6

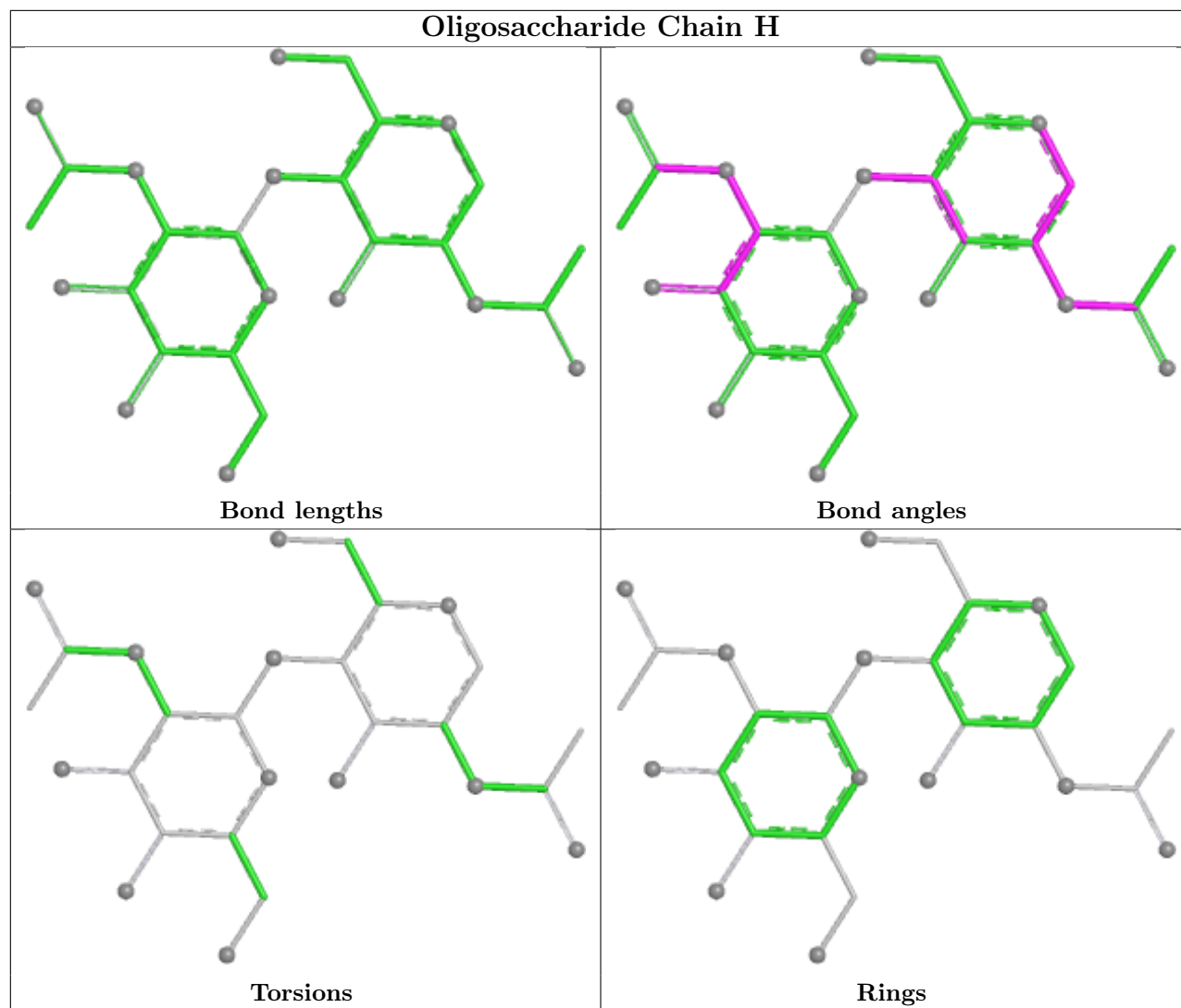
There are no ring outliers.

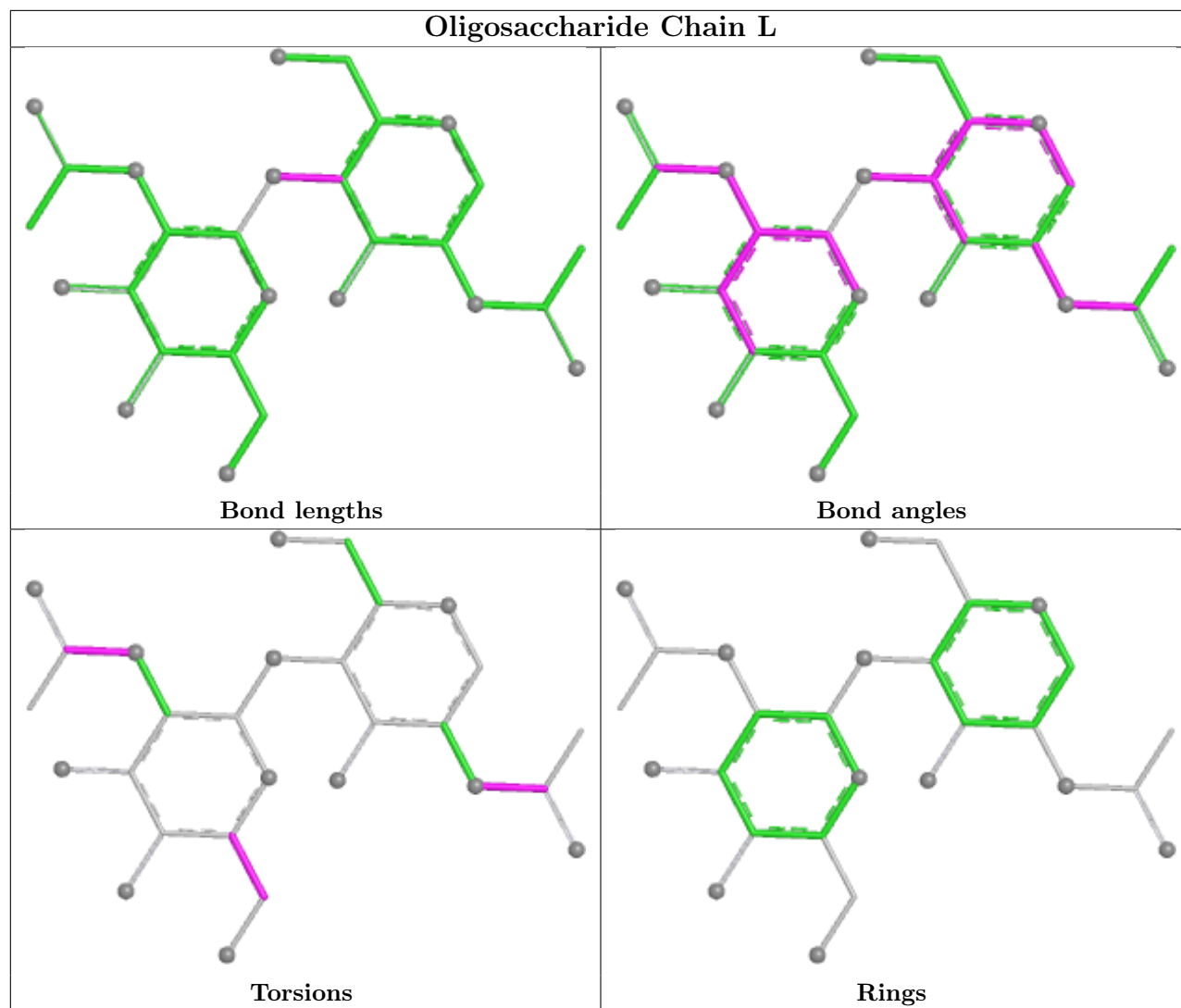
19 monomers are involved in 69 short contacts:

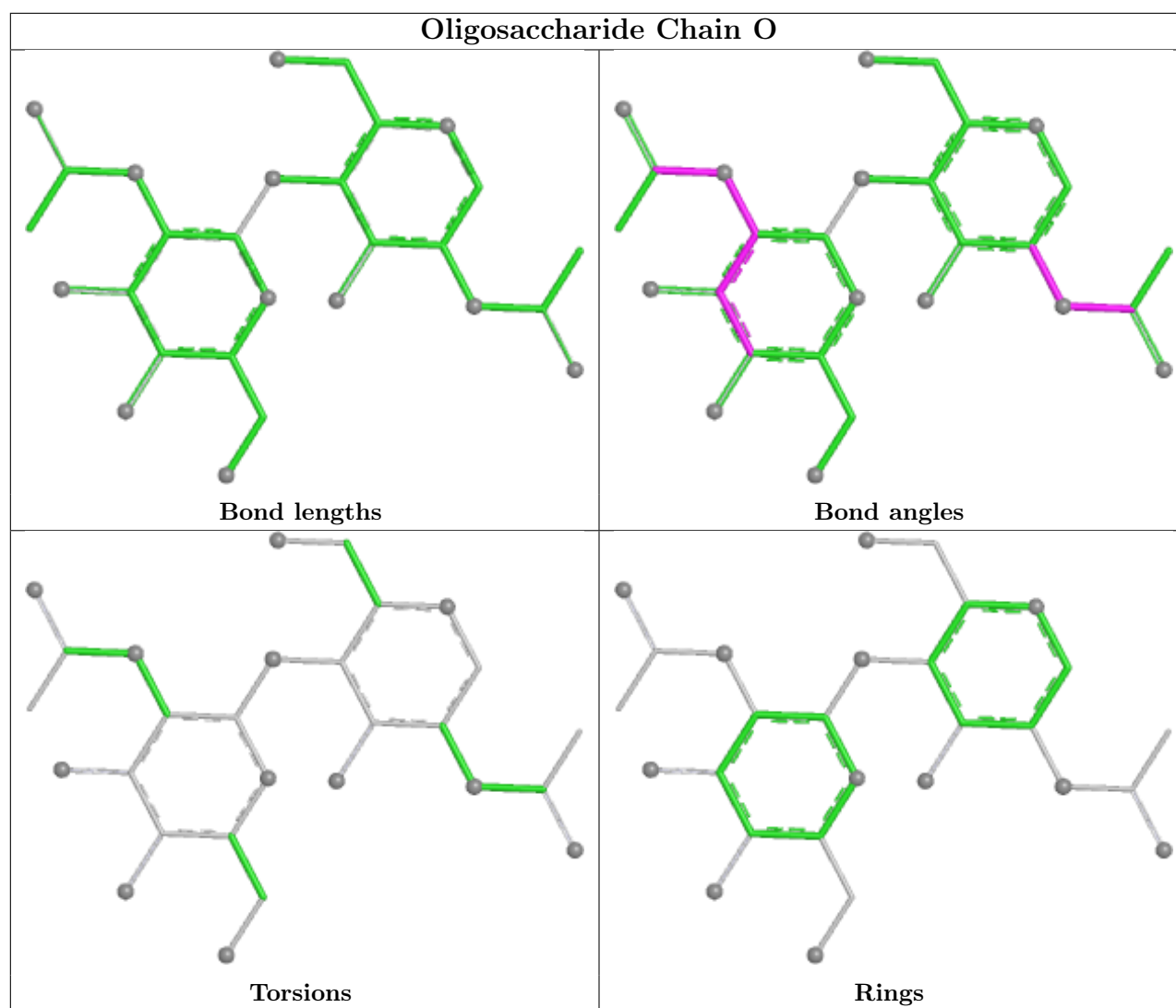
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	10	0
4	G	1	MAN	18	0
6	J	1	NAG	3	0
2	E	2	NAG	2	0
7	K	3	MAN	2	0
2	P	2	NAG	5	0
3	F	5	MAN	1	0
5	I	3	NAG	2	0
2	O	2	NAG	5	0
5	I	2	NAG	2	0
3	F	2	NAG	2	0
2	P	1	NAG	11	0
2	E	1	NAG	2	0
6	J	3	AH2	2	0
5	I	1	NAG	2	0
3	F	1	NAG	2	0
2	O	1	NAG	5	0
3	F	3	BMA	3	0
4	G	2	BMA	10	0

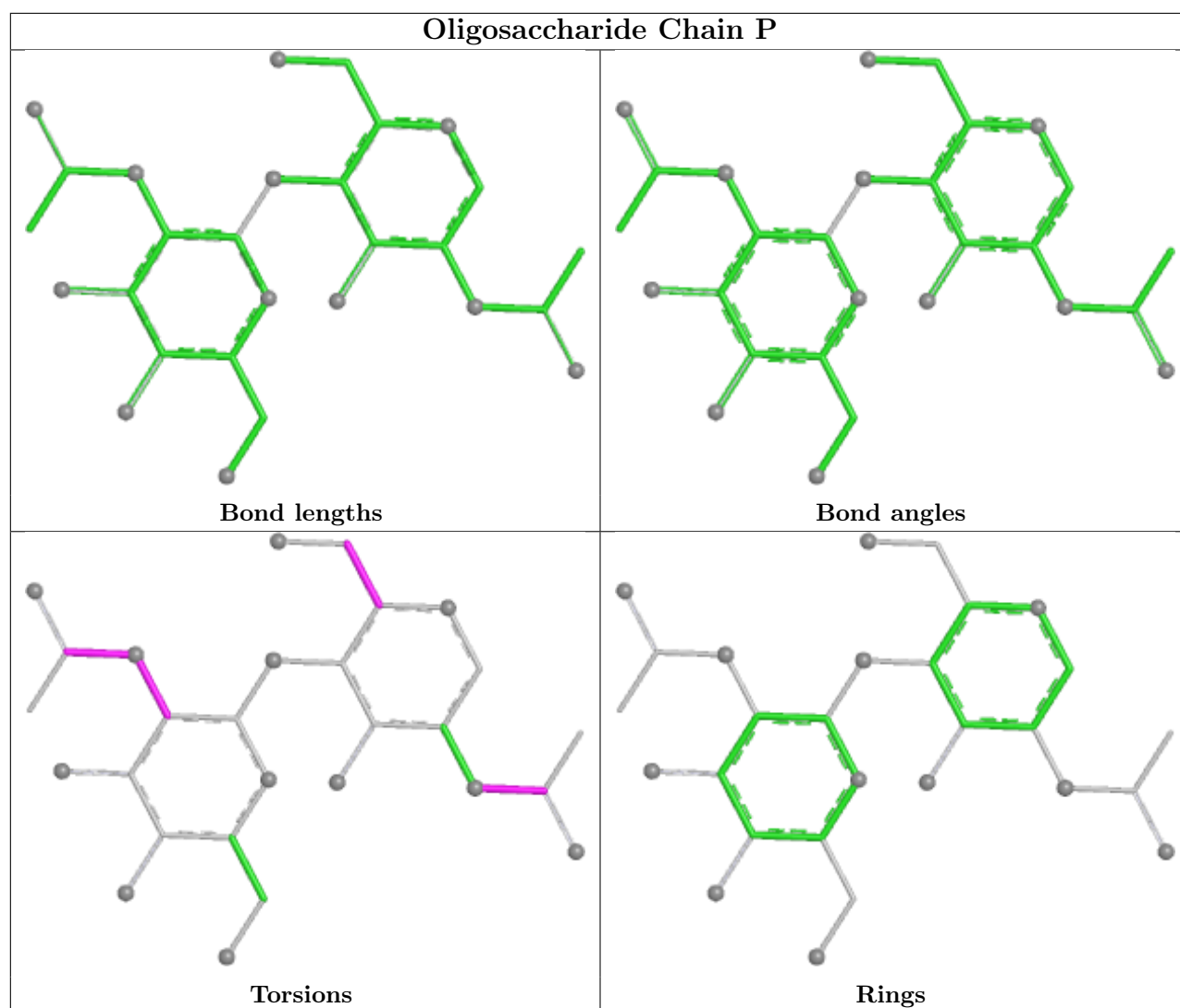
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

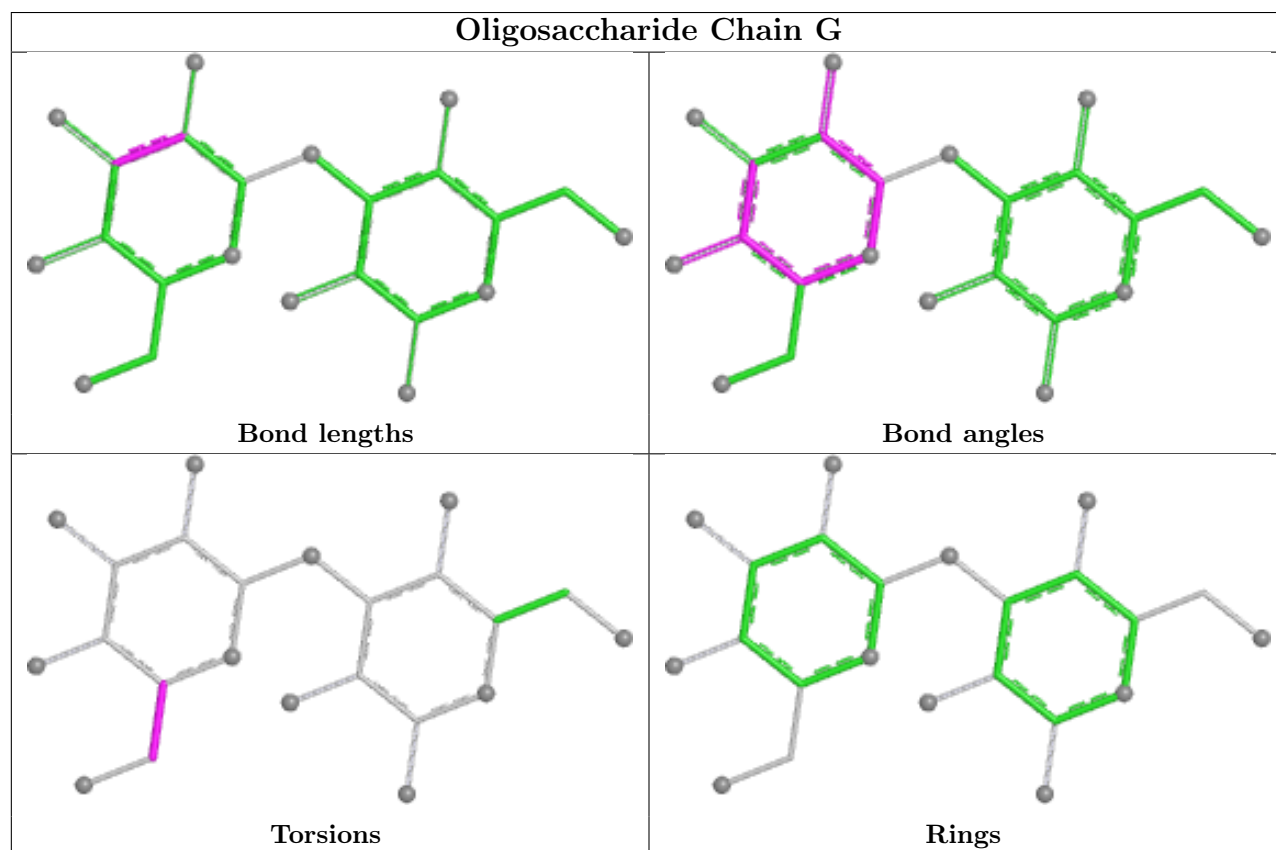
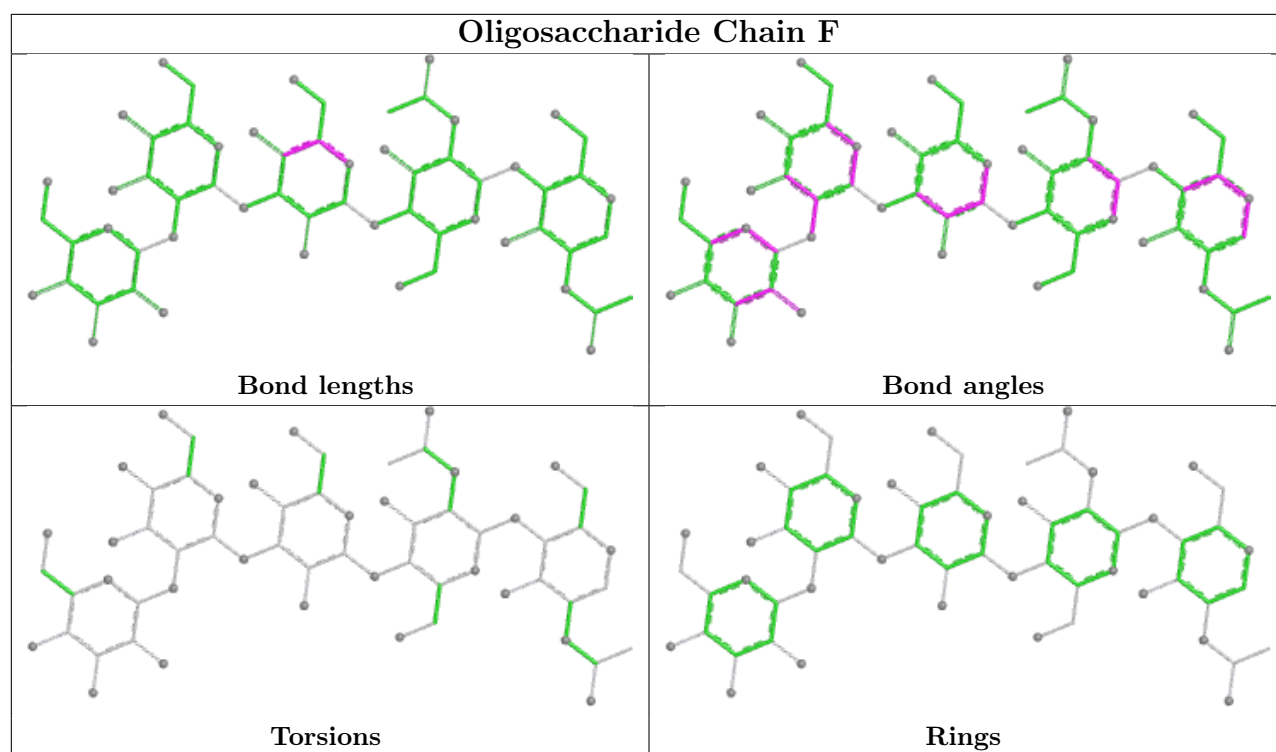


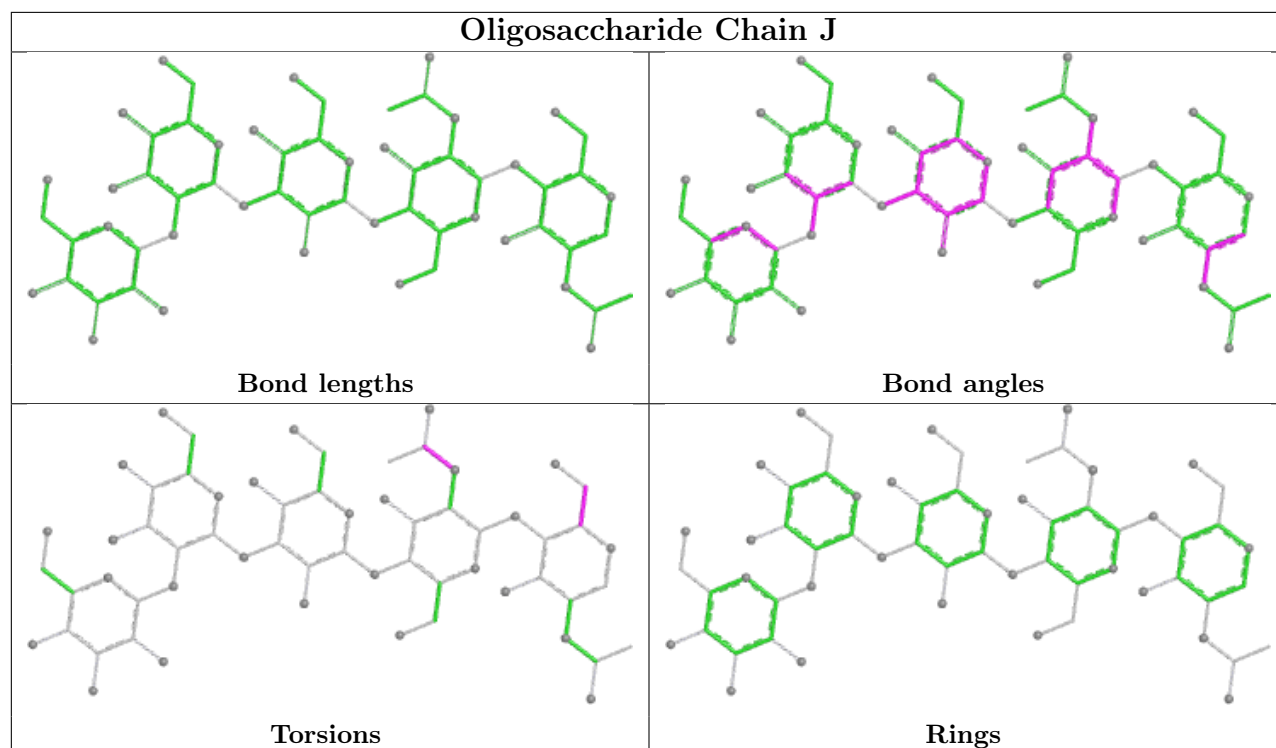
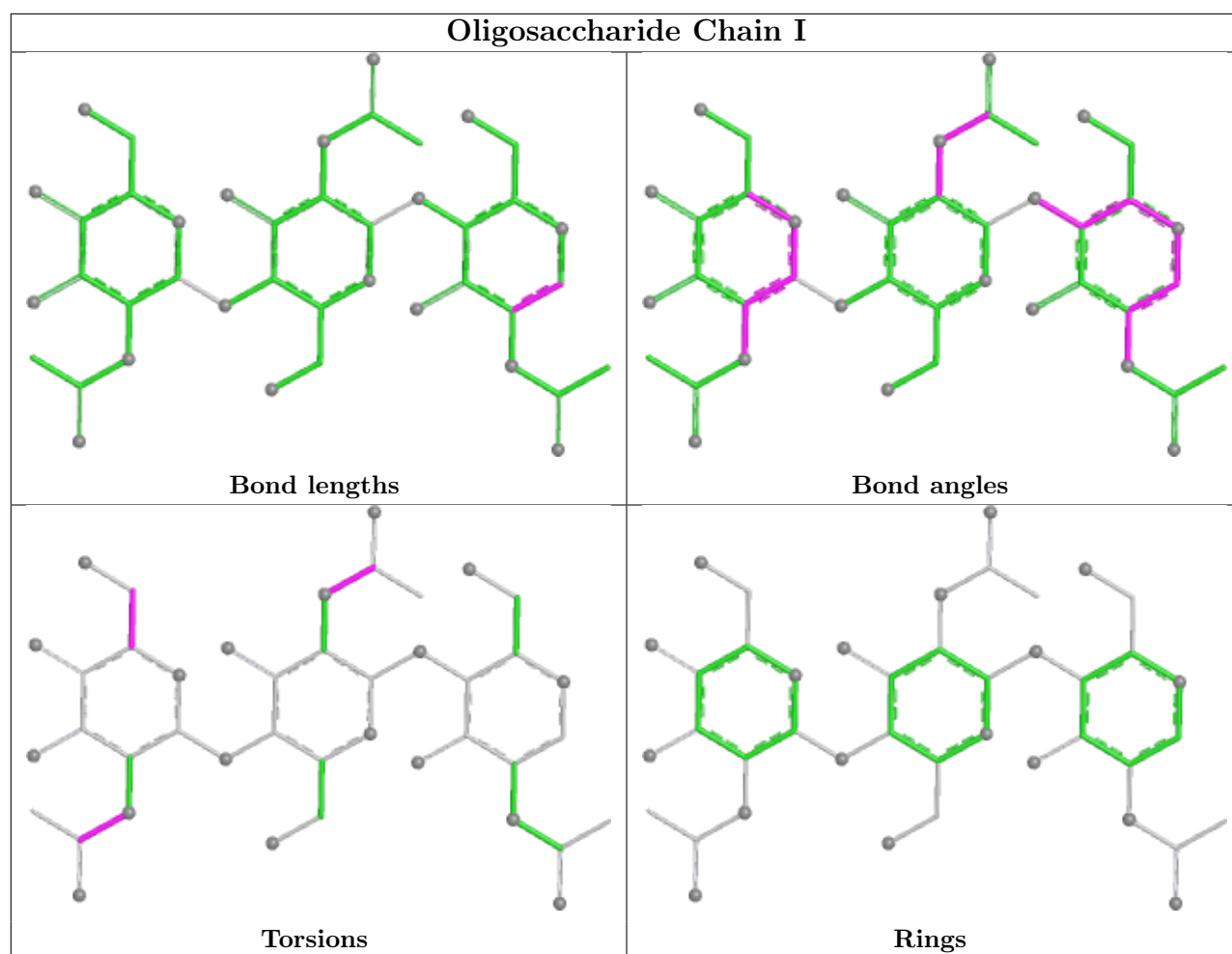


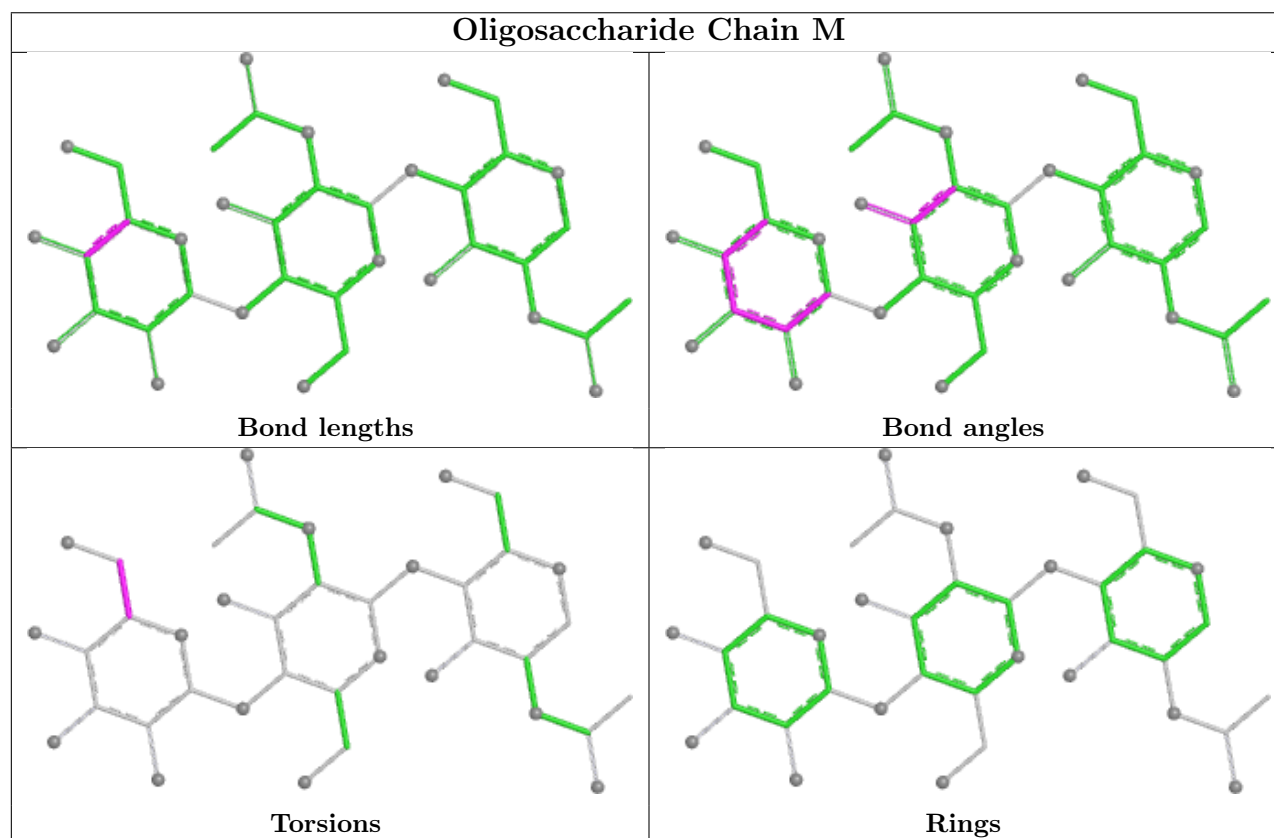
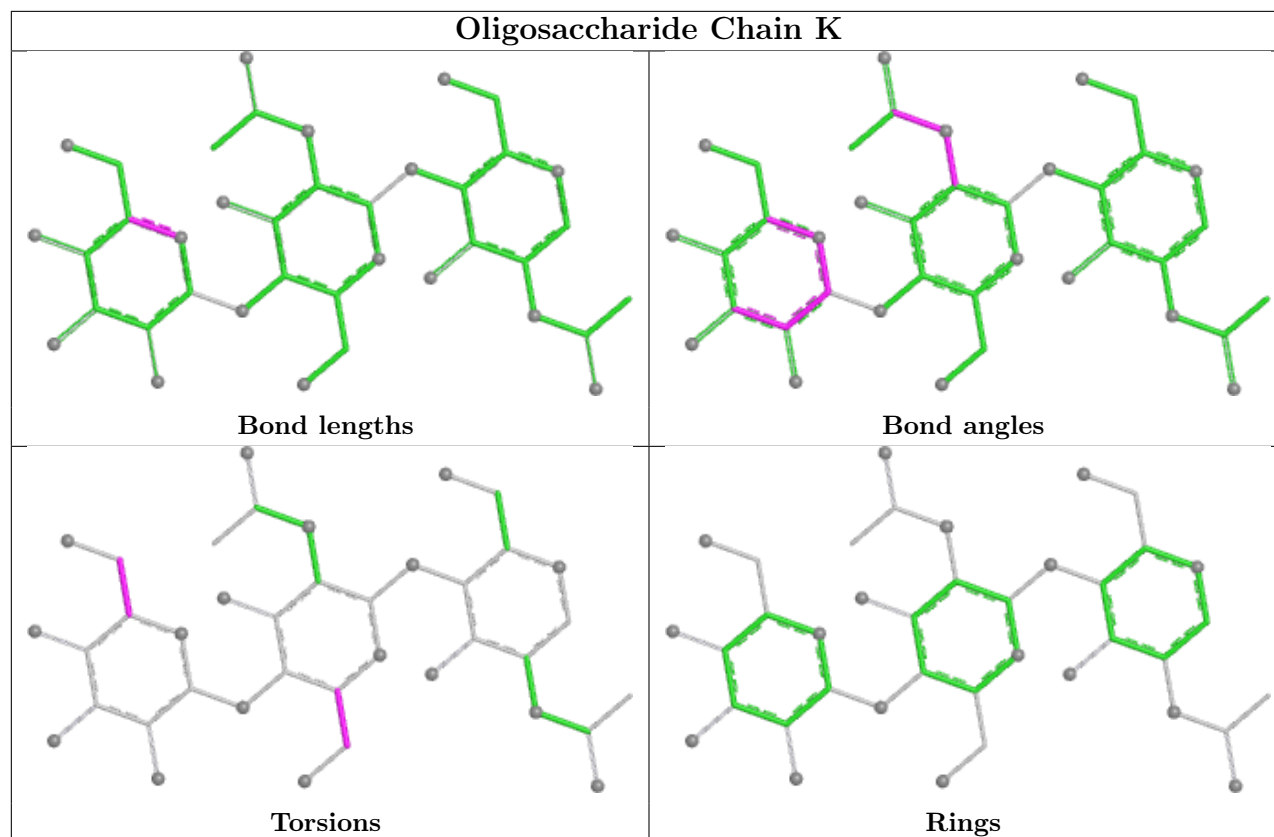


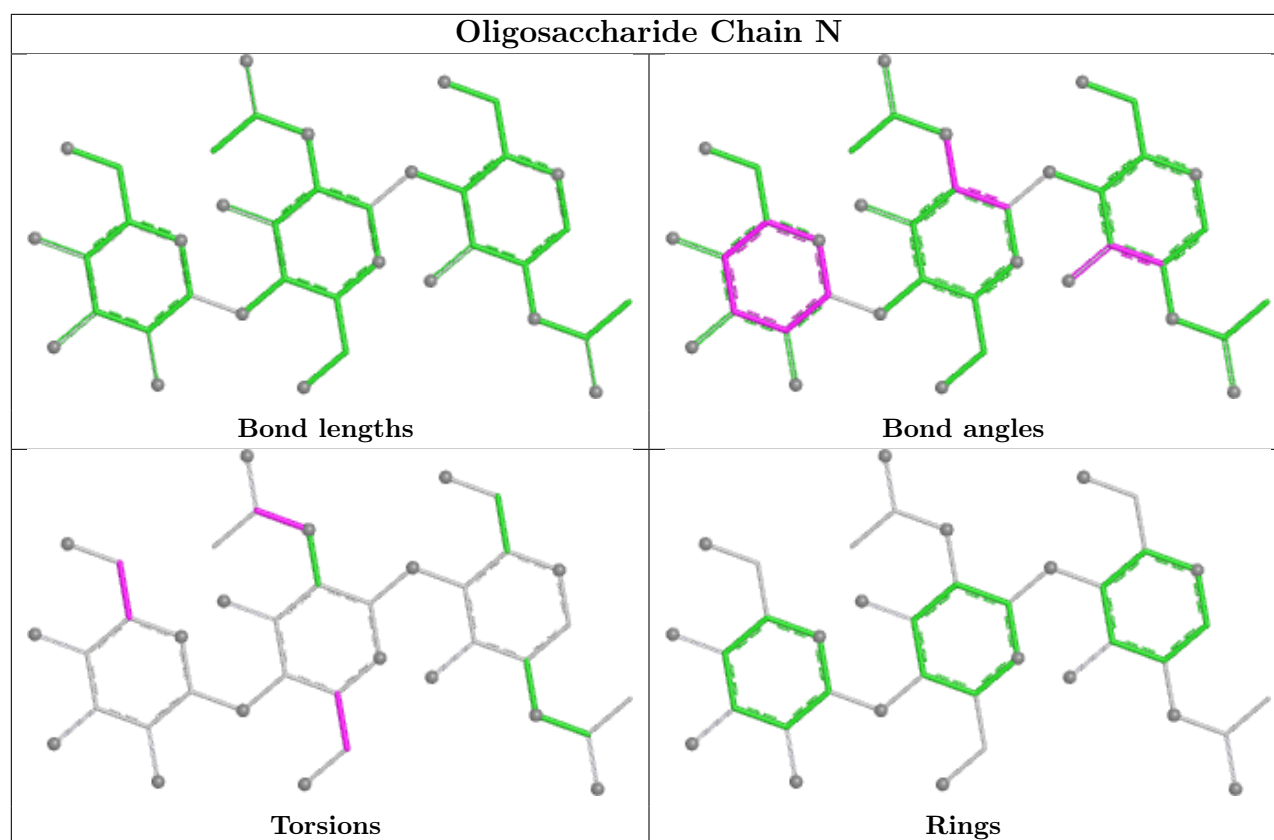












5.6 Ligand geometry [i](#)

50 ligands 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	$\# Z > 2$
11	NAG	D	909	1	14,14,15	0.43	0	17,19,21	1.08	1 (5%)
11	NAG	C	901	-	14,14,15	0.41	0	17,19,21	1.06	0
8	BKR	A	911	-	65,65,65	0.69	0	101,101,101	0.95	7 (6%)
9	XLS	A	912	-	8,8,9	0.73	0	10,10,11	2.81	4 (40%)
10	MAN	D	904	-	11,11,12	0.61	0	15,15,17	1.47	3 (20%)
11	NAG	C	902	-	14,14,15	0.43	0	17,19,21	0.72	0
11	NAG	C	909	1	14,14,15	0.46	0	17,19,21	0.97	1 (5%)
10	MAN	C	904	-	11,11,12	0.92	0	15,15,17	2.01	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	A	907	-	12,12,12	0.70	0	17,17,17	1.35	3 (17%)
11	NAG	A	905	1	14,14,15	0.40	0	17,19,21	1.35	4 (23%)
11	NAG	D	907	1	14,14,15	0.39	0	17,19,21	1.66	2 (11%)
10	MAN	B	903	-	11,11,12	0.86	1 (9%)	15,15,17	0.99	1 (6%)
11	NAG	D	908	1	14,14,15	0.83	1 (7%)	17,19,21	2.04	2 (11%)
11	NAG	B	914	1	14,14,15	0.38	0	17,19,21	1.26	1 (5%)
10	MAN	B	912	-	11,11,12	1.26	1 (9%)	15,15,17	1.66	2 (13%)
11	NAG	B	911	-	15,15,15	0.21	0	21,21,21	0.42	0
8	BKR	B	901	-	65,65,65	0.69	0	101,101,101	0.95	7 (6%)
10	MAN	D	905	-	11,11,12	0.85	1 (9%)	15,15,17	0.90	1 (6%)
11	NAG	B	913	1	14,14,15	0.43	0	17,19,21	1.21	1 (5%)
11	NAG	A	906	1	14,14,15	0.47	0	17,19,21	1.15	1 (5%)
11	NAG	D	906	1	14,14,15	0.50	0	17,19,21	1.14	3 (17%)
11	NAG	C	908	1	14,14,15	0.50	0	17,19,21	0.88	0
11	NAG	A	910	1	14,14,15	0.44	0	17,19,21	1.46	3 (17%)
10	MAN	A	908	-	11,11,12	0.58	0	15,15,17	1.06	1 (6%)
10	MAN	D	902	-	11,11,12	1.11	1 (9%)	15,15,17	2.25	2 (13%)
10	MAN	B	904	-	11,11,12	0.65	0	15,15,17	1.17	2 (13%)
11	NAG	A	909	1	14,14,15	0.39	0	17,19,21	0.95	2 (11%)
10	MAN	A	904	-	11,11,12	0.71	0	15,15,17	1.05	1 (6%)
10	MAN	C	907	-	11,11,12	0.58	0	15,15,17	1.07	2 (13%)
10	MAN	D	903	-	11,11,12	0.52	0	15,15,17	1.73	3 (20%)
10	MAN	C	903	-	11,11,12	0.70	0	15,15,17	1.37	2 (13%)
8	BKR	D	910	-	65,65,65	0.52	0	101,101,101	0.90	5 (4%)
9	XLS	B	902	-	8,8,9	0.72	0	10,10,11	2.82	4 (40%)
10	MAN	A	901	-	11,11,12	0.45	0	15,15,17	1.39	2 (13%)
11	NAG	B	916	-	14,14,15	0.39	0	17,19,21	0.71	1 (5%)
10	MAN	B	905	-	11,11,12	0.81	0	15,15,17	1.13	2 (13%)
10	MAN	A	903	-	11,11,12	0.77	0	15,15,17	1.19	1 (6%)
10	MAN	B	907	-	11,11,12	0.73	1 (9%)	15,15,17	1.02	2 (13%)
10	MAN	C	906	-	11,11,12	0.58	0	15,15,17	1.47	3 (20%)
11	NAG	C	910	1	14,14,15	0.48	0	17,19,21	0.81	0
10	MAN	C	905	-	11,11,12	0.43	0	15,15,17	1.09	1 (6%)
11	NAG	B	909	1	14,14,15	0.43	0	17,19,21	1.02	0
11	NAG	C	911	1	14,14,15	0.41	0	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	B	910	-	12,12,12	0.46	0	17,17,17	1.08	1 (5%)
10	MAN	A	902	-	11,11,12	0.65	0	15,15,17	1.07	2 (13%)
11	NAG	B	915	-	15,15,15	0.17	0	21,21,21	0.60	0
12	BMA	D	901	-	11,11,12	0.79	0	15,15,17	0.93	1 (6%)
11	NAG	B	908	1	14,14,15	0.41	0	17,19,21	1.04	3 (17%)
10	MAN	B	906	-	11,11,12	0.92	1 (9%)	15,15,17	1.48	3 (20%)
8	BKR	C	912	-	65,65,65	0.55	0	101,101,101	0.85	3 (2%)

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
11	NAG	D	909	1	-	3/6/23/26	0/1/1/1
11	NAG	C	901	-	-	3/6/23/26	0/1/1/1
8	BKR	A	911	-	-	5/37/123/123	0/7/7/7
9	XLS	A	912	-	-	7/10/10/12	-
10	MAN	D	904	-	-	2/2/19/22	0/1/1/1
11	NAG	C	902	-	-	3/6/23/26	0/1/1/1
11	NAG	C	909	1	-	2/6/23/26	0/1/1/1
10	MAN	C	904	-	-	2/2/19/22	0/1/1/1
10	MAN	A	907	-	-	2/2/22/22	0/1/1/1
11	NAG	A	905	1	-	0/6/23/26	0/1/1/1
11	NAG	D	907	1	-	4/6/23/26	0/1/1/1
10	MAN	B	903	-	-	2/2/19/22	0/1/1/1
11	NAG	D	908	1	-	4/6/23/26	0/1/1/1
11	NAG	B	914	1	-	2/6/23/26	0/1/1/1
10	MAN	B	912	-	-	0/2/19/22	1/1/1/1
11	NAG	B	911	-	-	4/6/26/26	0/1/1/1
8	BKR	B	901	-	-	5/37/123/123	0/7/7/7
10	MAN	D	905	-	-	2/2/19/22	0/1/1/1
11	NAG	B	913	1	-	0/6/23/26	0/1/1/1
11	NAG	A	906	1	-	0/6/23/26	0/1/1/1
11	NAG	D	906	1	-	2/6/23/26	0/1/1/1
11	NAG	C	908	1	-	0/6/23/26	0/1/1/1
11	NAG	A	910	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	A	908	-	-	0/2/19/22	0/1/1/1
10	MAN	D	902	-	-	2/2/19/22	0/1/1/1
10	MAN	B	904	-	-	2/2/19/22	0/1/1/1
11	NAG	A	909	1	-	0/6/23/26	0/1/1/1
10	MAN	A	904	-	-	2/2/19/22	0/1/1/1
10	MAN	C	907	-	-	1/2/19/22	0/1/1/1
10	MAN	D	903	-	-	2/2/19/22	0/1/1/1
10	MAN	C	903	-	-	0/2/19/22	1/1/1/1
8	BKR	D	910	-	-	8/37/123/123	0/7/7/7
9	XLS	B	902	-	-	7/10/10/12	-
10	MAN	A	901	-	-	0/2/19/22	0/1/1/1
11	NAG	B	916	-	-	0/6/23/26	0/1/1/1
10	MAN	B	905	-	-	0/2/19/22	0/1/1/1
10	MAN	A	903	-	-	0/2/19/22	0/1/1/1
10	MAN	B	907	-	-	2/2/19/22	0/1/1/1
10	MAN	C	906	-	-	1/2/19/22	0/1/1/1
11	NAG	C	910	1	-	0/6/23/26	0/1/1/1
10	MAN	C	905	-	-	0/2/19/22	0/1/1/1
11	NAG	B	909	1	-	2/6/23/26	0/1/1/1
11	NAG	C	911	1	-	4/6/23/26	0/1/1/1
10	MAN	B	910	-	-	2/2/22/22	0/1/1/1
10	MAN	A	902	-	-	0/2/19/22	0/1/1/1
11	NAG	B	915	-	-	0/6/26/26	0/1/1/1
12	BMA	D	901	-	-	0/2/19/22	0/1/1/1
11	NAG	B	908	1	-	2/6/23/26	0/1/1/1
10	MAN	B	906	-	-	2/2/19/22	0/1/1/1
8	BKR	C	912	-	-	7/37/123/123	0/7/7/7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	912	MAN	O5-C5	3.30	1.49	1.43
11	D	908	NAG	O5-C1	-2.57	1.39	1.43
10	D	902	MAN	O5-C5	2.53	1.48	1.43
10	B	903	MAN	O5-C5	2.43	1.48	1.43
10	B	906	MAN	C2-C3	-2.39	1.48	1.52

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	902	MAN	C1-O5-C5	7.43	122.14	112.19
11	D	908	NAG	O5-C1-C2	-6.89	100.62	111.29
9	B	902	XLS	C1-C2-C3	5.98	119.44	112.11
9	A	912	XLS	C1-C2-C3	5.98	119.43	112.11
11	D	907	NAG	O5-C1-C2	-5.66	102.54	111.29

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	901	BKR	C37-C29-N1-C30
8	A	911	BKR	C37-C29-N1-C30
9	B	902	XLS	O4-C4-C5-O5
9	A	912	XLS	O4-C4-C5-O5
11	B	914	NAG	C8-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	912	MAN	C1-C2-C3-C4-C5-O5
10	C	903	MAN	C1-C2-C3-C4-C5-O5

33 monomers are involved in 92 short contacts:

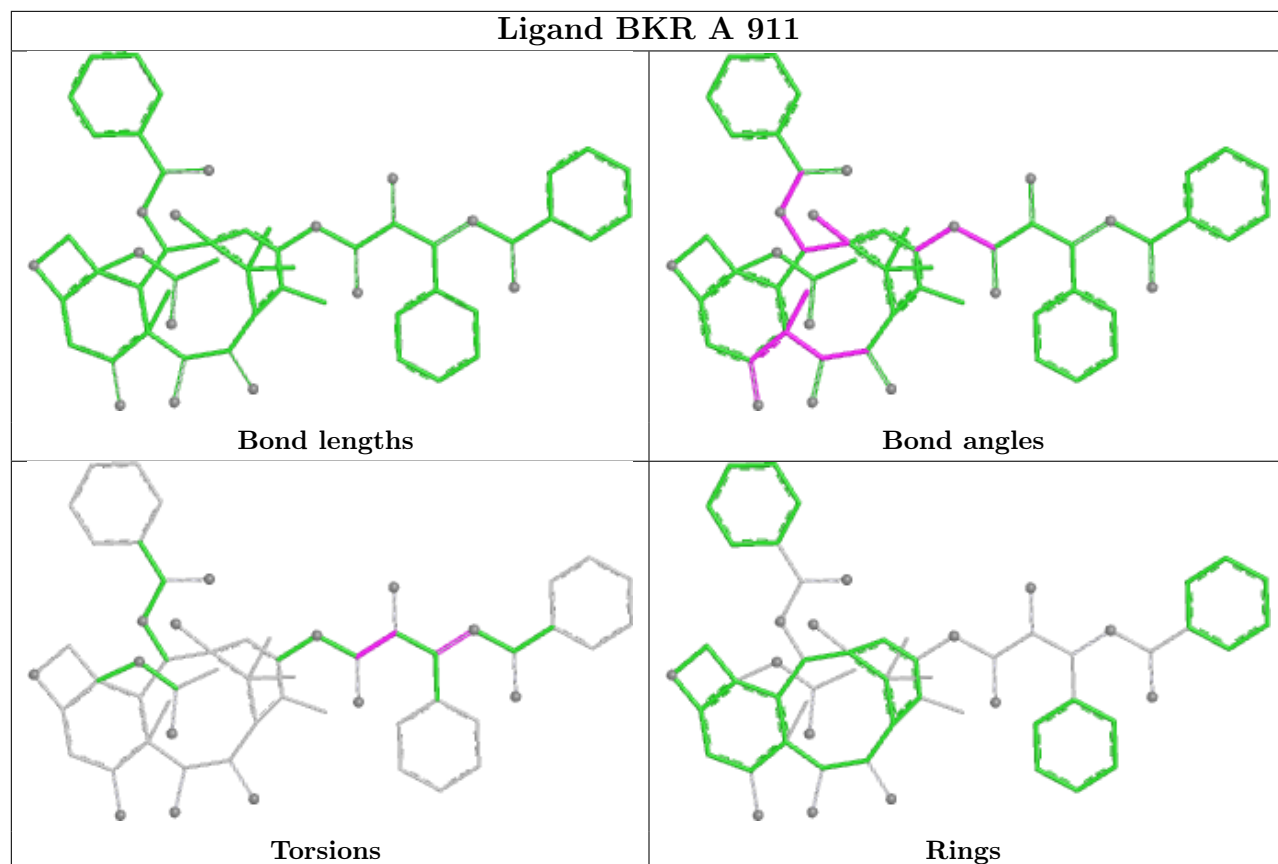
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	901	NAG	8	0
8	A	911	BKR	1	0
9	A	912	XLS	1	0
10	D	904	MAN	5	0
11	C	902	NAG	6	0
10	C	904	MAN	6	0
10	A	907	MAN	3	0
11	D	907	NAG	1	0
10	B	903	MAN	2	0
10	B	912	MAN	4	0
11	B	911	NAG	4	0
8	B	901	BKR	1	0
10	D	905	MAN	1	0
10	A	908	MAN	1	0
10	D	902	MAN	2	0
10	B	904	MAN	6	0
10	A	904	MAN	6	0
10	C	907	MAN	1	0

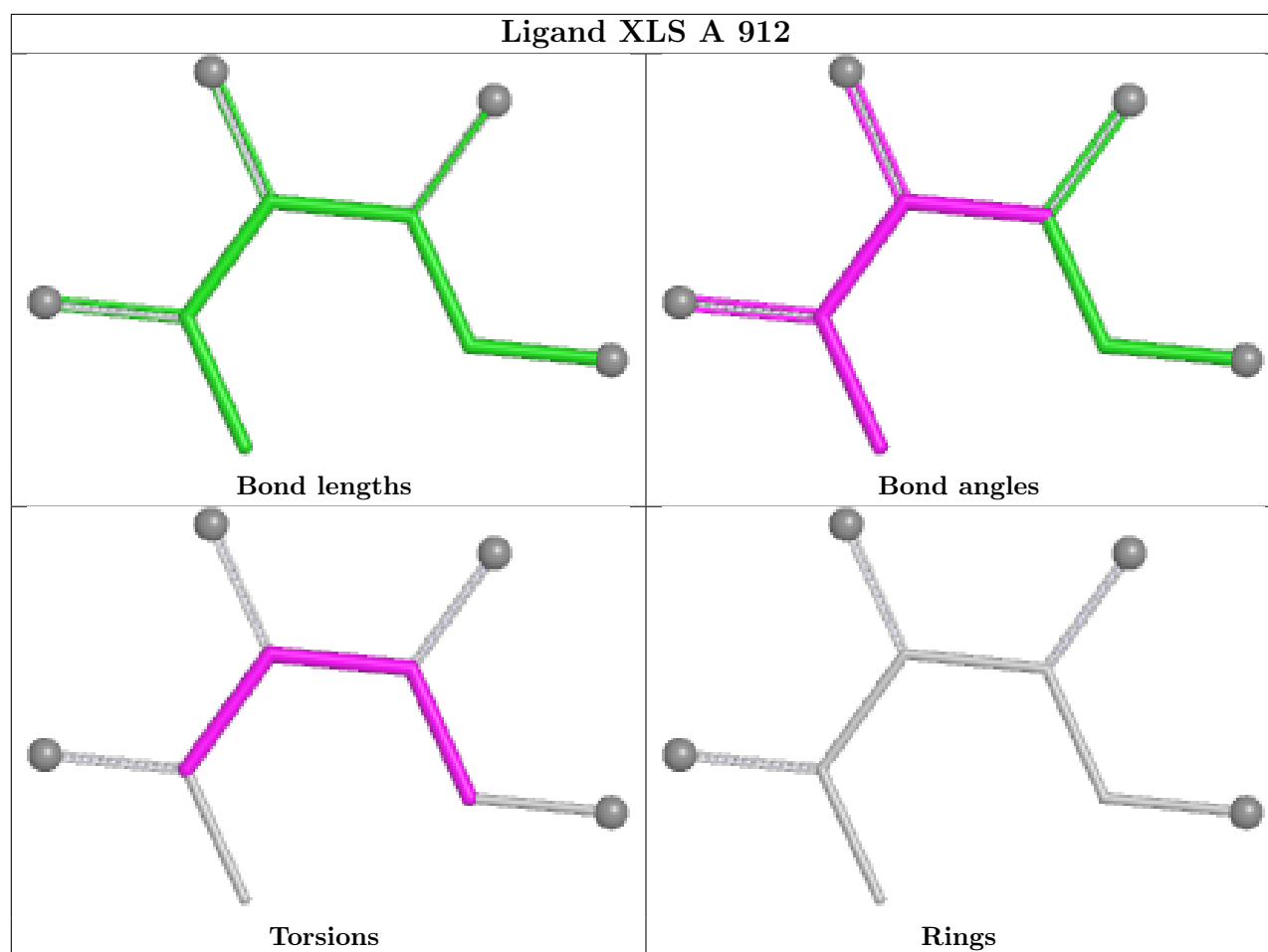
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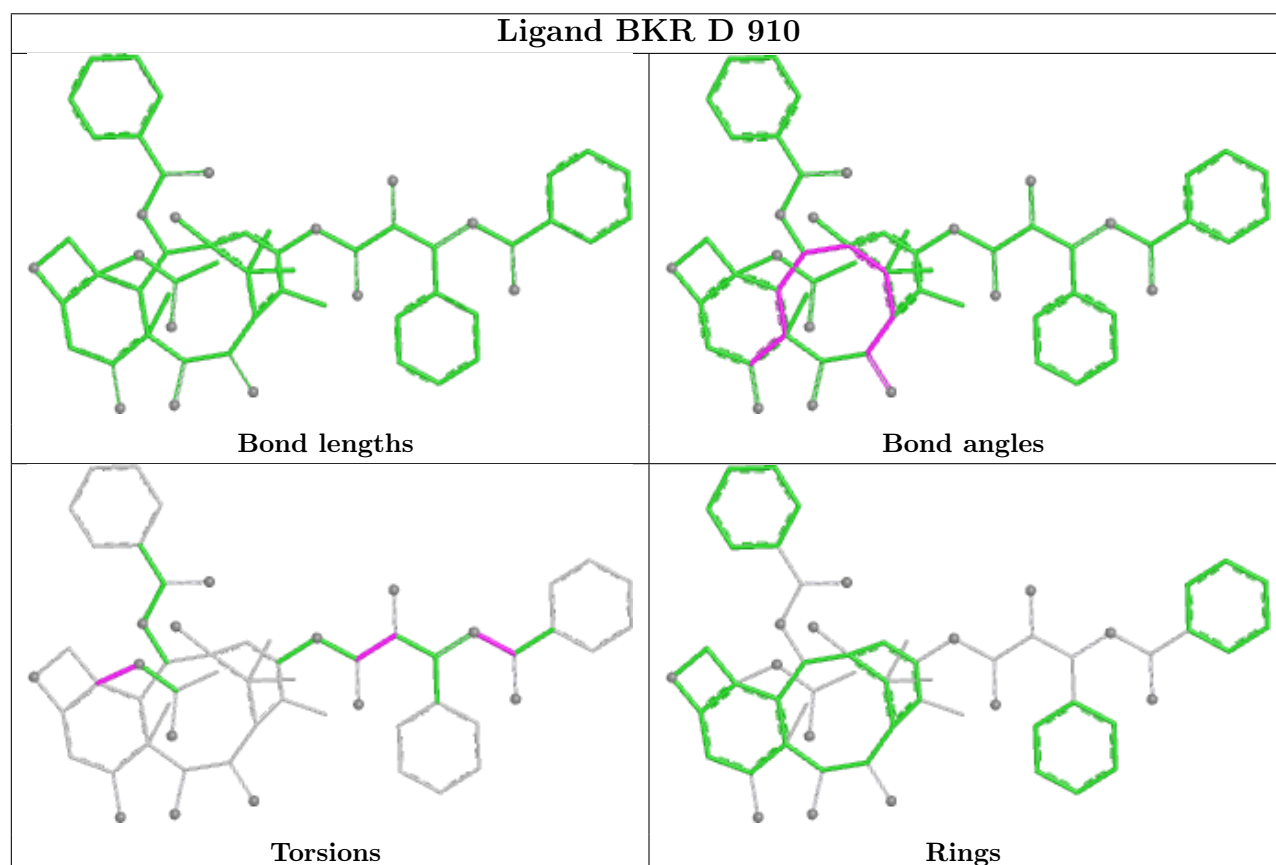
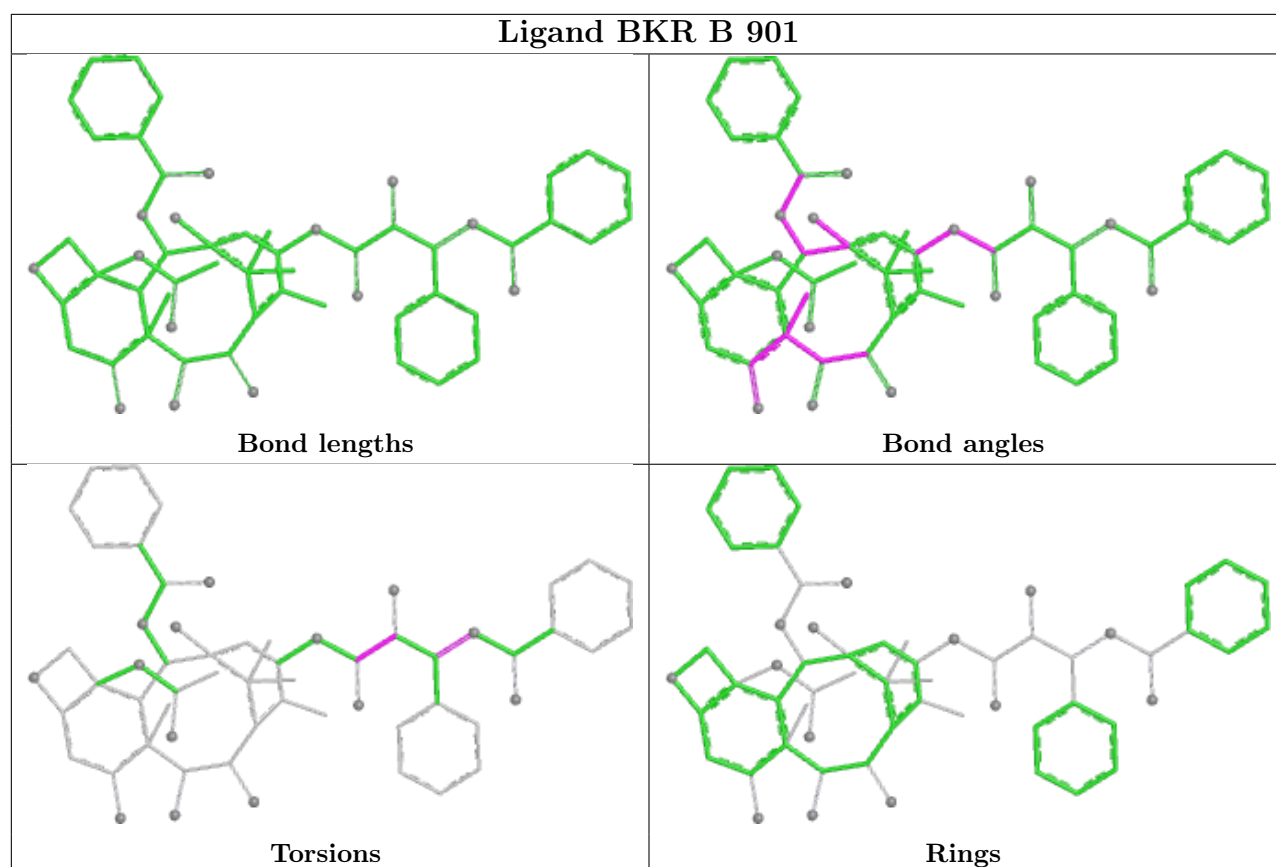
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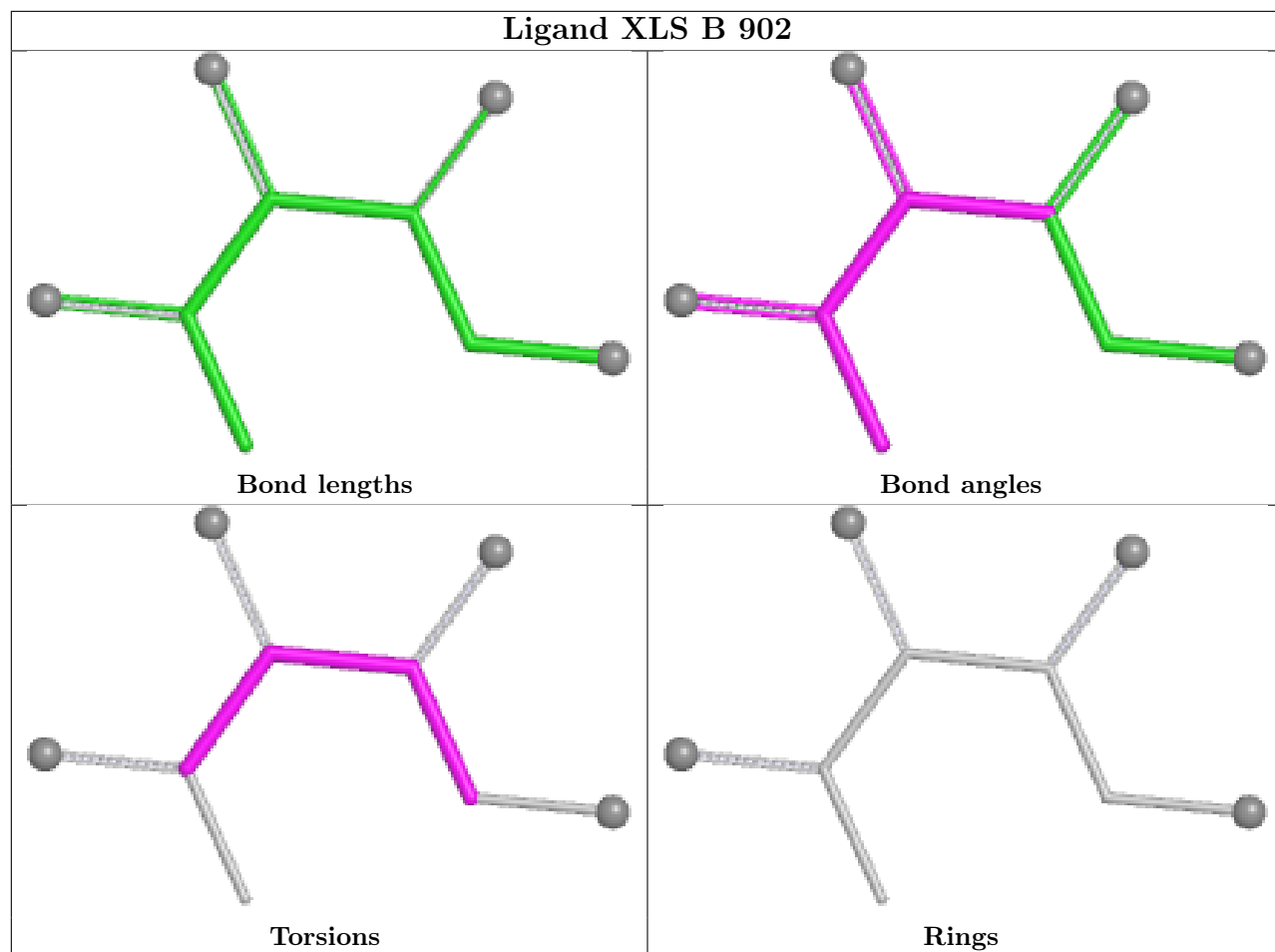
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	903	MAN	10	0
8	D	910	BKR	2	0
9	B	902	XLS	1	0
10	A	901	MAN	10	0
11	B	916	NAG	4	0
10	B	905	MAN	3	0
10	A	903	MAN	10	0
10	B	907	MAN	4	0
10	C	906	MAN	3	0
10	C	905	MAN	2	0
10	B	910	MAN	12	0
10	A	902	MAN	4	0
12	D	901	BMA	9	0
10	B	906	MAN	6	0
8	C	912	BKR	2	0

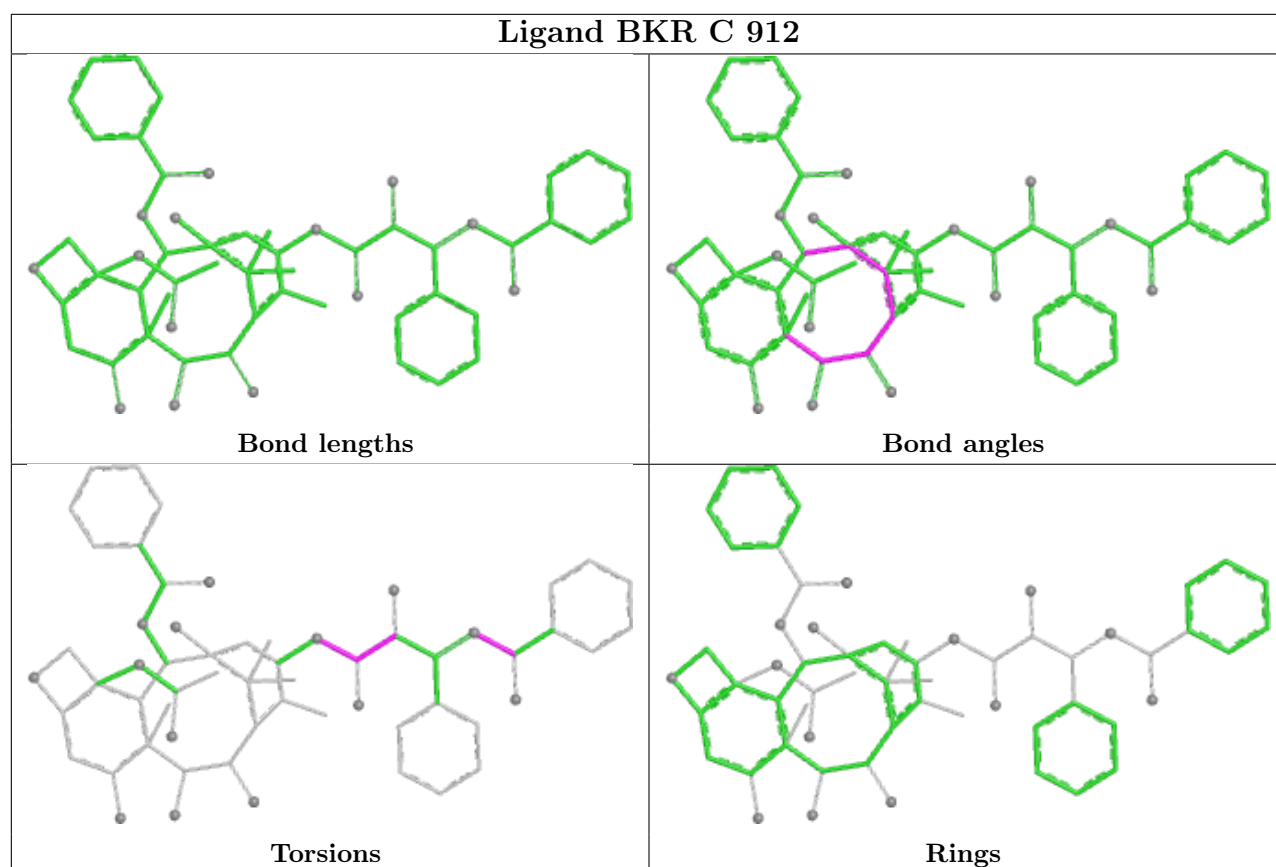
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	757/803 (94%)	-0.15	10 (1%) 75 77	18, 31, 50, 101	1 (0%)
1	B	756/803 (94%)	-0.22	6 (0%) 82 84	14, 30, 42, 84	3 (0%)
1	C	756/803 (94%)	0.79	78 (10%) 12 12	24, 50, 73, 121	2 (0%)
1	D	756/803 (94%)	0.87	61 (8%) 18 18	22, 48, 69, 96	2 (0%)
All	All	3025/3212 (94%)	0.32	155 (5%) 33 33	14, 39, 67, 121	8 (0%)

The worst 5 of 155 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	TYR	5.4
1	D	683	TYR	4.8
1	D	227	VAL	4.5
1	C	683	TYR	4.5
1	D	230	ALA	4.2

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	MAN	G	1	12/12	0.37	0.28	20,20,20,20	0
7	MAN	N	3	11/12	0.62	0.16	80,85,92,94	0

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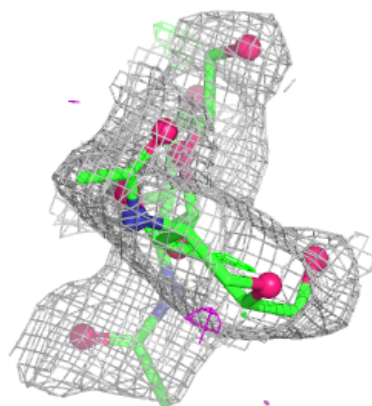
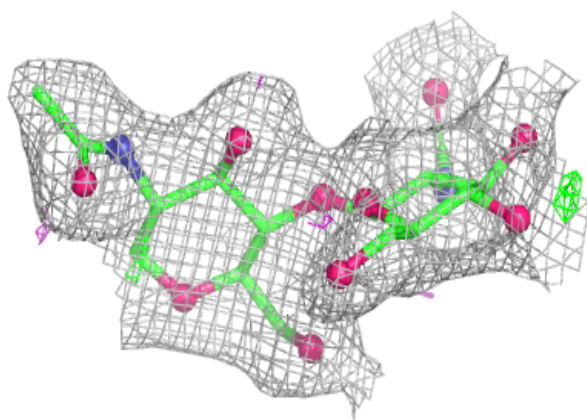
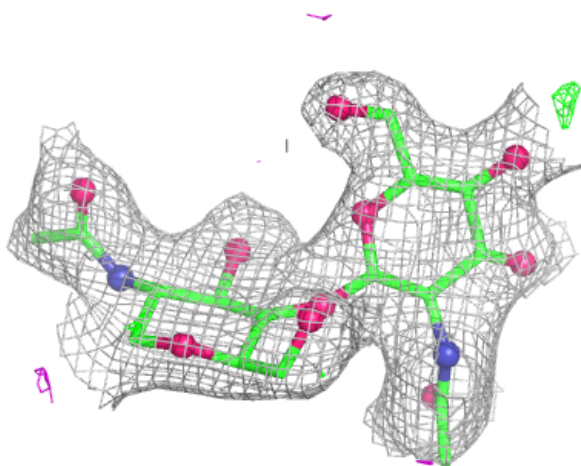
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	O	2	14/15	0.66	0.16	69,91,100,108	0
5	NAG	I	3	14/15	0.67	0.14	60,73,81,86	0
2	NAG	L	2	14/15	0.69	0.14	70,80,85,91	0
2	NAG	O	1	14/15	0.76	0.22	20,20,20,20	0
4	BMA	G	2	11/12	0.76	0.17	37,49,56,57	0
7	MAN	M	3	11/12	0.78	0.14	50,63,69,78	0
7	NAG	N	2	14/15	0.80	0.15	41,65,82,83	0
2	NAG	P	1	14/15	0.84	0.17	55,70,80,82	0
6	BMA	J	4	11/12	0.85	0.11	50,60,64,65	0
3	MAN	F	4	11/12	0.87	0.10	44,45,54,55	0
7	MAN	K	3	11/12	0.89	0.10	37,43,48,55	0
2	NAG	E	2	14/15	0.90	0.09	42,52,55,60	0
3	MAN	F	5	11/12	0.90	0.09	43,50,53,54	0
2	NAG	L	1	14/15	0.90	0.12	51,68,73,76	0
6	MAN	J	5	11/12	0.90	0.09	45,53,63,64	0
2	NAG	P	2	14/15	0.92	0.09	42,46,50,50	0
7	NAG	M	2	14/15	0.93	0.08	33,37,45,56	0
7	NAG	N	1	14/15	0.93	0.09	34,39,47,58	0
6	AH2	J	3	11/11	0.94	0.07	35,45,48,50	0
5	NAG	I	2	14/15	0.94	0.07	38,44,48,49	0
2	NAG	H	2	14/15	0.94	0.07	27,31,38,39	0
6	NAG	J	2	14/15	0.95	0.07	37,40,48,49	0
7	NAG	K	2	14/15	0.95	0.06	23,29,32,35	0
6	NAG	J	1	14/15	0.96	0.06	27,30,36,42	0
3	NAG	F	1	14/15	0.96	0.06	24,28,31,34	0
3	NAG	F	2	14/15	0.96	0.06	25,29,34,38	0
7	NAG	M	1	14/15	0.97	0.06	33,37,38,39	0
3	BMA	F	3	11/12	0.97	0.05	24,27,30,31	0
2	NAG	H	1	14/15	0.97	0.06	25,28,33,34	0
7	NAG	K	1	14/15	0.97	0.06	25,29,32,32	0
5	NAG	I	1	14/15	0.97	0.06	24,28,30,38	0
2	NAG	E	1	14/15	0.97	0.07	30,35,39,46	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.

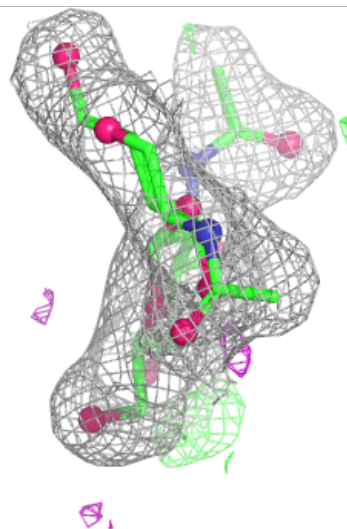
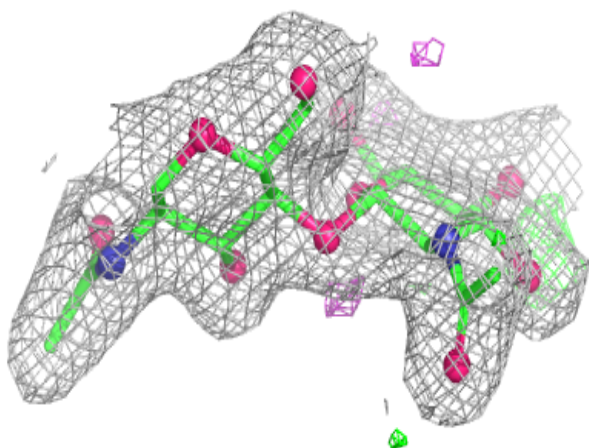
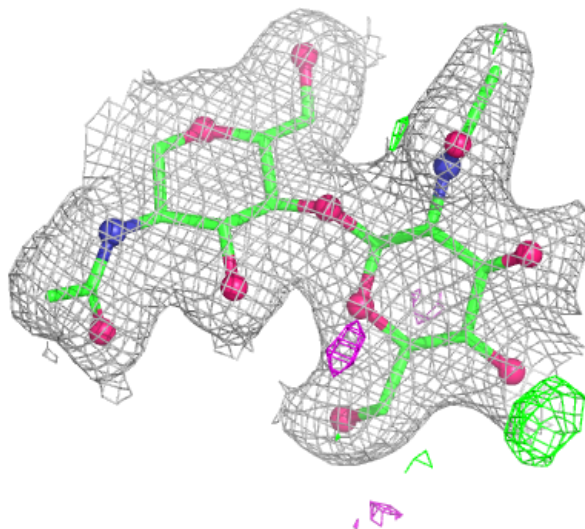
Electron density around Chain E:

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



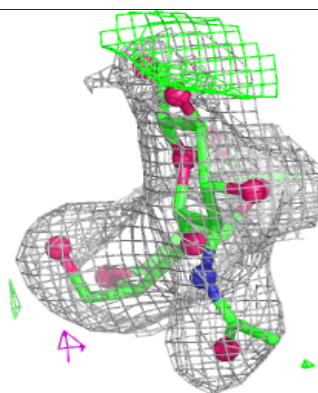
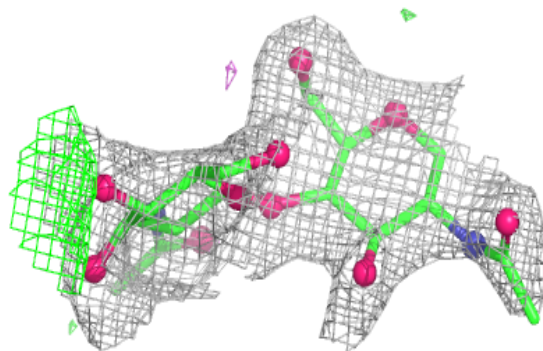
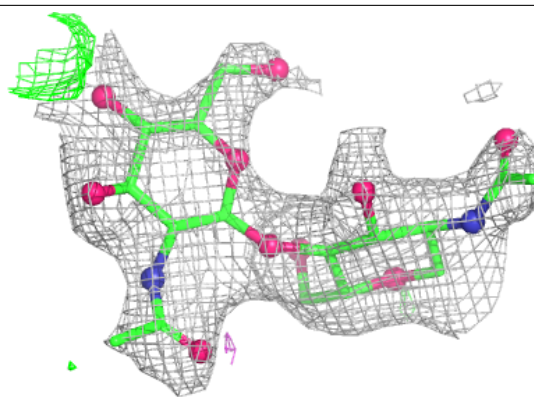
Electron density around Chain H:

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



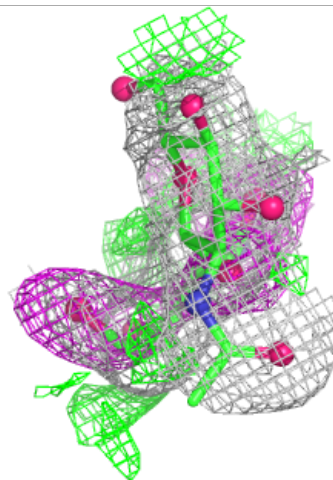
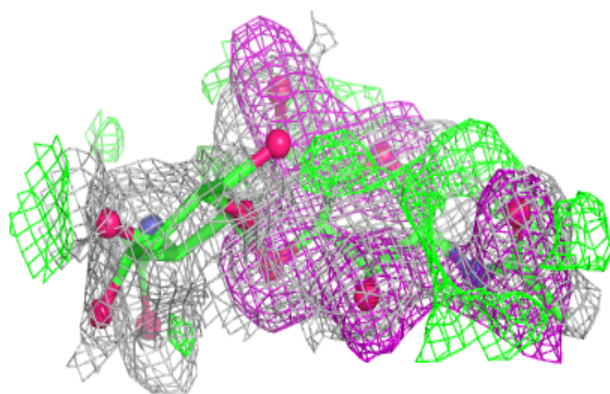
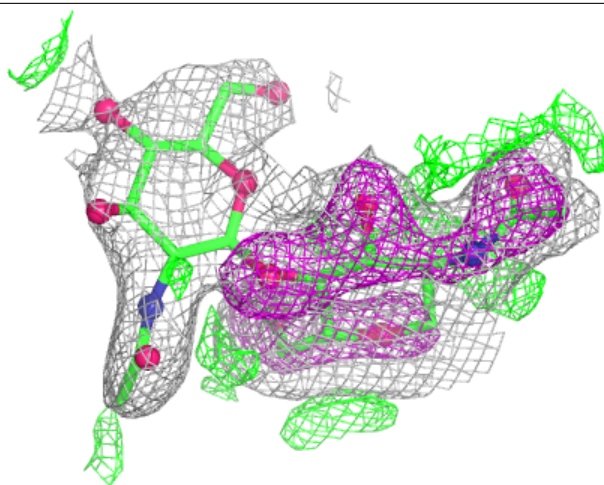
Electron density around Chain L:

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and green (positive)



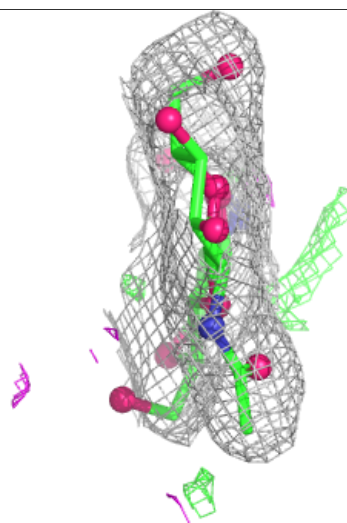
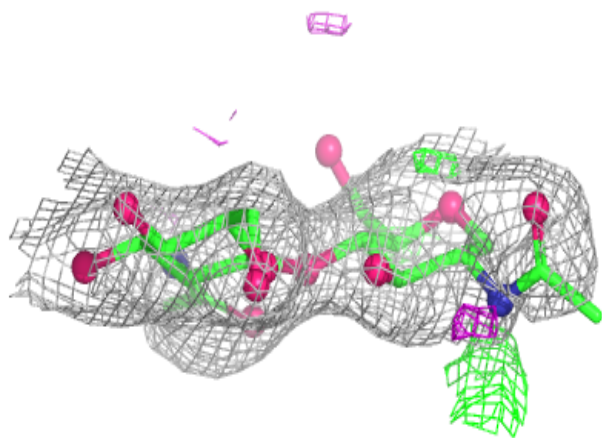
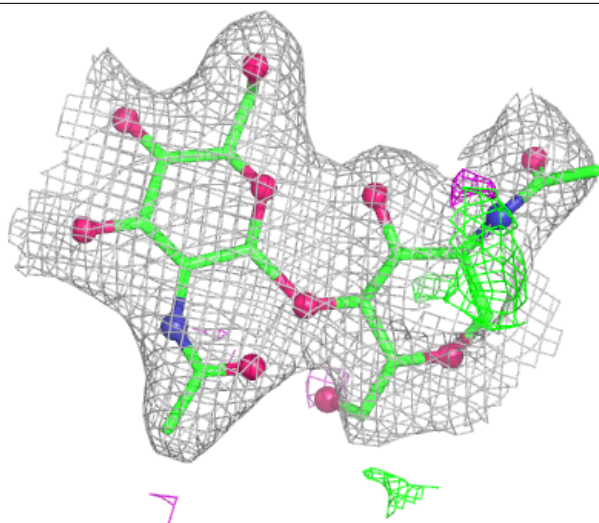
Electron density around Chain O:

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



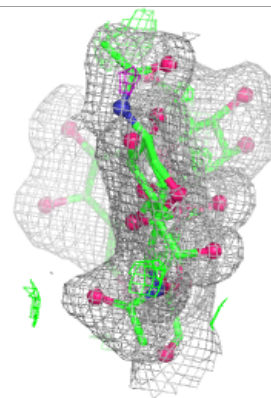
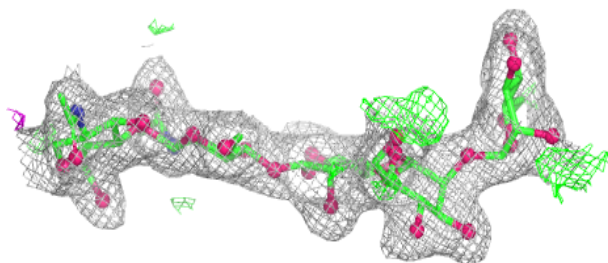
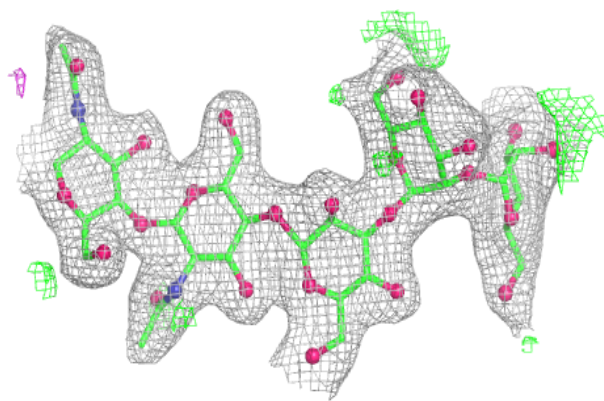
Electron density around Chain P:

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

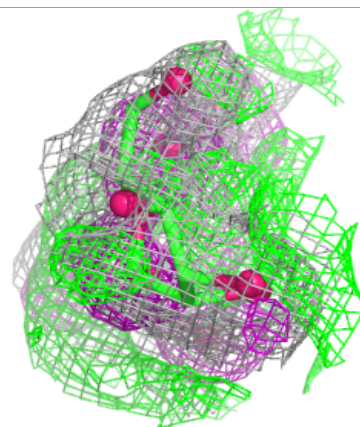
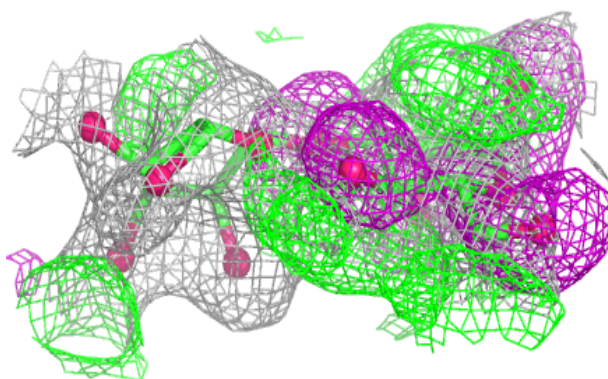
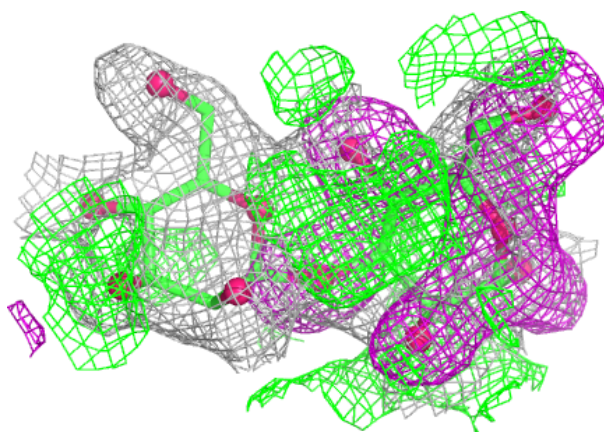


Electron density around Chain F:

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

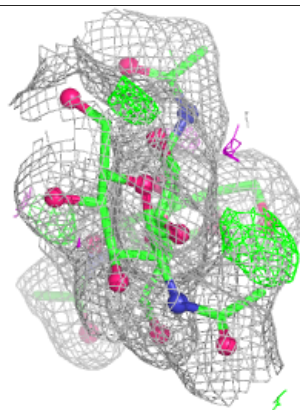
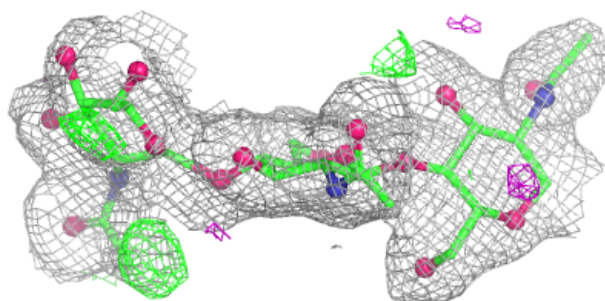
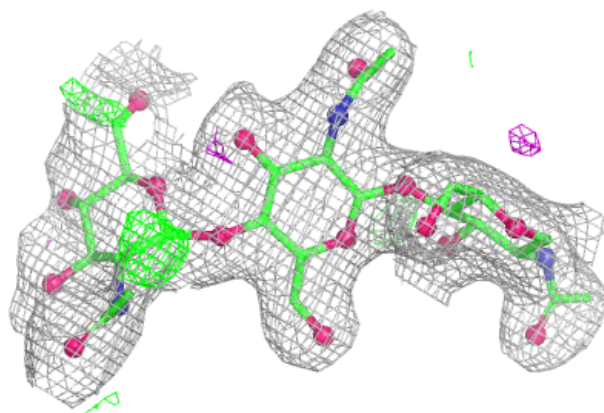
**Electron density around Chain G:**

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

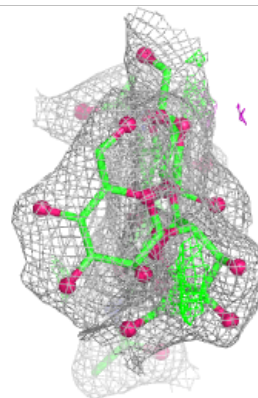
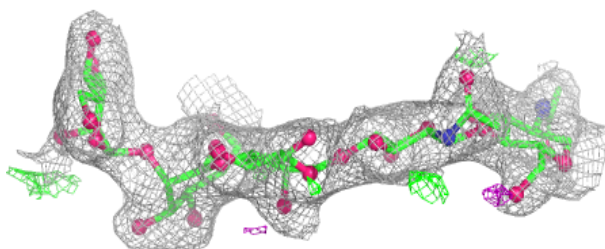
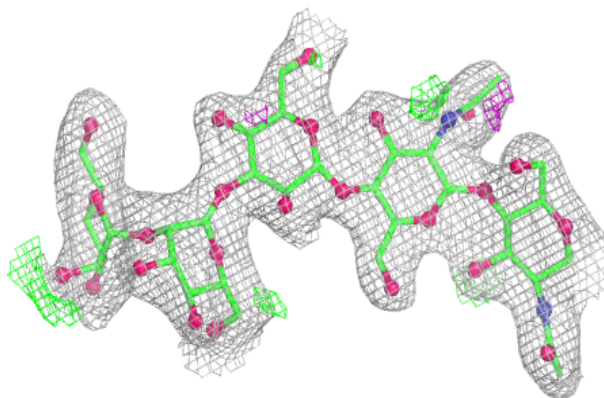


Electron density around Chain I:

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

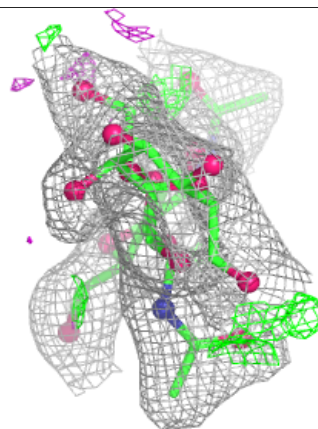
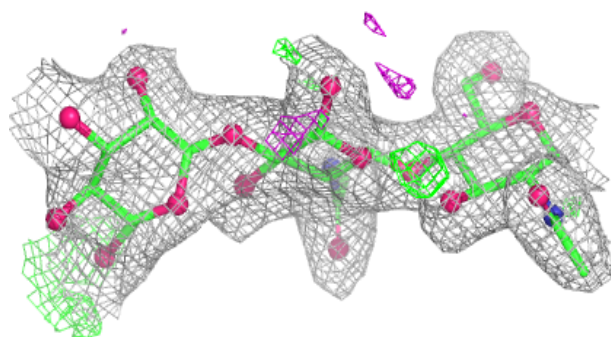
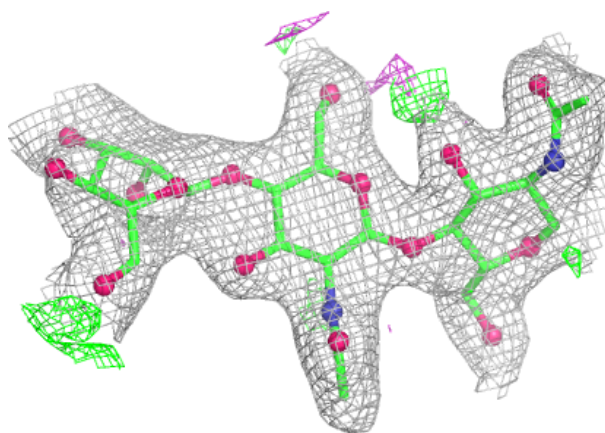
**Electron density around Chain J:**

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

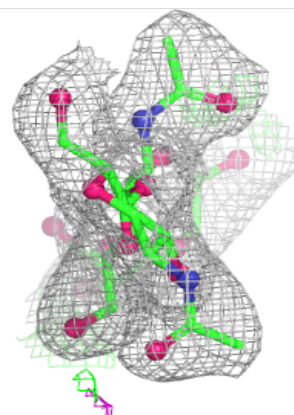
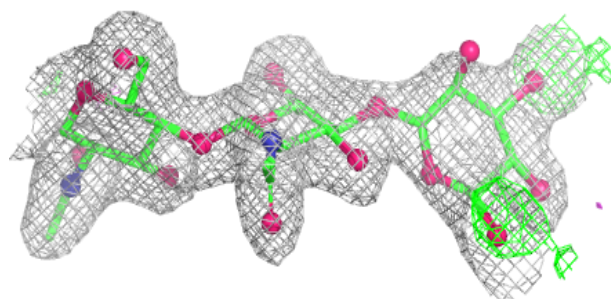
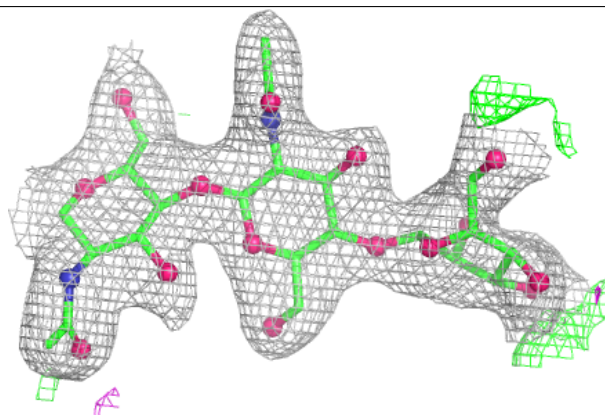


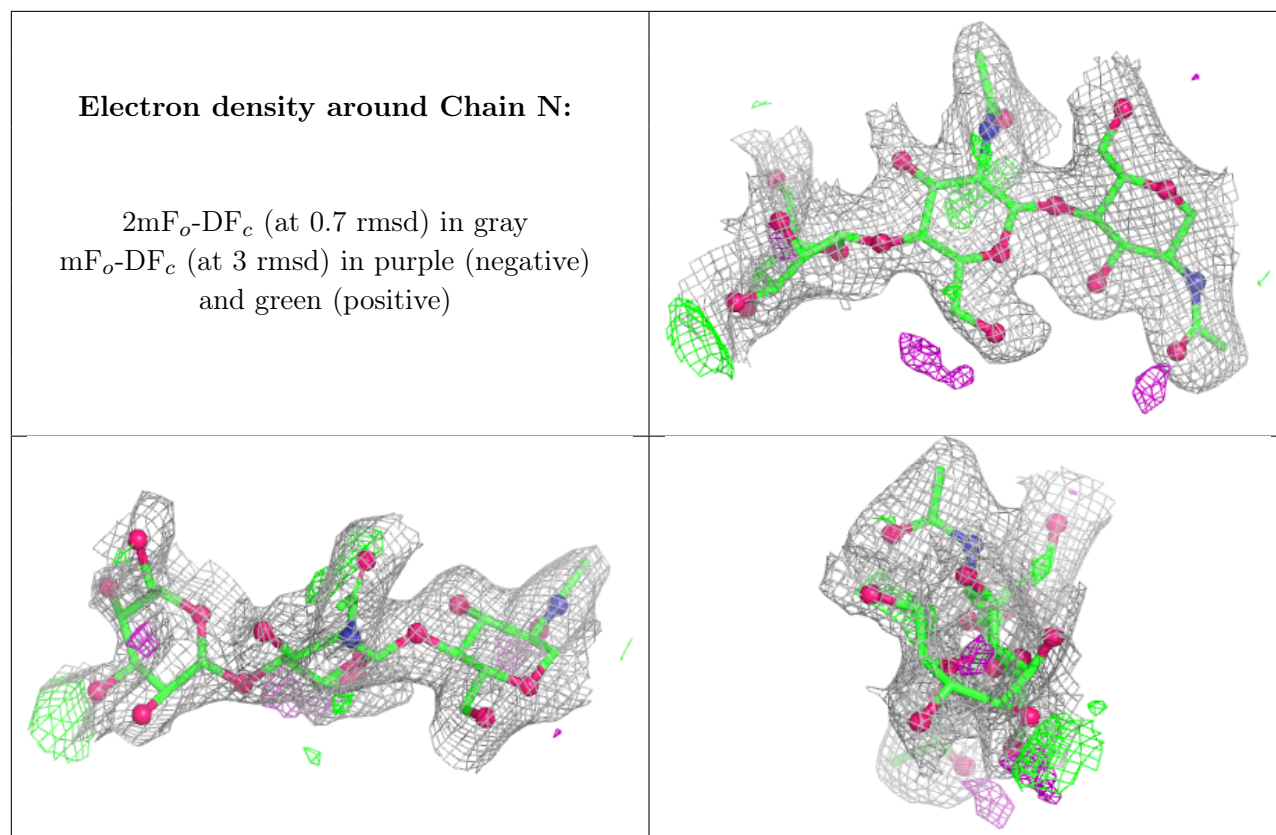
Electron density around Chain K:

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

**Electron density around Chain M:**

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





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	915	15/15	0.44	0.17	20,20,20,20	0
11	NAG	D	909	14/15	0.61	0.14	68,90,97,104	0
11	NAG	C	911	14/15	0.62	0.15	92,113,120,134	0
10	MAN	B	912	11/12	0.65	0.19	52,57,65,66	0
11	NAG	B	916	14/15	0.65	0.15	20,20,20,20	0
11	NAG	B	914	14/15	0.66	0.15	67,74,84,94	0
11	NAG	B	911	15/15	0.68	0.15	20,20,20,20	0
10	MAN	B	907	11/12	0.70	0.14	79,88,93,95	0
10	MAN	A	904	11/12	0.73	0.14	83,97,107,110	0
10	MAN	C	904	11/12	0.73	0.17	70,80,85,90	0
10	MAN	C	906	11/12	0.73	0.15	68,84,94,102	0
11	NAG	C	908	14/15	0.75	0.15	88,94,99,100	0
10	MAN	D	902	11/12	0.76	0.13	55,60,71,74	0
8	BKR	D	910	59/59	0.76	0.20	82,112,136,139	0

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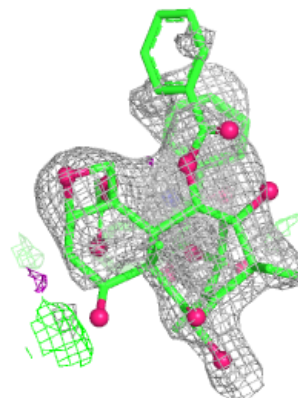
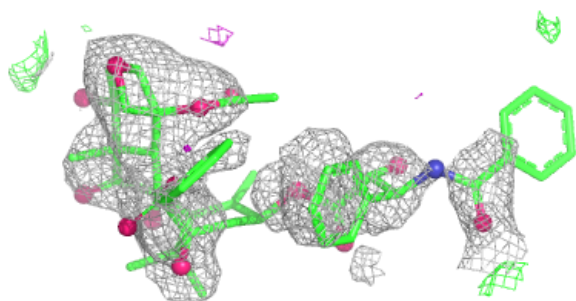
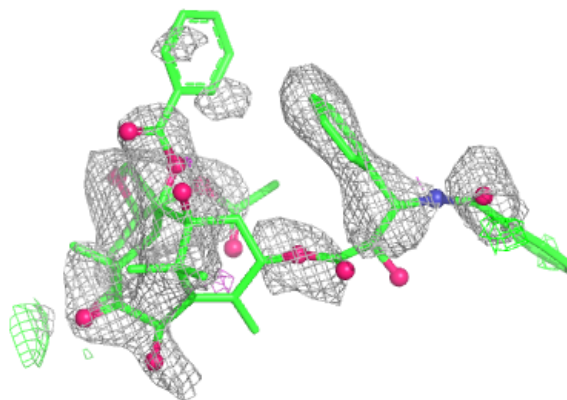
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	A	910	14/15	0.77	0.16	74,85,97,103	0
10	MAN	B	910	12/12	0.79	0.14	33,43,54,57	0
11	NAG	D	907	14/15	0.79	0.11	65,74,85,89	0
9	XLS	A	912	9/10	0.79	0.21	32,44,63,67	0
10	MAN	D	904	11/12	0.80	0.13	65,73,84,90	0
8	BKR	C	912	59/59	0.80	0.19	72,104,123,126	0
8	BKR	A	911	59/59	0.82	0.15	36,47,54,56	0
11	NAG	D	906	14/15	0.82	0.12	65,73,85,90	0
10	MAN	D	905	11/12	0.83	0.13	65,79,89,98	0
10	MAN	C	907	11/12	0.84	0.10	55,61,72,83	0
9	XLS	B	902	9/10	0.85	0.17	32,44,63,67	0
11	NAG	C	909	14/15	0.85	0.10	61,80,89,91	0
10	MAN	B	903	11/12	0.86	0.11	56,72,79,82	0
10	MAN	A	907	12/12	0.87	0.15	51,58,67,79	0
10	MAN	B	906	11/12	0.87	0.10	53,59,65,68	0
11	NAG	D	908	14/15	0.87	0.10	54,62,67,71	0
11	NAG	C	902	14/15	0.87	0.14	52,67,74,82	0
8	BKR	B	901	59/59	0.88	0.12	36,47,54,56	0
10	MAN	C	905	11/12	0.88	0.09	56,60,74,80	0
11	NAG	A	906	14/15	0.88	0.09	39,44,46,48	0
10	MAN	A	903	11/12	0.88	0.09	62,70,85,91	0
10	MAN	A	901	11/12	0.89	0.09	44,47,50,56	0
11	NAG	C	901	14/15	0.89	0.13	54,58,65,73	0
11	NAG	A	905	14/15	0.90	0.08	46,50,55,61	0
10	MAN	C	903	11/12	0.90	0.08	52,54,58,59	0
10	MAN	B	904	11/12	0.90	0.08	37,43,48,52	0
10	MAN	D	903	11/12	0.90	0.10	55,56,59,67	0
11	NAG	B	913	14/15	0.91	0.09	37,44,47,47	0
11	NAG	B	909	14/15	0.91	0.10	39,44,53,55	0
11	NAG	C	910	14/15	0.91	0.08	41,44,47,48	0
10	MAN	A	908	11/12	0.91	0.08	47,61,65,69	0
11	NAG	B	908	14/15	0.92	0.08	39,45,52,60	0
10	MAN	A	902	11/12	0.92	0.09	45,47,52,53	0
12	BMA	D	901	11/12	0.93	0.07	36,40,45,46	0
10	MAN	B	905	11/12	0.94	0.08	30,35,42,45	0
11	NAG	A	909	14/15	0.94	0.07	35,39,44,47	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.

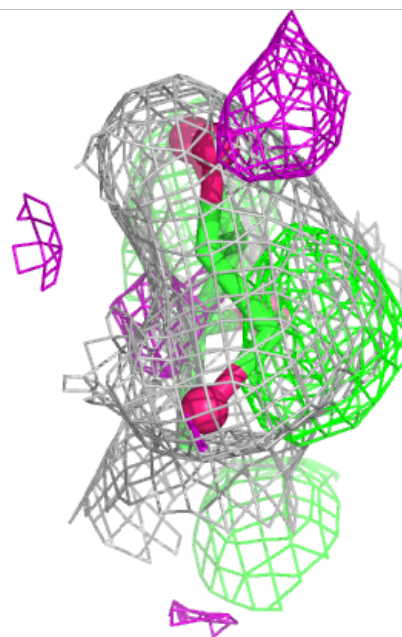
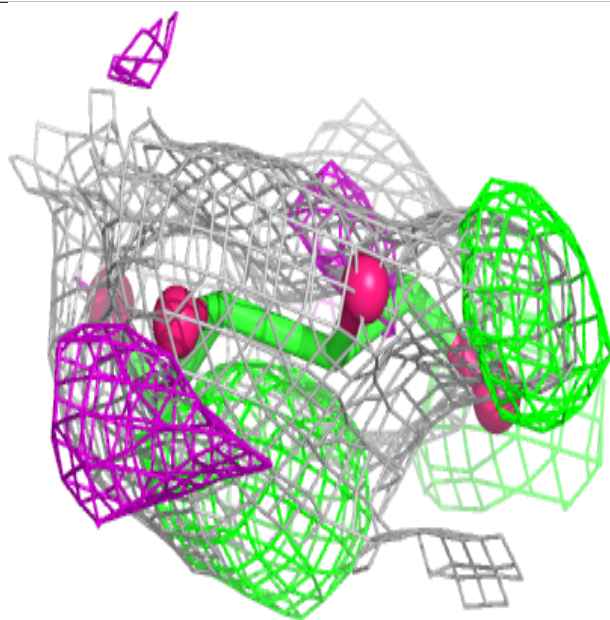
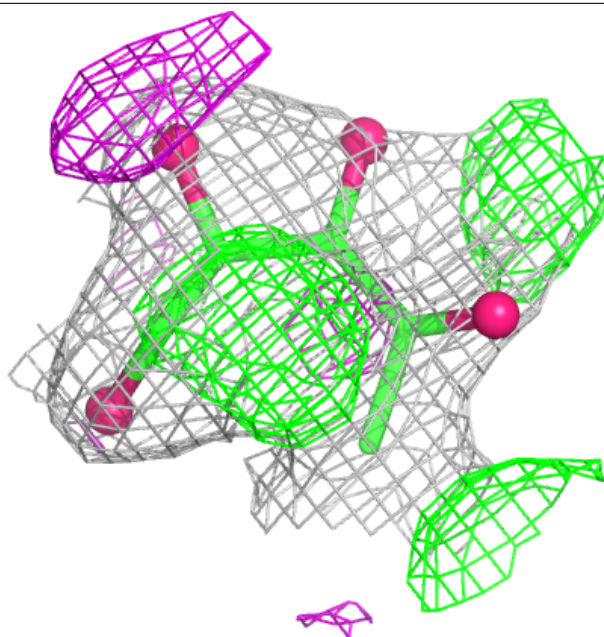
Electron density around BKR D 910:

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



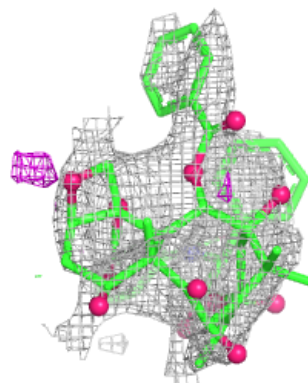
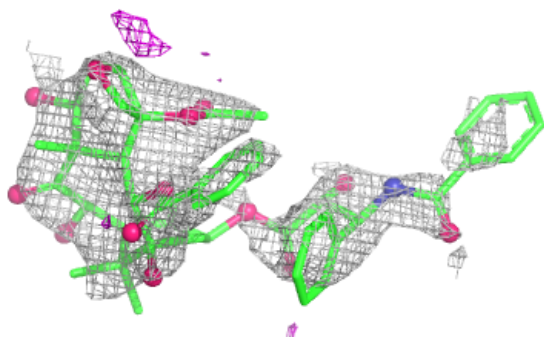
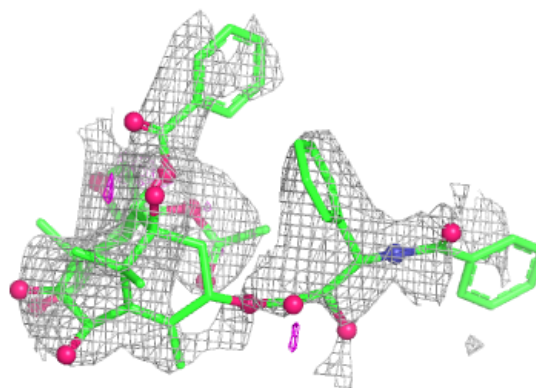
Electron density around XLS A 912:

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

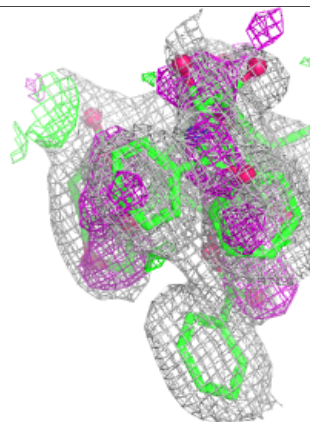
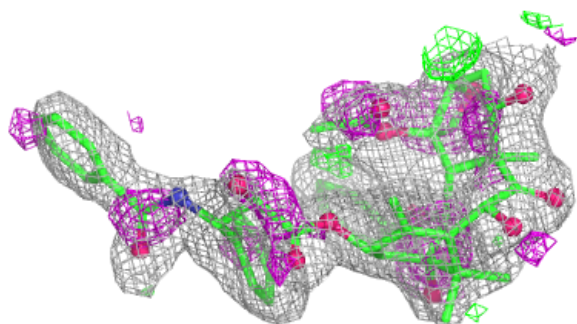
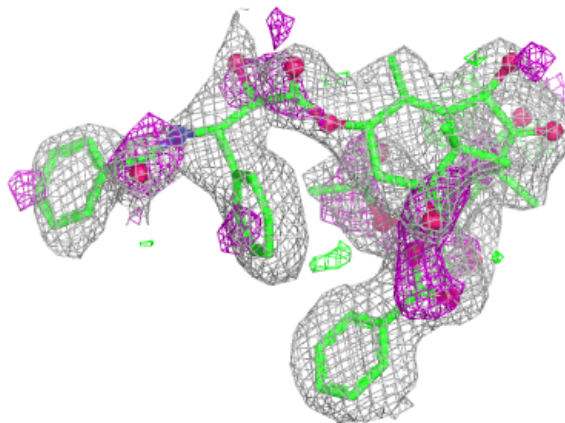


Electron density around BKR C 912:

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

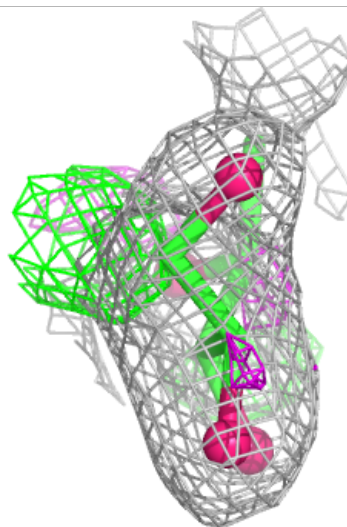
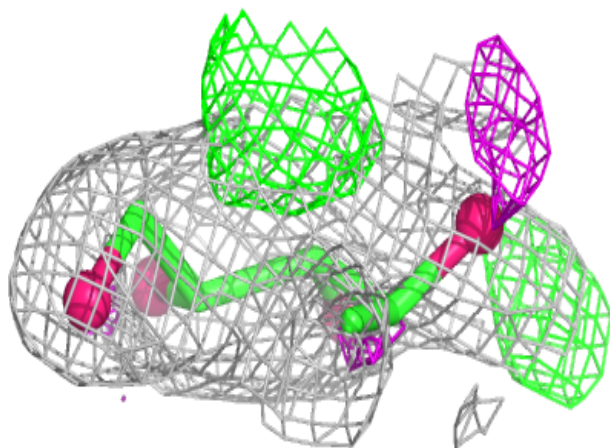
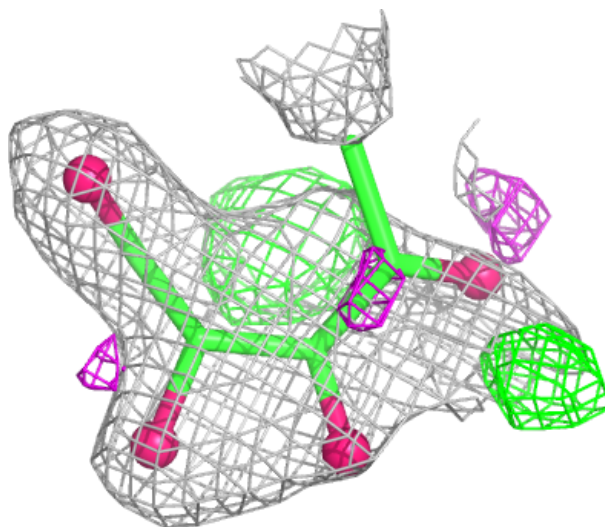
**Electron density around BKR A 911:**

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



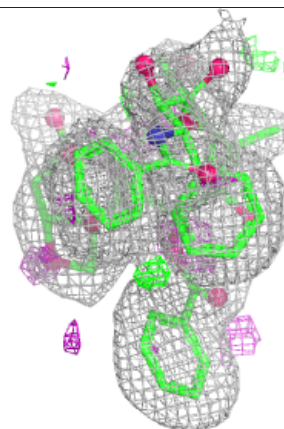
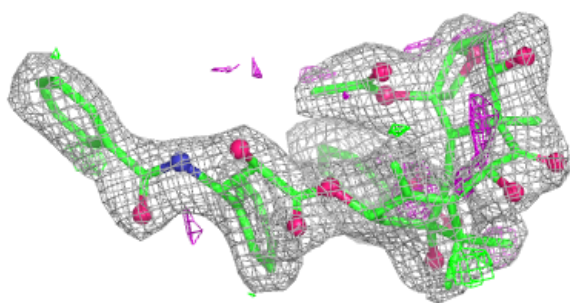
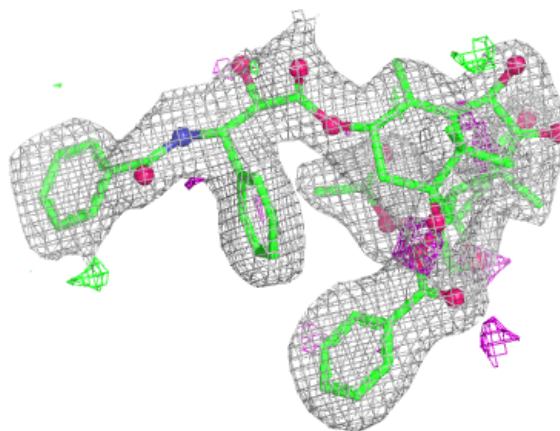
Electron density around XLS B 902:

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



Electron density around BKR B 901:

$2mF_o-DF_c$ (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.