wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 06:04 AM JST

PDB ID	:	7EY1
Title	:	Bifunctional xylosidase/glucosidase LXYL with intermediate substrate xylose
Authors	:	Gong, W.M.; Yang, L.Y.
Deposited on	:	2021-05-29
Resolution	:	2.46 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 (i) 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 (i)) were used in the production of this report:

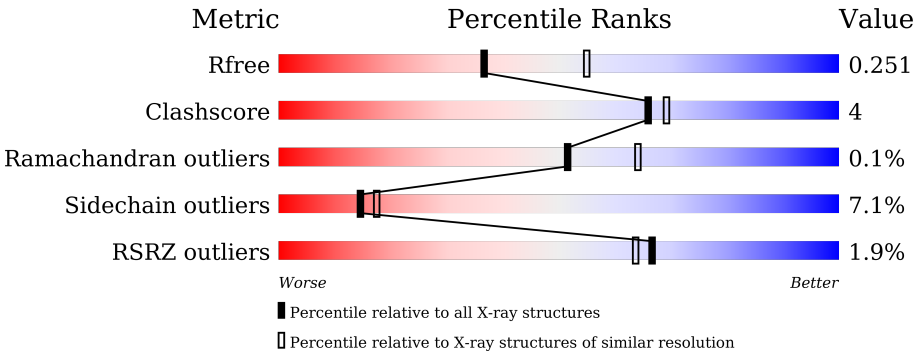
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	83% 10% • 6%
1	B	803	84% 9% • 6%
1	C	803	3% 81% 11% • 6%
1	D	803	3% 80% 13% • 6%
2	E	8	88% 12%
2	G	8	12% 75% 12%

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Mol	Chain	Length	Quality of chain
3	F	4	100%
4	I	3	100%
4	K	3	100%
4	M	3	67% 33%
5	J	4	75% 25%
6	L	8	88% 12%
7	N	2	100%

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
2	MAN	E	5	-	-	-	X
2	MAN	G	5	-	-	-	X
6	NAG	L	1	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 24651 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	A	756	Total	C	N	O	S	0	2	0
			5719	3621	957	1124	17			
1	B	756	Total	C	N	O	S	0	4	0
			5736	3633	958	1128	17			
1	C	756	Total	C	N	O	S	0	2	0
			5716	3621	955	1123	17			
1	D	756	Total	C	N	O	S	0	2	0
			5720	3624	956	1123	17			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			92	50	1	41			
2	G	8	Total	C	N	O	0	0	0
			92	50	1	41			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(4-3)-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
3	F	4	Total	C	N	O	0	0	0
			53	30	3	20			

- Molecule 4 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
4	I	3	Total C N O 39 22 2 15	0	0	0
4	K	3	Total C N O 39 22 2 15	0	0	0
4	M	3	Total C N O 39 22 2 15	0	0	0

- 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.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	J	4	Total C N O 48 26 1 21	0	0	0

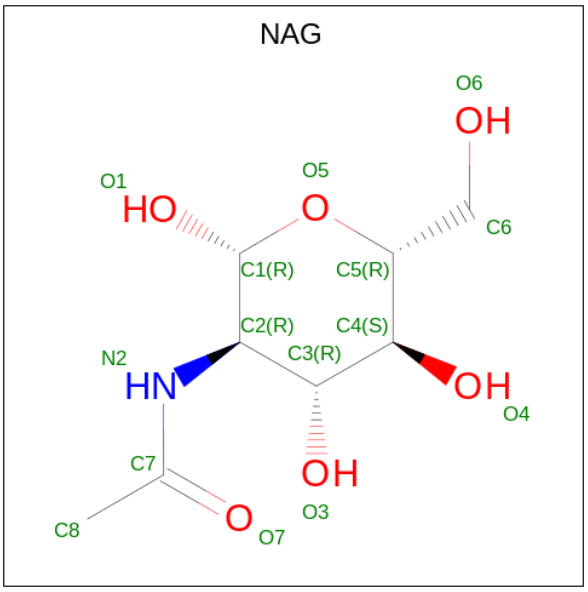
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(6-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	L	8	Total C N O 95 52 2 41	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	N	2	Total C O 22 12 10	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 13 8 1 4	0	0
8	A	1	Total C N O 15 8 1 6	0	0
8	A	1	Total C N O 13 8 1 4	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	A	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 13 8 1 4	0	0
8	B	1	Total C N O 15 8 1 6	0	0
8	B	1	Total C N O 13 8 1 4	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0
8	B	1	Total C N O 14 8 1 5	0	0

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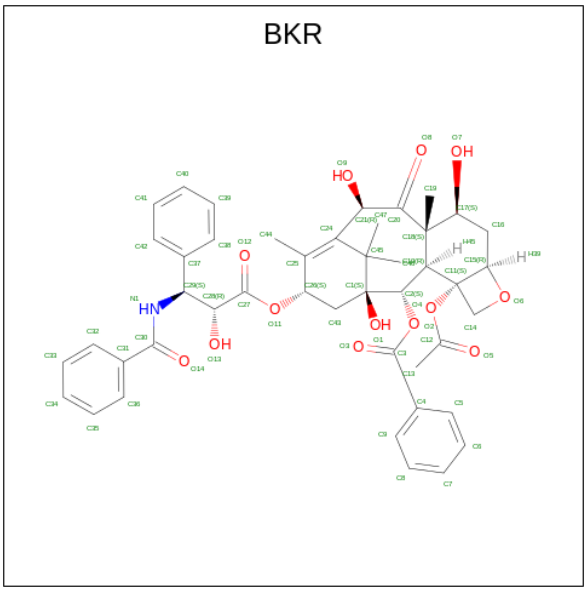
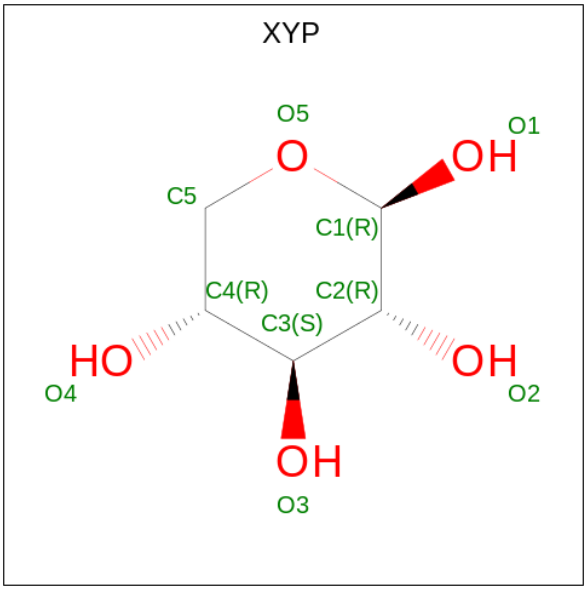
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O 13 8 1 4	0	0
8	C	1	Total C N O 15 8 1 6	0	0
8	C	1	Total C N O 13 8 1 4	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 13 8 1 4	0	0
8	D	1	Total C N O 15 8 1 6	0	0
8	D	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is Deacetyltaxol (three-letter code: BKR) (formula: $C_{45}H_{49}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



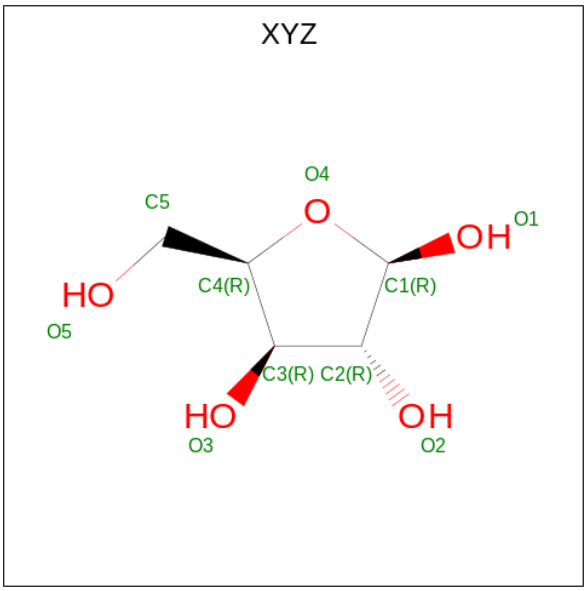
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N O 59 45 1 13	0	0
9	B	1	Total C N O 59 45 1 13	0	0

- Molecule 10 is beta-D-xylopyranose (three-letter code: XYP) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



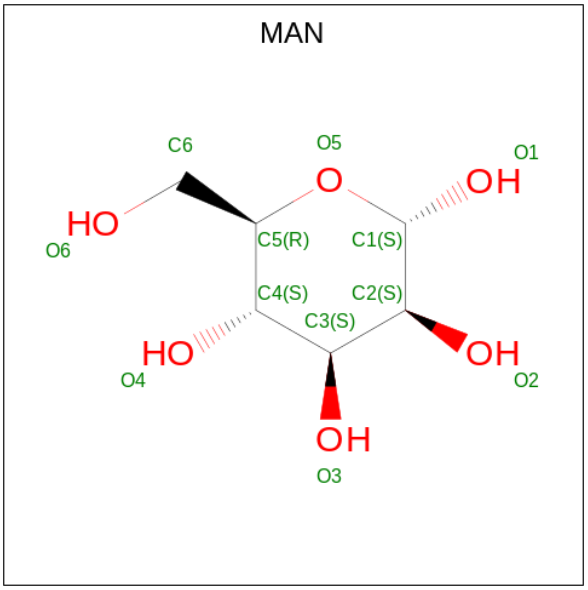
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 9 5 4	0	0

- Molecule 11 is beta-D-xylofuranose (three-letter code: XYZ) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



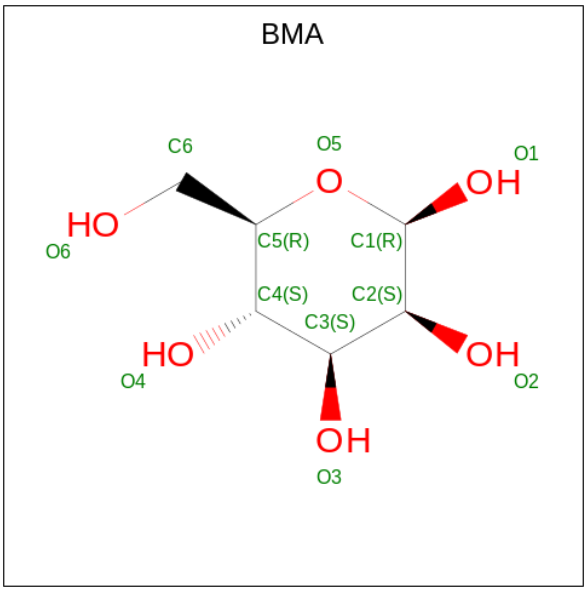
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C O 10 5 5	0	0

- Molecule 12 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

- Molecule 13 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 14 is water.

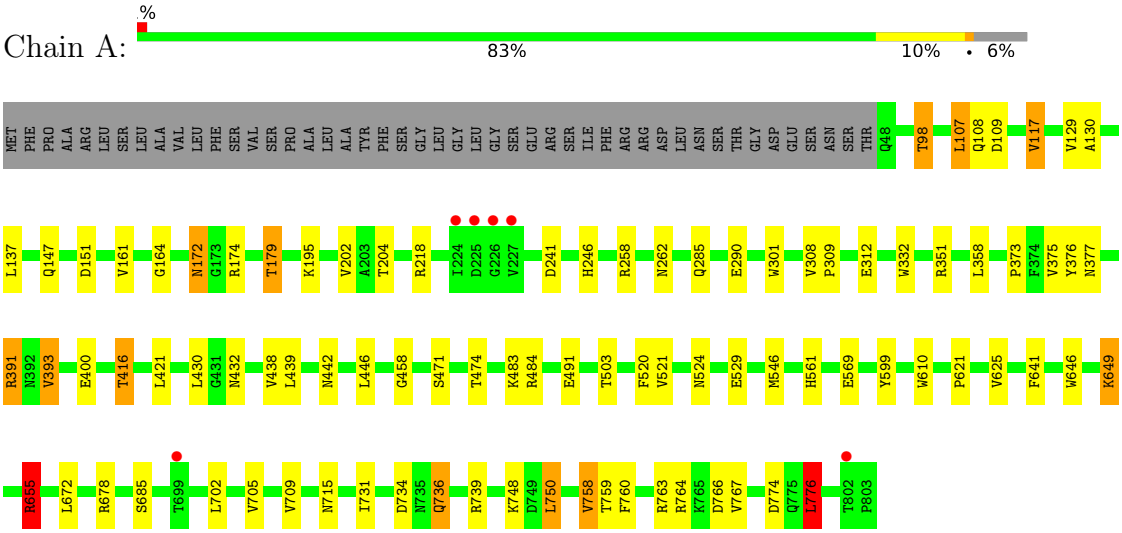
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	277	Total O 277 277	0	0
14	B	242	Total O 242 242	0	0
14	C	120	Total O 120 120	0	0
14	D	96	Total O 96 96	0	0

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.

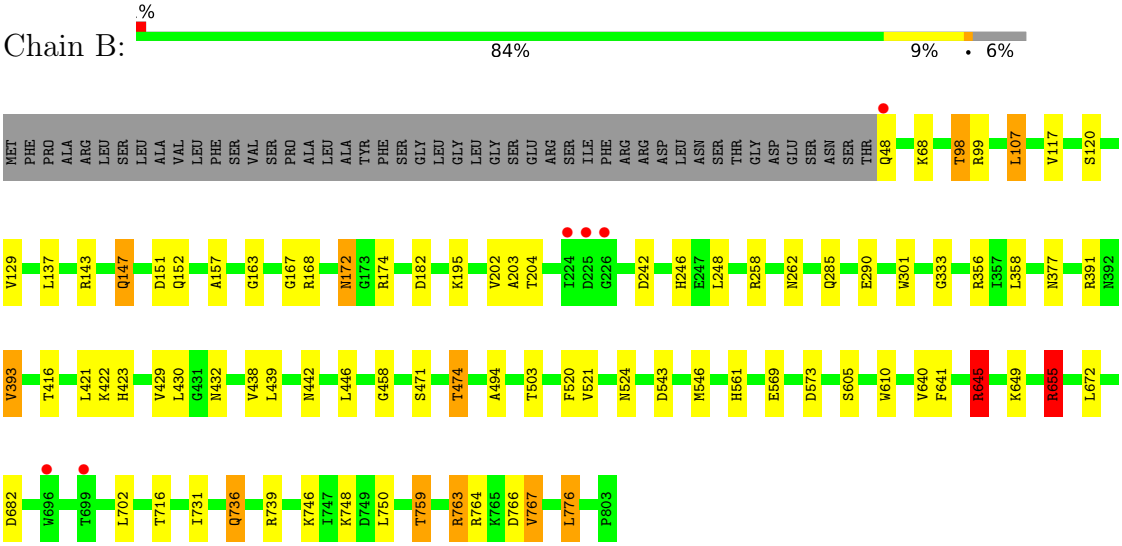
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain A:



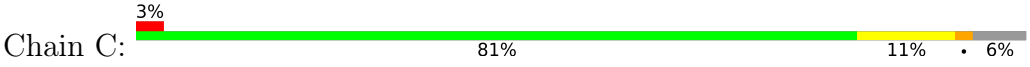
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

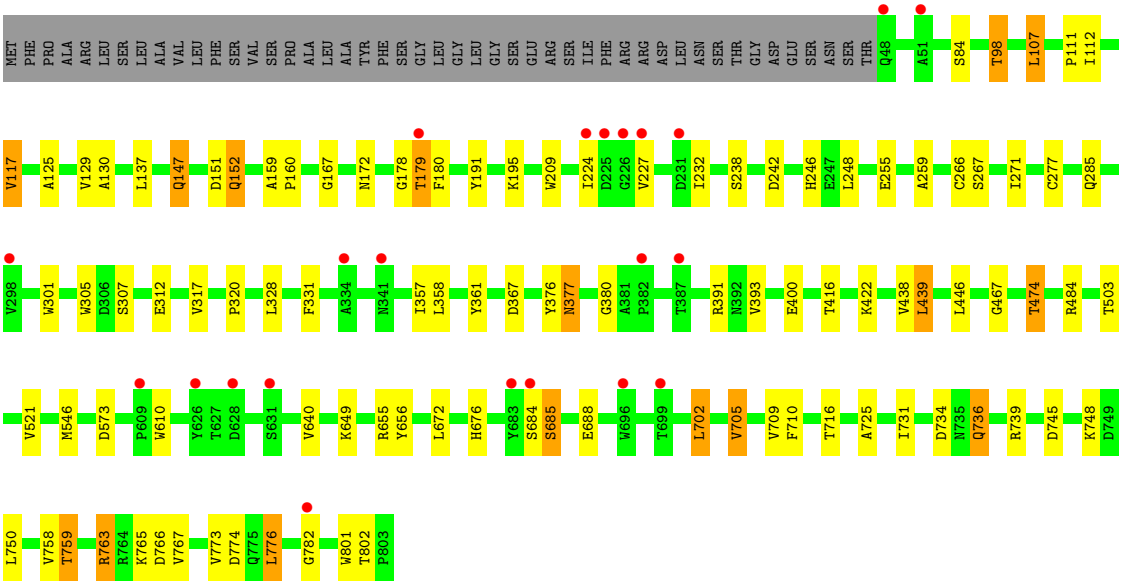
Chain B:



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

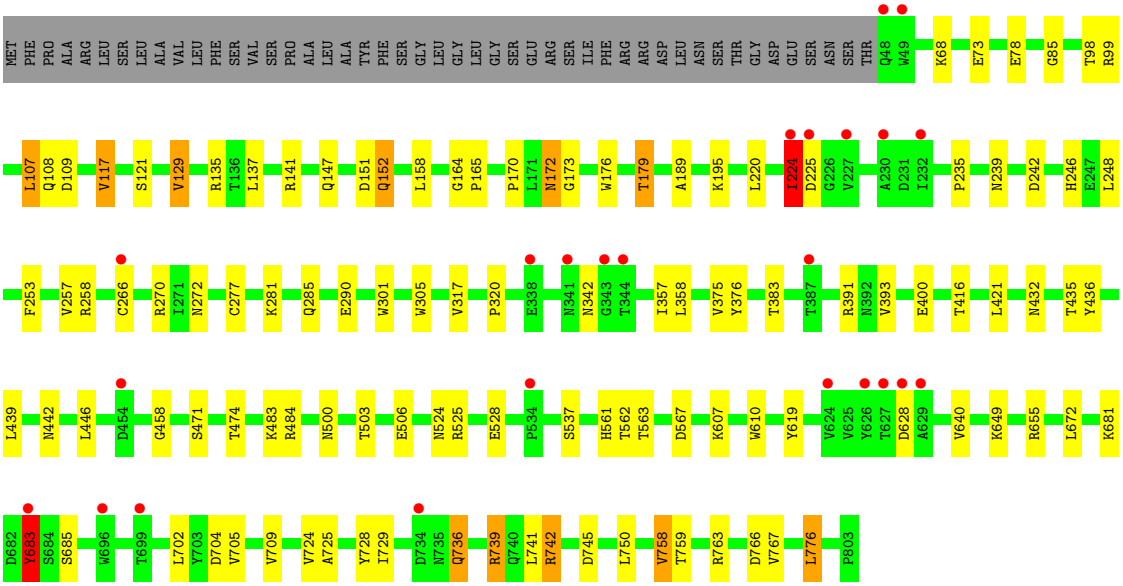
Chain C:





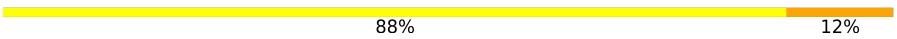
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain D:



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

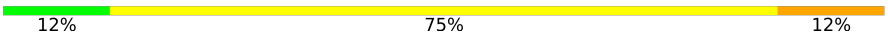
Chain E:



• Molecule 2: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1

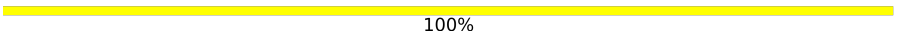
-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



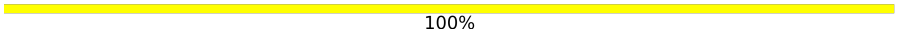
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(4-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



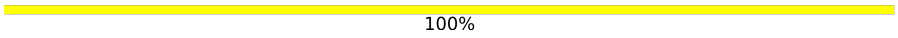
• Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



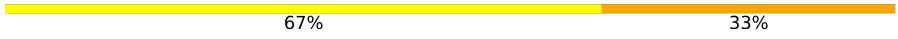
• Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



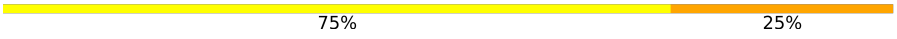
• Molecule 4: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



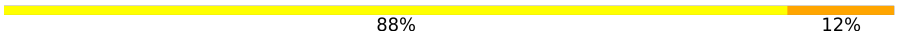
• Molecule 5: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



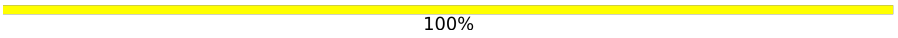
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(6-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



• Molecule 7: alpha-D-mannopyranose-(1-2)-beta-D-mannopyranose

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	228.51Å 88.17Å 218.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	218.50 – 2.46 36.03 – 2.46	Depositor EDS
% Data completeness (in resolution range)	98.7 (218.50-2.46) 98.8 (36.03-2.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.196 , 0.249 0.203 , 0.251	Depositor DCC
R_{free} test set	7844 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	30.1	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24651	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BKR, BMA, XYZ, MAN, XYP, NAG

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	0.72	1/5862 (0.0%)	0.88	16/8020 (0.2%)
1	B	0.74	1/5883 (0.0%)	0.89	21/8049 (0.3%)
1	C	0.67	1/5863 (0.0%)	0.84	9/8023 (0.1%)
1	D	0.68	0/5867	0.87	12/8027 (0.1%)
All	All	0.71	3/23475 (0.0%)	0.87	58/32119 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	178	GLY	C-O	-5.35	1.15	1.23
1	B	163	GLY	C-O	-5.29	1.15	1.23
1	A	491	GLU	CD-OE1	5.15	1.31	1.25

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	180	PHE	N-CA-CB	13.79	135.43	110.60
1	D	224	ILE	N-CA-C	11.84	142.98	111.00
1	A	391	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	C	391	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	B	763	ARG	NE-CZ-NH1	7.63	124.11	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5719	0	5511	31	0
1	B	5736	0	5528	39	0
1	C	5716	0	5507	47	0
1	D	5720	0	5519	54	0
2	E	92	0	78	2	0
2	G	92	0	78	3	0
3	F	53	0	46	0	0
4	I	39	0	34	0	0
4	K	39	0	34	0	0
4	M	39	0	34	1	0
5	J	48	0	42	2	0
6	L	95	0	78	9	0
7	N	22	0	17	0	0
8	A	97	0	89	6	0
8	B	97	0	89	8	0
8	C	83	0	75	5	0
8	D	70	0	64	1	0
9	A	59	0	0	4	0
9	B	59	0	0	1	0
10	A	9	0	0	1	0
11	B	10	0	7	0	0
12	B	11	0	10	0	0
13	C	11	0	10	0	0
14	A	277	0	0	2	0
14	B	242	0	0	5	0
14	C	120	0	0	1	0
14	D	96	0	0	2	0
All	All	24651	0	22850	189	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 4.

The worst 5 of 189 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)
8:A:901:NAG:C4	8:A:902:NAG:O1	1.86	1.21
1:D:224:ILE:HD12	1:D:224:ILE:O	1.38	1.18
8:B:903:NAG:C4	2:G:1:NAG:O1	1.92	1.18
8:B:901:NAG:C4	8:B:902:NAG:O1	1.91	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:903:NAG:C4	2:E:1:NAG:O1	1.90	1.18

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%)	722 (96%)	34 (4%)	0	100	100
1	B	758/803 (94%)	721 (95%)	36 (5%)	1 (0%)	51	64
1	C	756/803 (94%)	709 (94%)	46 (6%)	1 (0%)	51	64
1	D	756/803 (94%)	711 (94%)	45 (6%)	0	100	100
All	All	3026/3212 (94%)	2863 (95%)	161 (5%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	167	GLY
1	B	167	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	610/648 (94%)	567 (93%)	43 (7%)	15	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	613/648 (95%)	579 (94%)	34 (6%)	21 27
1	C	610/648 (94%)	566 (93%)	44 (7%)	14 17
1	D	611/648 (94%)	557 (91%)	54 (9%)	10 11
All	All	2444/2592 (94%)	2269 (93%)	175 (7%)	14 17

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	748	LYS
1	D	375	VAL
1	C	773	VAL
1	D	152	GLN
1	D	474	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	285	GLN
1	D	147	GLN
1	C	377	ASN
1	C	676	HIS
1	D	172	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

43 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2	15,15,15	0.52	0	21,21,21	1.12	2 (9%)
2	BMA	E	2	2	11,11,12	0.40	0	15,15,17	1.35	2 (13%)
2	MAN	E	3	2	11,11,12	0.83	0	15,15,17	2.40	4 (26%)
2	BMA	E	4	2	11,11,12	0.71	0	15,15,17	2.21	4 (26%)
2	MAN	E	5	2	11,11,12	0.61	0	15,15,17	1.78	4 (26%)
2	MAN	E	6	2	11,11,12	0.71	0	15,15,17	0.99	1 (6%)
2	MAN	E	7	2	11,11,12	0.64	0	15,15,17	2.40	4 (26%)
2	MAN	E	8	2	11,11,12	0.58	0	15,15,17	1.70	2 (13%)
3	NAG	F	1	3,1	14,14,15	0.71	0	17,19,21	1.36	2 (11%)
3	NAG	F	2	3	14,14,15	0.67	0	17,19,21	1.51	3 (17%)
3	MAN	F	3	3	11,11,12	1.84	2 (18%)	15,15,17	2.36	6 (40%)
3	NAG	F	4	3	14,14,15	2.73	4 (28%)	19,19,21	3.35	11 (57%)
2	NAG	G	1	2	15,15,15	0.49	0	21,21,21	1.55	4 (19%)
2	BMA	G	2	2	11,11,12	0.74	0	15,15,17	1.68	4 (26%)
2	MAN	G	3	2	11,11,12	0.27	0	15,15,17	0.72	0
2	BMA	G	4	2	11,11,12	0.77	1 (9%)	15,15,17	2.48	6 (40%)
2	MAN	G	5	2	11,11,12	0.61	0	15,15,17	2.20	4 (26%)
2	MAN	G	6	2	11,11,12	0.45	0	15,15,17	1.40	2 (13%)
2	MAN	G	7	2	11,11,12	0.88	0	15,15,17	2.73	6 (40%)
2	MAN	G	8	2	11,11,12	0.97	0	15,15,17	2.18	4 (26%)
4	NAG	I	1	4,1	14,14,15	0.59	0	17,19,21	1.28	2 (11%)
4	NAG	I	2	4	14,14,15	0.56	0	17,19,21	1.52	3 (17%)
4	MAN	I	3	4	11,11,12	0.94	0	15,15,17	2.48	6 (40%)
5	NAG	J	1	5	15,15,15	0.64	0	21,21,21	1.48	5 (23%)
5	BMA	J	2	5	11,11,12	1.10	2 (18%)	15,15,17	2.15	5 (33%)
5	MAN	J	3	5	11,11,12	0.51	0	15,15,17	2.37	7 (46%)
5	MAN	J	4	5	11,11,12	1.18	1 (9%)	15,15,17	1.18	0
4	NAG	K	1	4,1	14,14,15	0.53	0	17,19,21	1.17	2 (11%)
4	NAG	K	2	4	14,14,15	0.99	0	17,19,21	2.01	5 (29%)
4	MAN	K	3	4	11,11,12	1.54	2 (18%)	15,15,17	2.29	4 (26%)
6	NAG	L	1	6	14,14,15	1.27	3 (21%)	17,19,21	2.12	3 (17%)
6	NAG	L	2	6	14,14,15	0.45	0	17,19,21	1.19	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	L	3	6	11,11,12	0.38	0	15,15,17	0.92	1 (6%)
6	MAN	L	4	6	11,11,12	0.99	0	15,15,17	2.52	3 (20%)
6	MAN	L	5	6	11,11,12	0.89	0	15,15,17	1.79	3 (20%)
6	MAN	L	6	6	11,11,12	1.18	0	15,15,17	2.98	6 (40%)
6	MAN	L	7	6	11,11,12	0.60	0	15,15,17	1.74	3 (20%)
6	MAN	L	8	6	12,12,12	1.23	1 (8%)	17,17,17	1.75	4 (23%)
4	NAG	M	1	4,1	14,14,15	0.39	0	17,19,21	1.11	2 (11%)
4	NAG	M	2	4	14,14,15	0.55	0	17,19,21	1.78	4 (23%)
4	MAN	M	3	4	11,11,12	1.02	0	15,15,17	2.09	4 (26%)
7	BMA	N	1	7	11,11,12	1.12	1 (9%)	15,15,17	2.87	8 (53%)
7	MAN	N	2	7	11,11,12	1.37	2 (18%)	15,15,17	3.53	8 (53%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2	-	0/6/26/26	0/1/1/1
2	BMA	E	2	2	-	2/2/19/22	0/1/1/1
2	MAN	E	3	2	-	2/2/19/22	1/1/1/1
2	BMA	E	4	2	-	2/2/19/22	0/1/1/1
2	MAN	E	5	2	-	2/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	0/1/1/1
2	MAN	E	7	2	-	2/2/19/22	0/1/1/1
2	MAN	E	8	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	1/2/19/22	0/1/1/1
3	NAG	F	4	3	-	2/6/22/26	0/1/1/1
2	NAG	G	1	2	-	0/6/26/26	0/1/1/1
2	BMA	G	2	2	-	0/2/19/22	0/1/1/1
2	MAN	G	3	2	-	0/2/19/22	0/1/1/1
2	BMA	G	4	2	-	1/2/19/22	0/1/1/1
2	MAN	G	5	2	-	0/2/19/22	0/1/1/1
2	MAN	G	6	2	-	0/2/19/22	0/1/1/1
2	MAN	G	7	2	-	2/2/19/22	0/1/1/1
2	MAN	G	8	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
4	MAN	I	3	4	-	2/2/19/22	0/1/1/1
5	NAG	J	1	5	-	2/6/26/26	0/1/1/1
5	BMA	J	2	5	-	2/2/19/22	0/1/1/1
5	MAN	J	3	5	-	2/2/19/22	0/1/1/1
5	MAN	J	4	5	-	1/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	MAN	K	3	4	-	2/2/19/22	0/1/1/1
6	NAG	L	1	6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
6	MAN	L	4	6	-	0/2/19/22	0/1/1/1
6	MAN	L	5	6	-	2/2/19/22	0/1/1/1
6	MAN	L	6	6	-	2/2/19/22	0/1/1/1
6	MAN	L	7	6	-	0/2/19/22	0/1/1/1
6	MAN	L	8	6	-	1/2/22/22	0/1/1/1
4	NAG	M	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	MAN	M	3	4	-	2/2/19/22	0/1/1/1
7	BMA	N	1	7	-	2/2/19/22	0/1/1/1
7	MAN	N	2	7	-	1/2/19/22	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	NAG	C3-C2	7.42	1.59	1.53
3	F	4	NAG	C4-C3	4.18	1.60	1.52
3	F	4	NAG	C2-N2	3.95	1.52	1.45
3	F	3	MAN	C2-C3	3.86	1.58	1.52
7	N	1	BMA	O5-C1	-2.95	1.39	1.43

The worst 5 of 166 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	6	MAN	C1-O5-C5	8.09	123.15	112.19
6	L	4	MAN	C1-O5-C5	7.87	122.85	112.19
2	E	7	MAN	C1-O5-C5	7.52	122.38	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	N	1	BMA	O2-C2-C3	6.62	123.41	110.14
3	F	4	NAG	O5-C1-C2	6.52	116.06	109.52

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	5	MAN	O5-C5-C6-O6
2	E	3	MAN	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	M	3	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

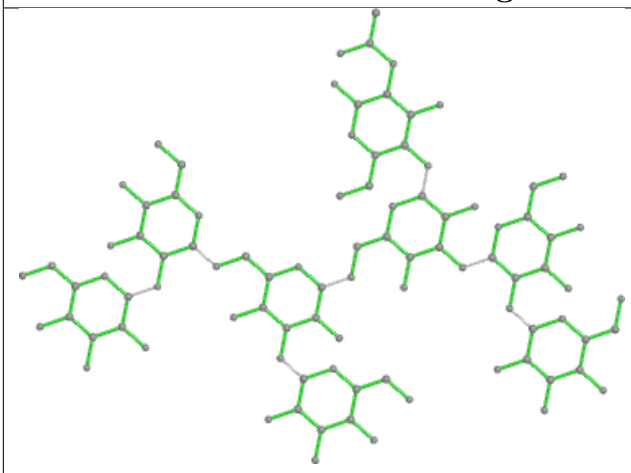
Mol	Chain	Res	Type	Atoms
2	E	3	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 17 short contacts:

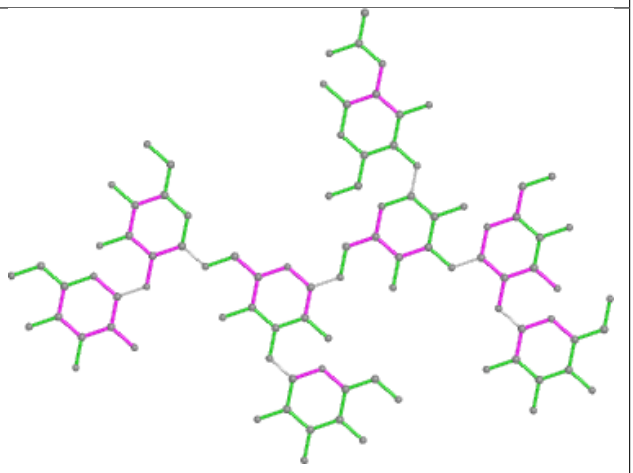
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	2	0
6	L	1	NAG	9	0
2	G	1	NAG	3	0
5	J	1	NAG	2	0
4	M	2	NAG	1	0

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

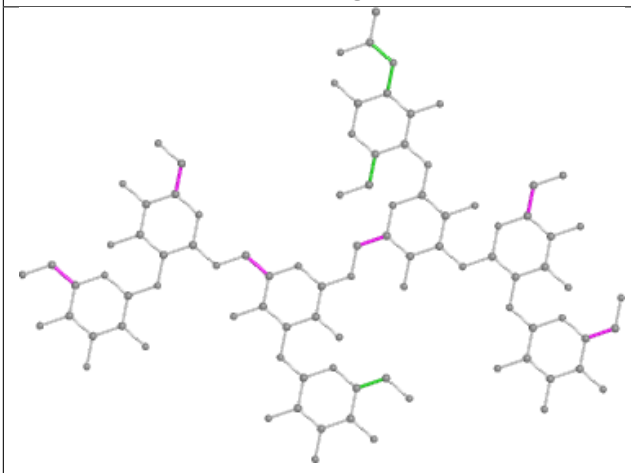
Oligosaccharide Chain E



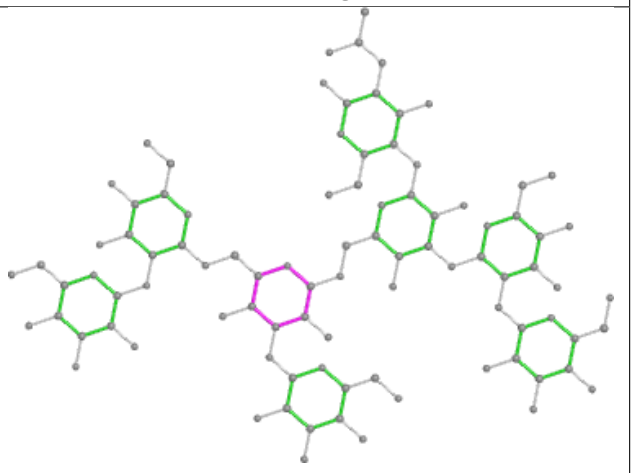
Bond lengths



Bond angles

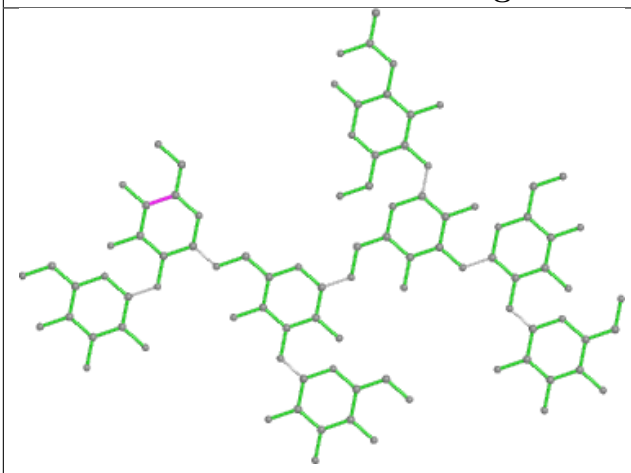


Torsions

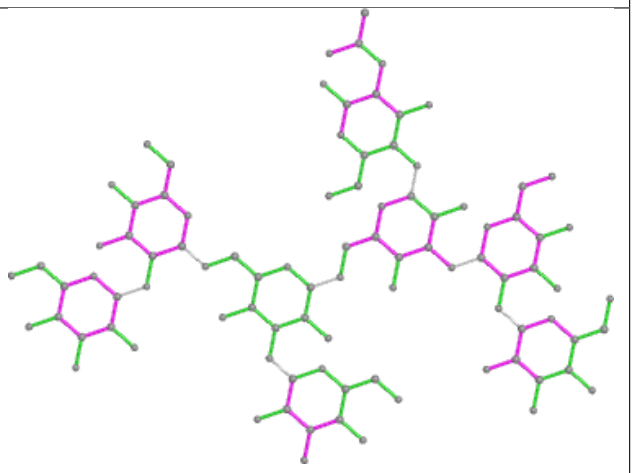


Rings

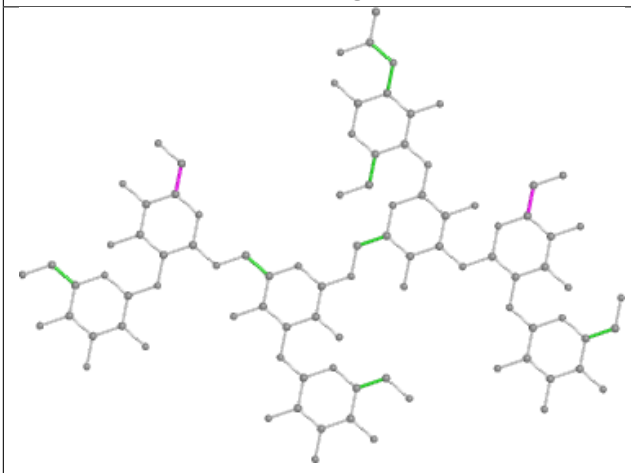
Oligosaccharide Chain G



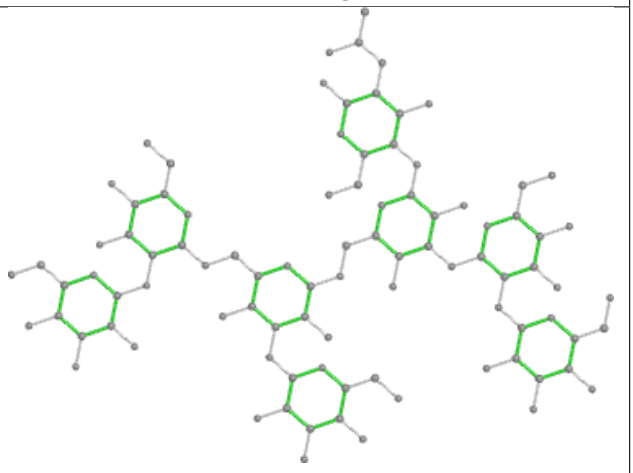
Bond lengths



Bond angles

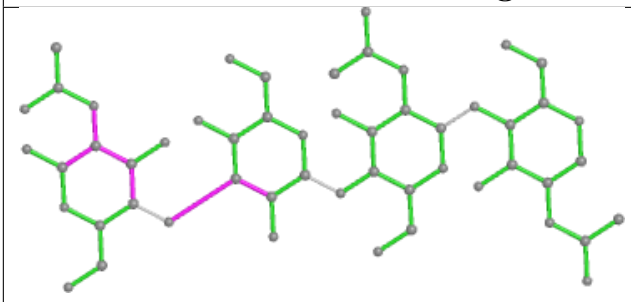


Torsions

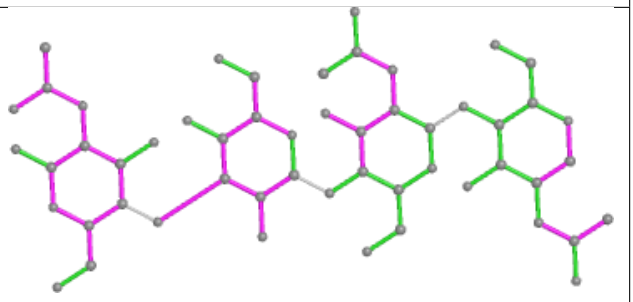


Rings

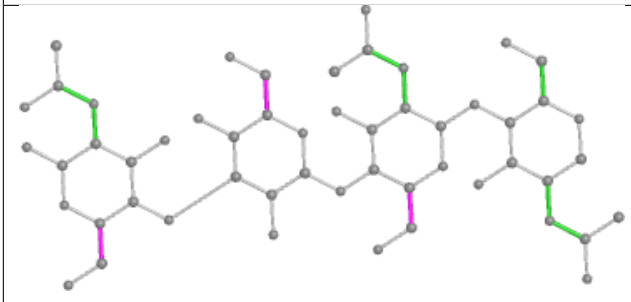
Oligosaccharide Chain F



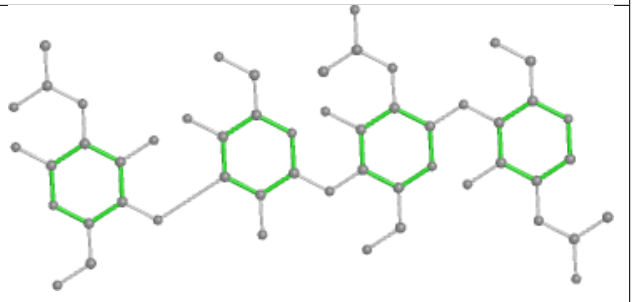
Bond lengths



Bond angles

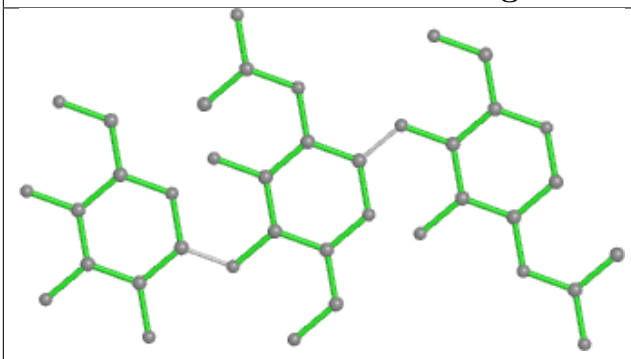


Torsions

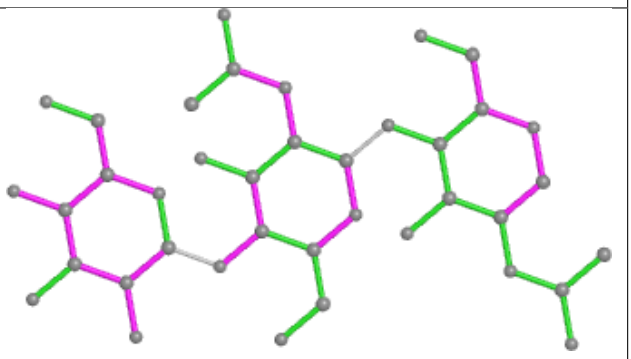


Rings

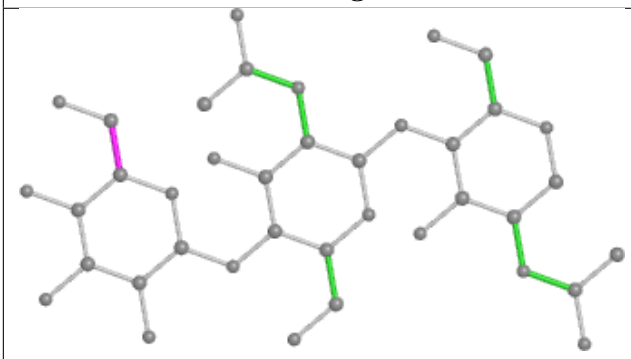
Oligosaccharide Chain I



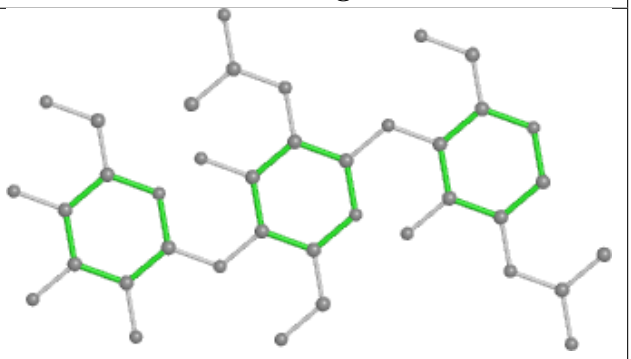
Bond lengths



Bond angles

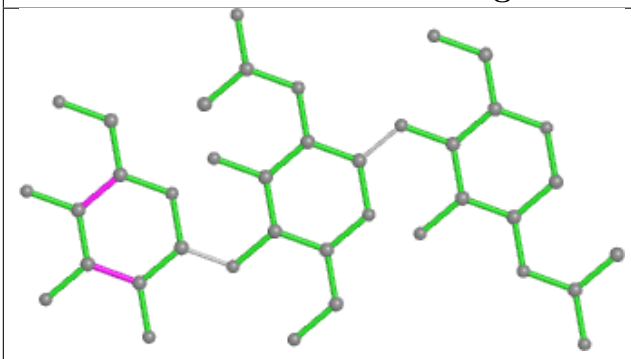


Torsions

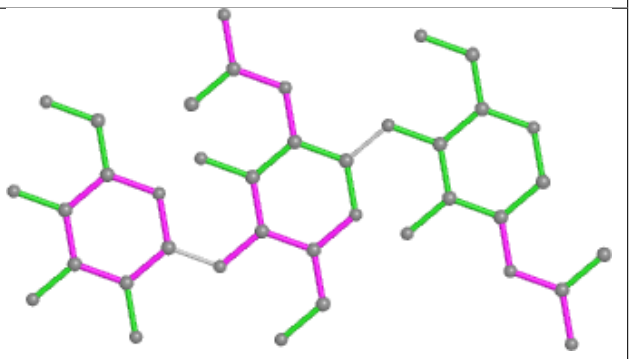


Rings

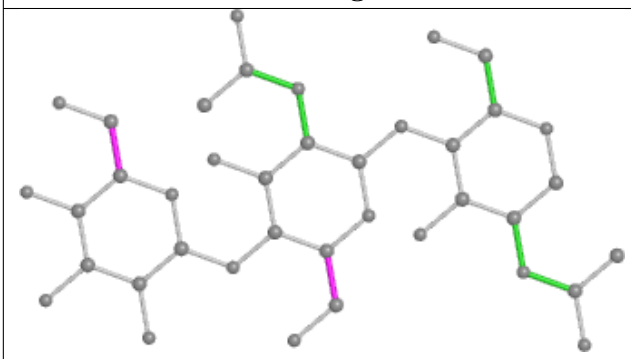
Oligosaccharide Chain K



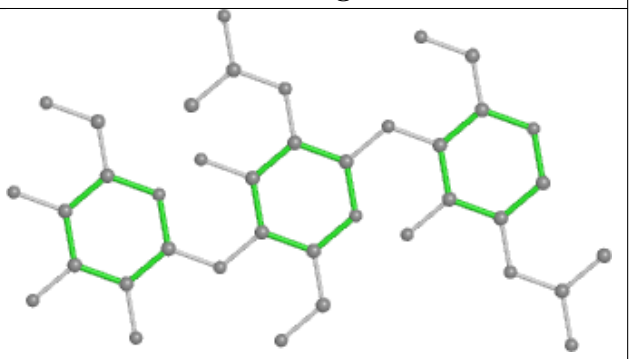
Bond lengths



Bond angles

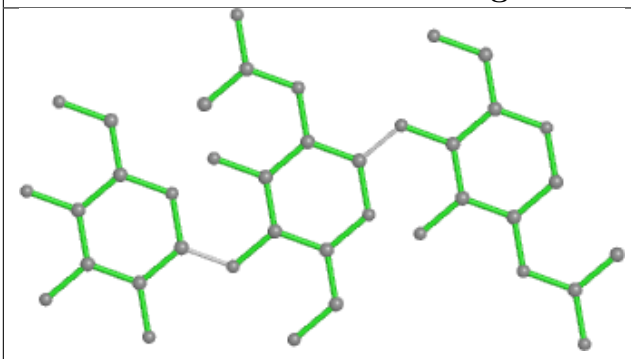


Torsions

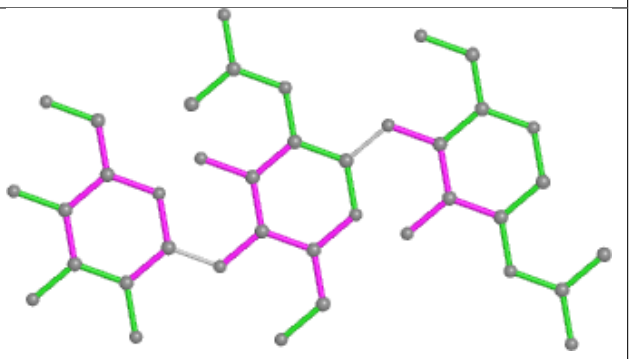


Rings

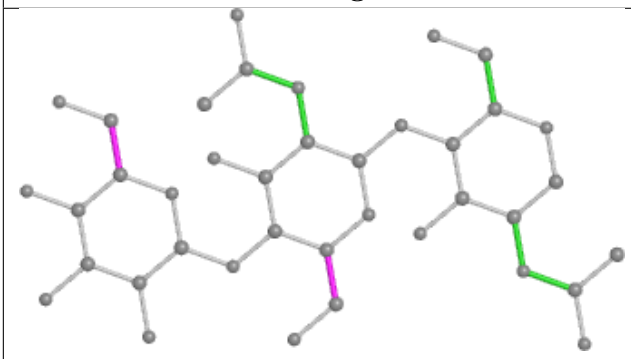
Oligosaccharide Chain M



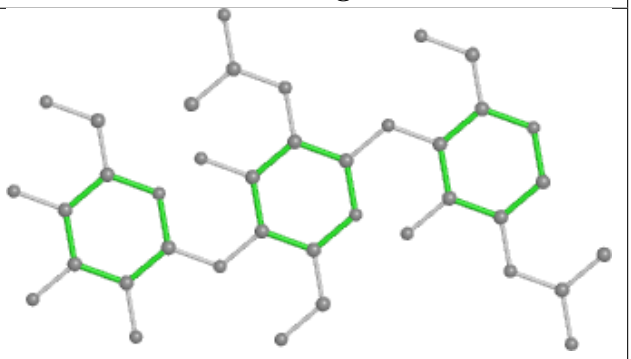
Bond lengths



Bond angles

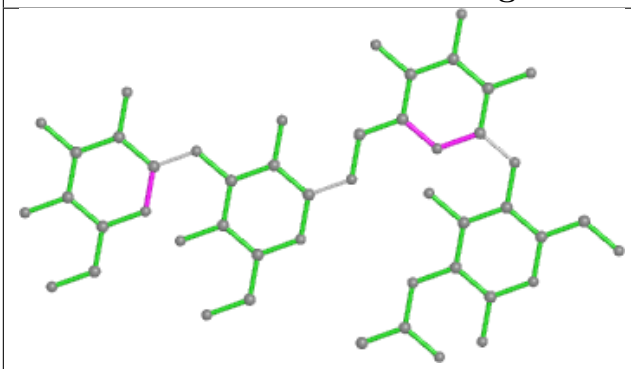


Torsions

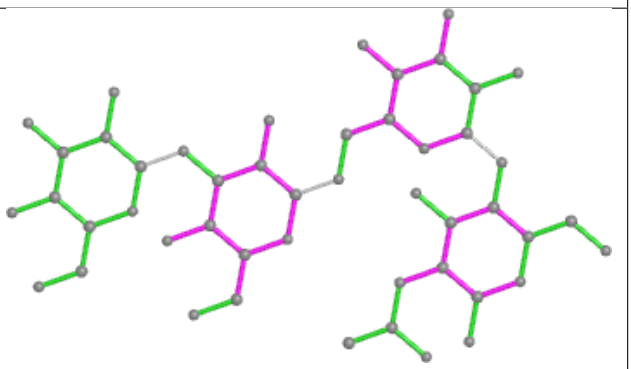


Rings

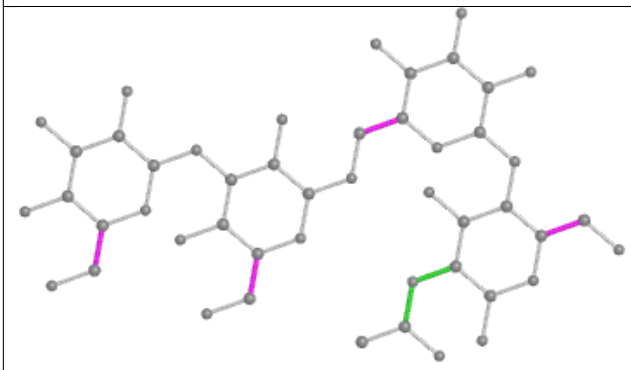
Oligosaccharide Chain J



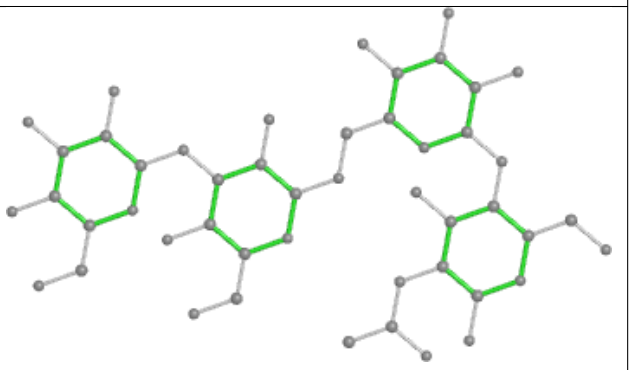
Bond lengths



Bond angles

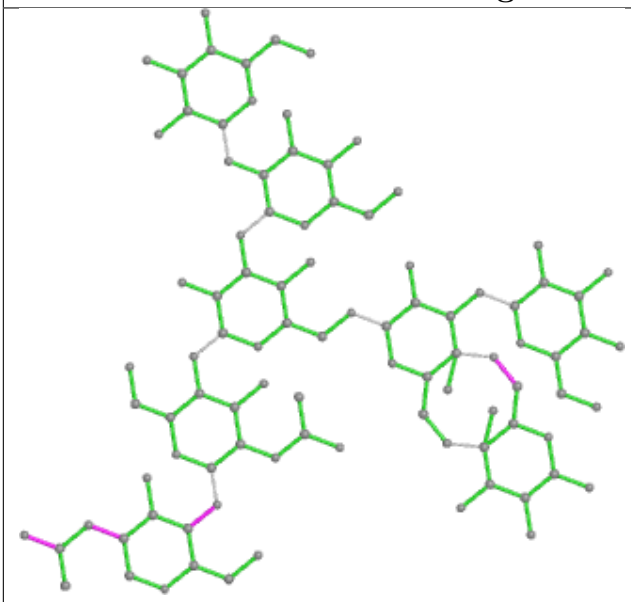


Torsions

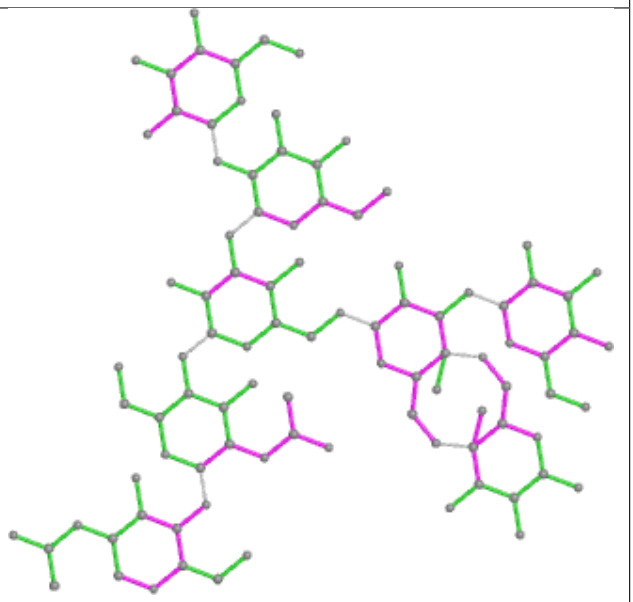


Rings

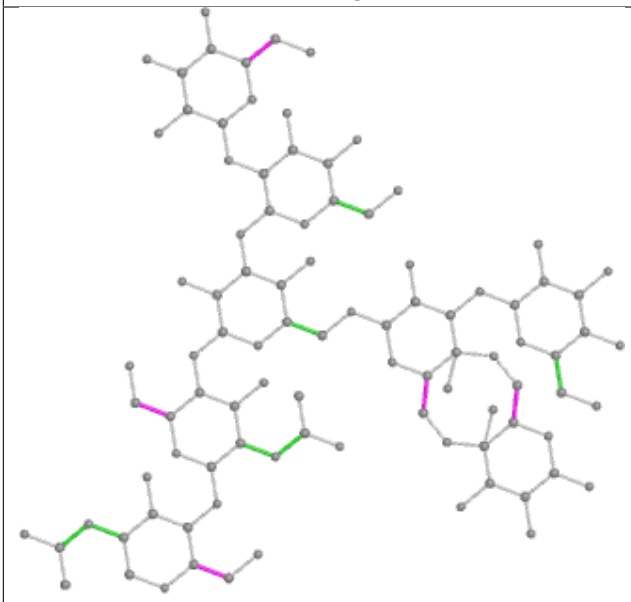
Oligosaccharide Chain L



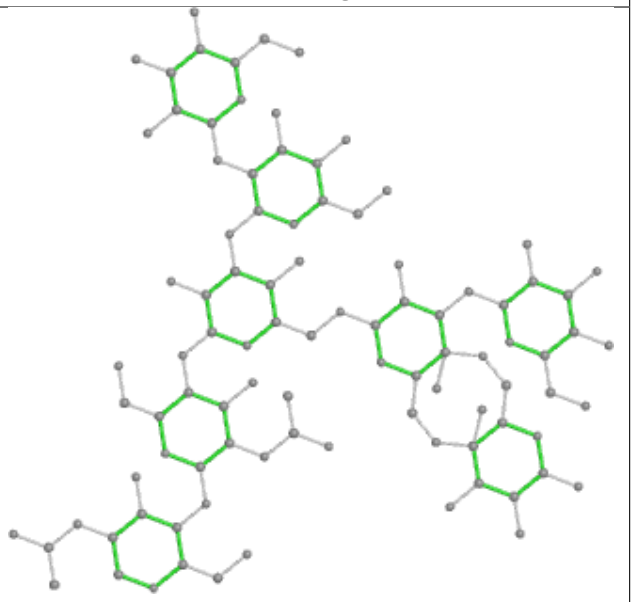
Bond lengths



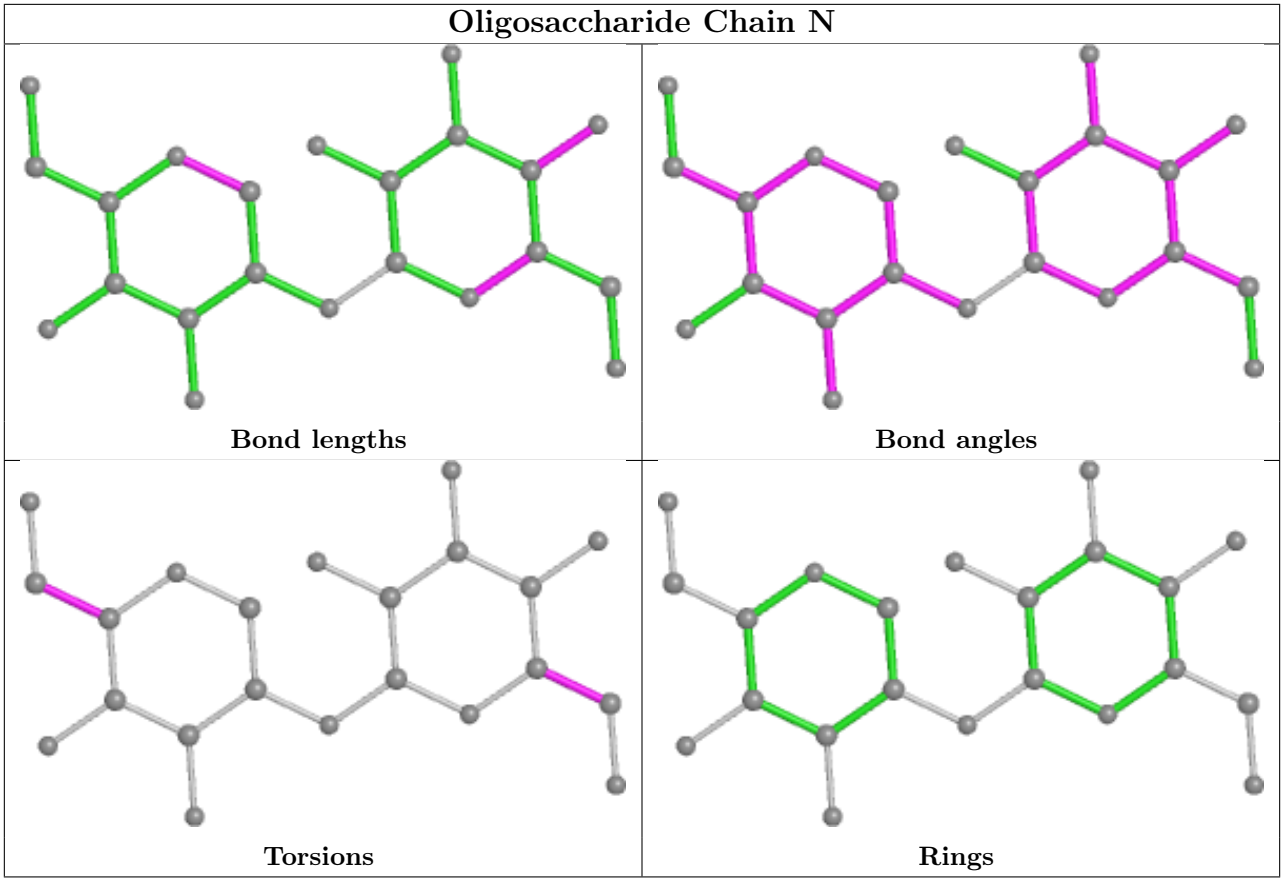
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

31 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	$\#\|Z\| > 2$
8	NAG	C	907	1	14,14,15	0.52	0	17,19,21	1.19	2 (11%)
9	BKR	A	908	10	65,65,65	1.43	9 (13%)	101,101,101	1.93	23 (22%)
8	NAG	A	904	1	14,14,15	0.68	1 (7%)	17,19,21	1.10	1 (5%)
8	NAG	A	903	1	13,13,15	1.80	1 (7%)	14,17,21	2.55	5 (35%)
8	NAG	C	906	1	14,14,15	0.48	0	17,19,21	1.14	1 (5%)
8	NAG	C	901	1	13,13,15	1.12	1 (7%)	14,17,21	2.37	8 (57%)
8	NAG	D	901	1	13,13,15	1.32	1 (7%)	14,17,21	2.56	8 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	XYZ	B	909	9	10,10,10	1.10	1 (10%)	13,14,14	2.06	5 (38%)
8	NAG	B	905	1	14,14,15	0.60	0	17,19,21	1.60	4 (23%)
9	BKR	B	908	11	65,65,65	1.56	5 (7%)	101,101,101	1.57	19 (18%)
8	NAG	B	903	1	13,13,15	0.60	0	14,17,21	2.25	5 (35%)
8	NAG	B	904	1	14,14,15	0.60	0	17,19,21	1.20	1 (5%)
8	NAG	A	902	-	15,15,15	0.77	0	21,21,21	2.09	4 (19%)
8	NAG	A	906	1	14,14,15	0.45	0	17,19,21	1.27	1 (5%)
12	MAN	B	910	1	11,11,12	0.83	0	15,15,17	2.40	6 (40%)
8	NAG	D	905	1	14,14,15	0.62	0	17,19,21	1.41	2 (11%)
8	NAG	B	901	1	13,13,15	1.63	2 (15%)	14,17,21	1.25	2 (14%)
8	NAG	A	905	1	14,14,15	0.68	0	17,19,21	1.53	3 (17%)
8	NAG	A	907	1	14,14,15	0.42	0	17,19,21	1.46	2 (11%)
10	XYP	A	909	9	9,9,10	0.22	0	10,12,14	0.53	0
8	NAG	B	906	1	14,14,15	0.40	0	17,19,21	1.13	1 (5%)
8	NAG	D	902	-	15,15,15	0.70	0	21,21,21	2.16	5 (23%)
8	NAG	B	907	1	14,14,15	0.52	0	17,19,21	1.37	2 (11%)
8	NAG	C	902	-	15,15,15	0.99	0	21,21,21	1.53	4 (19%)
8	NAG	B	902	-	15,15,15	0.90	1 (6%)	21,21,21	1.90	7 (33%)
8	NAG	A	901	1	13,13,15	0.92	1 (7%)	14,17,21	1.30	3 (21%)
8	NAG	D	904	1	14,14,15	0.42	0	17,19,21	1.58	5 (29%)
13	BMA	C	904	-	11,11,12	0.73	0	15,15,17	1.86	3 (20%)
8	NAG	D	903	1	14,14,15	1.25	1 (7%)	17,19,21	1.92	3 (17%)
8	NAG	C	905	1	14,14,15	0.72	0	17,19,21	1.50	2 (11%)
8	NAG	C	903	1	13,13,15	0.63	0	14,17,21	2.05	4 (28%)

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
8	NAG	C	907	1	-	0/6/23/26	0/1/1/1
9	BKR	A	908	10	-	9/37/123/123	0/7/7/7
8	NAG	A	904	1	-	0/6/23/26	0/1/1/1
8	NAG	A	903	1	-	1/6/19/26	0/1/1/1
8	NAG	C	906	1	-	2/6/23/26	0/1/1/1
8	NAG	C	901	1	-	1/6/19/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	D	901	1	-	2/6/19/26	0/1/1/1
11	XYZ	B	909	9	-	2/2/18/18	0/1/1/1
8	NAG	B	905	1	-	1/6/23/26	0/1/1/1
9	BKR	B	908	11	-	7/37/123/123	0/7/7/7
8	NAG	B	903	1	-	0/6/19/26	0/1/1/1
8	NAG	B	904	1	-	0/6/23/26	0/1/1/1
8	NAG	A	902	-	-	0/6/26/26	0/1/1/1
8	NAG	A	906	1	-	0/6/23/26	0/1/1/1
12	MAN	B	910	1	-	2/2/19/22	0/1/1/1
8	NAG	D	905	1	-	2/6/23/26	0/1/1/1
8	NAG	B	901	1	-	0/6/19/26	0/1/1/1
8	NAG	A	905	1	-	1/6/23/26	0/1/1/1
8	NAG	A	907	1	-	3/6/23/26	0/1/1/1
10	XYP	A	909	9	-	-	0/1/1/1
8	NAG	B	906	1	-	0/6/23/26	0/1/1/1
8	NAG	D	902	-	-	0/6/26/26	0/1/1/1
8	NAG	B	907	1	-	2/6/23/26	0/1/1/1
8	NAG	C	902	-	-	0/6/26/26	0/1/1/1
8	NAG	B	902	-	-	0/6/26/26	0/1/1/1
8	NAG	A	901	1	-	0/6/19/26	0/1/1/1
8	NAG	D	904	1	-	2/6/23/26	0/1/1/1
13	BMA	C	904	-	-	1/2/19/22	0/1/1/1
8	NAG	D	903	1	-	3/6/23/26	0/1/1/1
8	NAG	C	905	1	-	4/6/23/26	0/1/1/1
8	NAG	C	903	1	-	2/6/19/26	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	908	BKR	O2-C3	6.27	1.47	1.34
9	B	908	BKR	O11-C27	5.96	1.48	1.34
8	A	903	NAG	O5-C1	-5.85	1.34	1.43
9	A	908	BKR	O2-C3	4.97	1.44	1.34
9	A	908	BKR	O11-C27	4.92	1.45	1.34

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	908	BKR	C14-C11-C10	-7.80	107.85	120.30
9	A	908	BKR	O4-C12-C13	6.21	121.98	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	902	NAG	C1-C2-N2	-6.12	103.64	110.73
8	B	903	NAG	O5-C5-C4	-5.85	101.17	110.65
13	C	904	BMA	C1-O5-C5	5.72	119.94	112.19

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	903	NAG	C4-C5-C6-O6
8	C	903	NAG	O5-C5-C6-O6
8	D	901	NAG	C4-C5-C6-O6
8	D	901	NAG	O5-C5-C6-O6
8	D	903	NAG	C3-C2-N2-C7

There are no ring outliers.

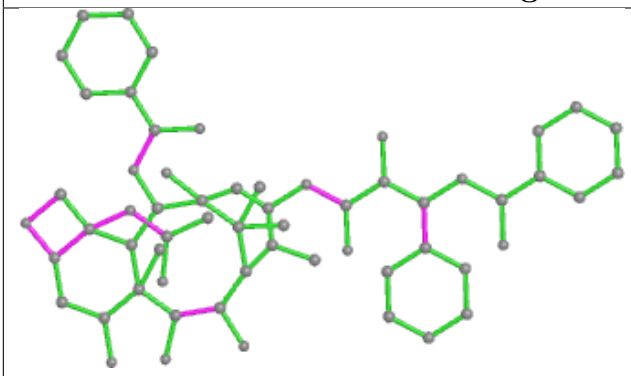
14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	908	BKR	4	0
8	A	903	NAG	2	0
8	C	901	NAG	2	0
8	D	901	NAG	1	0
9	B	908	BKR	1	0
8	B	903	NAG	3	0
8	A	902	NAG	2	0
8	B	901	NAG	4	0
10	A	909	XYP	1	0
8	D	902	NAG	1	0
8	C	902	NAG	2	0
8	B	902	NAG	3	0
8	A	901	NAG	4	0
8	C	903	NAG	2	0

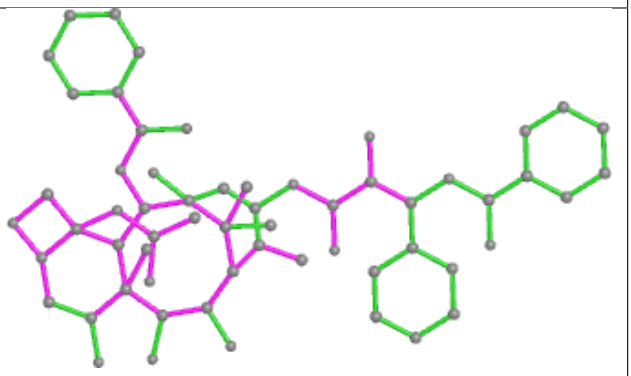
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

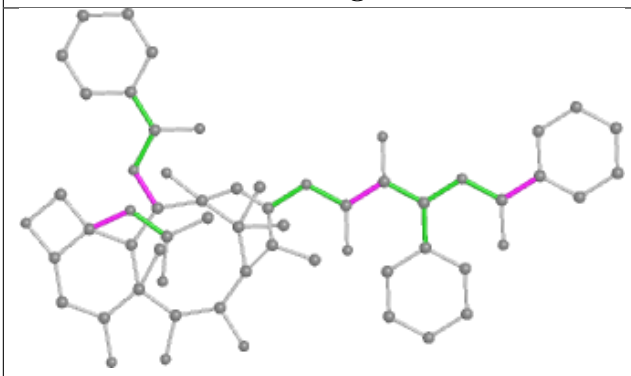
Ligand BKR A 908



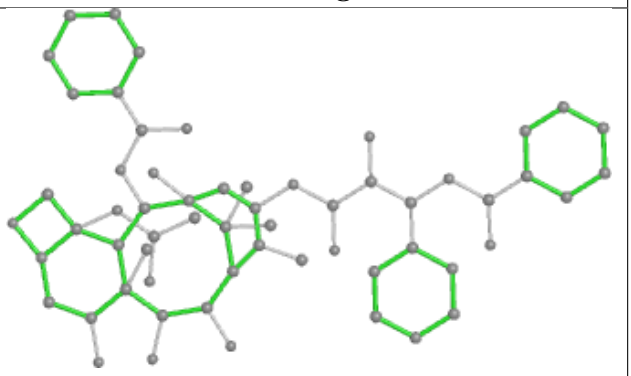
Bond lengths



Bond angles

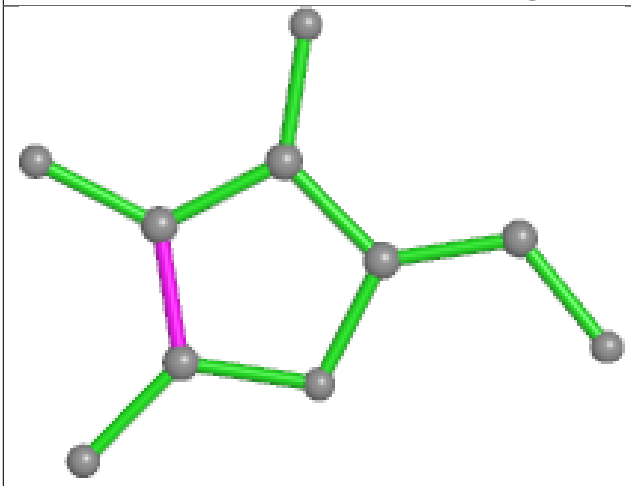


Torsions

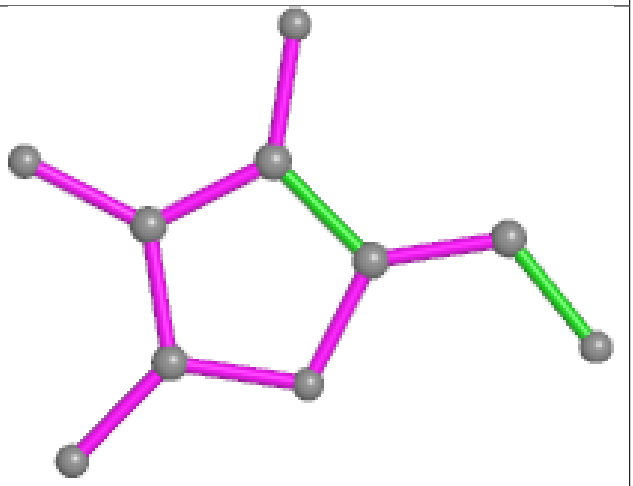


Rings

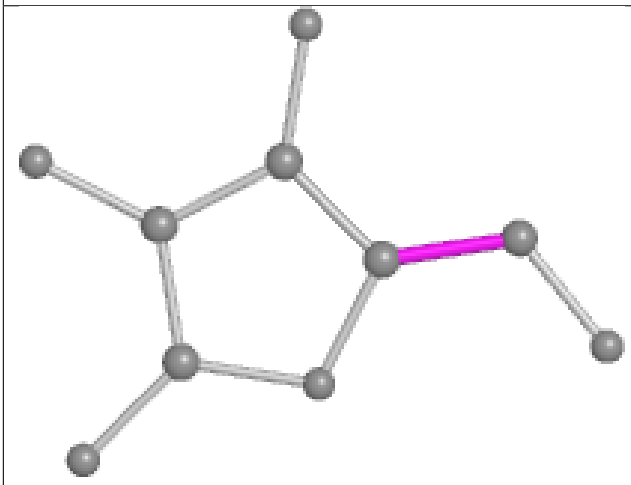
Ligand XYZ B 909



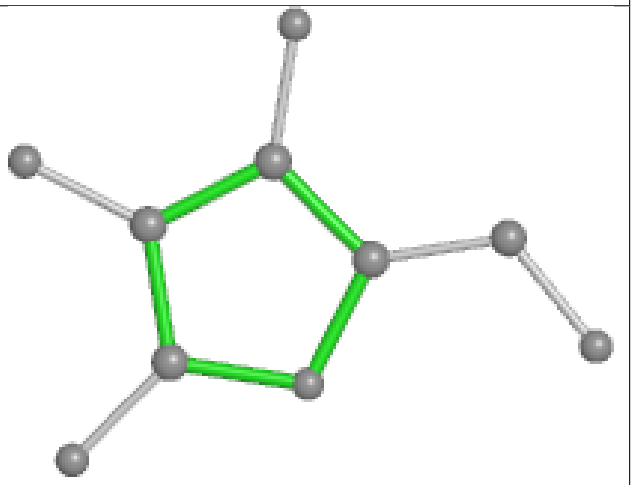
Bond lengths



Bond angles

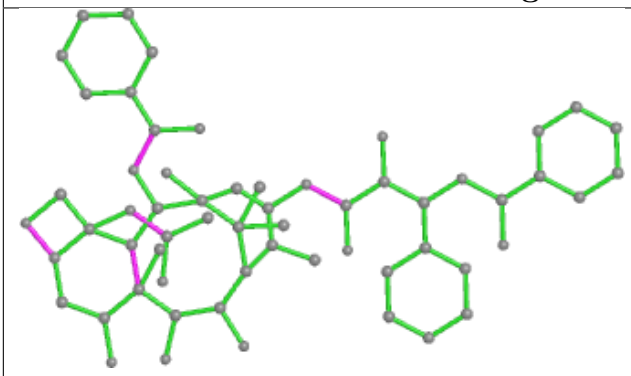


Torsions

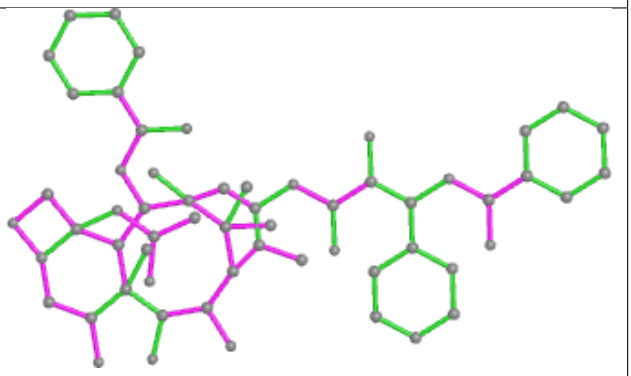


Rings

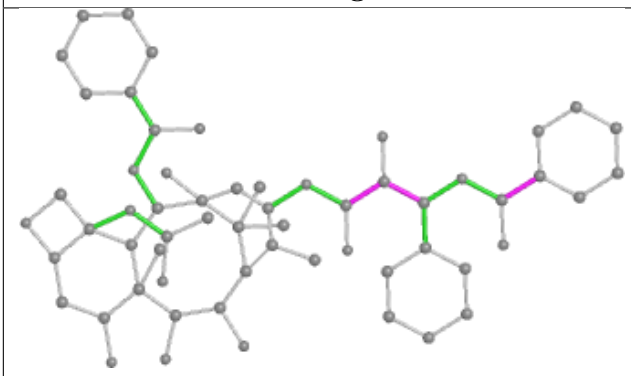
Ligand BKR B 908



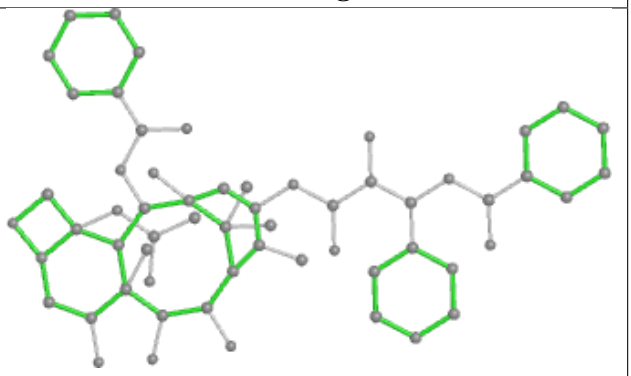
Bond lengths



Bond angles

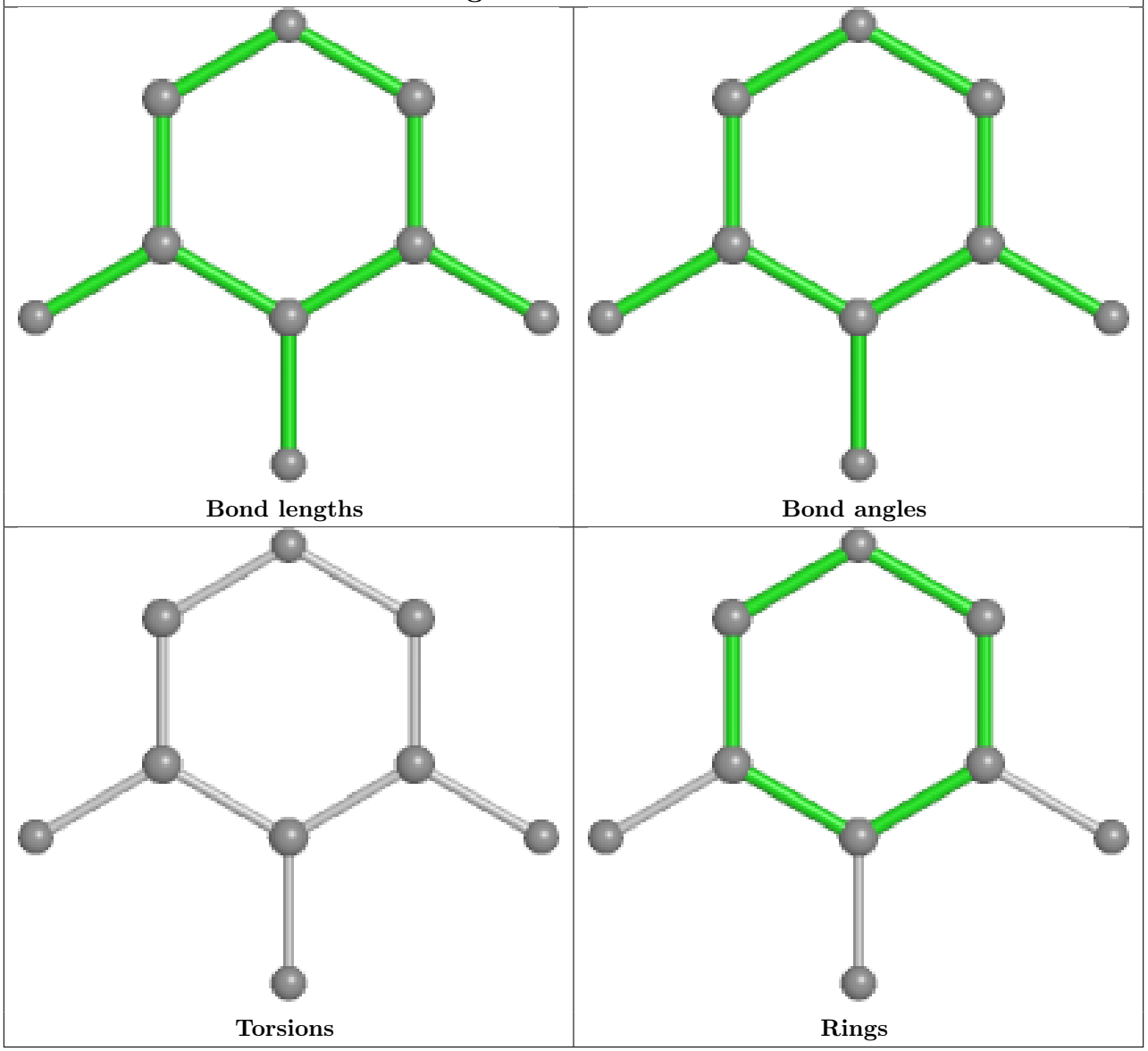


Torsions



Rings

Ligand XYP A 909



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^{th} 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	756/803 (94%)	-0.41	6 (0%)	86	86	16, 24, 41, 97	0
1	B	756/803 (94%)	-0.50	6 (0%)	86	86	14, 23, 36, 70	0
1	C	756/803 (94%)	-0.05	22 (2%)	51	47	20, 40, 62, 106	0
1	D	756/803 (94%)	-0.05	24 (3%)	47	44	24, 39, 59, 90	0
All	All	3024/3212 (94%)	-0.25	58 (1%)	66	64	14, 31, 56, 106	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	225	ASP	6.5
1	C	226	GLY	5.0
1	C	227	VAL	4.4
1	D	699	THR	4.3
1	A	225	ASP	4.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	M	3	11/12	0.39	0.38	78,89,93,94	0
3	NAG	F	4	14/15	0.57	0.30	63,75,81,86	0

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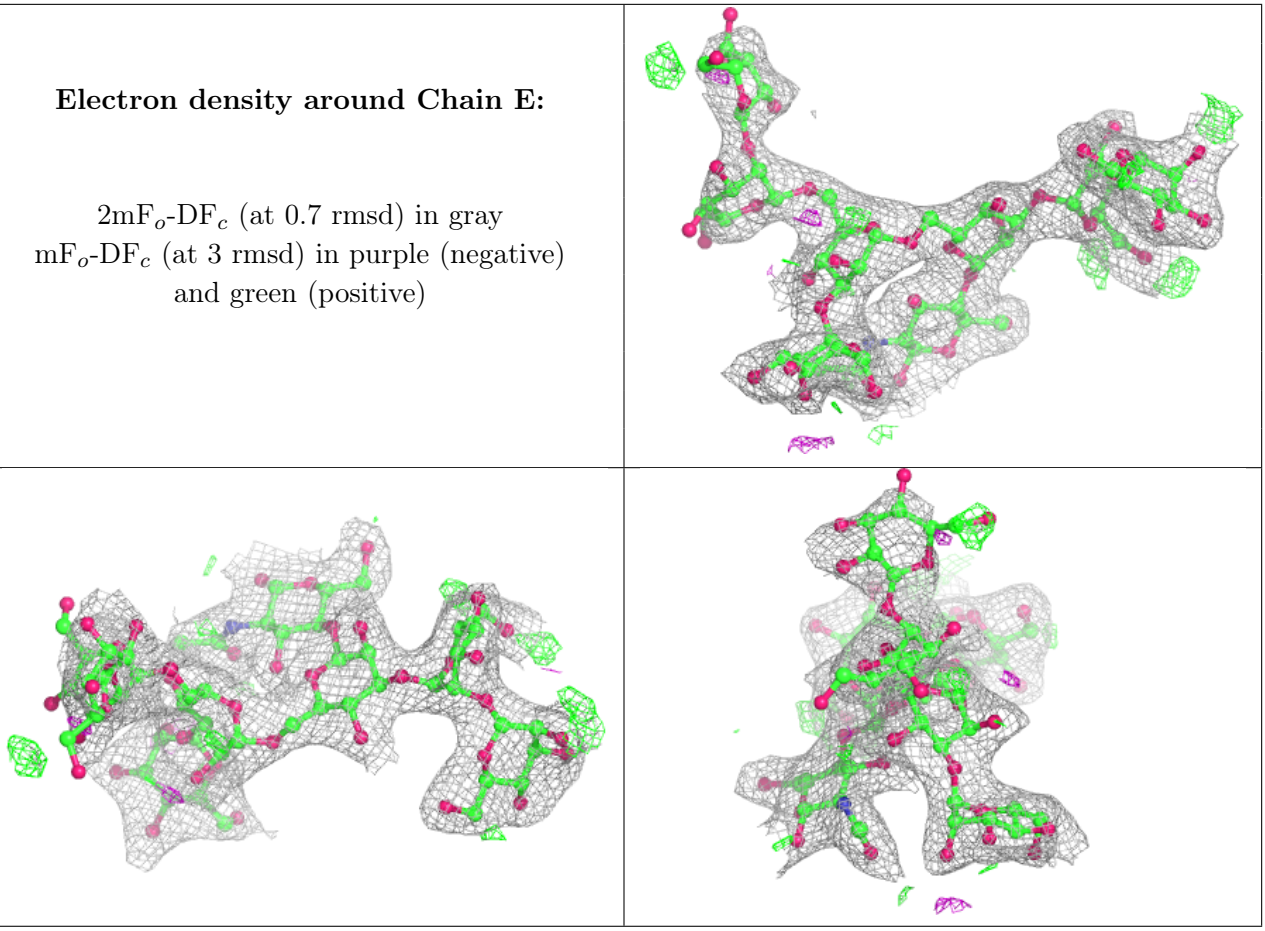
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MAN	K	3	11/12	0.68	0.28	58,67,72,74	0
6	MAN	L	8	12/12	0.75	0.36	70,79,92,98	0
5	MAN	J	3	11/12	0.77	0.22	52,61,75,78	0
2	MAN	E	5	11/12	0.78	0.49	79,93,103,107	0
6	MAN	L	5	11/12	0.79	0.21	58,66,70,71	0
2	MAN	G	5	11/12	0.79	0.46	75,81,91,94	0
7	BMA	N	1	11/12	0.79	0.18	58,72,82,84	0
7	MAN	N	2	11/12	0.80	0.29	46,55,61,61	0
6	MAN	L	6	11/12	0.83	0.18	47,55,64,70	0
3	MAN	F	3	11/12	0.83	0.31	54,60,68,72	0
6	NAG	L	1	14/15	0.85	0.21	39,52,56,58	0
4	MAN	I	3	11/12	0.85	0.18	37,46,50,51	0
4	NAG	M	2	14/15	0.85	0.18	43,62,73,77	0
5	BMA	J	2	11/12	0.87	0.16	49,53,56,58	0
2	MAN	G	7	11/12	0.87	0.19	37,43,49,49	0
2	MAN	E	7	11/12	0.89	0.20	41,43,46,48	0
2	BMA	G	4	11/12	0.90	0.33	50,56,63,65	0
6	MAN	L	4	11/12	0.91	0.18	54,61,66,67	0
5	NAG	J	1	15/15	0.91	0.16	41,54,62,68	0
2	BMA	E	4	11/12	0.91	0.46	71,81,89,90	0
2	MAN	G	3	11/12	0.92	0.17	33,35,47,51	0
5	MAN	J	4	11/12	0.92	0.18	50,61,64,69	0
2	MAN	E	8	11/12	0.92	0.17	39,44,47,48	0
2	MAN	G	6	11/12	0.93	0.17	30,36,38,40	0
4	NAG	M	1	14/15	0.93	0.12	32,37,44,52	0
4	NAG	K	2	14/15	0.93	0.19	33,41,51,64	0
6	MAN	L	7	11/12	0.94	0.16	50,53,56,57	0
2	MAN	G	8	11/12	0.94	0.18	39,42,45,45	0
3	NAG	F	2	14/15	0.94	0.12	22,31,40,49	0
2	MAN	E	3	11/12	0.94	0.14	36,38,51,59	0
6	BMA	L	3	11/12	0.95	0.13	36,38,45,46	0
4	NAG	I	2	14/15	0.96	0.14	23,28,37,40	0
6	NAG	L	2	14/15	0.96	0.14	35,39,44,52	0
2	MAN	E	6	11/12	0.96	0.18	35,38,44,45	0
4	NAG	K	1	14/15	0.96	0.11	28,30,35,35	0
2	NAG	E	1	15/15	0.96	0.12	27,30,31,33	0
2	BMA	G	2	11/12	0.97	0.13	24,26,30,32	0
4	NAG	I	1	14/15	0.97	0.11	18,21,24,26	0
2	BMA	E	2	11/12	0.97	0.19	29,34,40,40	0
2	NAG	G	1	15/15	0.97	0.12	22,24,27,31	0
3	NAG	F	1	14/15	0.98	0.08	21,22,25,27	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

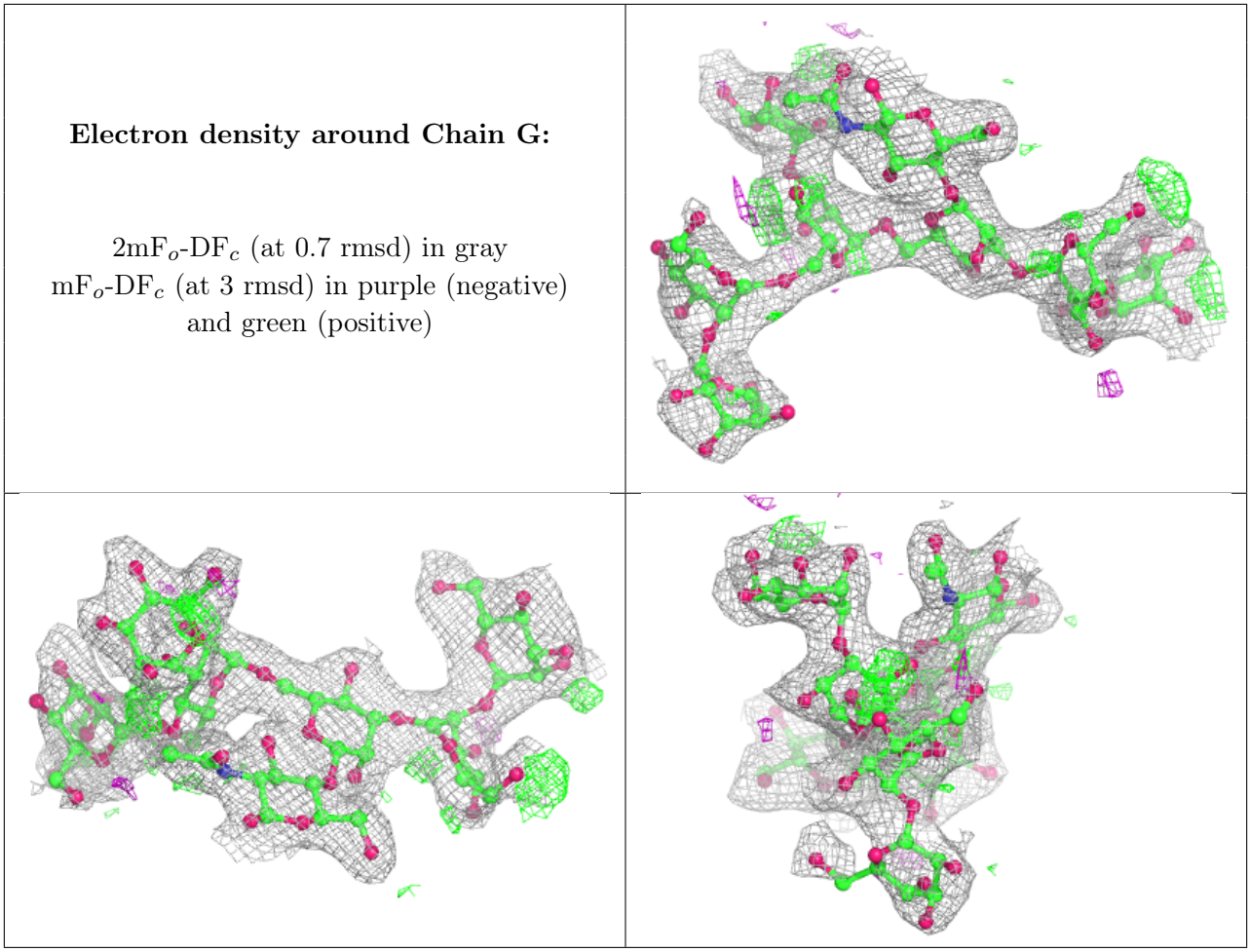
Electron density around Chain E:

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



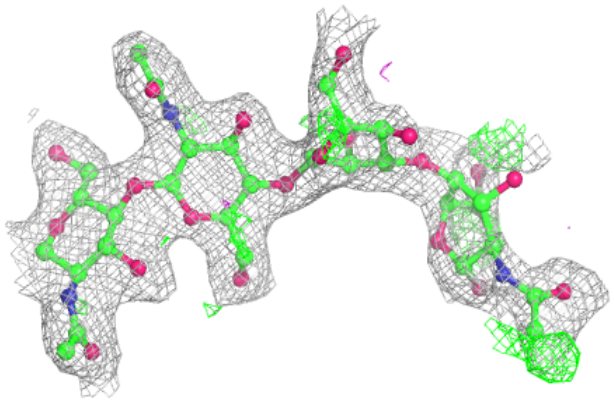
Electron density around Chain G:

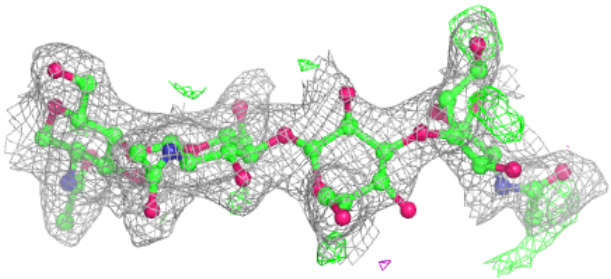
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

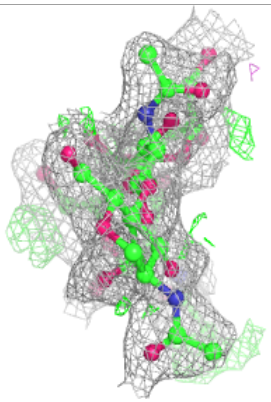


Electron density around Chain F:

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

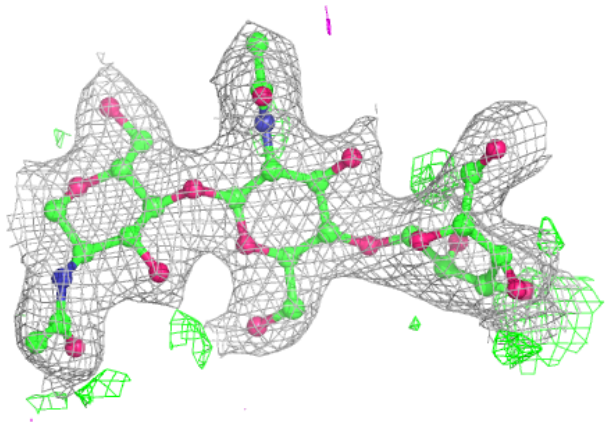


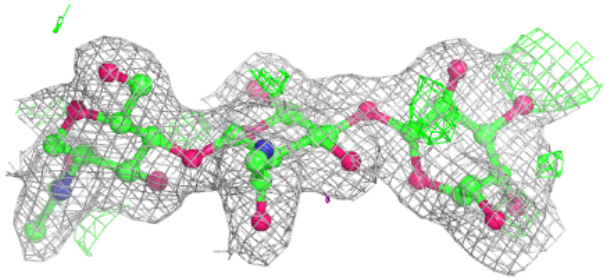


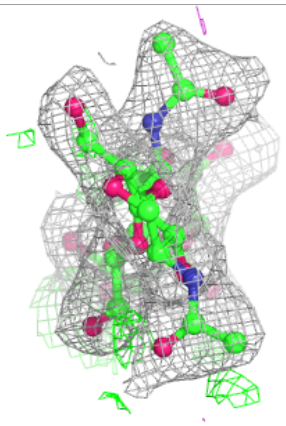


Electron density around Chain I:

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

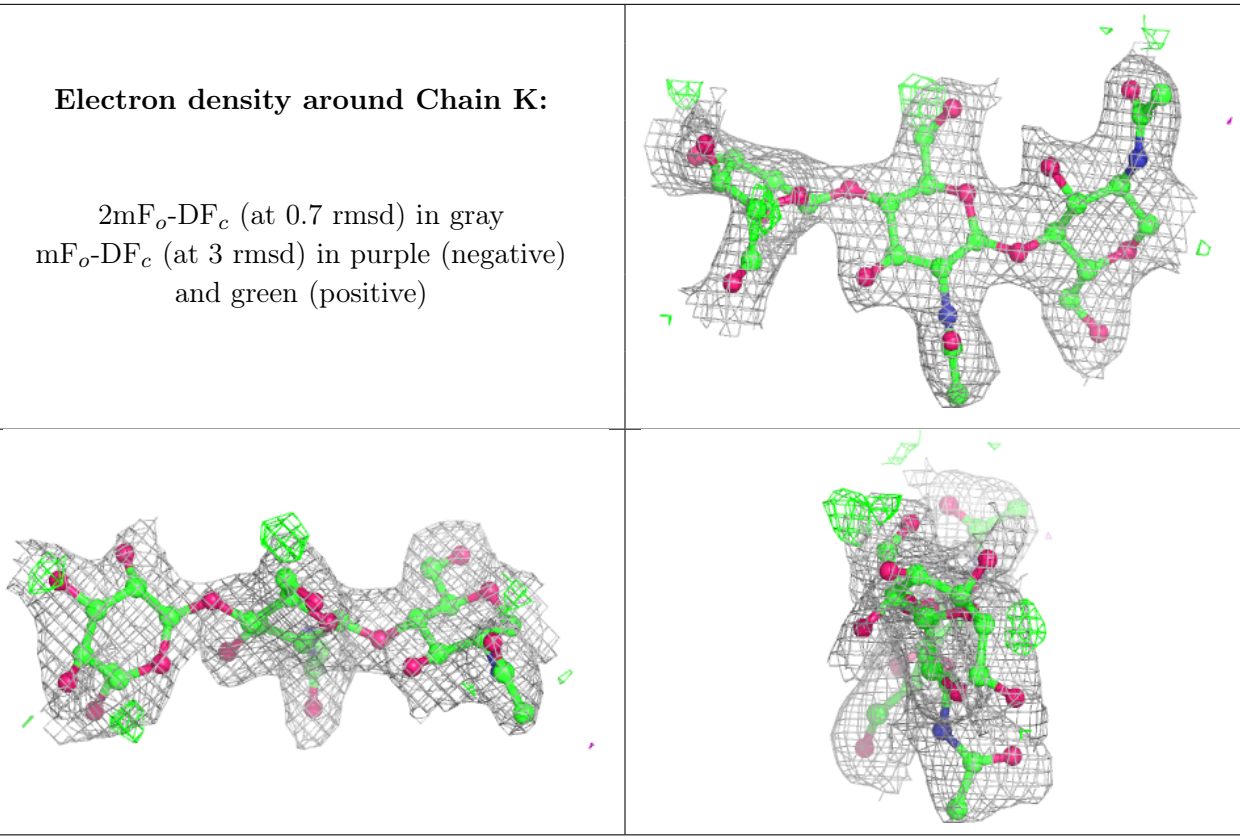






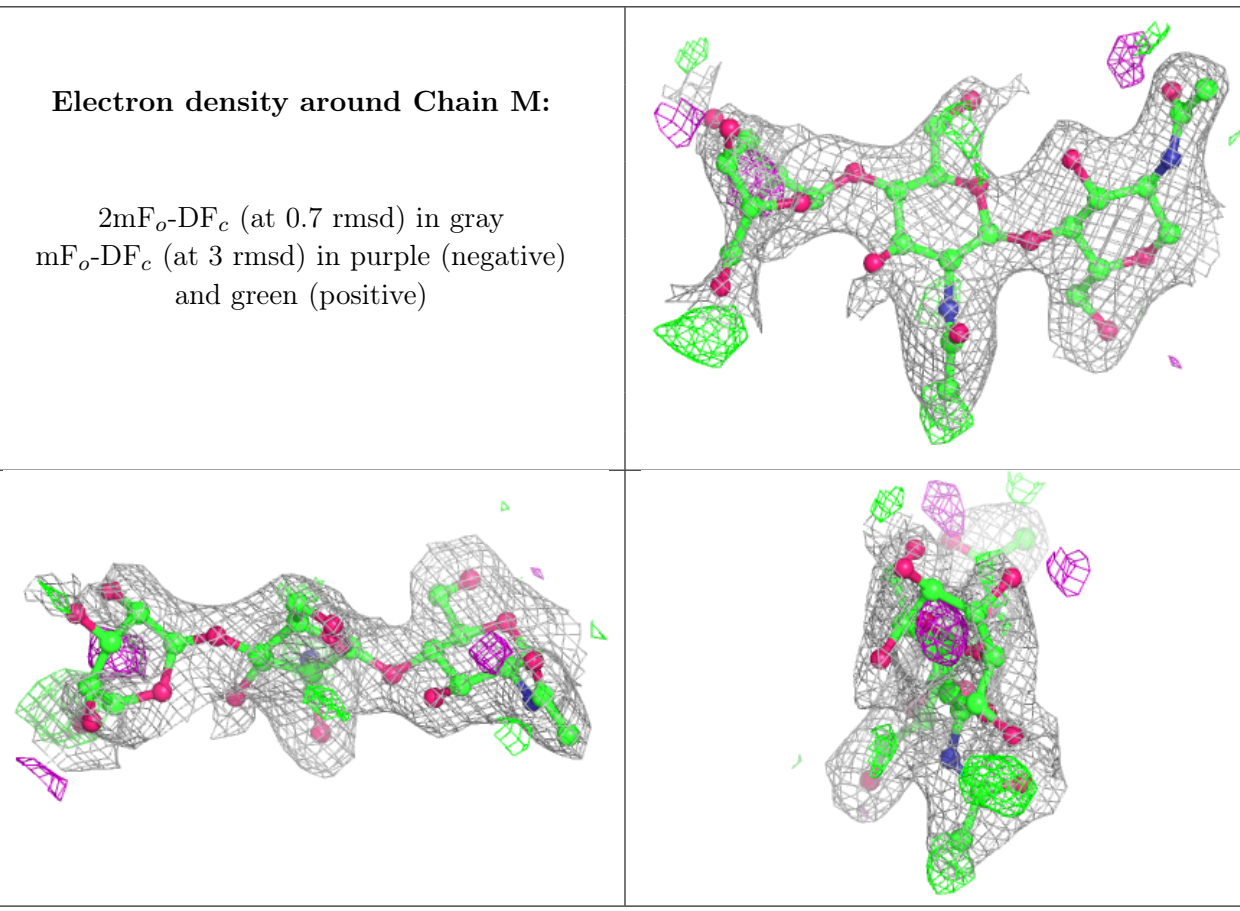
Electron density around Chain K:

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



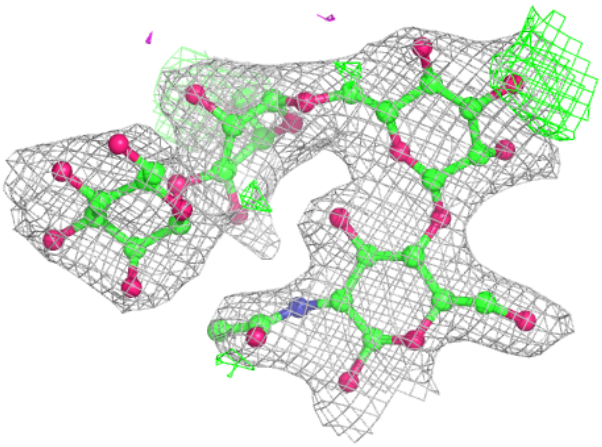
Electron density around Chain M:

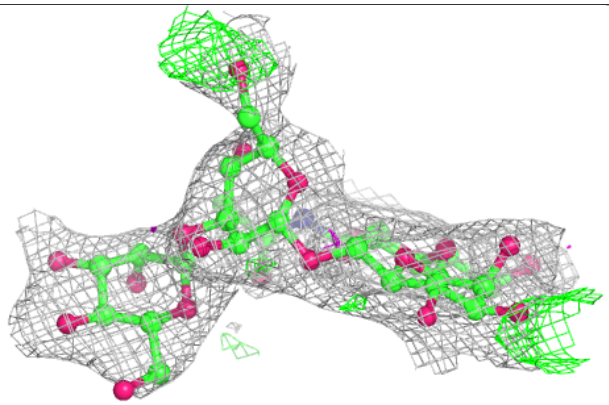
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

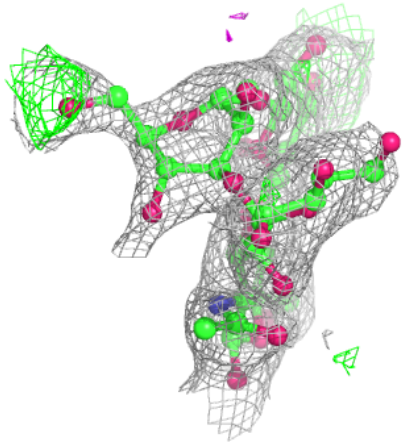


Electron density around Chain J:

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

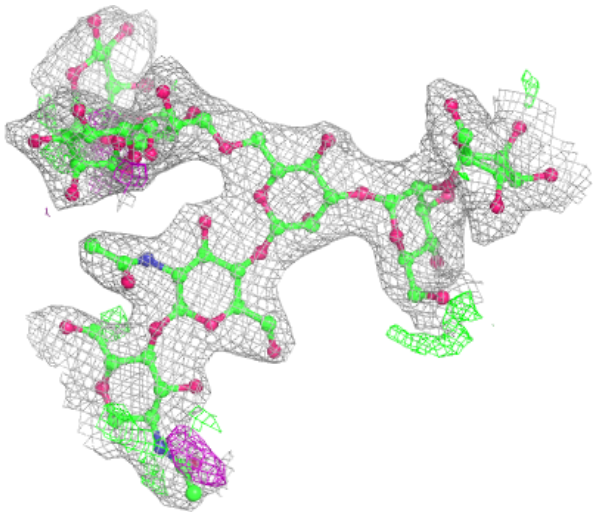


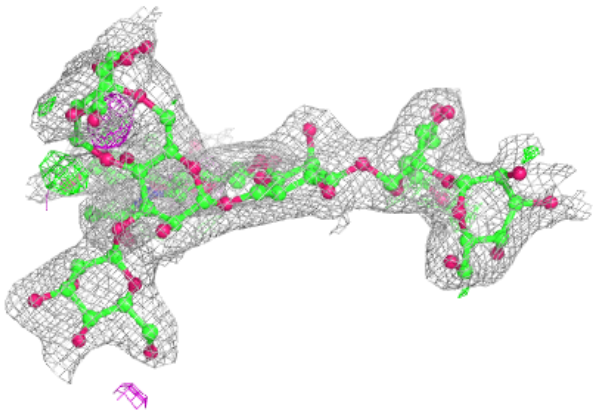


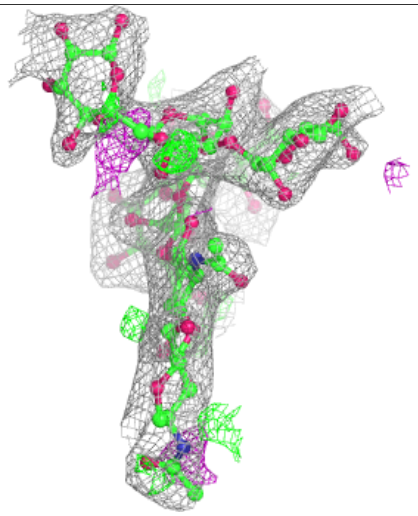


Electron density around Chain L:

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

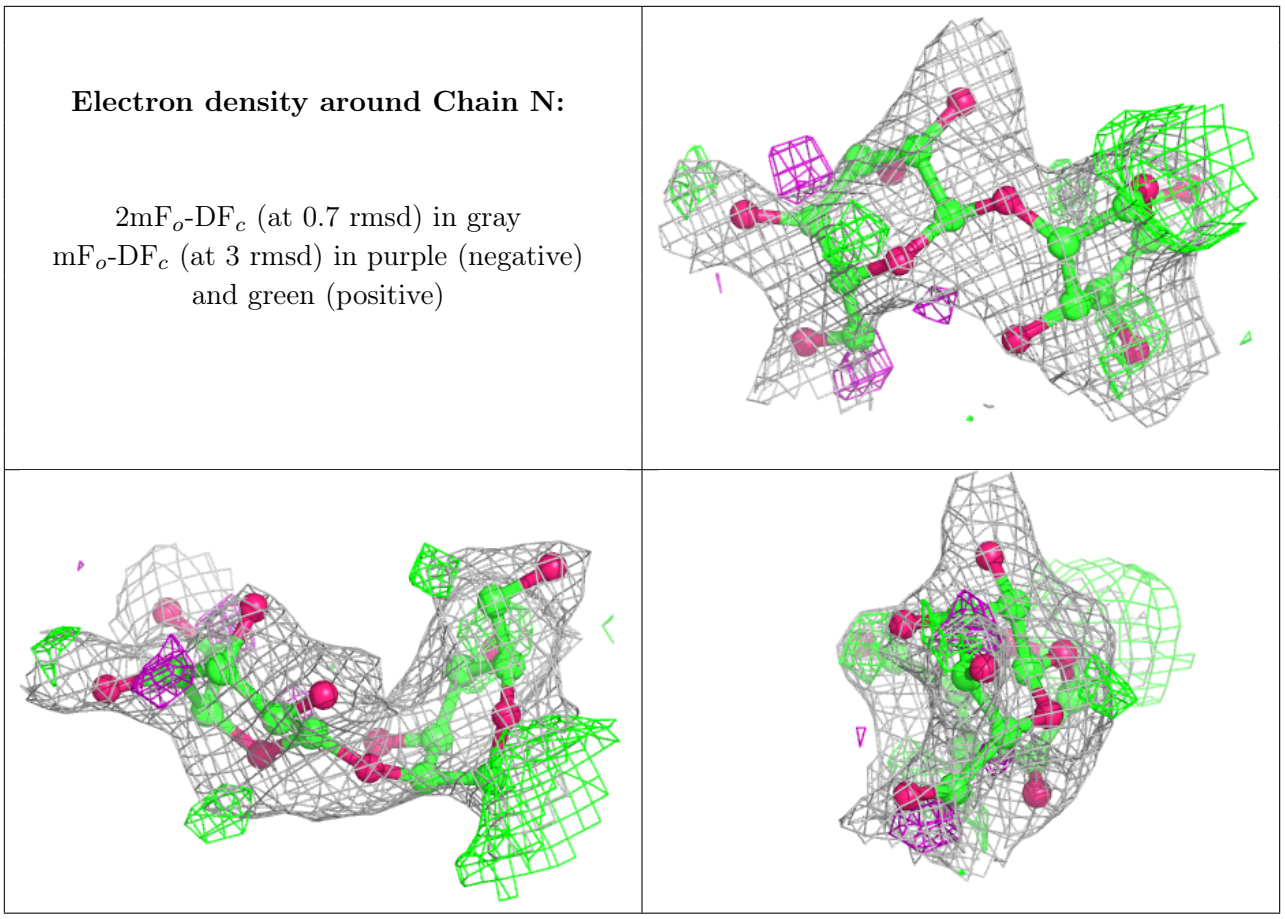






Electron density around Chain N:

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



6.4 Ligands

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^{th} 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
10	XYP	A	909	9/10	0.62	0.38	38,52,58,59	0
11	XYZ	B	909	10/10	0.75	0.26	20,20,20,20	0
9	BKR	A	908	59/59	0.76	0.33	59,79,94,96	0
8	NAG	D	902	15/15	0.78	0.27	60,71,75,76	0
8	NAG	C	902	15/15	0.78	0.25	51,60,65,66	0
8	NAG	A	907	14/15	0.81	0.29	59,65,68,78	0
8	NAG	C	905	14/15	0.81	0.46	76,90,95,96	0
13	BMA	C	904	11/12	0.81	0.20	46,55,67,69	0
8	NAG	B	907	14/15	0.84	0.41	66,73,75,75	0
8	NAG	D	903	14/15	0.84	0.34	68,71,79,83	0
9	BKR	B	908	59/59	0.85	0.26	44,56,61,64	0
8	NAG	D	904	14/15	0.89	0.31	57,68,70,72	0

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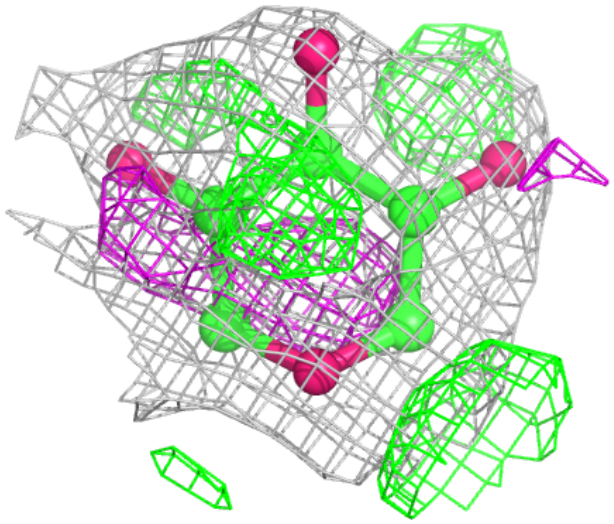
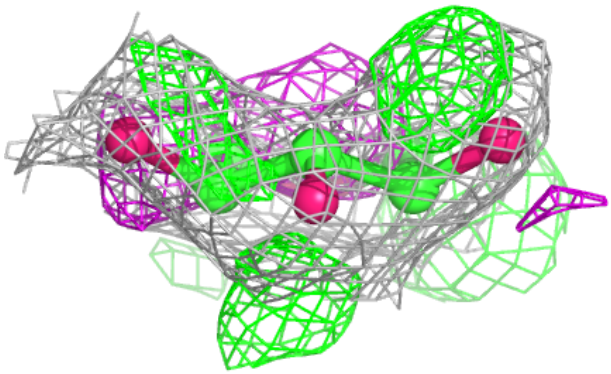
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	MAN	B	910	11/12	0.89	0.25	53,59,66,66	0
8	NAG	C	906	14/15	0.89	0.34	57,64,68,68	0
8	NAG	C	901	13/15	0.90	0.18	49,60,64,65	0
8	NAG	D	901	13/15	0.91	0.18	49,55,61,62	0
8	NAG	D	905	14/15	0.92	0.24	40,51,59,59	0
8	NAG	A	905	14/15	0.93	0.26	35,39,43,50	0
8	NAG	A	902	15/15	0.93	0.14	27,30,33,38	0
8	NAG	A	904	14/15	0.93	0.22	37,43,46,46	0
8	NAG	C	907	14/15	0.94	0.16	38,40,42,45	0
8	NAG	C	903	13/15	0.94	0.15	48,51,65,68	0
8	NAG	B	904	14/15	0.95	0.19	30,32,34,37	0
8	NAG	B	905	14/15	0.95	0.27	36,39,45,46	0
8	NAG	A	906	14/15	0.95	0.20	31,34,37,38	0
8	NAG	B	902	15/15	0.95	0.16	33,36,39,43	0
8	NAG	A	901	13/15	0.96	0.10	17,20,21,21	0
8	NAG	A	903	13/15	0.96	0.11	23,25,30,35	0
8	NAG	B	901	13/15	0.96	0.10	19,21,26,26	0
8	NAG	B	903	13/15	0.97	0.09	22,23,27,30	0
8	NAG	B	906	14/15	0.97	0.17	29,34,35,35	0

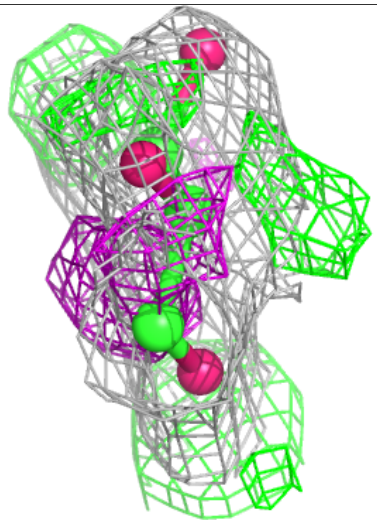
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around XYP A 909:

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

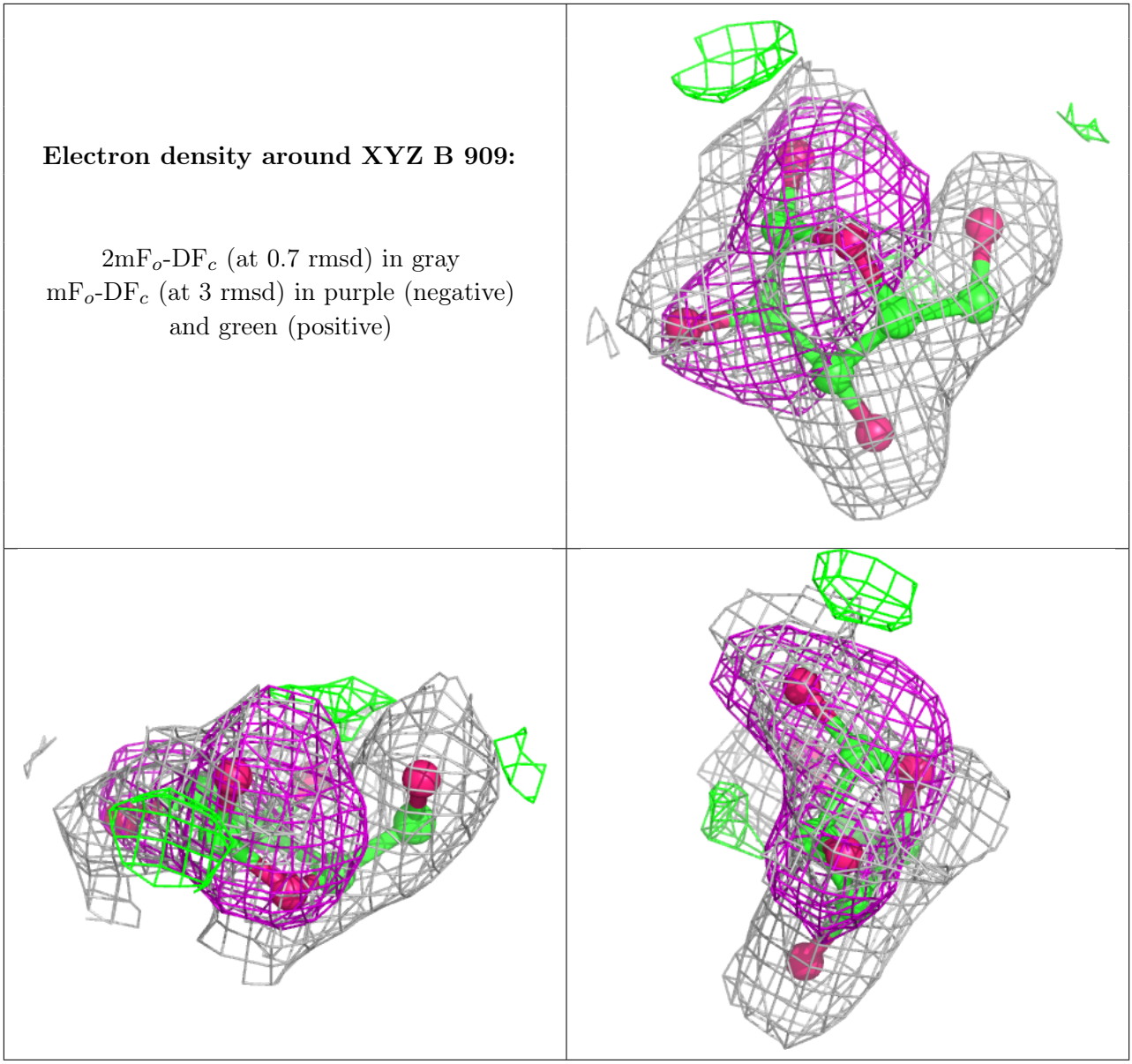






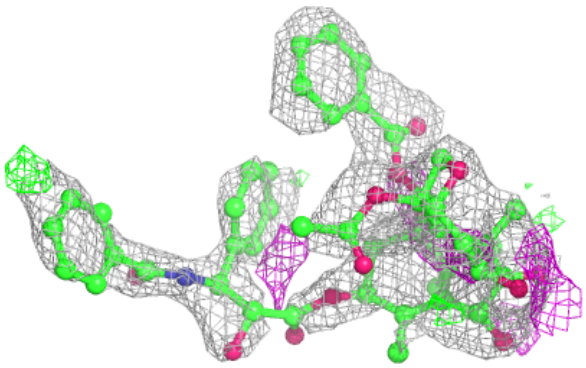
Electron density around XYZ B 909:

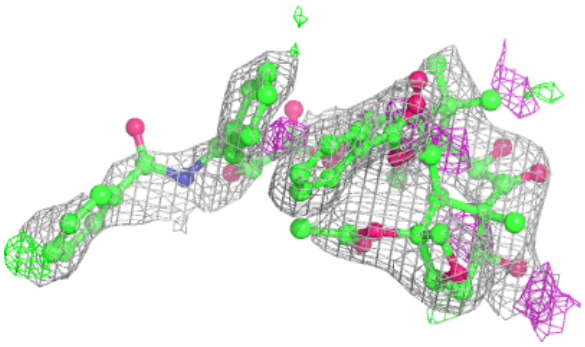
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

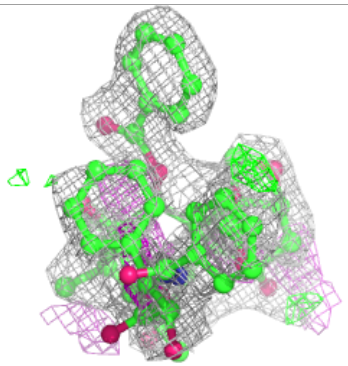


Electron density around BKR A 908:

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

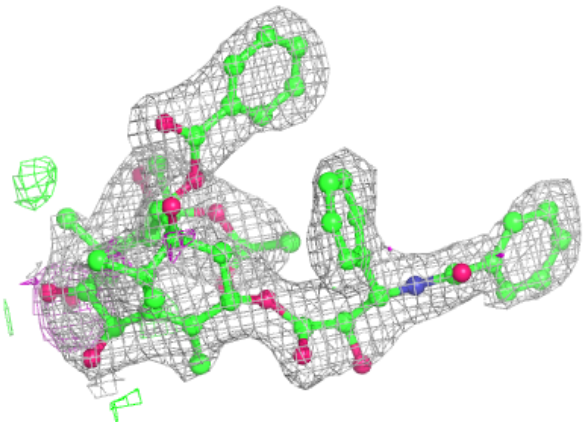


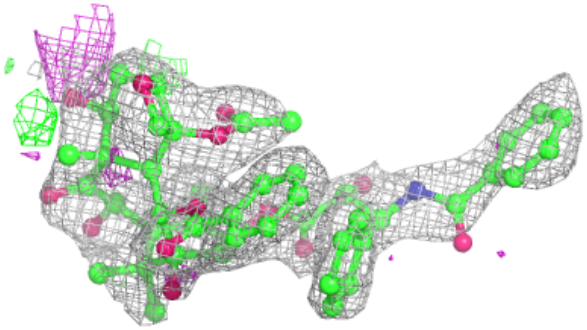


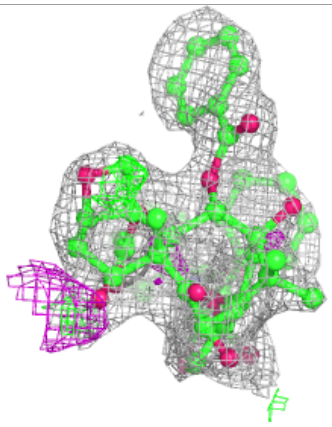


Electron density around BKR B 908:

$2mF_o$-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.