wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 08:27 PM JST

PDB ID	:	8GYY
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 (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:

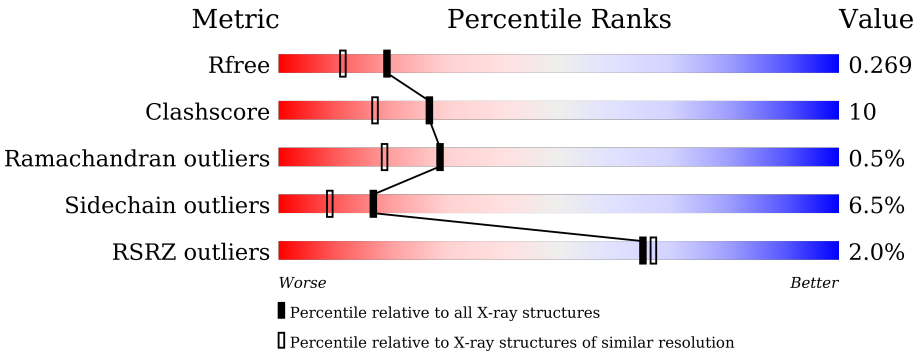
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.07 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}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (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 <=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	80% 12% • 6%
1	B	803	81% 11% • 6%
1	C	803	3% 75% 17% • 6%
1	D	803	3% 73% 19% • 6%
2	E	2	100%
2	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	L	2	100%
2	O	2	50% 50%
2	P	2	100%
3	F	5	20% 80%
4	G	2	50% 50%
5	I	3	100%
6	J	5	60% 40%
7	K	3	33% 33% 33%
7	M	3	33% 67%
7	N	3	33% 67%

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	B	916	-	-	-	X
11	NAG	C	901	-	-	X	-
11	NAG	C	911	-	-	-	X
12	BMA	D	901	-	-	X	-
2	NAG	H	2	-	-	X	-
2	NAG	P	1	-	-	X	-
4	MAN	G	1	-	-	X	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.

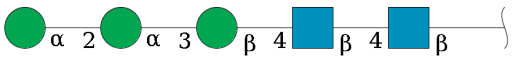
- Molecule 1 is a protein called Beta-D-xylosidase/beta-D-glucosidase.

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.

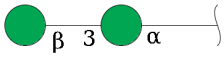
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	O	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	P	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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.



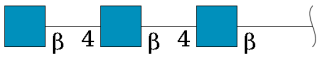
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



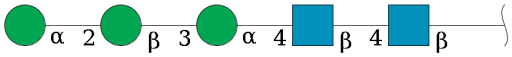
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total	C	O	0	0	0
			23	12	11			

- 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.



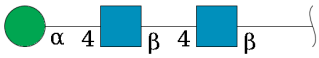
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			42	24	3	15			

- 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.



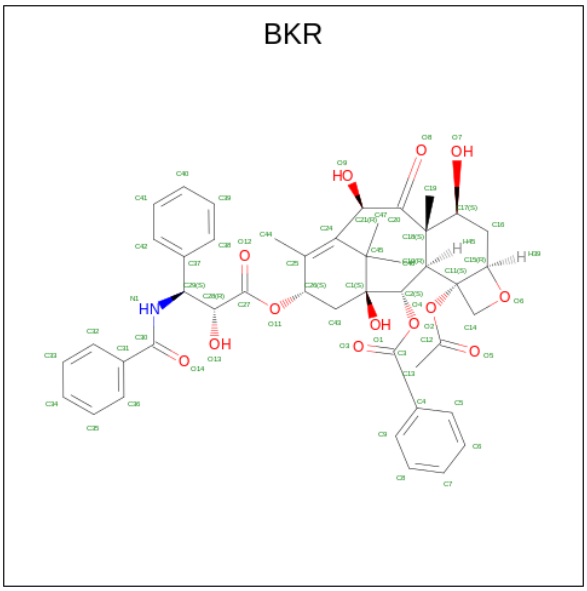
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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 39 22 2 15	0	0	0
7	M	3	Total C N O 39 22 2 15	0	0	0
7	N	3	Total C N O 39 22 2 15	0	0	0

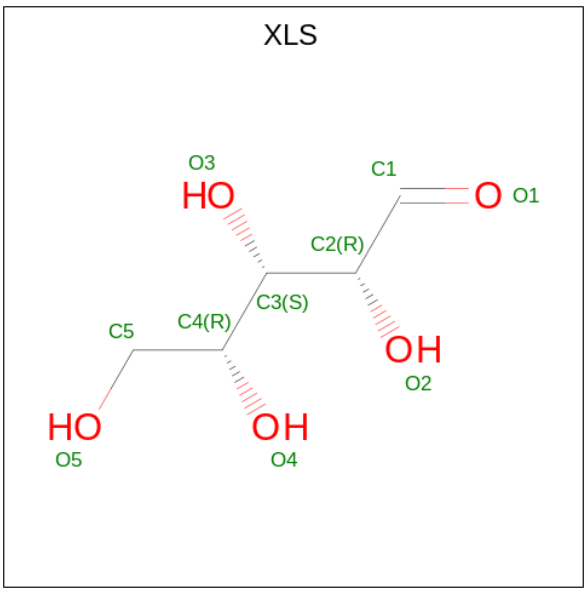
- Molecule 8 is Deacetyltaxol (three-letter code: BKR) (formula: $C_{45}H_{49}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



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

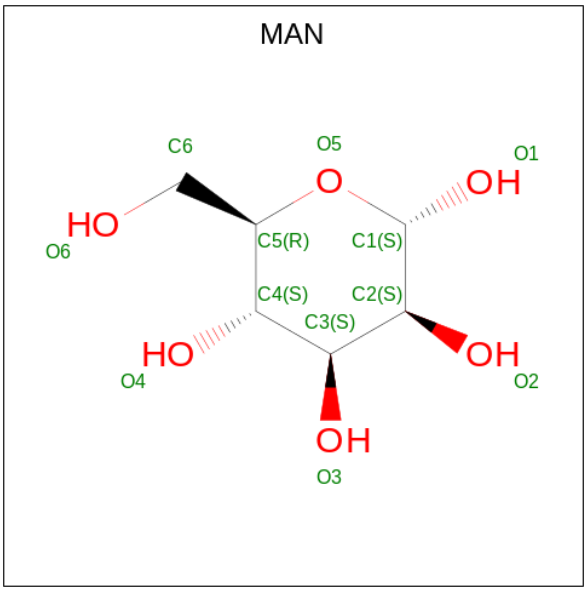
- Molecule 9 is D-xylose (three-letter code: XLS) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of

Interest" by depositor).



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

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

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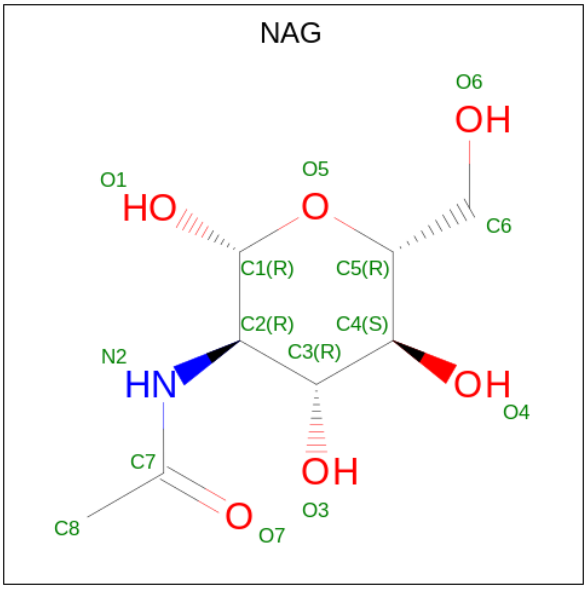
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 11 6 5	0	0
10	B	1	Total C O 11 6 5	0	0
10	B	1	Total C O 11 6 5	0	0
10	B	1	Total C O 11 6 5	0	0
10	B	1	Total C O 12 6 6	0	0
10	B	1	Total C O 11 6 5	0	0
10	A	1	Total C O 11 6 5	0	0
10	A	1	Total C O 11 6 5	0	0
10	A	1	Total C O 11 6 5	0	0
10	A	1	Total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

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



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

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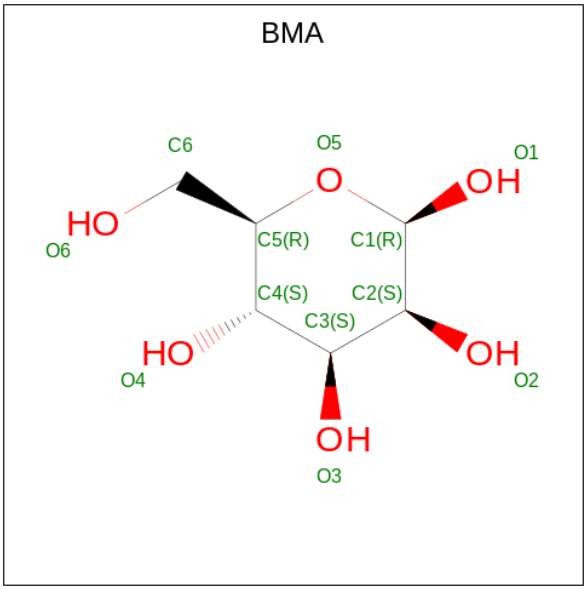
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C N O 14 8 1 5	0	0
11	C	1	Total C N O 14 8 1 5	0	0
11	C	1	Total C N O 14 8 1 5	0	0
11	C	1	Total C N O 14 8 1 5	0	0
11	C	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0
11	D	1	Total C N O 14 8 1 5	0	0
11	D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

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



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

- Molecule 13 is water.

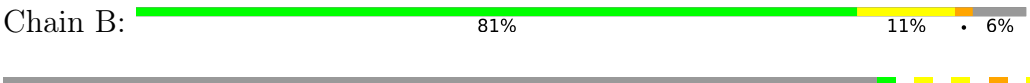
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	479	Total O 479 479	0	0
13	A	436	Total O 436 436	0	0
13	C	198	Total O 198 198	0	0
13	D	181	Total O 181 181	0	0

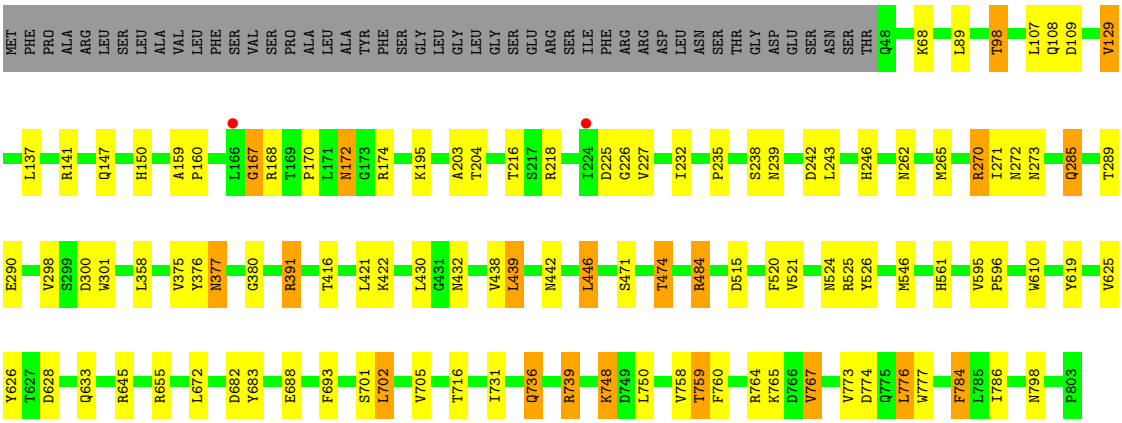
3 Residue-property plots (i)

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

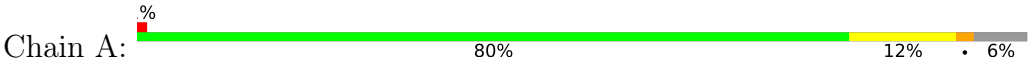
Chain B:

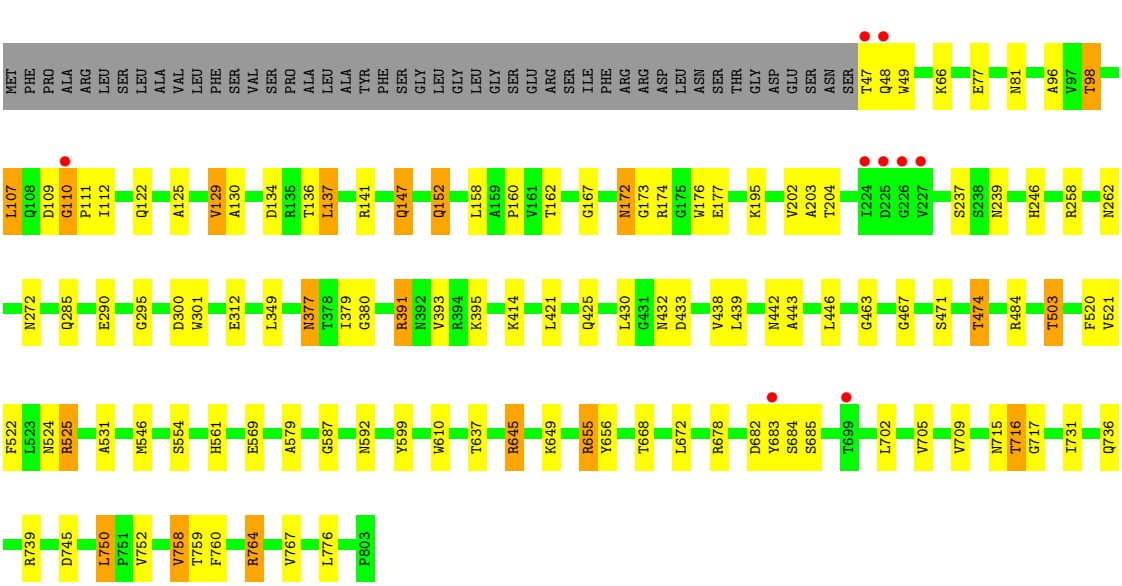




• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

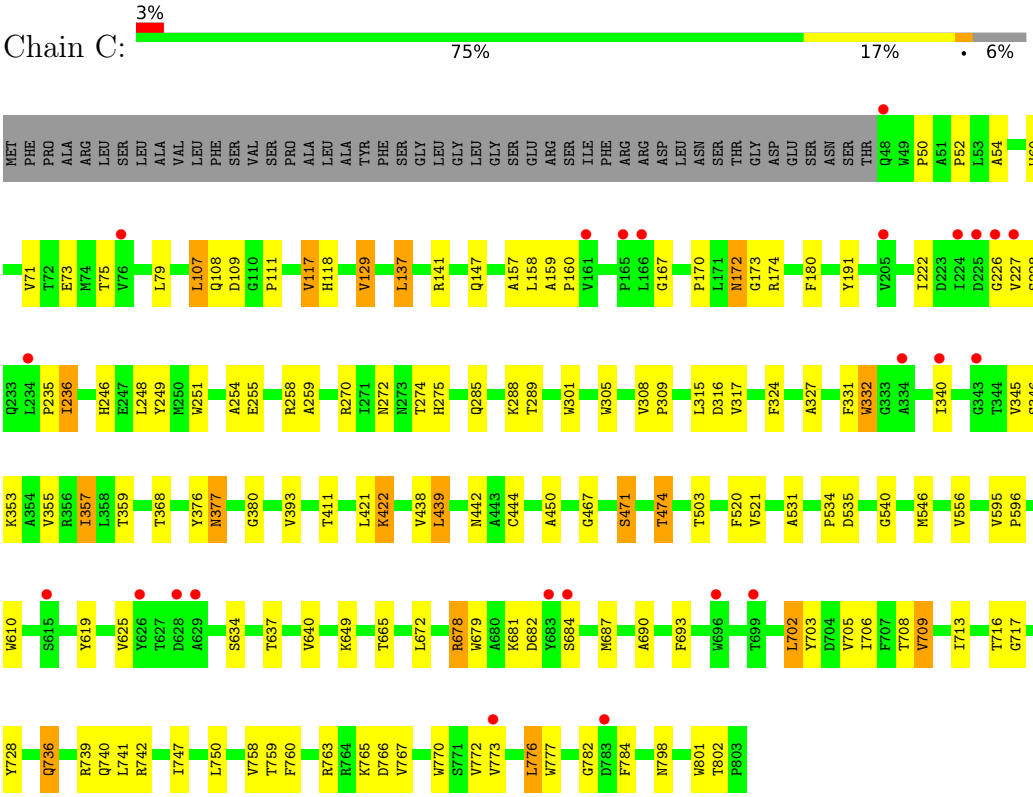
Chain A:





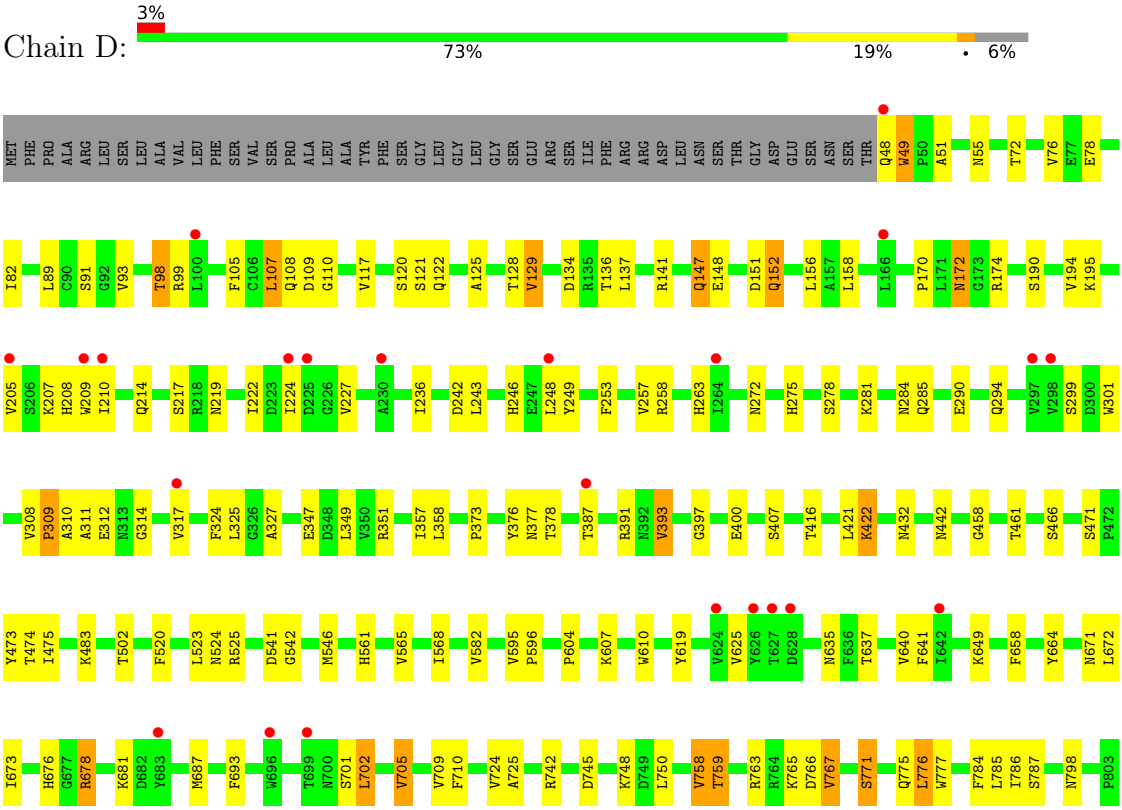
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain C:



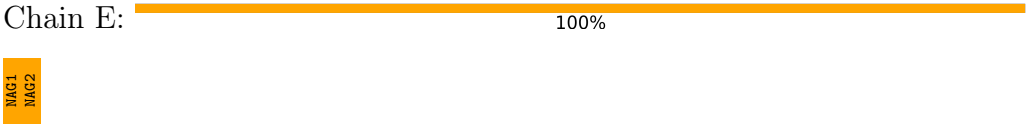
• Molecule 1: Beta-D-xylosidase/beta-D-glucosidase

Chain D:



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

Chain E:

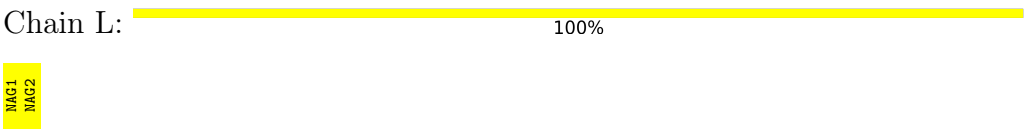


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

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

Chain L:

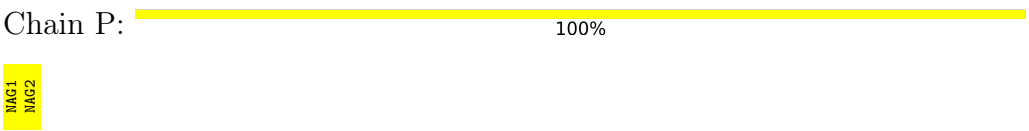


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain P:



• 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:

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

Chain G:

• 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

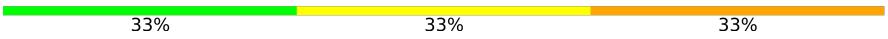
Chain I:

• 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:

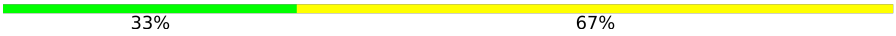
• Molecule 7: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• 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:



• 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:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	228.43Å 89.23Å 218.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.97 – 2.07 35.94 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.97-2.07) 95.1 (35.94-2.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.219 , 0.259 0.231 , 0.269	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 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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: AH2, BKR, NAG, BMA, MAN, XLS

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	0.42	0/5865	0.74	0/8025
1	B	0.44	0/5883	0.75	0/8049
1	C	0.38	0/5864	0.72	0/8023
1	D	0.39	0/5867	0.75	0/8027
All	All	0.41	0/23479	0.74	0/32124

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.

There are no bond angle outliers.

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5721	0	5518	72	0
1	B	5738	0	5526	85	0
1	C	5717	0	5510	100	0
1	D	5720	0	5519	119	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	18	0
10	B	78	0	72	28	0
10	C	55	0	50	14	0
10	D	44	0	39	7	0
11	A	56	0	52	1	0
11	B	100	0	95	7	0
11	C	84	0	78	11	0
11	D	56	0	52	1	0
12	D	11	0	10	9	0
13	A	436	0	0	8	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	474	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 10.

The worst 5 of 474 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%)	41	32
1	B	757/803 (94%)	719 (95%)	37 (5%)	1 (0%)	51	45
1	C	756/803 (94%)	693 (92%)	56 (7%)	7 (1%)	17	8
1	D	756/803 (94%)	685 (91%)	67 (9%)	4 (0%)	29	19
All	All	3025/3212 (94%)	2817 (93%)	194 (6%)	14 (0%)	29	19

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 (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 7
1	B	612/648 (94%)	577 (94%)	35 (6%)	20 12
1	C	610/648 (94%)	574 (94%)	36 (6%)	19 11
1	D	611/648 (94%)	565 (92%)	46 (8%)	13 6
All	All	2443/2592 (94%)	2283 (94%)	160 (6%)	17 9

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	49	TRP
1	D	582	VAL
1	D	107	LEU
1	D	299	SER
1	D	702	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	246	HIS
1	C	676	HIS
1	D	671	ASN
1	C	262	ASN
1	C	377	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)

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	2,1	14,14,15	0.66	0	17,19,21	3.18	4 (23%)
2	NAG	E	2	2	14,14,15	0.51	0	17,19,21	1.13	2 (11%)
3	NAG	F	1	3,1	14,14,15	0.49	0	17,19,21	0.97	2 (11%)
3	NAG	F	2	3	14,14,15	0.42	0	17,19,21	1.21	1 (5%)
3	BMA	F	3	3	11,11,12	1.14	1 (9%)	15,15,17	1.59	2 (13%)
3	MAN	F	4	3	11,11,12	0.54	0	15,15,17	1.56	2 (13%)
3	MAN	F	5	3	11,11,12	0.64	0	15,15,17	1.52	2 (13%)
4	MAN	G	1	4	12,12,12	0.34	0	17,17,17	0.50	0
4	BMA	G	2	4	11,11,12	1.06	1 (9%)	15,15,17	1.84	4 (26%)
2	NAG	H	1	2,1	14,14,15	0.40	0	17,19,21	1.09	2 (11%)
2	NAG	H	2	2	14,14,15	0.45	0	17,19,21	1.17	2 (11%)
5	NAG	I	1	5,1	14,14,15	0.76	1 (7%)	17,19,21	1.60	3 (17%)
5	NAG	I	2	5	14,14,15	0.44	0	17,19,21	0.80	1 (5%)
5	NAG	I	3	5	14,14,15	0.34	0	17,19,21	1.71	3 (17%)
6	NAG	J	1	6,1	14,14,15	0.47	0	17,19,21	1.13	1 (5%)
6	NAG	J	2	6	14,14,15	0.44	0	17,19,21	1.14	2 (11%)
6	AH2	J	3	6	11,11,11	0.70	0	15,15,15	1.95	6 (40%)
6	BMA	J	4	6	11,11,12	0.49	0	15,15,17	1.44	2 (13%)
6	MAN	J	5	6	11,11,12	0.83	0	15,15,17	1.10	2 (13%)
7	NAG	K	1	7,1	14,14,15	0.41	0	17,19,21	0.69	0
7	NAG	K	2	7	14,14,15	0.38	0	17,19,21	1.33	1 (5%)
7	MAN	K	3	7	11,11,12	0.84	1 (9%)	15,15,17	1.46	2 (13%)
2	NAG	L	1	2,1	14,14,15	0.77	1 (7%)	17,19,21	2.52	4 (23%)
2	NAG	L	2	2	14,14,15	0.52	0	17,19,21	1.35	3 (17%)
7	NAG	M	1	7,1	14,14,15	0.30	0	17,19,21	0.61	0
7	NAG	M	2	7	14,14,15	0.49	0	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	M	3	7	11,11,12	1.06	2 (18%)	15,15,17	1.46	2 (13%)
7	NAG	N	1	7,1	14,14,15	0.28	0	17,19,21	0.93	1 (5%)
7	NAG	N	2	7	14,14,15	0.40	0	17,19,21	0.80	0
7	MAN	N	3	7	11,11,12	0.95	0	15,15,17	1.27	3 (20%)
2	NAG	O	1	2,1	14,14,15	0.38	0	17,19,21	0.67	0
2	NAG	O	2	2	14,14,15	0.51	0	17,19,21	1.21	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	1.01	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2,1	-	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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	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	2,1	-	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	6,1	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
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	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2,1	-	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 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	BMA	C2-C3	-2.54	1.48	1.52
2	L	1	NAG	O4-C4	2.34	1.48	1.43
5	I	1	NAG	C1-C2	2.32	1.55	1.52
3	F	3	BMA	C4-C5	-2.32	1.48	1.53
7	K	3	MAN	O5-C5	2.24	1.48	1.43

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	NAG	O4-C4-C5	9.86	133.79	109.30
2	L	1	NAG	O4-C4-C3	7.94	128.70	110.35
2	E	1	NAG	O5-C1-C2	-5.76	102.20	111.29
7	K	2	NAG	C2-N2-C7	4.97	129.98	122.90
3	F	4	MAN	C1-O5-C5	4.91	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

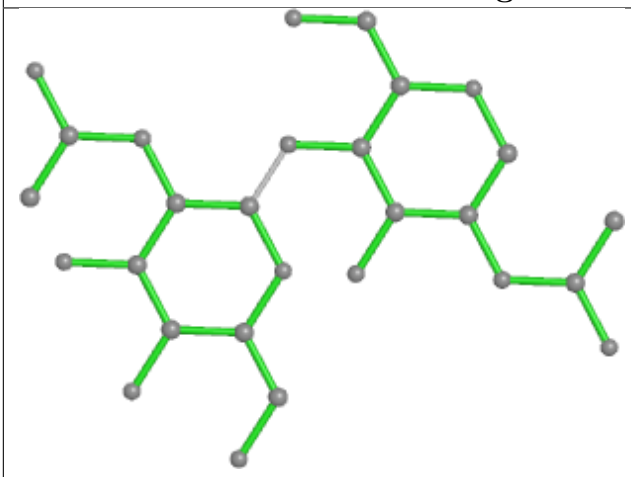
There are no ring outliers.

19 monomers are involved in 69 short contacts:

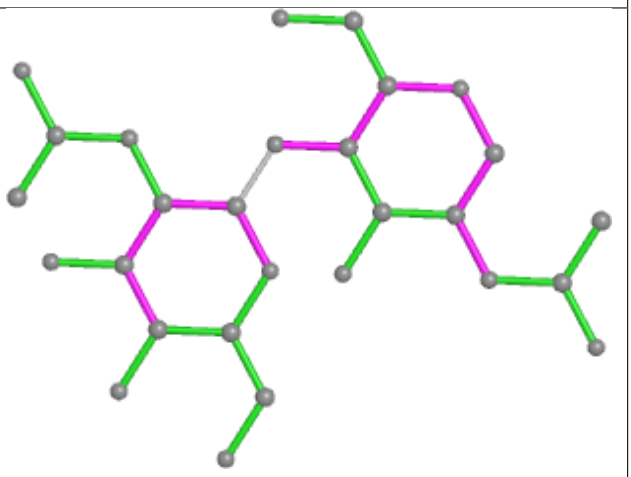
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	NAG	2	0
2	P	2	NAG	5	0
3	F	1	NAG	2	0
5	I	1	NAG	2	0
4	G	2	BMA	10	0
3	F	5	MAN	1	0
5	I	3	NAG	2	0
3	F	2	NAG	2	0
2	P	1	NAG	11	0
2	E	1	NAG	2	0
2	O	1	NAG	5	0
3	F	3	BMA	3	0
2	H	2	NAG	10	0
4	G	1	MAN	18	0
2	E	2	NAG	2	0
6	J	1	NAG	3	0
2	O	2	NAG	5	0
7	K	3	MAN	2	0
6	J	3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

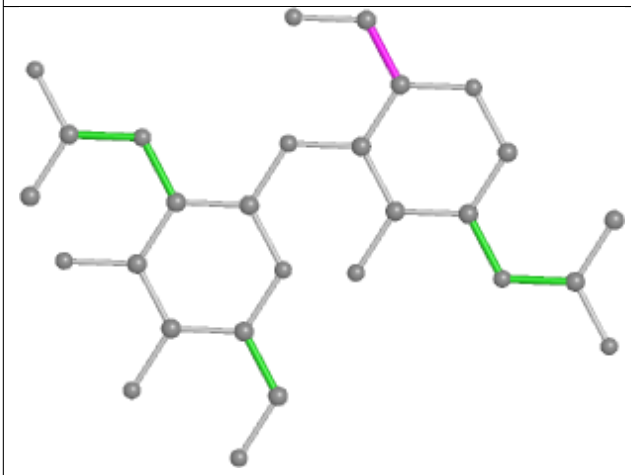
Oligosaccharide Chain E



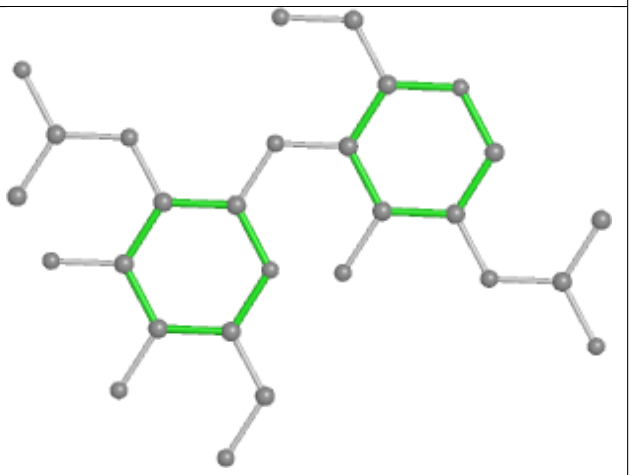
Bond lengths



Bond angles

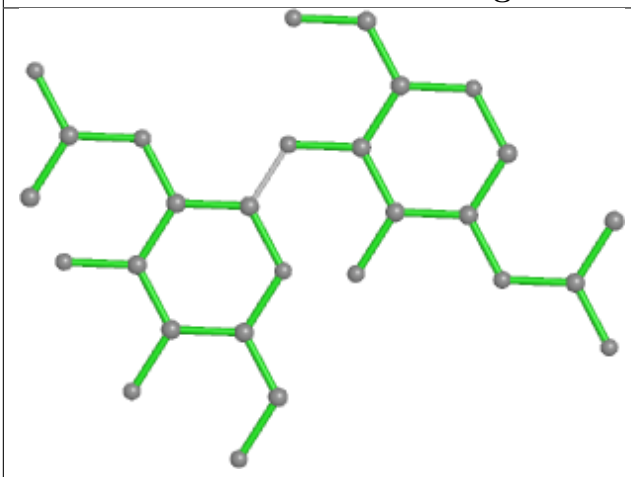


Torsions

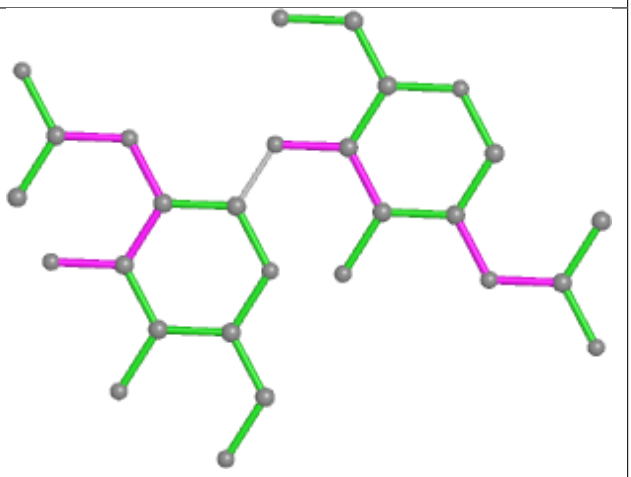


Rings

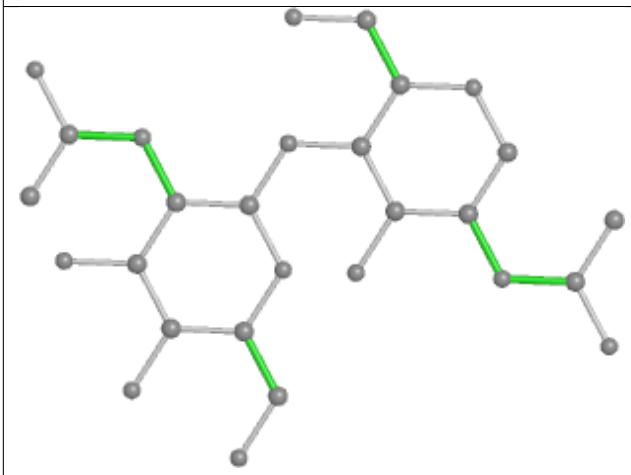
Oligosaccharide Chain H



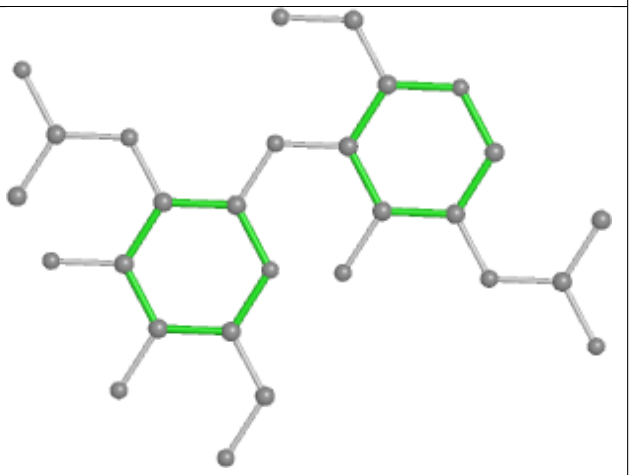
Bond lengths



Bond angles

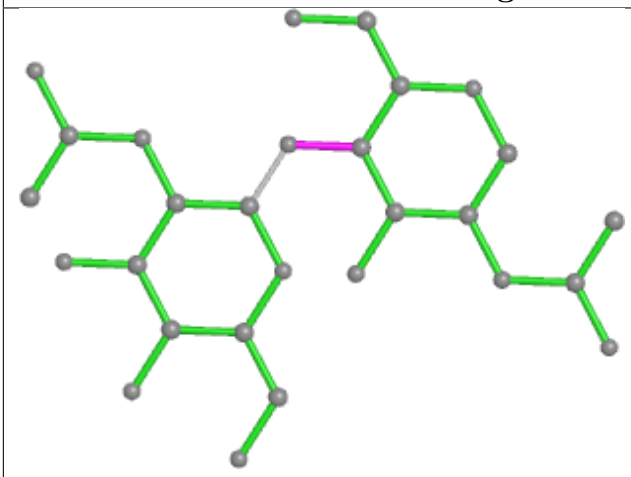


Torsions

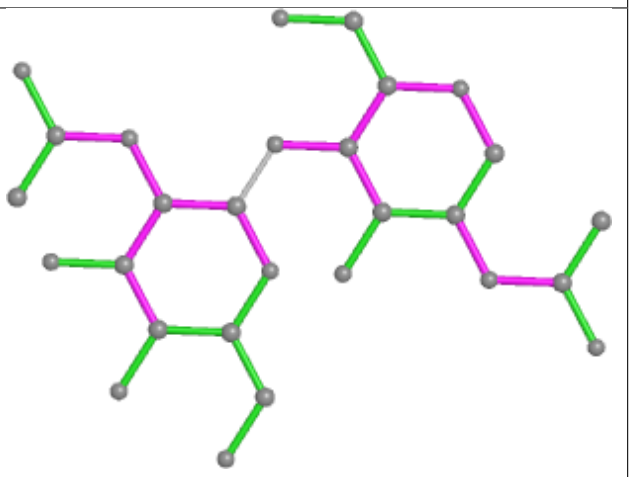


Rings

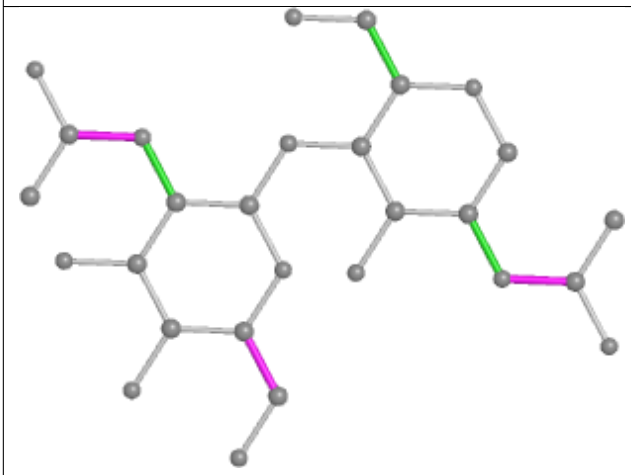
Oligosaccharide Chain L



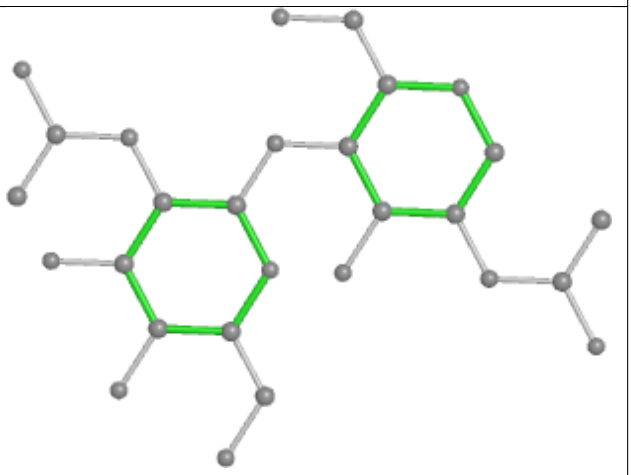
Bond lengths



Bond angles

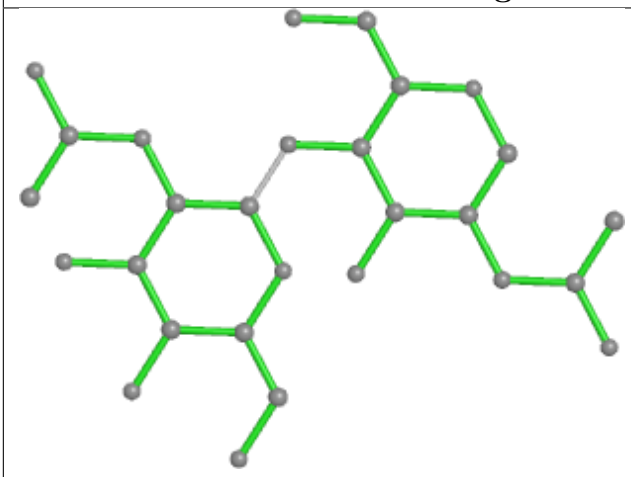


Torsions

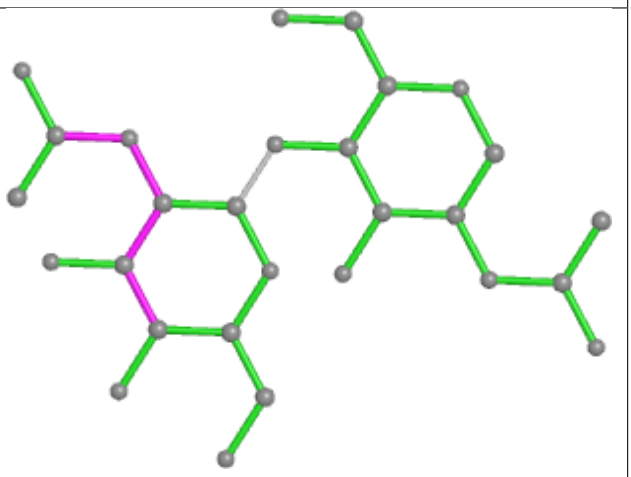


Rings

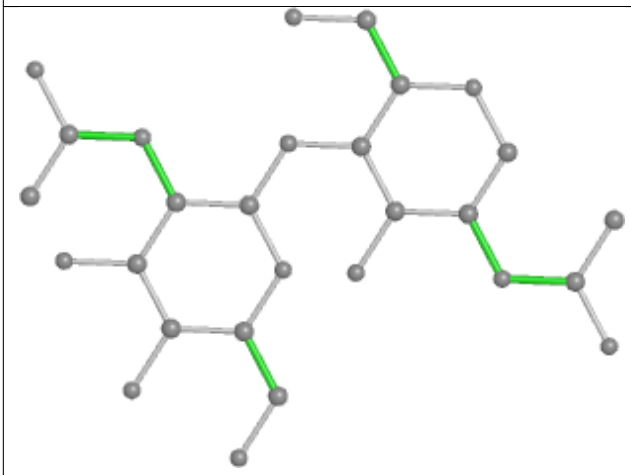
Oligosaccharide Chain O



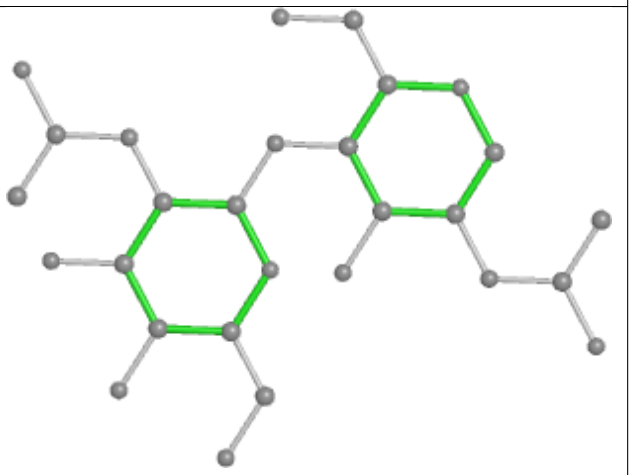
Bond lengths



Bond angles

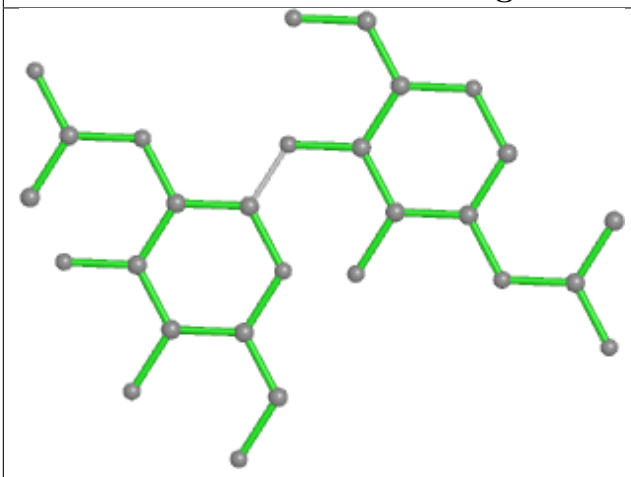


Torsions

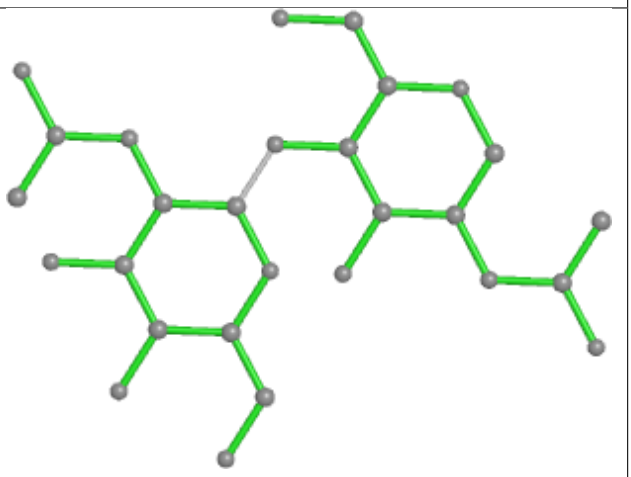


Rings

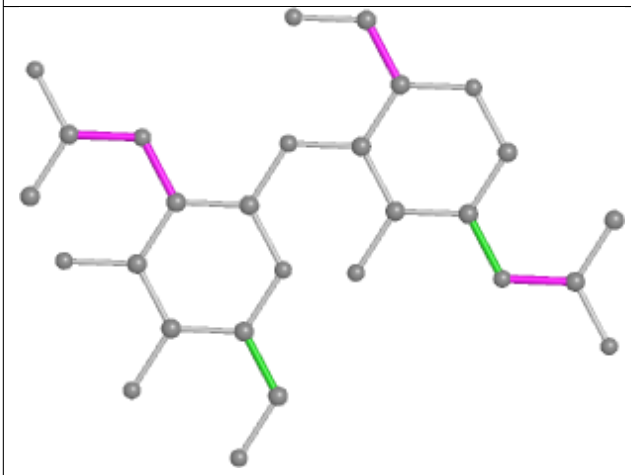
Oligosaccharide Chain P



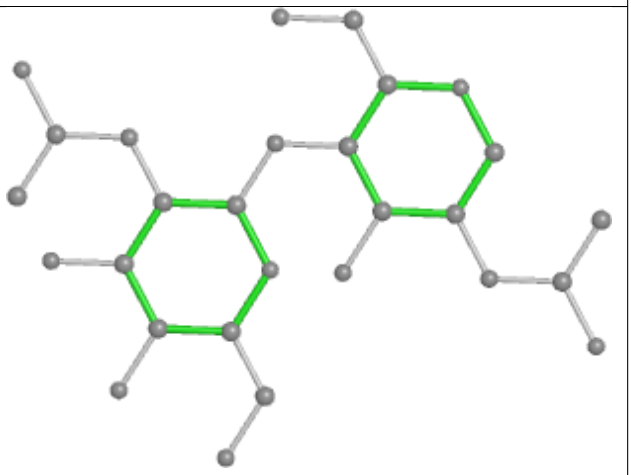
Bond lengths



Bond angles

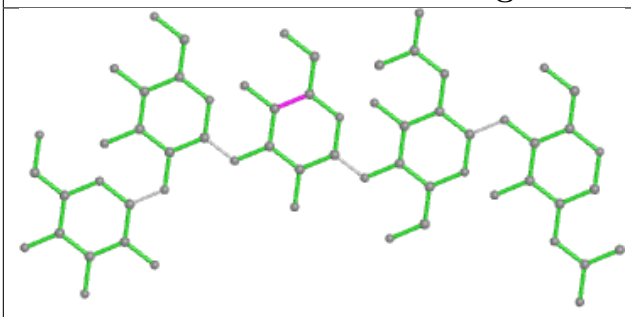


Torsions

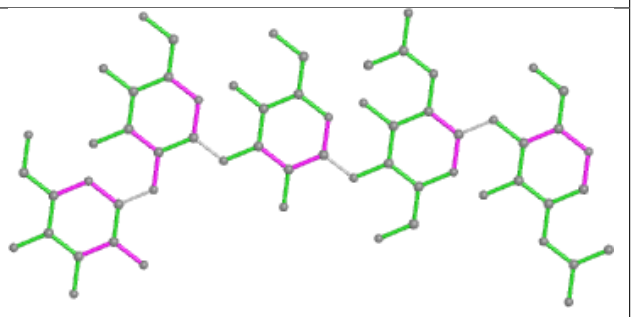


Rings

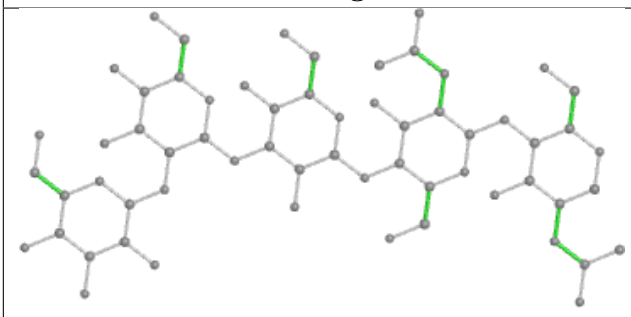
Oligosaccharide Chain F



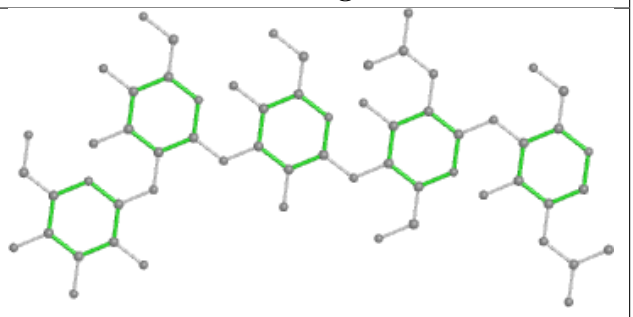
Bond lengths



Bond angles

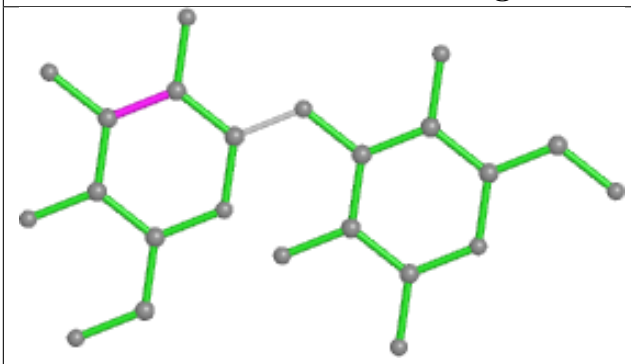


Torsions

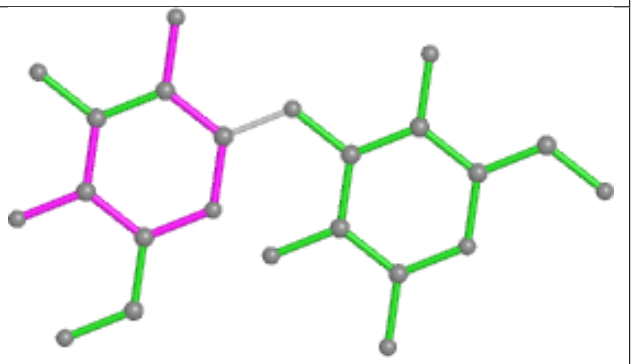


Rings

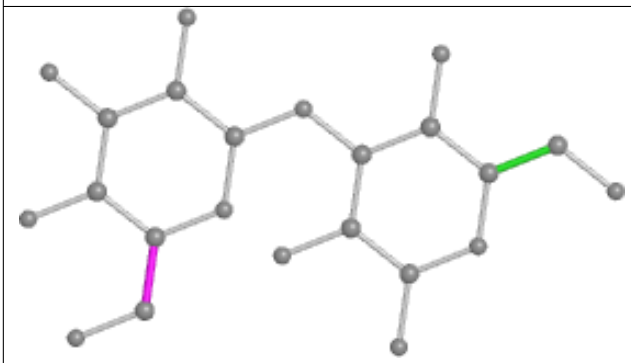
Oligosaccharide Chain G



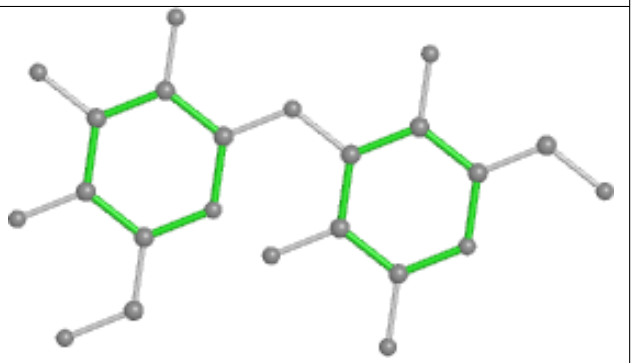
Bond lengths



Bond angles

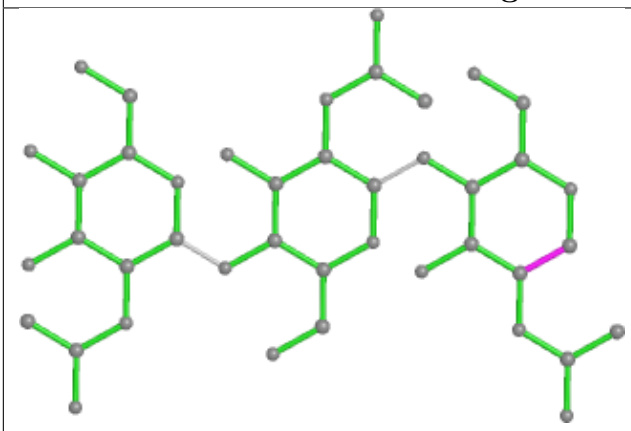


Torsions

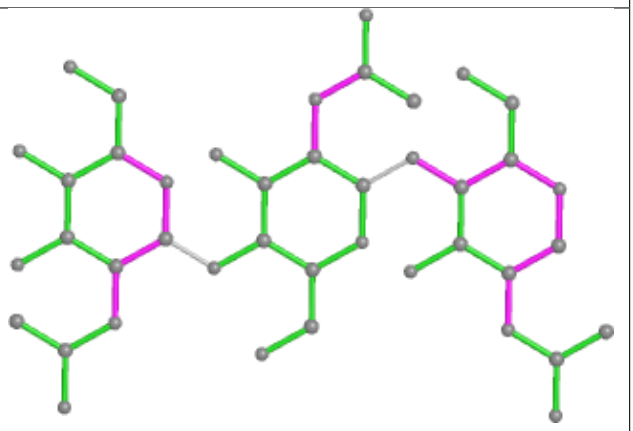


Rings

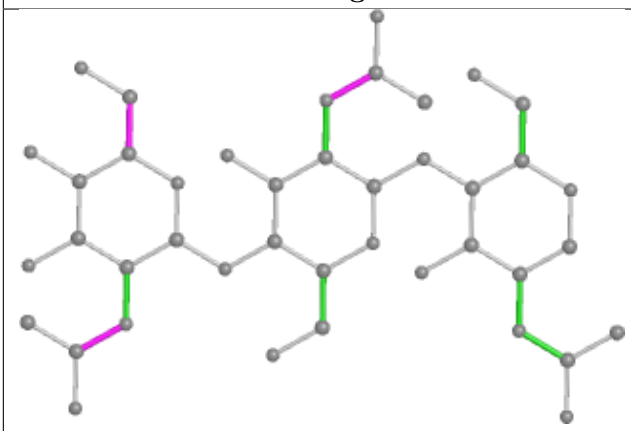
Oligosaccharide Chain I



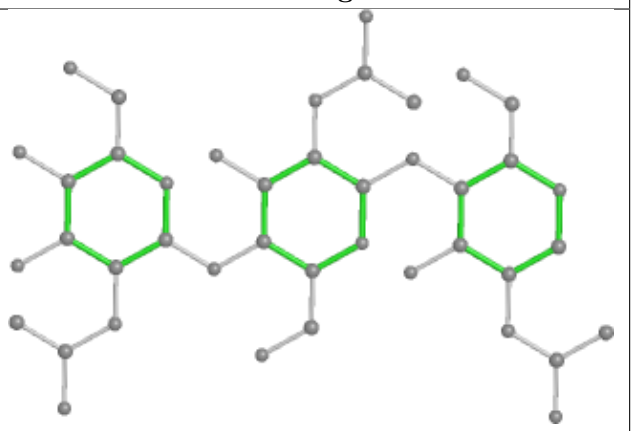
Bond lengths



Bond angles

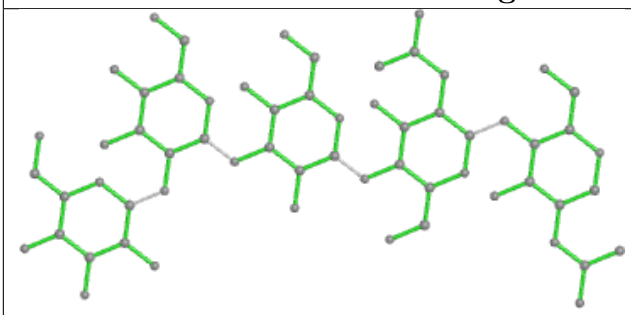


Torsions

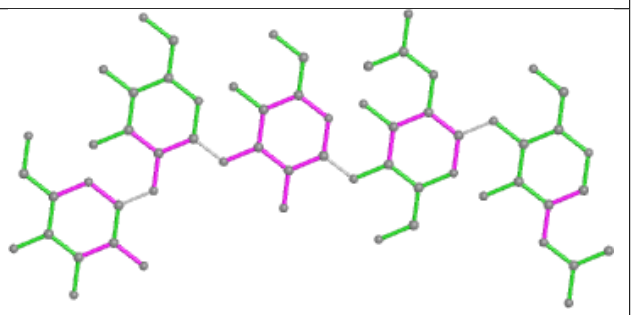


Rings

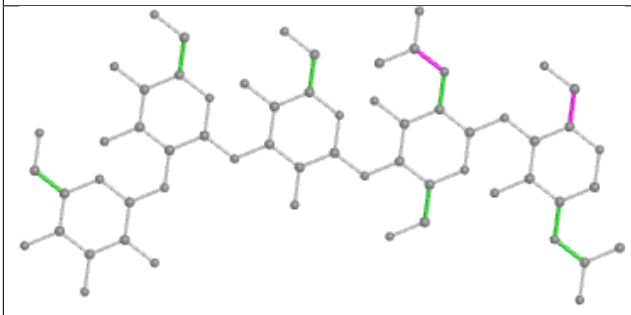
Oligosaccharide Chain J



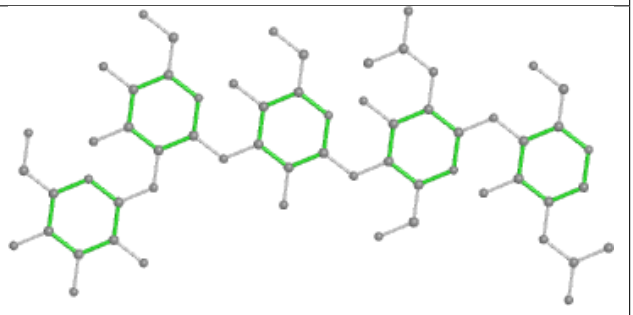
Bond lengths



Bond angles

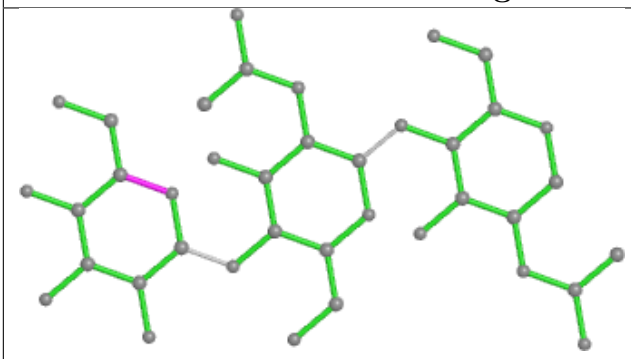


Torsions

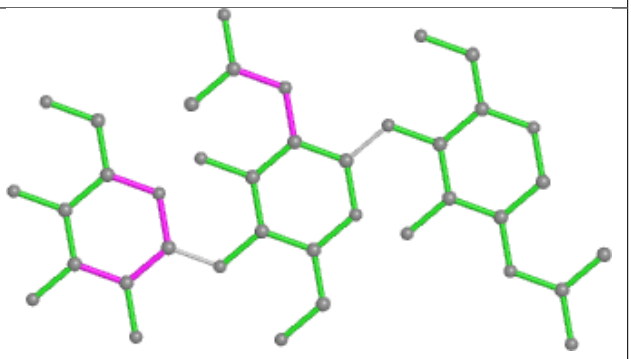


Rings

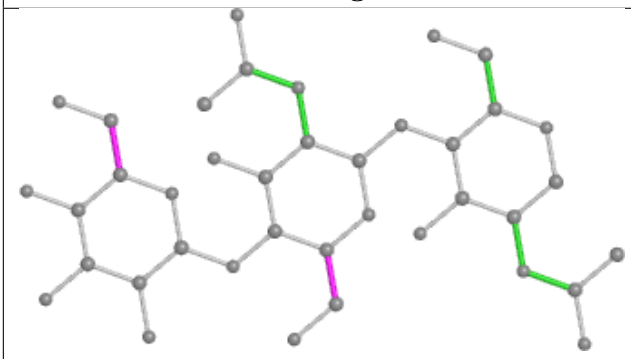
Oligosaccharide Chain K



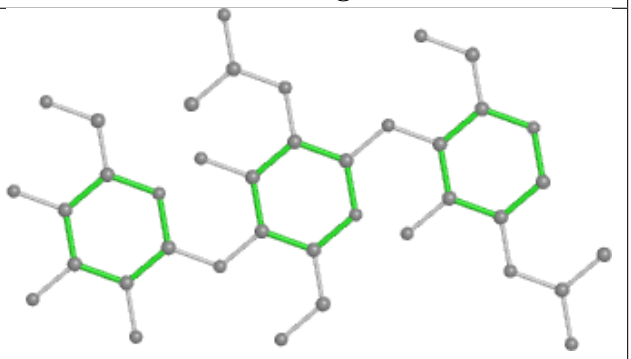
Bond lengths



Bond angles

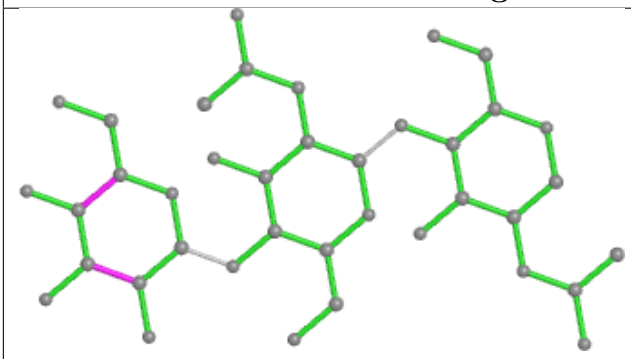


Torsions

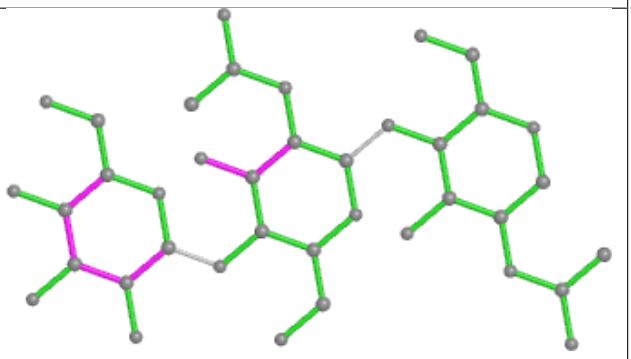


Rings

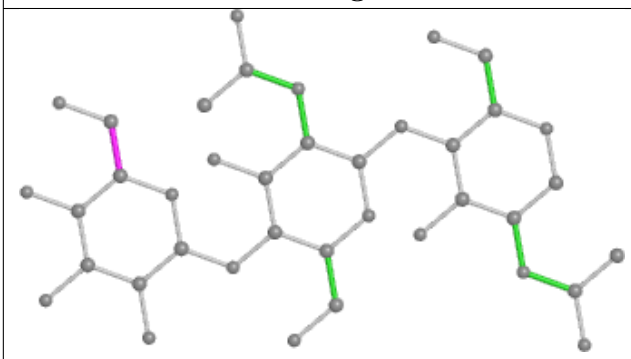
Oligosaccharide Chain M



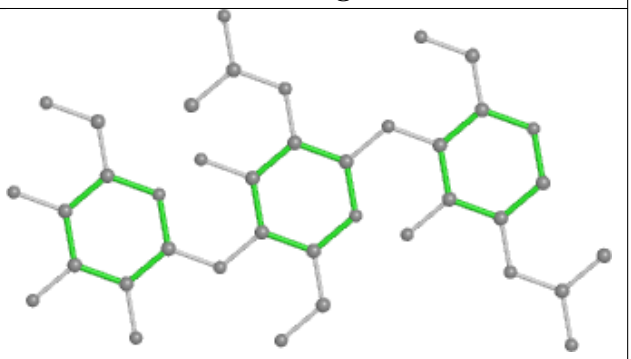
Bond lengths



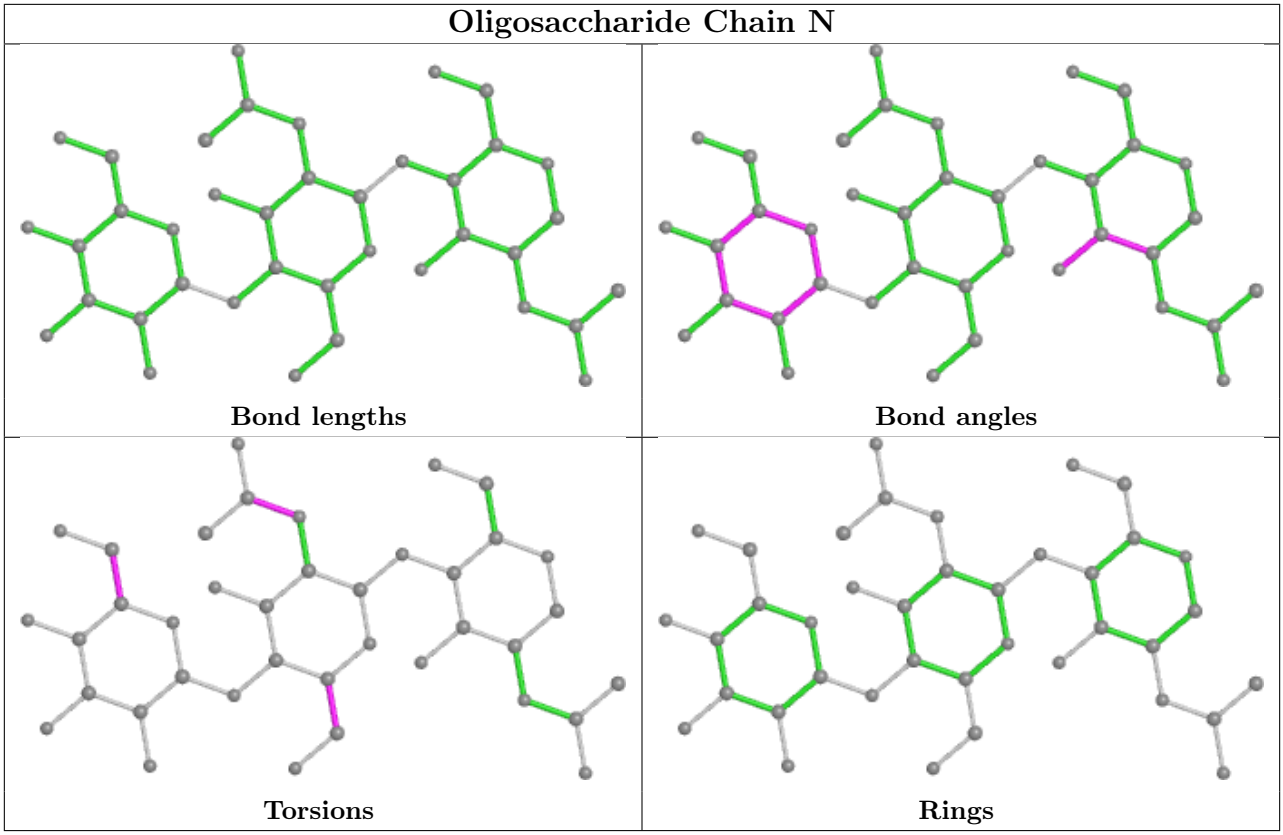
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
9	XLS	B	902	-	7,8,9	0.74	0	7,10,11	1.54	1 (14%)
11	NAG	B	909	1	14,14,15	0.43	0	17,19,21	1.01	0
11	NAG	C	901	-	14,14,15	0.42	0	17,19,21	1.05	0
9	XLS	A	912	-	7,8,9	0.74	0	7,10,11	1.53	1 (14%)
11	NAG	D	909	1	14,14,15	0.41	0	17,19,21	1.05	1 (5%)
10	MAN	B	907	-	11,11,12	0.76	1 (9%)	15,15,17	1.10	2 (13%)
11	NAG	D	907	1	14,14,15	0.39	0	17,19,21	1.60	2 (11%)
11	NAG	C	911	1	14,14,15	0.39	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	B	912	-	11,11,12	1.24	1 (9%)	15,15,17	1.70	2 (13%)
10	MAN	D	903	-	11,11,12	0.53	0	15,15,17	1.96	3 (20%)
8	BKR	C	912	-	65,65,65	0.53	0	101,101,101	0.84	3 (2%)
10	MAN	C	903	-	11,11,12	0.72	1 (9%)	15,15,17	1.46	2 (13%)
10	MAN	B	906	-	11,11,12	0.95	1 (9%)	15,15,17	1.66	4 (26%)
10	MAN	A	902	-	11,11,12	0.64	0	15,15,17	1.27	2 (13%)
10	MAN	A	904	-	11,11,12	0.70	0	15,15,17	1.07	1 (6%)
10	MAN	B	903	-	11,11,12	0.84	1 (9%)	15,15,17	1.01	1 (6%)
11	NAG	B	915	-	15,15,15	0.17	0	21,21,21	0.60	0
11	NAG	B	916	-	14,14,15	0.38	0	17,19,21	0.67	0
10	MAN	A	908	-	11,11,12	0.58	0	15,15,17	1.11	2 (13%)
10	MAN	D	905	-	11,11,12	0.85	1 (9%)	15,15,17	0.94	1 (6%)
8	BKR	A	911	-	65,65,65	0.68	0	101,101,101	0.92	7 (6%)
10	MAN	D	904	-	11,11,12	0.61	0	15,15,17	1.56	3 (20%)
11	NAG	B	913	1	14,14,15	0.42	0	17,19,21	1.18	1 (5%)
11	NAG	B	908	1	14,14,15	0.39	0	17,19,21	1.01	1 (5%)
11	NAG	A	905	1	14,14,15	0.40	0	17,19,21	1.31	3 (17%)
12	BMA	D	901	-	11,11,12	0.82	0	15,15,17	0.96	1 (6%)
10	MAN	C	907	-	11,11,12	0.59	0	15,15,17	1.18	2 (13%)
10	MAN	B	904	-	11,11,12	0.67	0	15,15,17	1.24	3 (20%)
10	MAN	C	905	-	11,11,12	0.43	0	15,15,17	1.25	1 (6%)
11	NAG	C	902	-	14,14,15	0.44	0	17,19,21	0.71	0
11	NAG	C	909	1	14,14,15	0.44	0	17,19,21	0.95	1 (5%)
10	MAN	C	904	-	11,11,12	0.92	0	15,15,17	2.07	4 (26%)
10	MAN	B	910	-	12,12,12	0.46	0	17,17,17	1.10	1 (5%)
11	NAG	B	911	-	15,15,15	0.21	0	21,21,21	0.41	0
11	NAG	C	910	1	14,14,15	0.47	0	17,19,21	0.79	0
8	BKR	B	901	-	65,65,65	0.68	0	101,101,101	0.92	7 (6%)
10	MAN	C	906	-	11,11,12	0.59	0	15,15,17	1.52	3 (20%)
10	MAN	B	905	-	11,11,12	0.83	0	15,15,17	1.21	2 (13%)
8	BKR	D	910	-	65,65,65	0.51	0	101,101,101	0.88	5 (4%)
11	NAG	A	910	1	14,14,15	0.42	0	17,19,21	1.42	2 (11%)
11	NAG	A	909	1	14,14,15	0.38	0	17,19,21	0.93	2 (11%)
11	NAG	D	906	1	14,14,15	0.47	0	17,19,21	1.08	2 (11%)
11	NAG	A	906	1	14,14,15	0.46	0	17,19,21	1.11	1 (5%)
11	NAG	C	908	1	14,14,15	0.47	0	17,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	A	903	-	11,11,12	0.77	0	15,15,17	1.21	1 (6%)
11	NAG	D	908	1	14,14,15	0.86	1 (7%)	17,19,21	2.01	2 (11%)
11	NAG	B	914	1	14,14,15	0.37	0	17,19,21	1.19	1 (5%)
10	MAN	A	901	-	11,11,12	0.46	0	15,15,17	1.55	3 (20%)
10	MAN	D	902	-	11,11,12	1.11	2 (18%)	15,15,17	2.28	2 (13%)
10	MAN	A	907	-	12,12,12	0.70	0	17,17,17	1.36	3 (17%)

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
9	XLS	B	902	-	-	7/10/10/12	-
11	NAG	B	909	1	-	2/6/23/26	0/1/1/1
11	NAG	C	901	-	-	3/6/23/26	0/1/1/1
9	XLS	A	912	-	-	7/10/10/12	-
11	NAG	D	909	1	-	2/6/23/26	0/1/1/1
10	MAN	B	907	-	-	2/2/19/22	0/1/1/1
11	NAG	D	907	1	-	4/6/23/26	0/1/1/1
11	NAG	C	911	1	-	4/6/23/26	0/1/1/1
10	MAN	B	912	-	-	0/2/19/22	1/1/1/1
10	MAN	D	903	-	-	2/2/19/22	0/1/1/1
8	BKR	C	912	-	-	7/37/123/123	0/7/7/7
10	MAN	C	903	-	-	0/2/19/22	1/1/1/1
10	MAN	B	906	-	-	2/2/19/22	0/1/1/1
10	MAN	A	902	-	-	0/2/19/22	0/1/1/1
10	MAN	A	904	-	-	2/2/19/22	0/1/1/1
10	MAN	B	903	-	-	2/2/19/22	0/1/1/1
11	NAG	B	915	-	-	0/6/26/26	0/1/1/1
11	NAG	B	916	-	-	0/6/23/26	0/1/1/1
10	MAN	A	908	-	-	0/2/19/22	0/1/1/1
10	MAN	D	905	-	-	2/2/19/22	0/1/1/1
8	BKR	A	911	-	-	4/37/123/123	0/7/7/7
10	MAN	D	904	-	-	2/2/19/22	0/1/1/1
11	NAG	B	913	1	-	0/6/23/26	0/1/1/1
11	NAG	B	908	1	-	2/6/23/26	0/1/1/1

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	912	MAN	O5-C5	3.17	1.49	1.43
11	D	908	NAG	O5-C1	-2.71	1.39	1.43
10	B	906	MAN	C2-C3	-2.51	1.48	1.52
10	D	902	MAN	O5-C5	2.43	1.48	1.43
10	B	903	MAN	O5-C5	2.33	1.48	1.43

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	902	MAN	C1-O5-C5	7.34	122.14	112.19
11	D	908	NAG	O5-C1-C2	-6.75	100.62	111.29
11	D	907	NAG	O5-C1-C2	-5.54	102.54	111.29
10	B	912	MAN	C1-O5-C5	5.24	119.28	112.19
10	D	903	MAN	C1-O5-C5	4.74	118.62	112.19

There are no chirality outliers.

5 of 99 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

34 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	902	XLS	1	0
11	C	901	NAG	8	0
9	A	912	XLS	1	0
10	B	907	MAN	4	0
11	D	907	NAG	1	0
10	B	912	MAN	4	0
8	C	912	BKR	2	0
10	C	903	MAN	11	0
10	B	906	MAN	6	0
10	A	902	MAN	4	0
10	A	904	MAN	5	0
10	B	903	MAN	2	0
11	B	916	NAG	3	0
10	A	908	MAN	1	0
10	D	905	MAN	1	0
8	A	911	BKR	1	0
10	D	904	MAN	5	0
12	D	901	BMA	9	0

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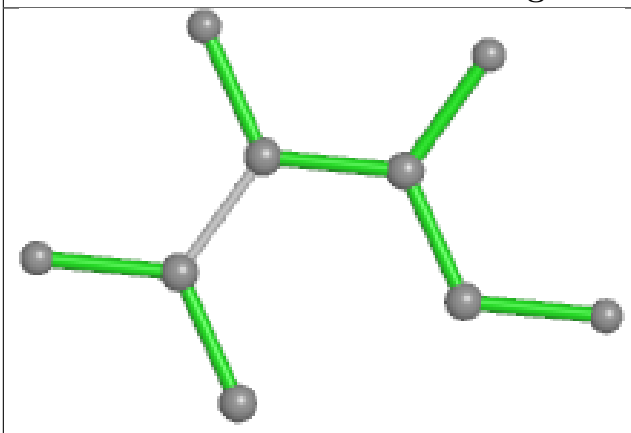
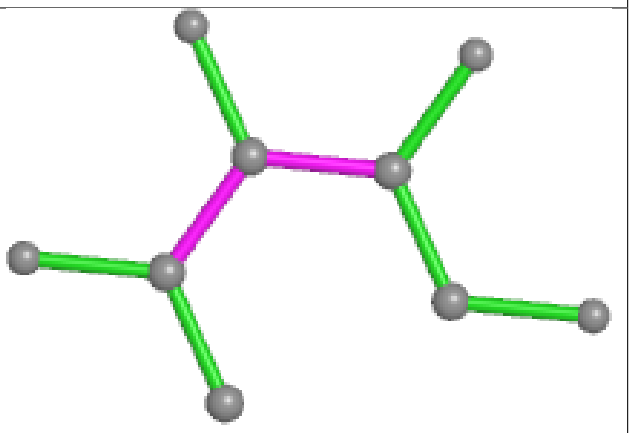
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	907	MAN	1	0
10	B	904	MAN	6	0
10	C	905	MAN	2	0
11	C	902	NAG	6	0
10	C	904	MAN	7	0
10	B	910	MAN	12	0
11	B	911	NAG	4	0
8	B	901	BKR	1	0
10	C	906	MAN	3	0
10	B	905	MAN	3	0
8	D	910	BKR	2	0
11	A	910	NAG	1	0
10	A	903	MAN	9	0
10	A	901	MAN	10	0
10	D	902	MAN	2	0
10	A	907	MAN	3	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.

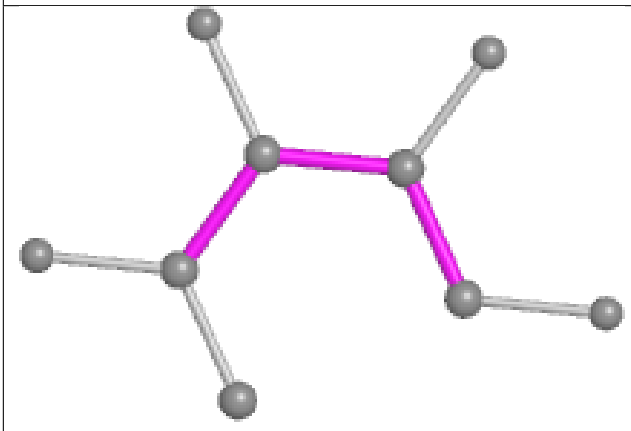
Ligand XLS B 902



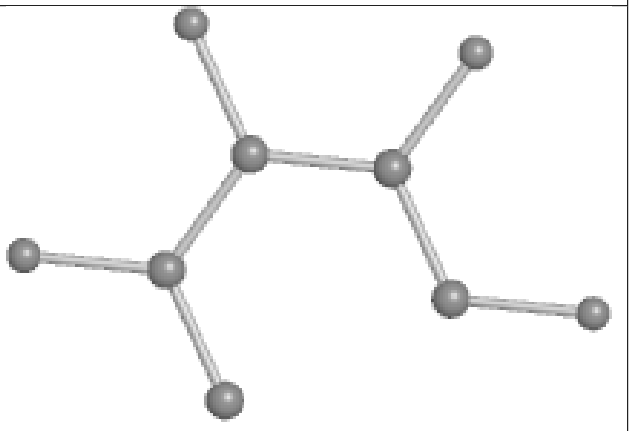
Bond lengths



Bond angles

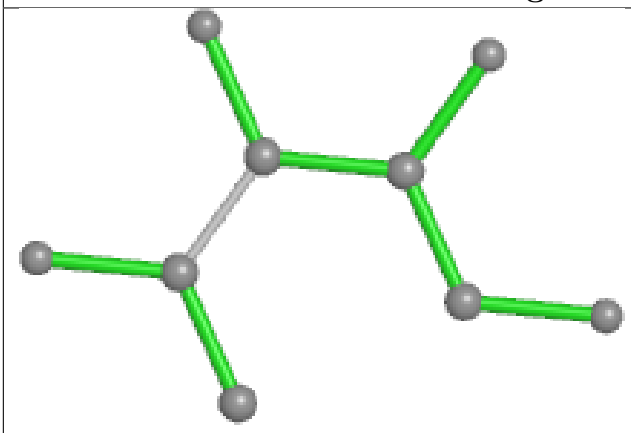


Torsions

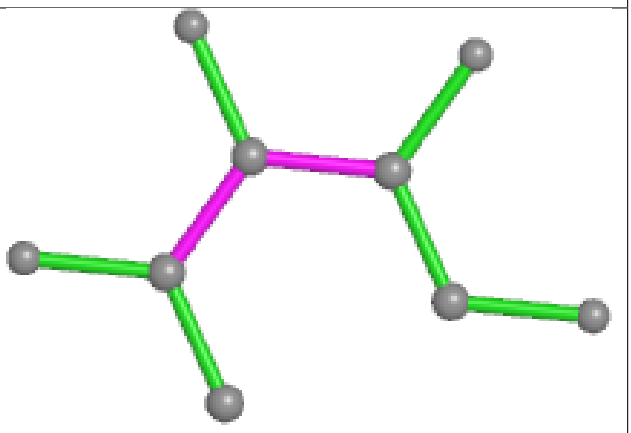


Rings

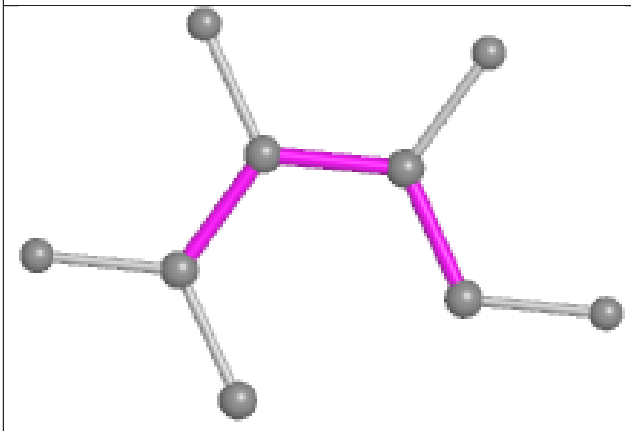
Ligand XLS A 912



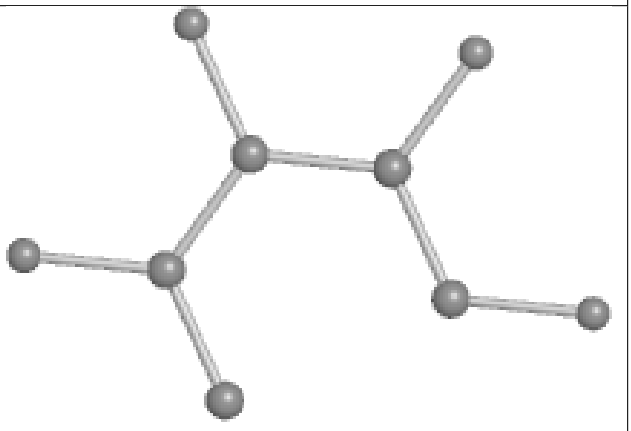
Bond lengths



Bond angles

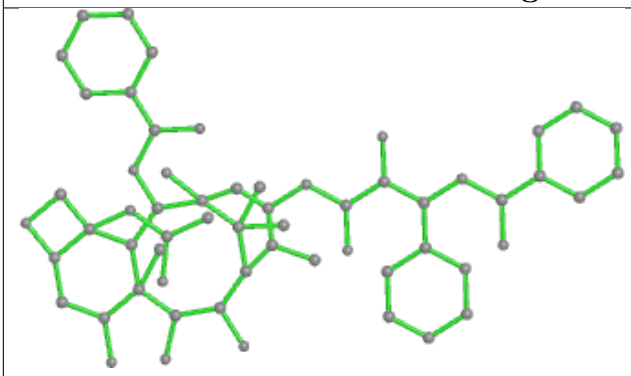


Torsions

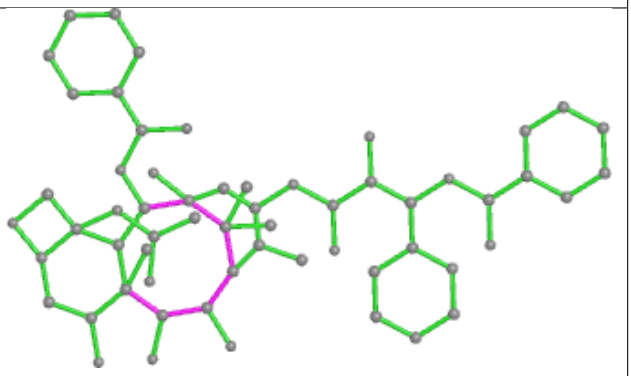


Rings

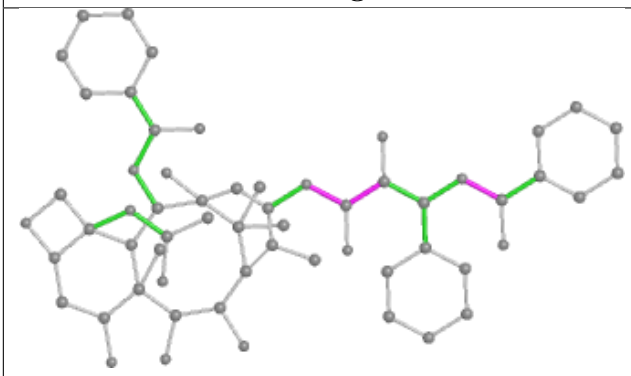
Ligand BKR C 912



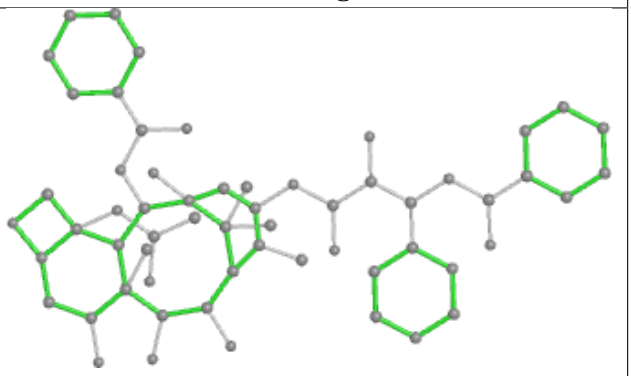
Bond lengths



Bond angles

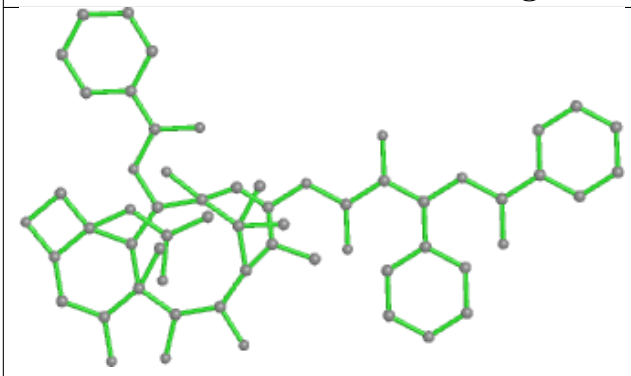


Torsions



Rings

Ligand BKR A 911



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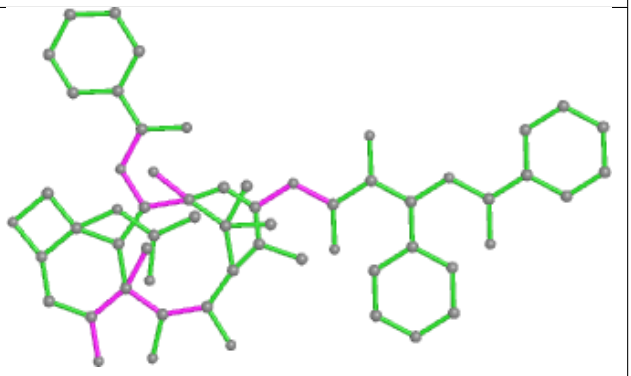
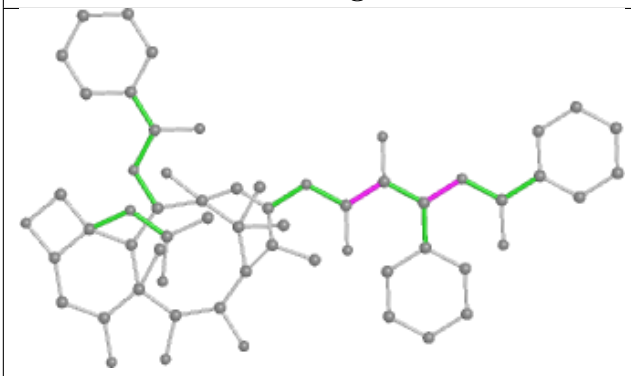
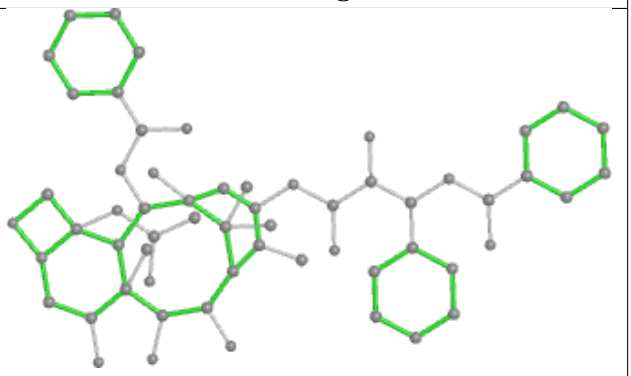


Bond angles

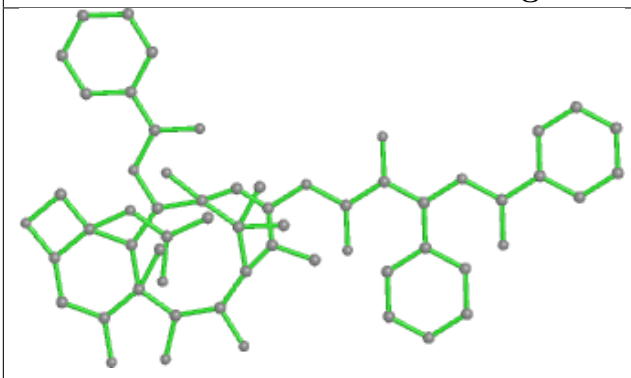


Torsions

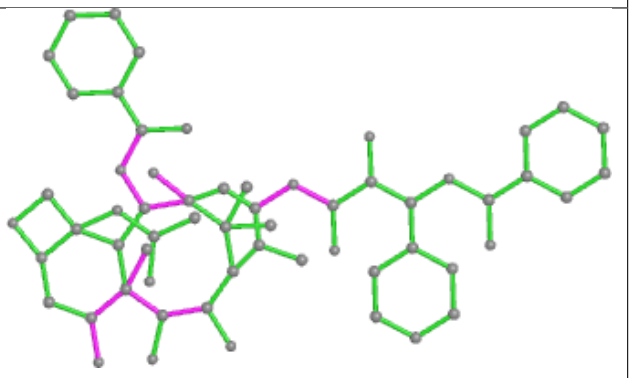


Rings

Ligand BKR B 901



Bond lengths



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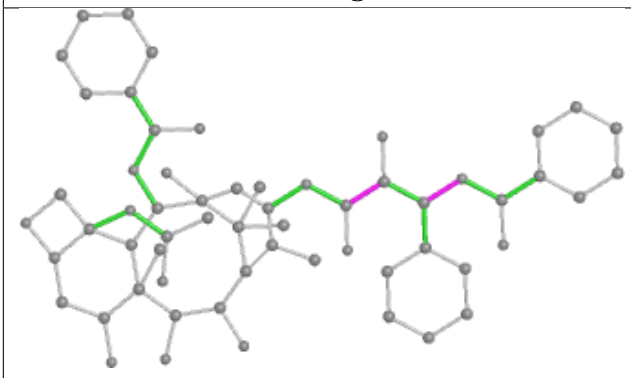
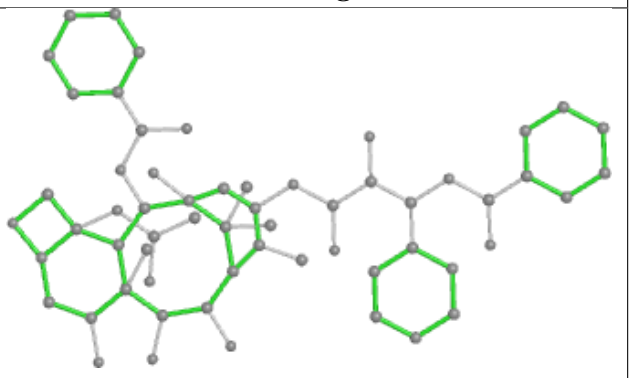
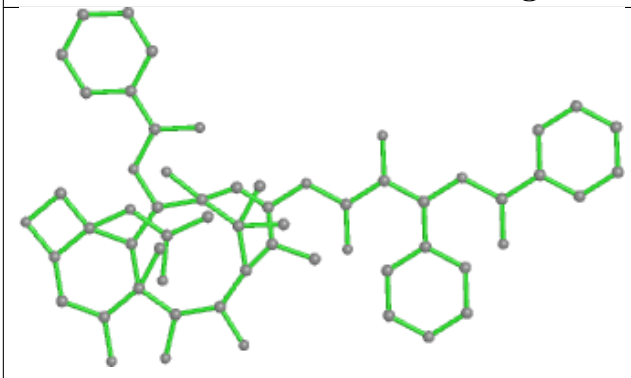


Torsions

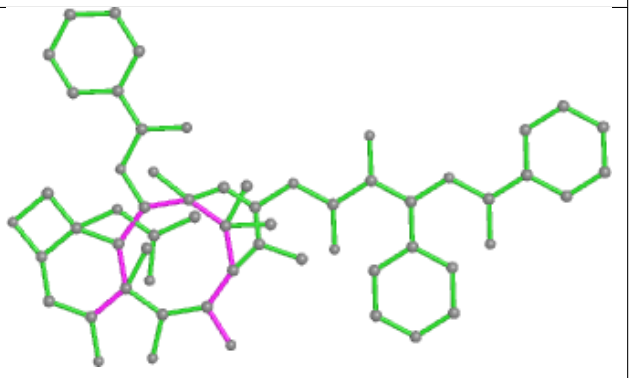


Rings

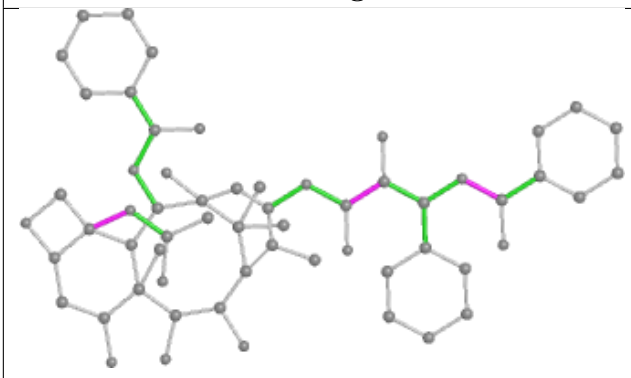
Ligand BKR D 910



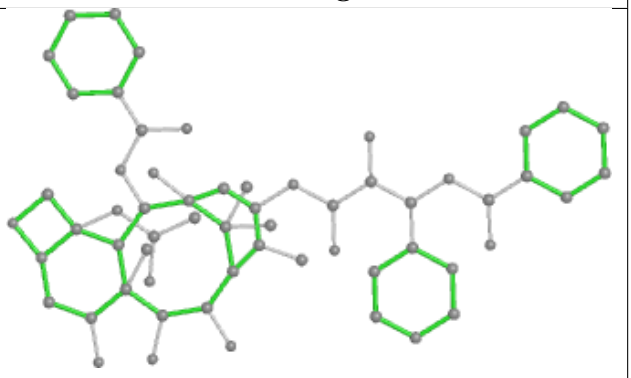
Bond lengths



Bond angles



Torsions



Rings

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	757/803 (94%)	-0.39	9 (1%)	79	80	20, 31, 50, 101	0
1	B	756/803 (94%)	-0.50	2 (0%)	94	94	20, 30, 42, 84	0
1	C	756/803 (94%)	0.07	26 (3%)	45	47	28, 50, 73, 121	0
1	D	756/803 (94%)	0.07	23 (3%)	50	53	28, 48, 69, 96	0
All	All	3025/3212 (94%)	-0.19	60 (1%)	65	67	20, 39, 67, 121	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	GLY	5.4
1	C	683	TYR	4.8
1	C	225	ASP	4.1
1	A	683	TYR	4.0
1	A	225	ASP	3.9

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	G	1	12/12	0.53	0.42	20,20,20,20	0
7	MAN	N	3	11/12	0.69	0.26	80,85,92,94	0

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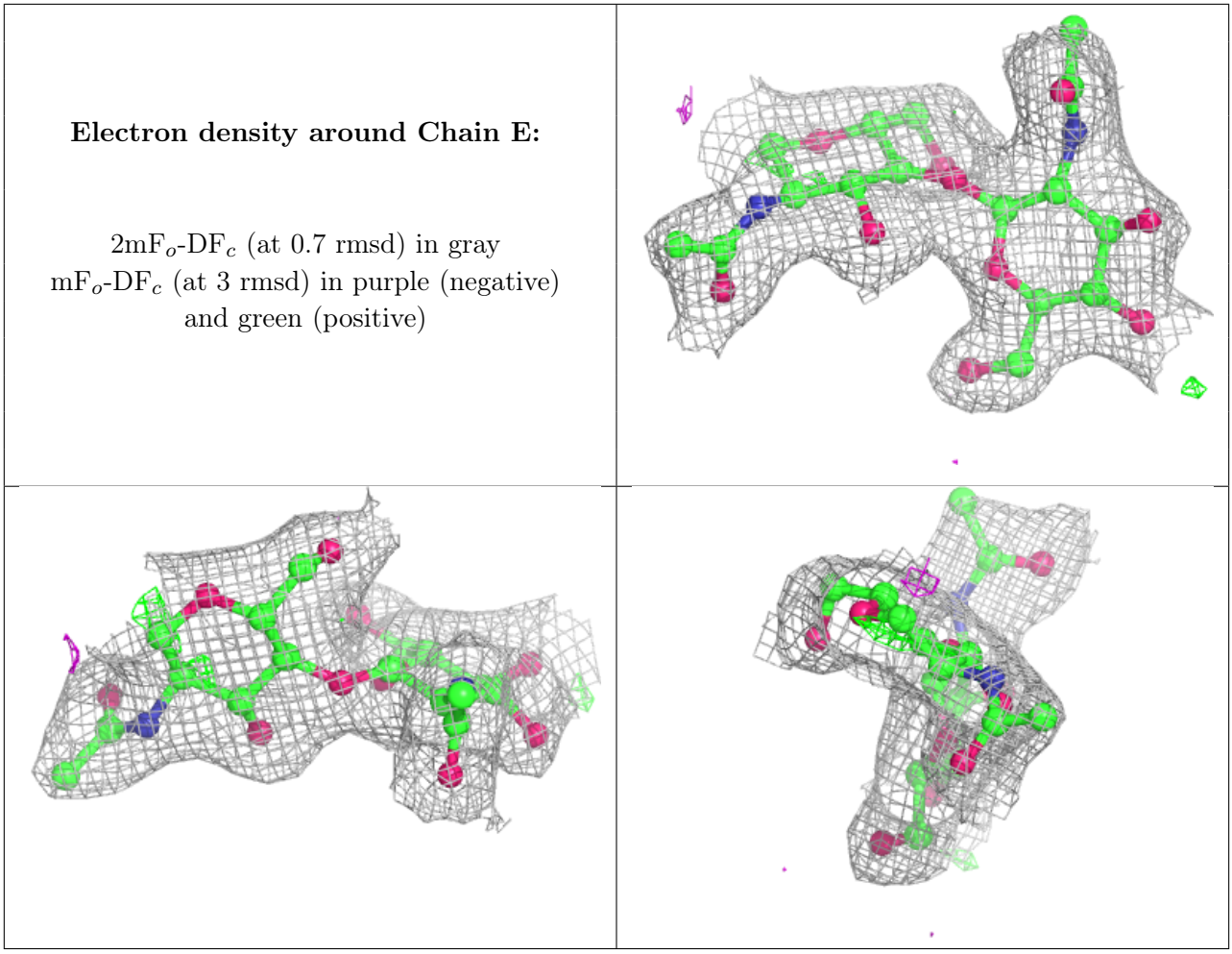
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	I	3	14/15	0.74	0.20	60,73,81,86	0
2	NAG	L	2	14/15	0.74	0.24	70,80,85,91	0
4	BMA	G	2	11/12	0.76	0.14	37,49,56,57	0
7	MAN	M	3	11/12	0.78	0.17	50,63,69,78	0
2	NAG	O	1	14/15	0.79	0.29	20,20,20,20	0
2	NAG	O	2	14/15	0.86	0.23	69,91,100,108	0
7	NAG	N	2	14/15	0.88	0.14	41,65,82,83	0
2	NAG	P	1	14/15	0.88	0.14	55,70,80,82	0
6	BMA	J	4	11/12	0.89	0.12	50,60,64,65	0
2	NAG	L	1	14/15	0.90	0.14	51,68,73,76	0
7	MAN	K	3	11/12	0.91	0.14	37,43,48,55	0
3	MAN	F	4	11/12	0.92	0.11	44,45,54,55	0
3	MAN	F	5	11/12	0.92	0.12	43,50,53,54	0
2	NAG	P	2	14/15	0.93	0.11	42,46,50,50	0
6	MAN	J	5	11/12	0.94	0.12	45,53,63,64	0
6	AH2	J	3	11/11	0.94	0.10	35,45,48,50	0
7	NAG	M	2	14/15	0.94	0.09	33,37,45,56	0
2	NAG	H	2	14/15	0.95	0.08	27,31,38,39	0
2	NAG	E	2	14/15	0.95	0.14	42,52,55,60	0
7	NAG	N	1	14/15	0.95	0.09	34,39,47,58	0
2	NAG	H	1	14/15	0.95	0.07	25,28,33,34	0
6	NAG	J	1	14/15	0.95	0.09	27,30,36,42	0
7	NAG	K	2	14/15	0.96	0.07	23,29,32,35	0
3	BMA	F	3	11/12	0.96	0.08	24,27,30,31	0
7	NAG	M	1	14/15	0.96	0.06	33,37,38,39	0
6	NAG	J	2	14/15	0.96	0.08	37,40,48,49	0
5	NAG	I	1	14/15	0.96	0.07	24,28,30,38	0
5	NAG	I	2	14/15	0.96	0.07	38,44,48,49	0
2	NAG	E	1	14/15	0.96	0.09	30,35,39,46	0
7	NAG	K	1	14/15	0.96	0.06	25,29,32,32	0
3	NAG	F	1	14/15	0.97	0.08	24,28,31,34	0
3	NAG	F	2	14/15	0.97	0.07	25,29,34,38	0

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

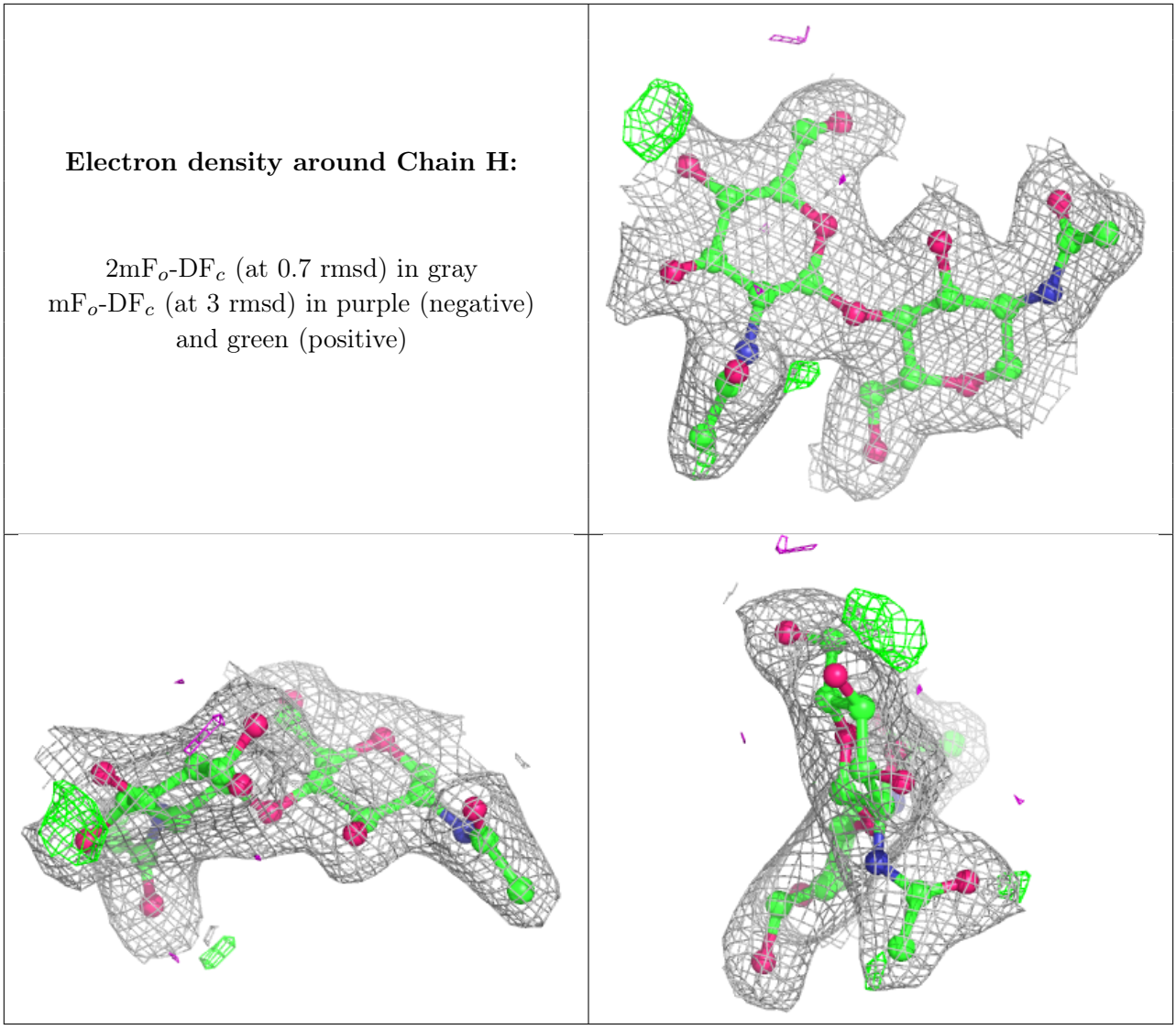
Electron density around Chain E:

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



Electron density around Chain H:

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



Electron density around Chain L:

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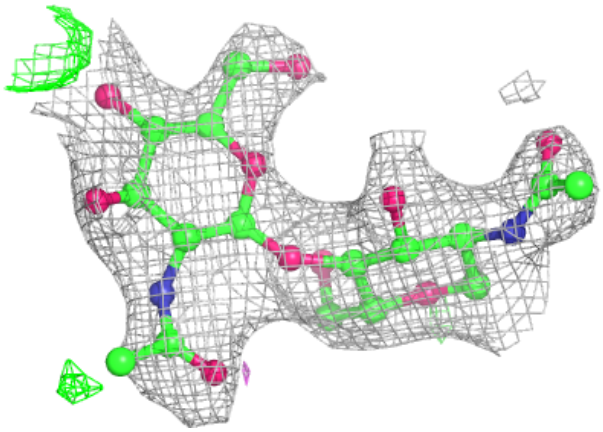
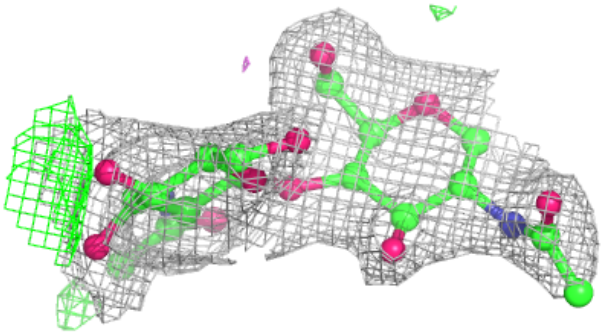
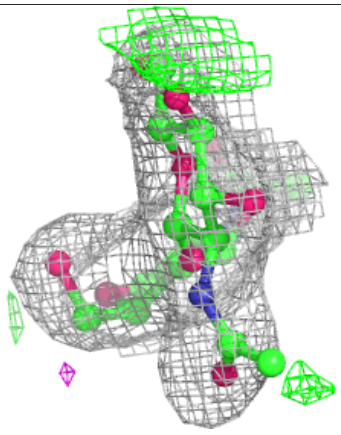
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around Chain O:

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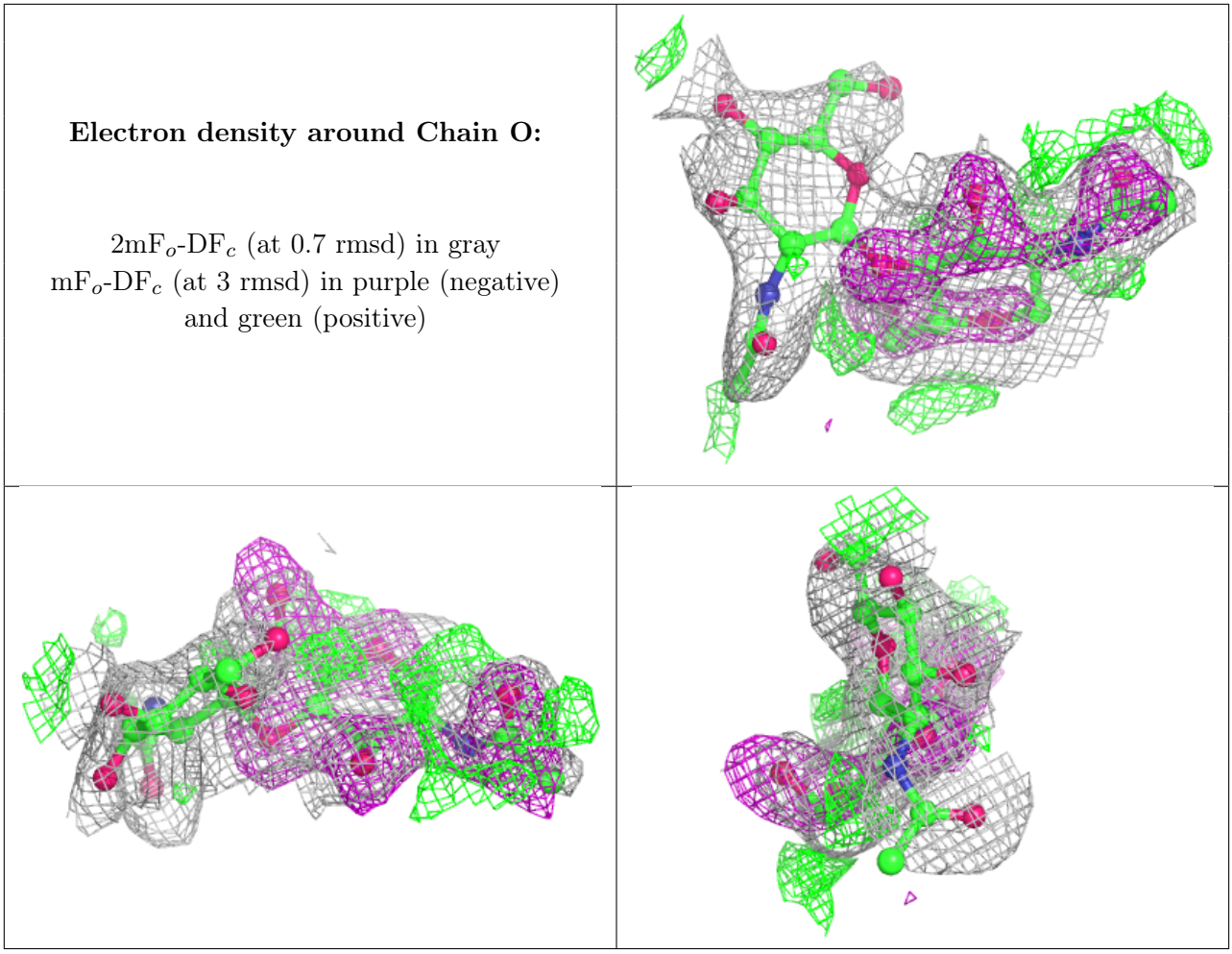
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain P:

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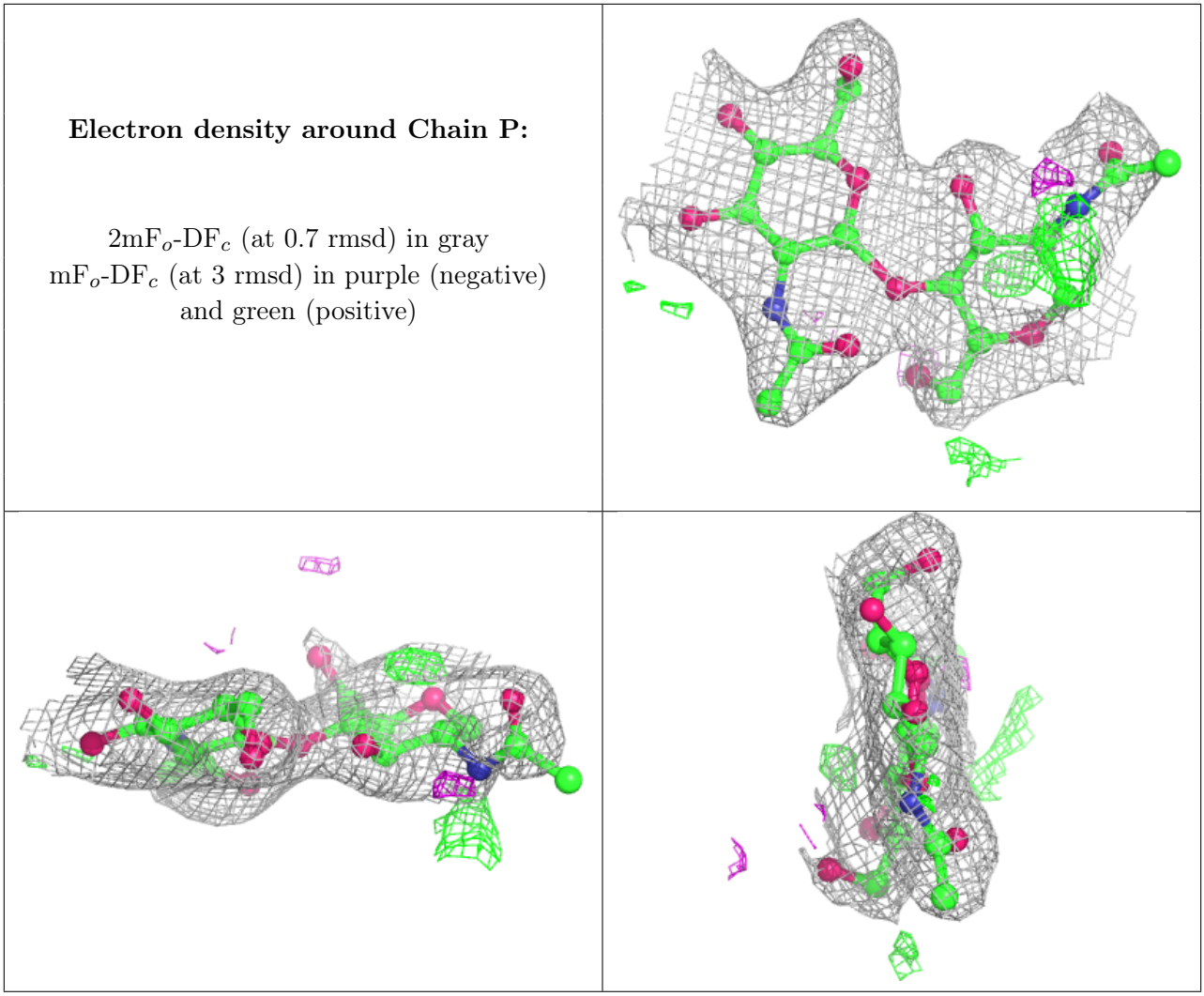
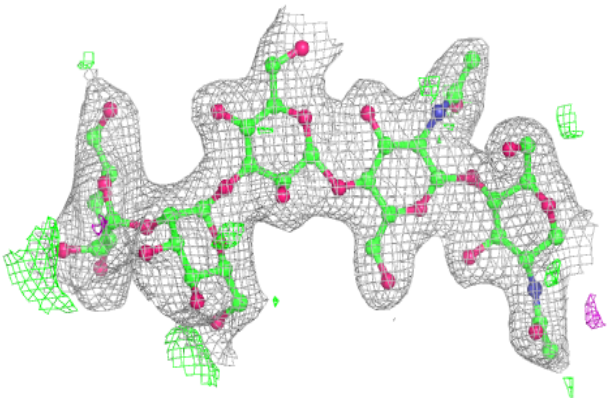
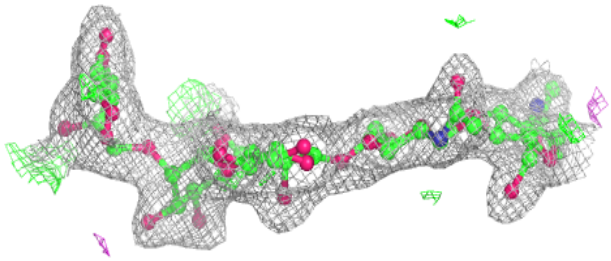
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

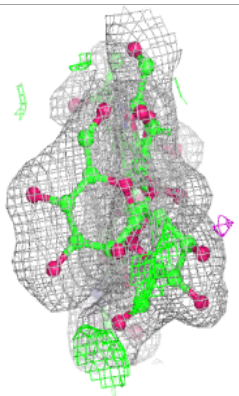


Electron density around Chain F:

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

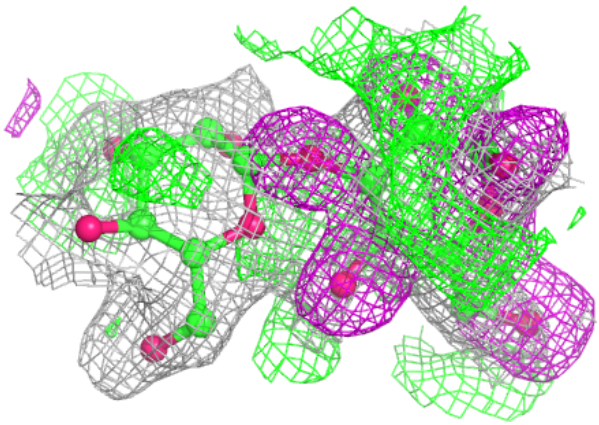


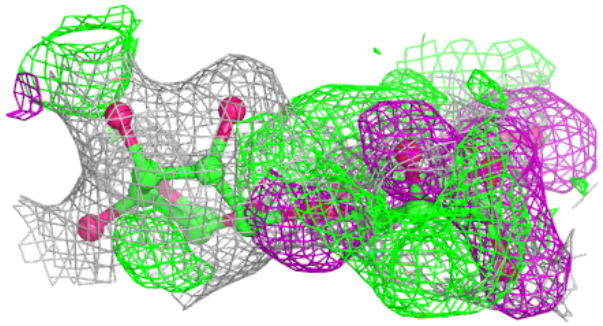


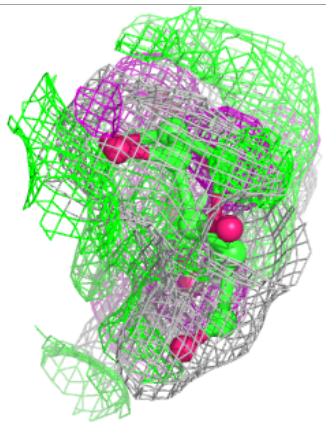


Electron density around Chain G:

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

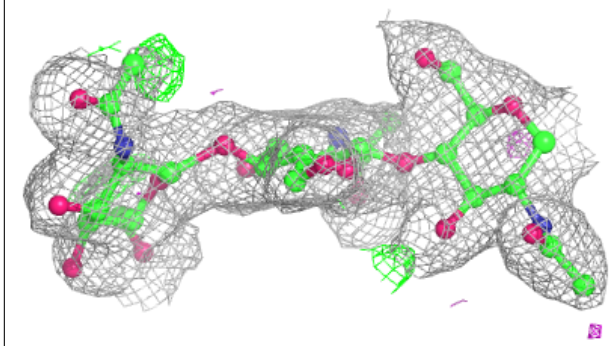


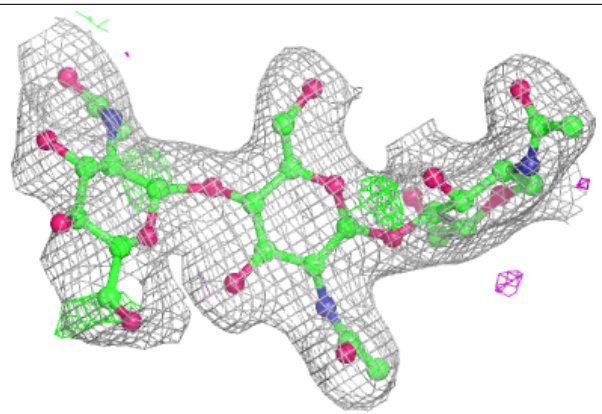




Electron density around Chain I:

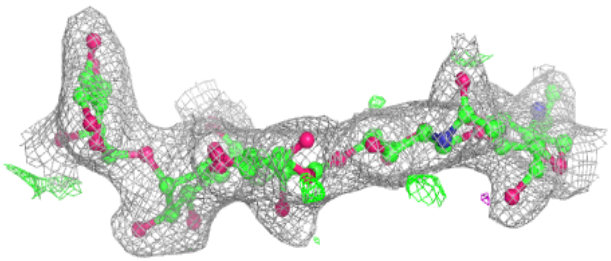
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

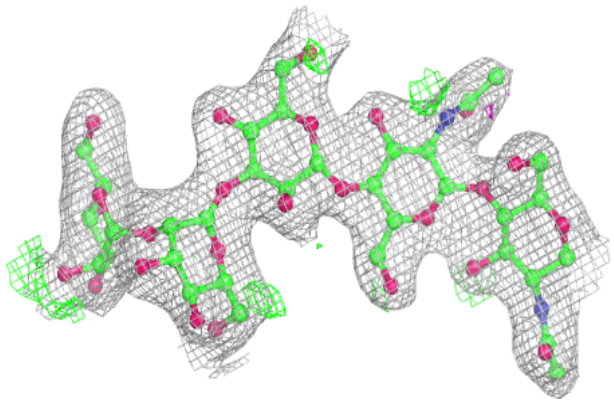


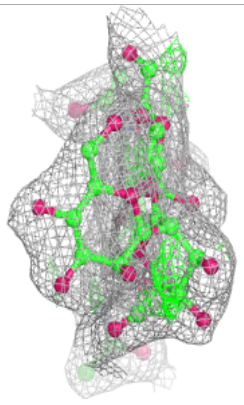


Electron density around Chain J:

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

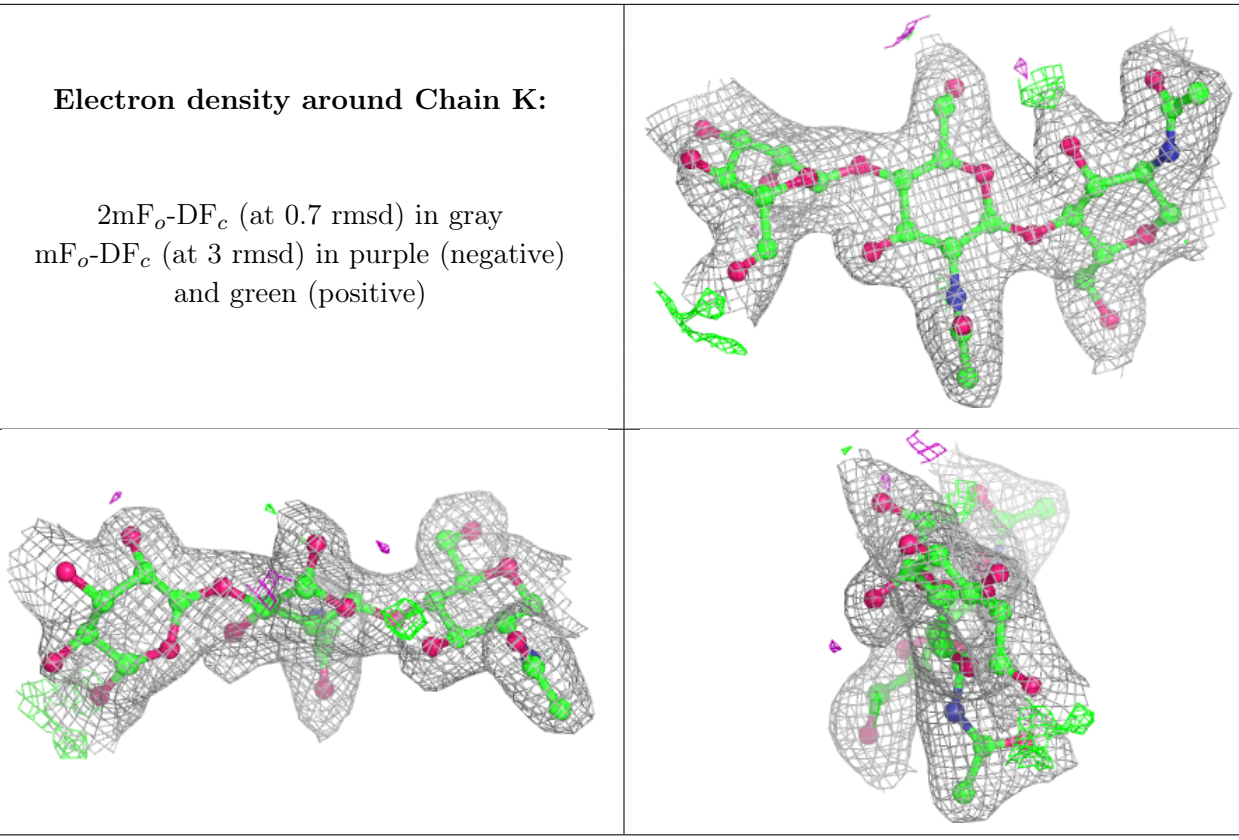






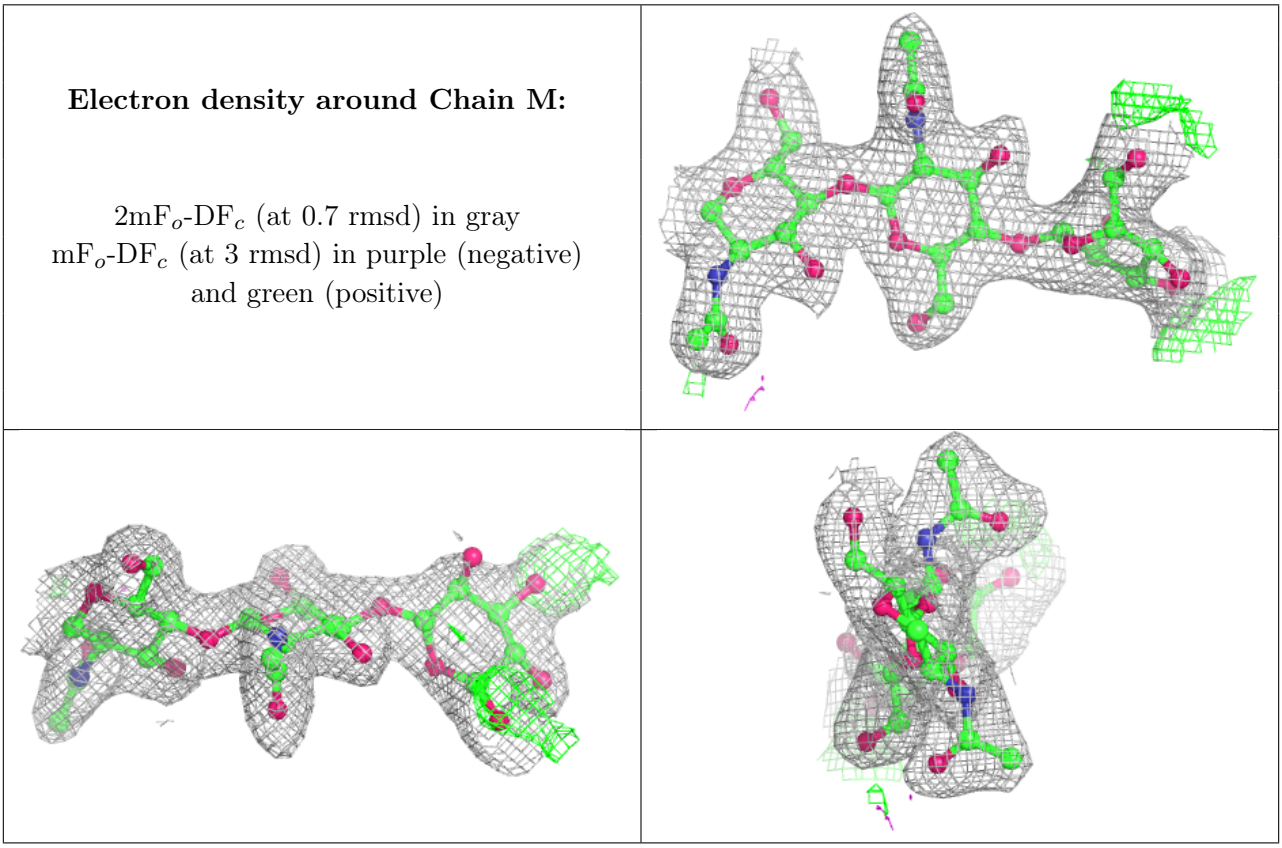
Electron density around Chain K:

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



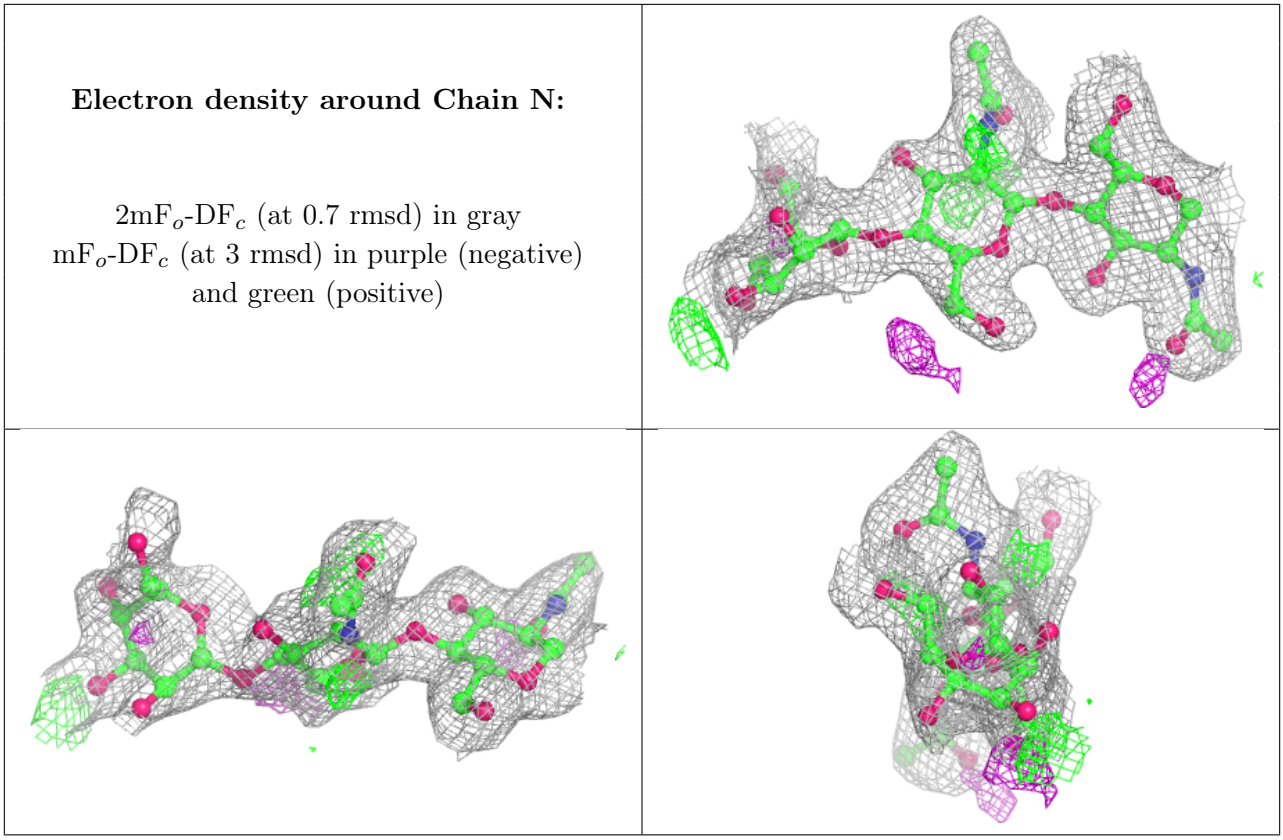
Electron density around Chain M:

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



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	MAN	B	912	11/12	0.56	0.18	52,57,65,66	0
11	NAG	B	915	15/15	0.66	0.38	20,20,20,20	0
10	MAN	D	905	11/12	0.72	0.20	65,79,89,98	0
10	MAN	C	904	11/12	0.72	0.22	70,80,85,90	0
11	NAG	B	911	15/15	0.73	0.34	20,20,20,20	0
9	XLS	A	912	9/10	0.74	0.27	32,44,63,67	0
8	BKR	D	910	59/59	0.74	0.31	82,112,136,139	0
10	MAN	B	903	11/12	0.75	0.16	56,72,79,82	0
10	MAN	D	904	11/12	0.76	0.20	65,73,84,90	0
10	MAN	A	904	11/12	0.76	0.42	83,97,107,110	0
11	NAG	C	911	14/15	0.76	0.46	92,113,120,134	0
8	BKR	C	912	59/59	0.77	0.29	72,104,123,126	0
11	NAG	C	908	14/15	0.78	0.31	88,94,99,100	0
10	MAN	C	906	11/12	0.79	0.17	68,84,94,102	0

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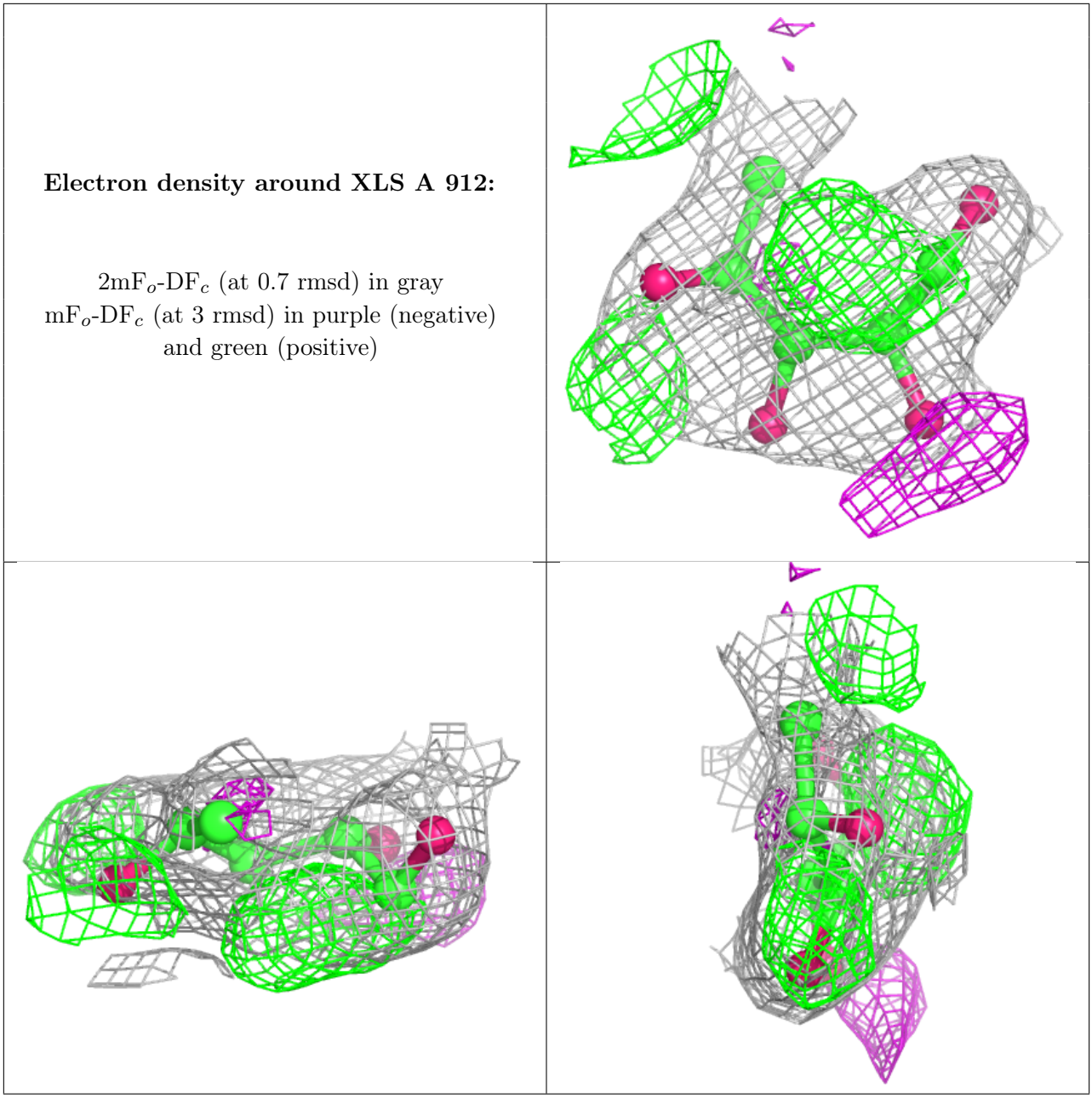
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	B	916	14/15	0.79	0.41	20,20,20,20	0
8	BKR	A	911	59/59	0.82	0.24	36,47,54,56	0
11	NAG	D	909	14/15	0.82	0.34	68,90,97,104	0
9	XLS	B	902	9/10	0.83	0.19	32,44,63,67	0
10	MAN	B	907	11/12	0.83	0.33	79,88,93,95	0
10	MAN	B	910	12/12	0.83	0.12	33,43,54,57	0
11	NAG	D	907	14/15	0.84	0.28	65,74,85,89	0
11	NAG	D	906	14/15	0.84	0.28	65,73,85,90	0
11	NAG	A	910	14/15	0.85	0.26	74,85,97,103	0
11	NAG	B	914	14/15	0.85	0.28	67,74,84,94	0
10	MAN	D	902	11/12	0.87	0.15	55,60,71,74	0
11	NAG	C	909	14/15	0.88	0.31	61,80,89,91	0
10	MAN	D	903	11/12	0.88	0.12	55,56,59,67	0
10	MAN	C	907	11/12	0.88	0.11	55,61,72,83	0
11	NAG	C	902	14/15	0.88	0.15	52,67,74,82	0
11	NAG	D	908	14/15	0.88	0.19	54,62,67,71	0
10	MAN	A	908	11/12	0.88	0.18	47,61,65,69	0
10	MAN	A	903	11/12	0.89	0.27	62,70,85,91	0
10	MAN	C	905	11/12	0.91	0.12	56,60,74,80	0
8	BKR	B	901	59/59	0.91	0.14	36,47,54,56	0
10	MAN	A	907	12/12	0.91	0.15	51,58,67,79	0
11	NAG	C	901	14/15	0.91	0.14	54,58,65,73	0
11	NAG	B	913	14/15	0.92	0.11	37,44,47,47	0
10	MAN	C	903	11/12	0.92	0.09	52,54,58,59	0
11	NAG	B	909	14/15	0.93	0.19	39,44,53,55	0
10	MAN	B	906	11/12	0.93	0.21	53,59,65,68	0
11	NAG	B	908	14/15	0.94	0.13	39,45,52,60	0
11	NAG	A	906	14/15	0.94	0.19	39,44,46,48	0
10	MAN	A	901	11/12	0.94	0.12	44,47,50,56	0
10	MAN	B	904	11/12	0.94	0.11	37,43,48,52	0
10	MAN	B	905	11/12	0.95	0.09	30,35,42,45	0
11	NAG	A	909	14/15	0.95	0.14	35,39,44,47	0
10	MAN	A	902	11/12	0.95	0.10	45,47,52,53	0
12	BMA	D	901	11/12	0.95	0.08	36,40,45,46	0
11	NAG	A	905	14/15	0.96	0.15	46,50,55,61	0
11	NAG	C	910	14/15	0.96	0.13	41,44,47,48	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.

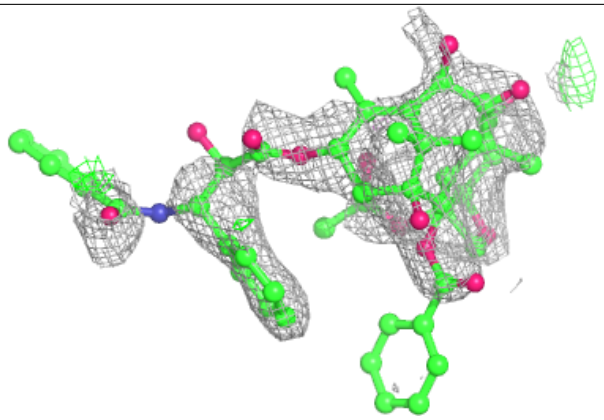
Electron density around XLS A 912:

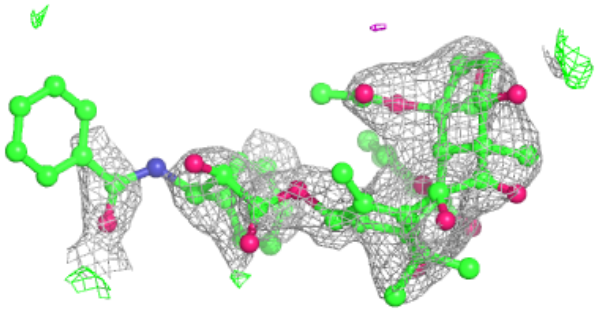
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

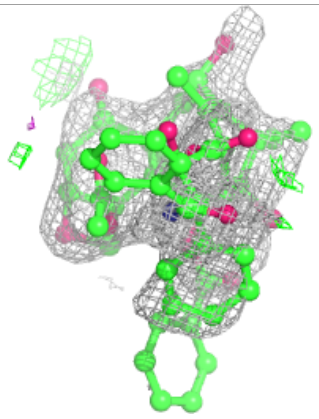


Electron density around BKR D 910:

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

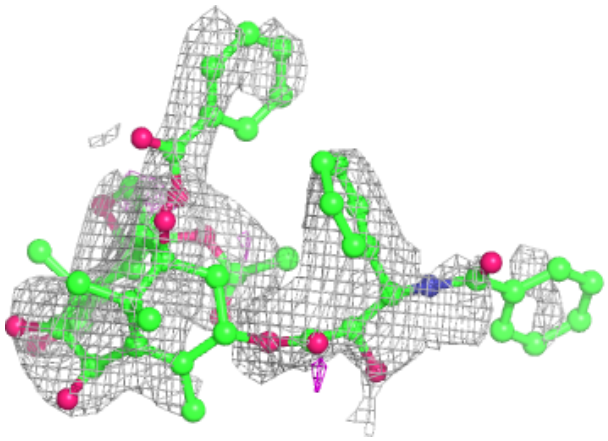


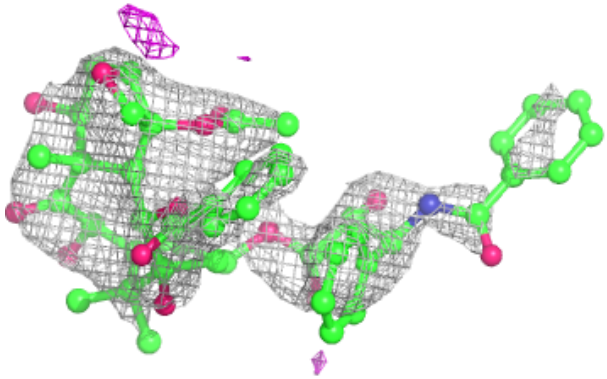


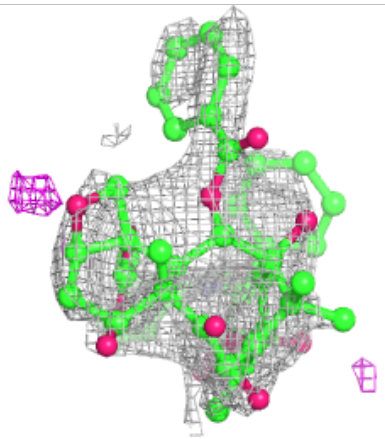


Electron density around BKR C 912:

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

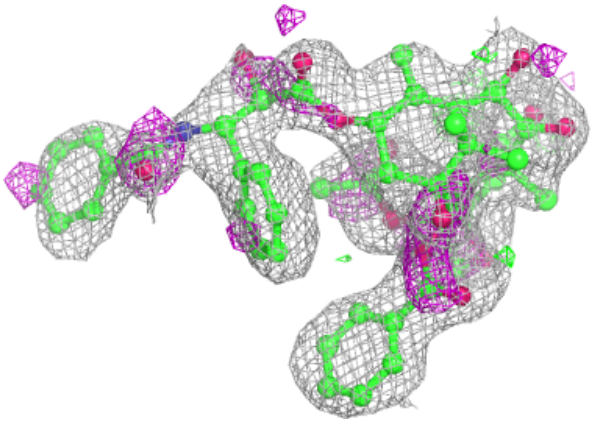


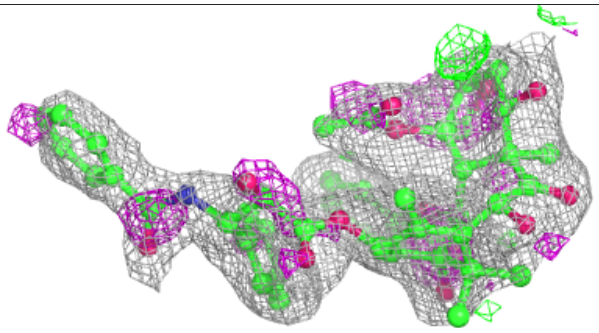


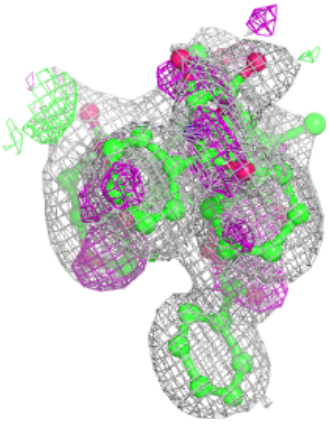


Electron density around BKR A 911:

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

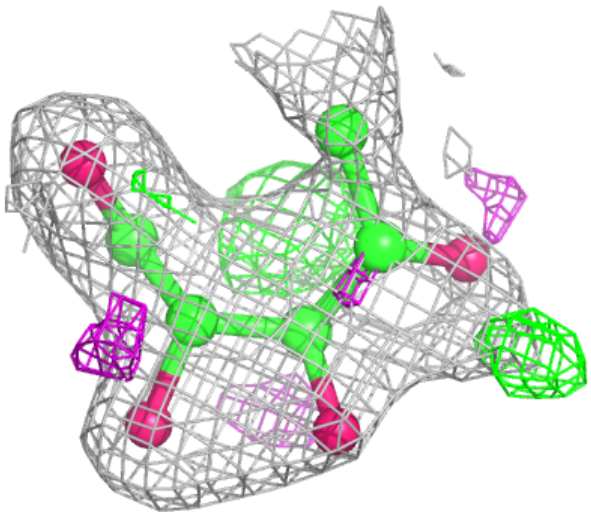


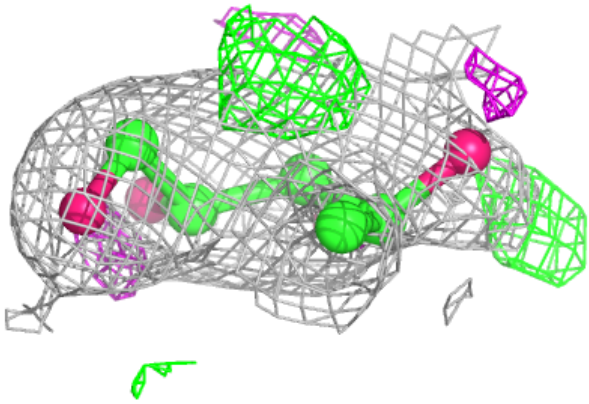


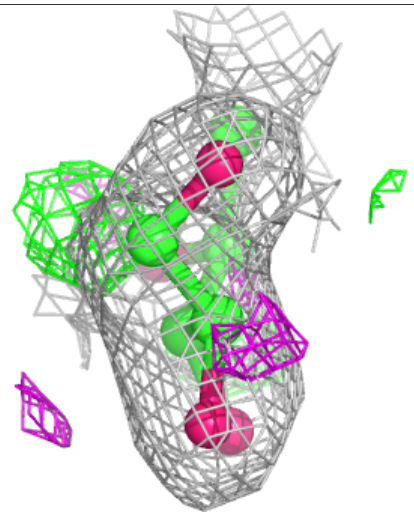


Electron density around XLS B 902:

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

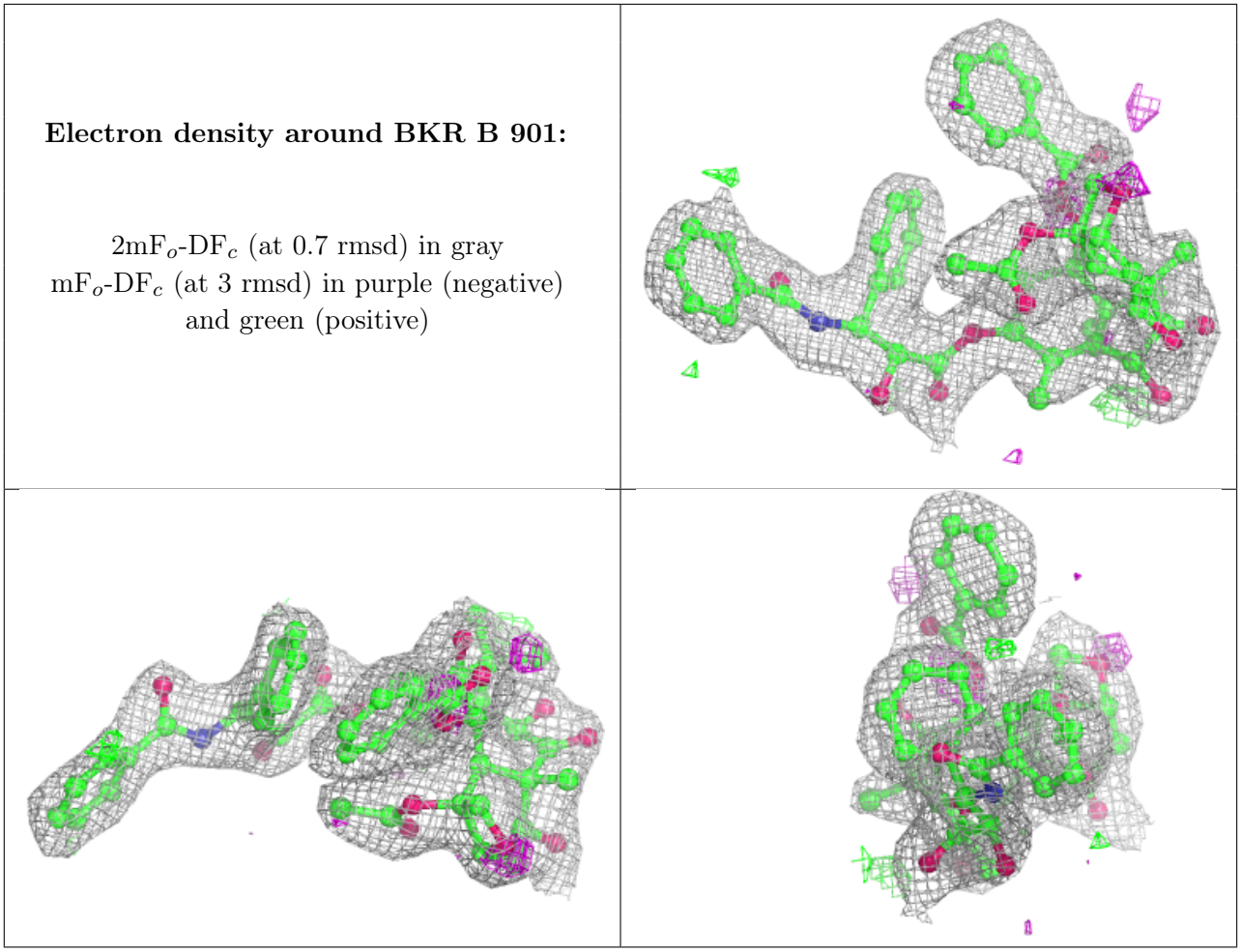






Electron density around BKR B 901:

$2mF_o$-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 (i)

There are no such residues in this entry.