Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 11:35 am BST

PDB ID	:	8ONH
Title	:	Variant Surface Glycoprotein VSG11wt-Oil
Authors	:	Zeelen, J.P.; Stebbins, C.E.; Foti, K.; Gkeka, A.; Vlachou, E.P.
Deposited on	:	2023-04-03
Resolution	:	2.59 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

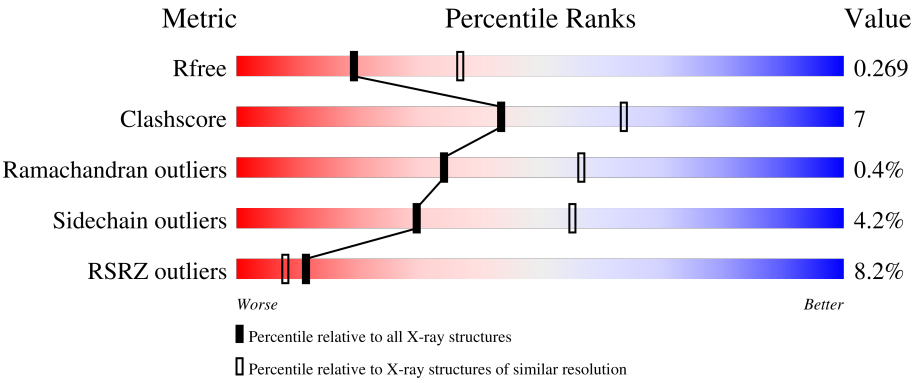
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	410	77% 12% • 11%
1	B	410	2% 78% 10% • 11%
1	C	410	3% 74% 14% • 11%
1	D	410	8% 64% 13% • 22%
1	E	410	4% 54% 15% 30%

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Mol	Chain	Length	Quality of chain
1	F	410	7% 55% 13% 31%
1	G	410	6% 68% 19% 11%
1	H	410	9% 49% 20% 30%
1	I	410	21% 59% 21% 16%
1	J	410	2% 73% 16% 11%
1	K	410	4% 77% 11% 11%
1	L	410	3% 78% 9% 13%
1	M	410	5% 61% 9% 30%
1	N	410	12% 71% 13% 14%
1	O	410	10% 57% 15% 27%
1	P	410	4% 56% 8% 36%
1	Q	410	8% 54% 12% 34%
1	R	410	7% 66% 9% 24%
2	S	6	67% 17% 17%
2	Z	6	100%
3	T	5	20% 20% 60%
4	U	3	33% 67%
5	V	3	100%
5	X	3	33% 67%
5	Y	3	33% 67%
6	W	5	60% 20% 20%
6	c	5	100%
7	a	5	80% 20%
7	b	5	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	V	1	-	-	-	X
5	NAG	V	2	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 43982 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 Variant surface glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2749	1699	490	547	13			
1	B	366	Total	C	N	O	S	0	0	0
			2704	1665	480	546	13			
1	C	366	Total	C	N	O	S	0	0	0
			2721	1679	485	544	13			
1	D	321	Total	C	N	O	S	0	0	0
			2332	1436	417	466	13			
1	E	285	Total	C	N	O	S	0	0	0
			2046	1250	363	421	12			
1	F	282	Total	C	N	O	S	0	0	0
			2044	1246	363	422	13			
1	G	365	Total	C	N	O	S	0	0	0
			2704	1672	475	544	13			
1	H	287	Total	C	N	O	S	0	0	0
			2057	1260	363	422	12			
1	I	343	Total	C	N	O	S	0	0	0
			2461	1517	433	500	11			
1	J	366	Total	C	N	O	S	0	0	0
			2741	1692	489	547	13			
1	K	365	Total	C	N	O	S	0	0	0
			2698	1668	478	539	13			
1	L	358	Total	C	N	O	S	0	0	0
			2660	1644	470	533	13			
1	M	287	Total	C	N	O	S	0	0	0
			2079	1270	372	425	12			
1	N	353	Total	C	N	O	S	0	0	0
			2618	1608	471	526	13			
1	O	301	Total	C	N	O	S	0	0	0
			2172	1332	382	445	13			
1	P	261	Total	C	N	O	S	0	0	0
			1882	1147	335	387	13			

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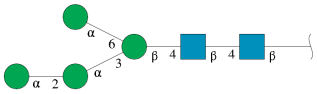
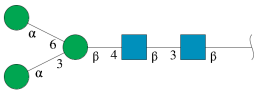
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	272	Total	C	N	O	S	0	0	0
			1967	1200	350	405	12			
1	R	310	Total	C	N	O	S	0	0	0
			2215	1363	390	449	13			

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



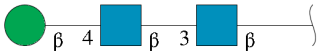
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	S	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	Z	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



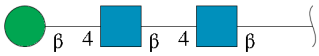
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	T	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



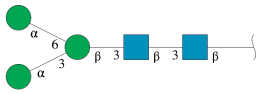
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	U	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



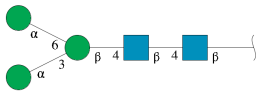
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	V	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

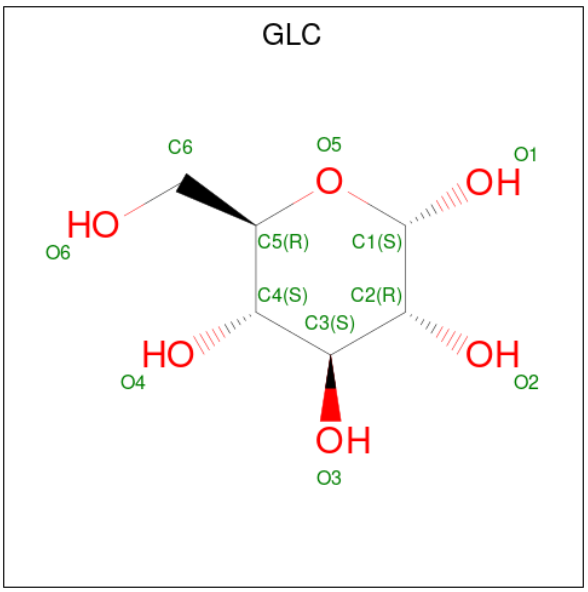
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	a	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	b	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 11 6 5	0	0
8	B	1	Total C O 11 6 5	0	0
8	C	1	Total C O 11 6 5	0	0
8	D	1	Total C O 11 6 5	0	0
8	E	1	Total C O 11 6 5	0	0
8	F	1	Total C O 11 6 5	0	0
8	H	1	Total C O 11 6 5	0	0
8	I	1	Total C O 11 6 5	0	0
8	J	1	Total C O 11 6 5	0	0
8	K	1	Total C O 11 6 5	0	0
8	L	1	Total C O 11 6 5	0	0
8	M	1	Total C O 11 6 5	0	0
8	N	1	Total C O 11 6 5	0	0

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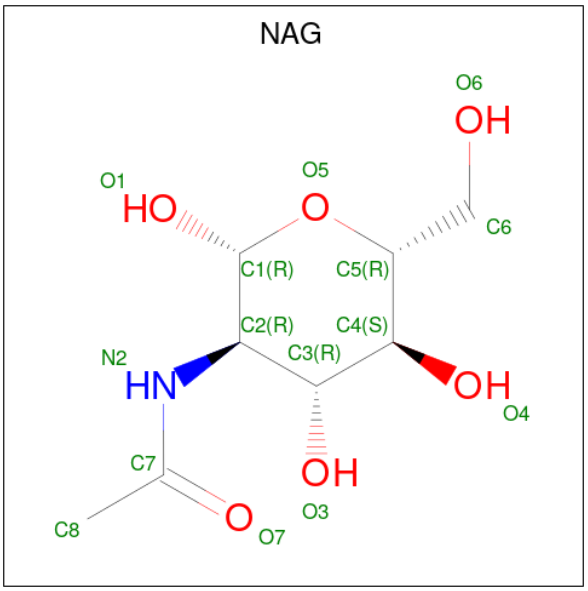
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	O	1	Total C O 11 6 5	0	0
8	P	1	Total C O 11 6 5	0	0
8	Q	1	Total C O 11 6 5	0	0
8	R	1	Total C O 11 6 5	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total C N O 14 8 1 5	0	0
9	O	1	Total C N O 14 8 1 5	0	0
9	Q	1	Total C N O 14 8 1 5	0	0
9	R	1	Total C N O 14 8 1 5	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	53	Total O 53 53	0	0

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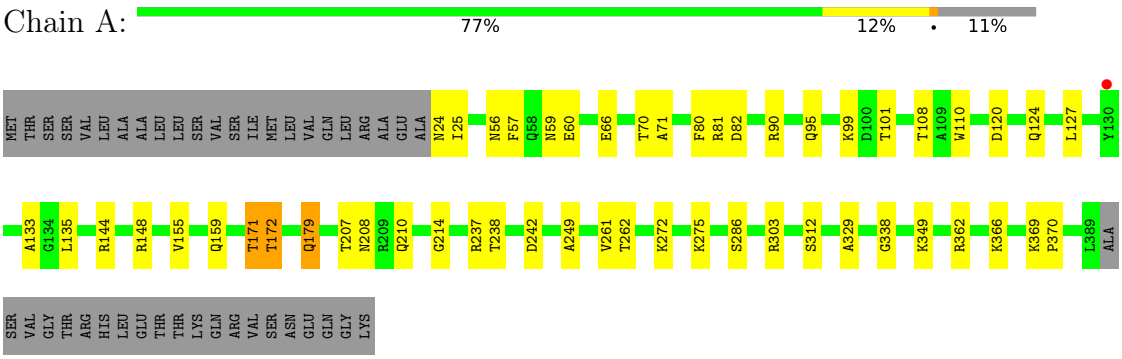
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	43	Total O 43 43	0	0
10	C	28	Total O 28 28	0	0
10	D	19	Total O 19 19	0	0
10	E	4	Total O 4 4	0	0
10	F	12	Total O 12 12	0	0
10	J	51	Total O 51 51	0	0
10	K	13	Total O 13 13	0	0
10	L	15	Total O 15 15	0	0
10	M	20	Total O 20 20	0	0
10	N	19	Total O 19 19	0	0
10	P	2	Total O 2 2	0	0
10	R	5	Total O 5 5	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.

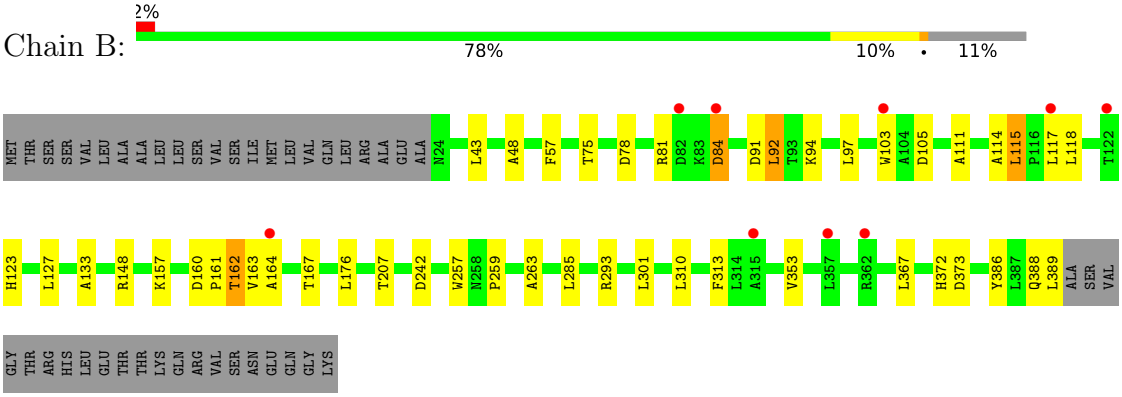
• Molecule 1: Variant surface glycoprotein

Chain A:



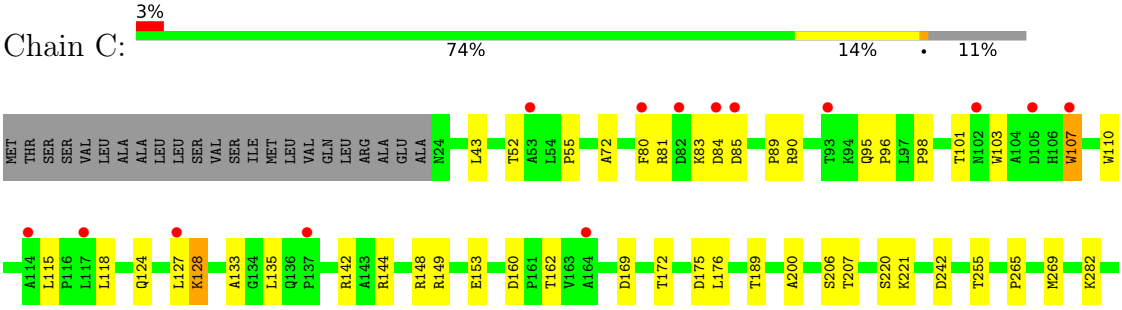
• Molecule 1: Variant surface glycoprotein

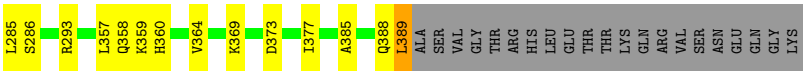
Chain B:



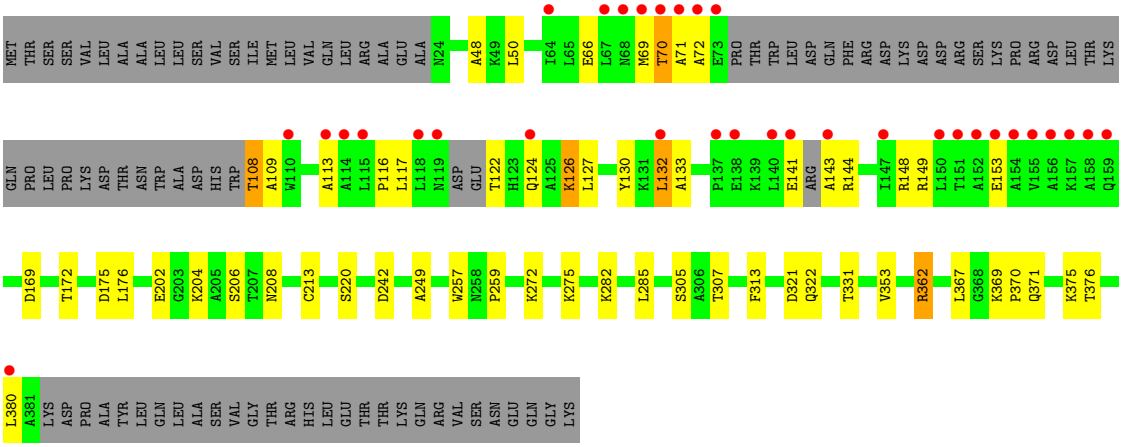
• Molecule 1: Variant surface glycoprotein

Chain C:

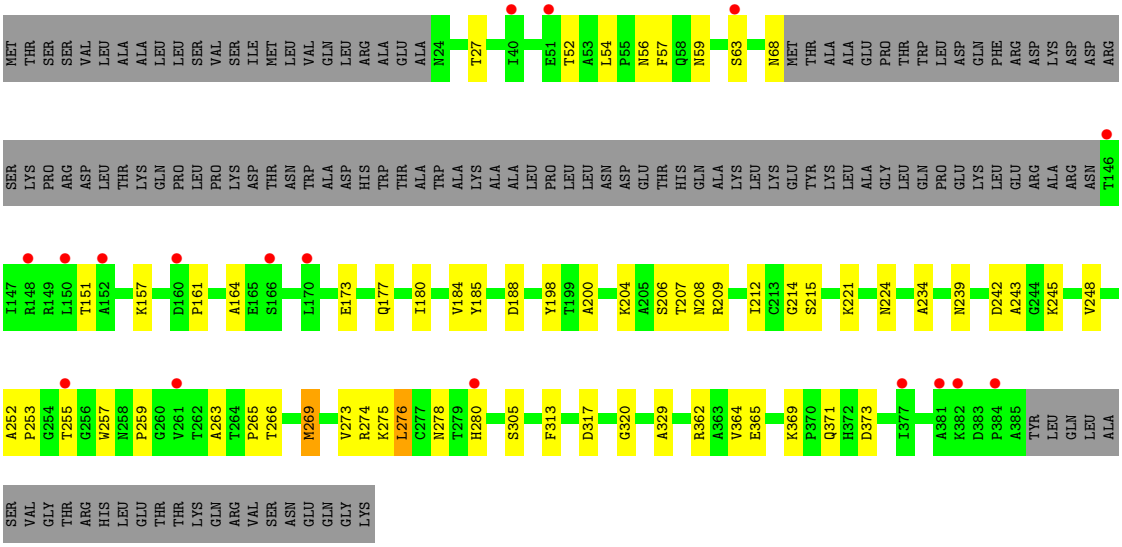




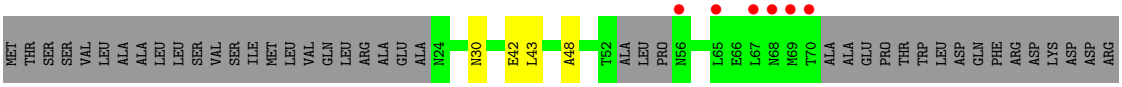
• Molecule 1: Variant surface glycoprotein

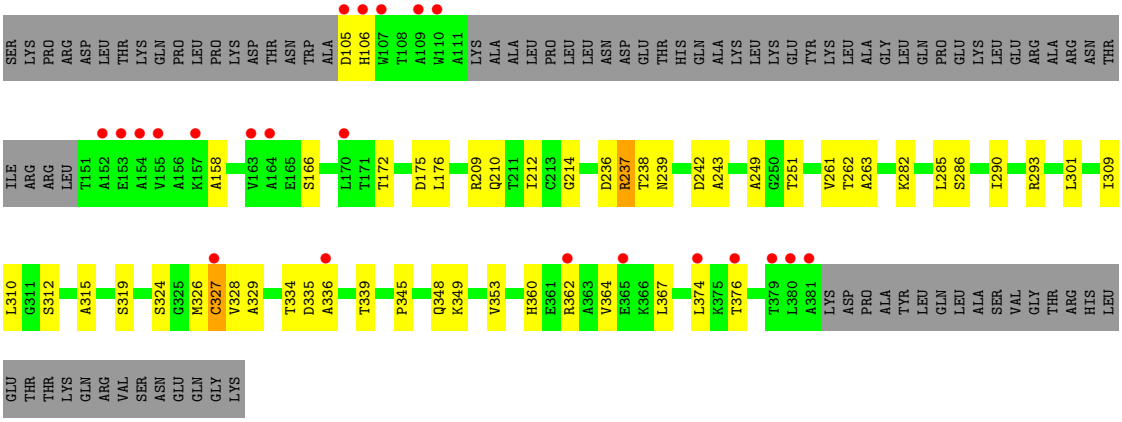


• Molecule 1: Variant surface glycoprotein



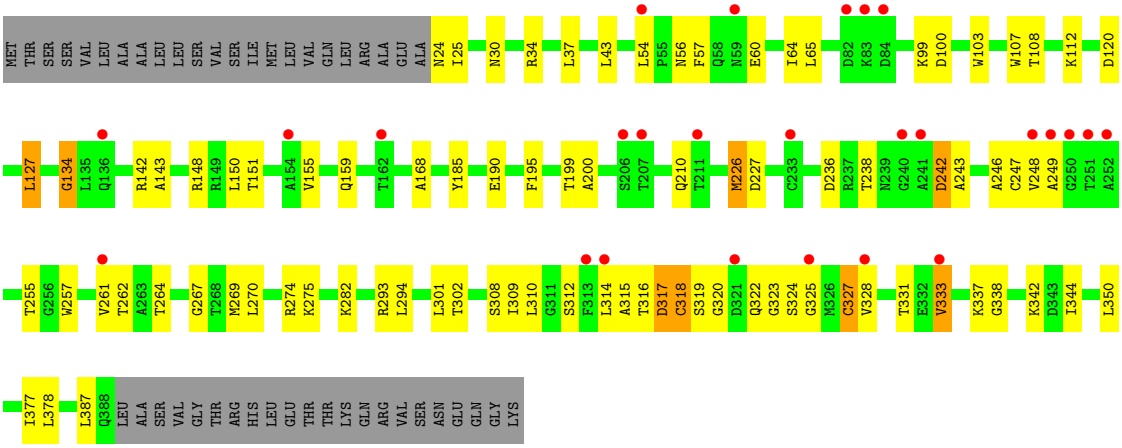
• Molecule 1: Variant surface glycoprotein





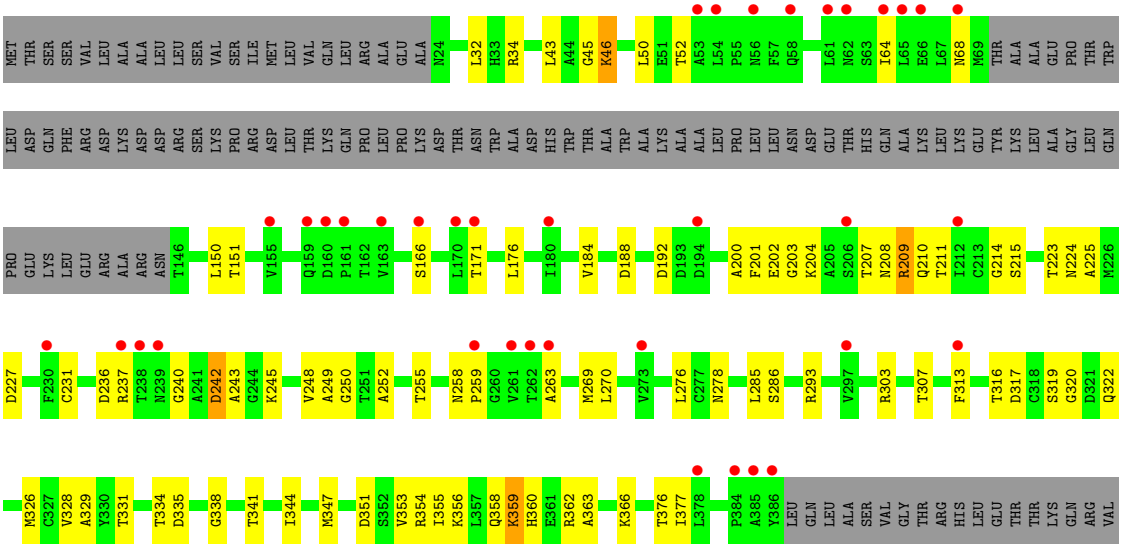
• Molecule 1: Variant surface glycoprotein

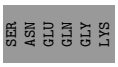
Chain G:



• Molecule 1: Variant surface glycoprotein

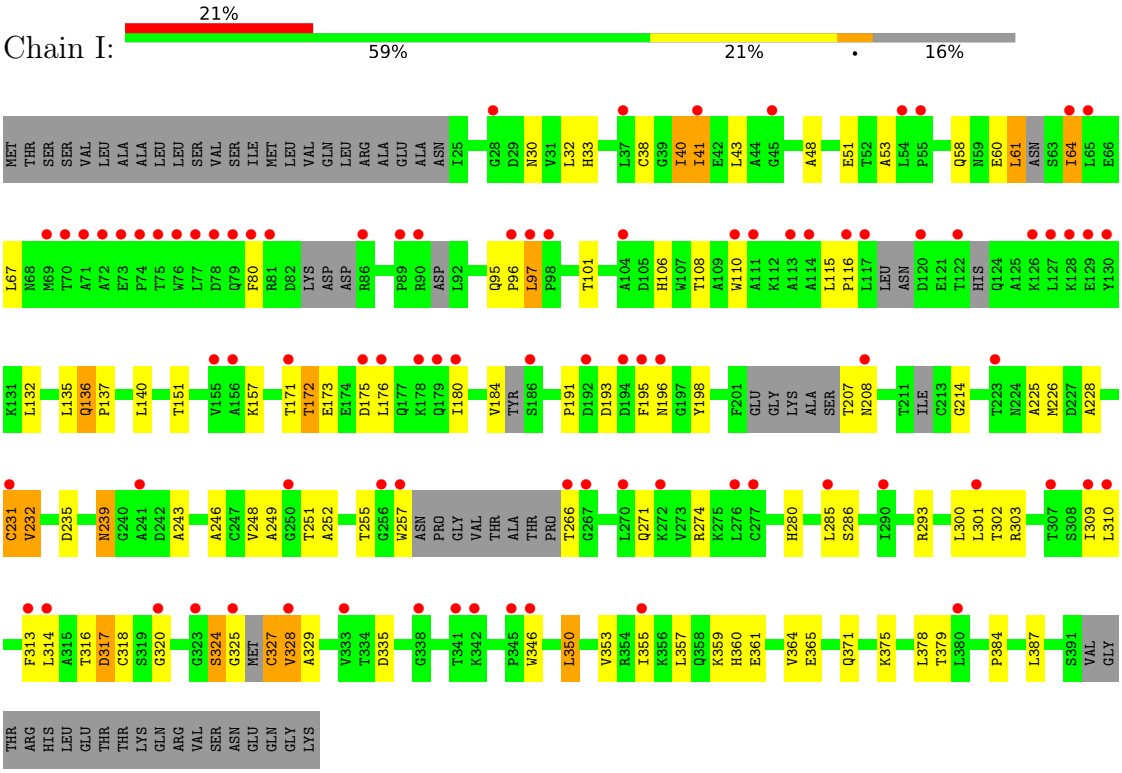
Chain H:





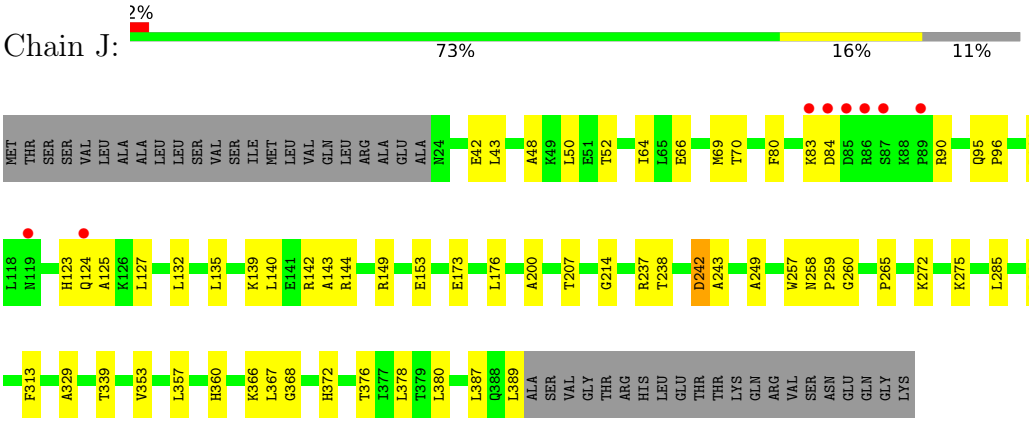
• Molecule 1: Variant surface glycoprotein

Chain I:



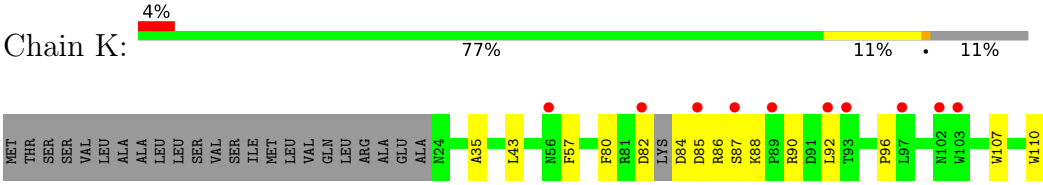
• Molecule 1: Variant surface glycoprotein

Chain J:

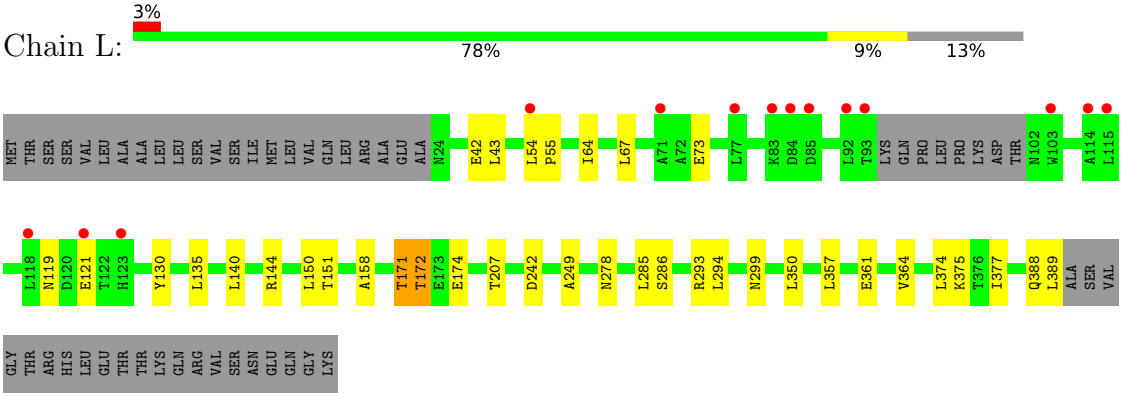


• Molecule 1: Variant surface glycoprotein

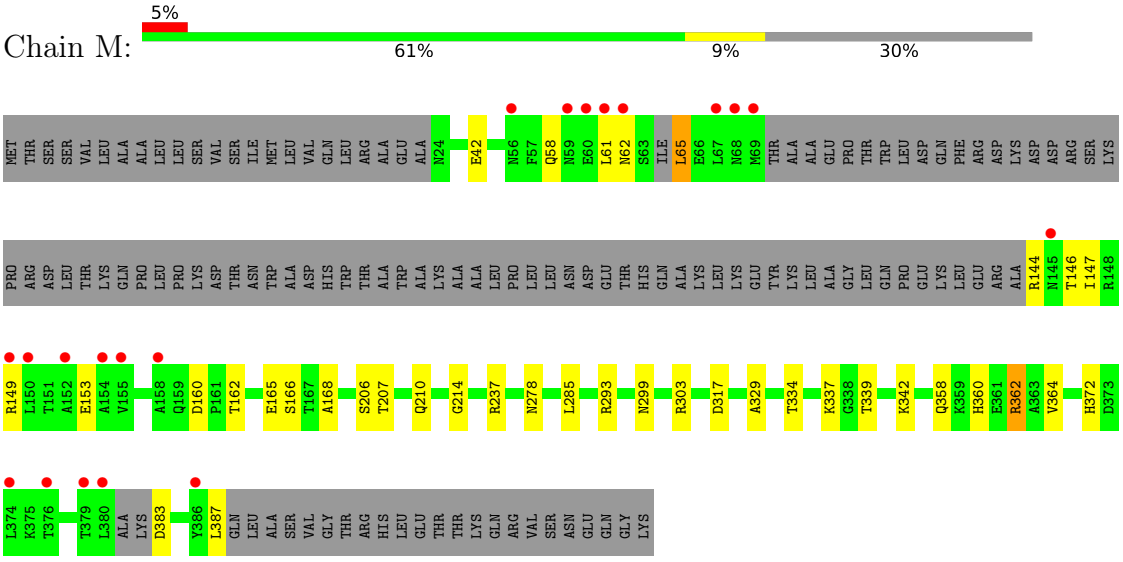
Chain K:



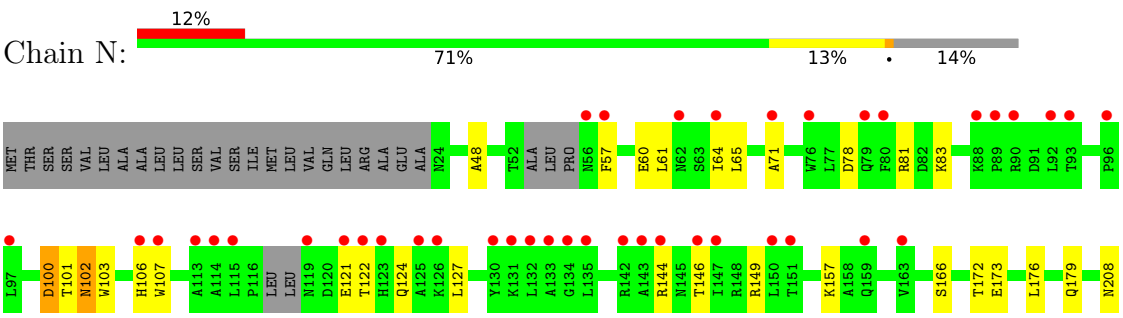
• Molecule 1: Variant surface glycoprotein

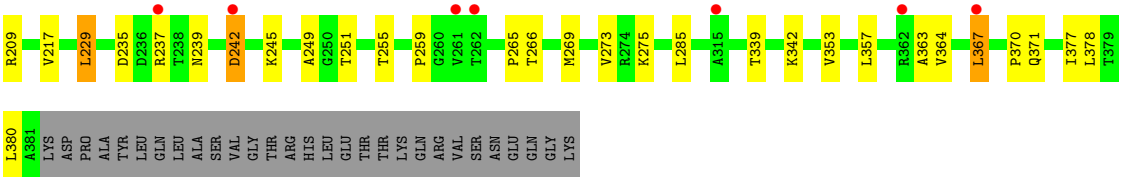


• Molecule 1: Variant surface glycoprotein

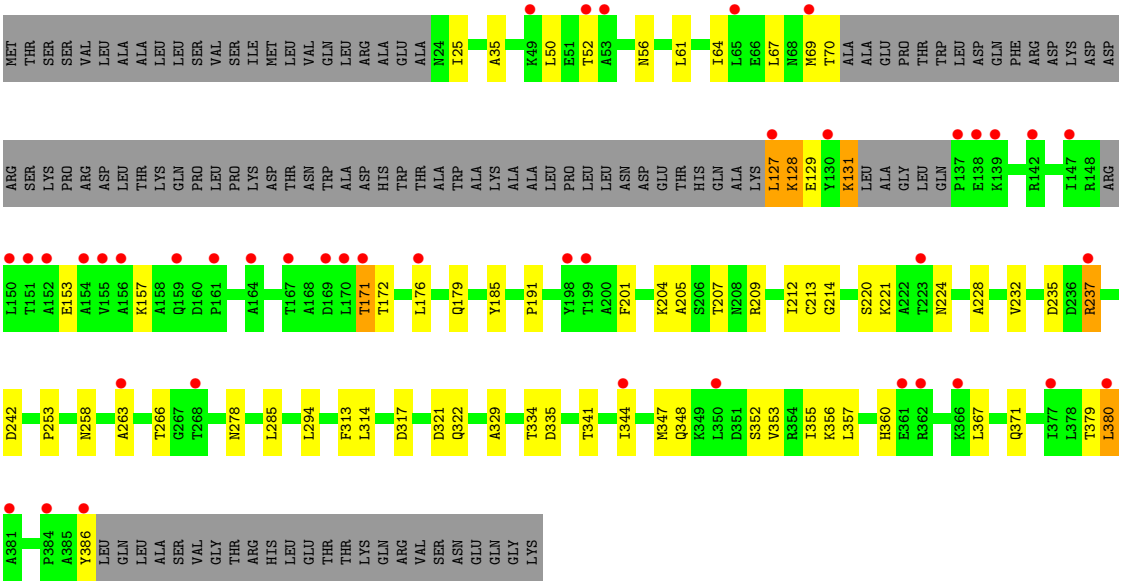


• Molecule 1: Variant surface glycoprotein

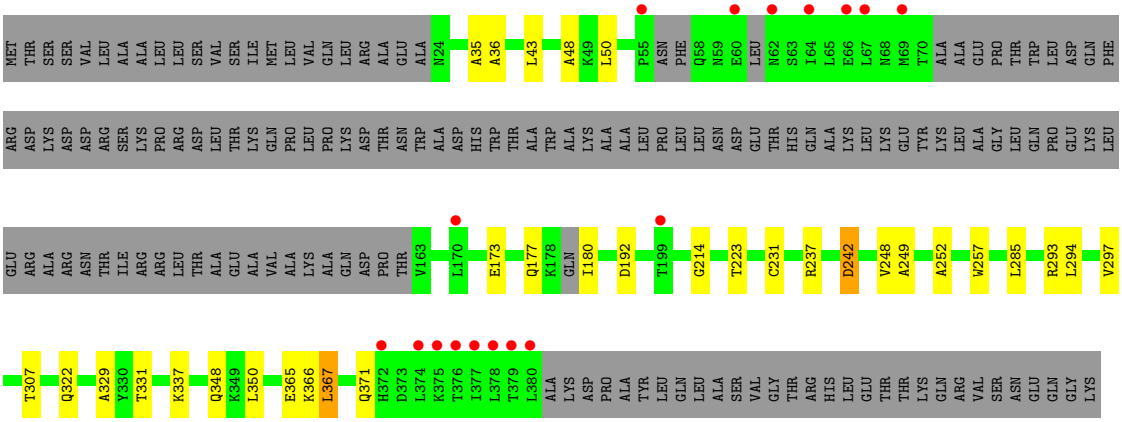




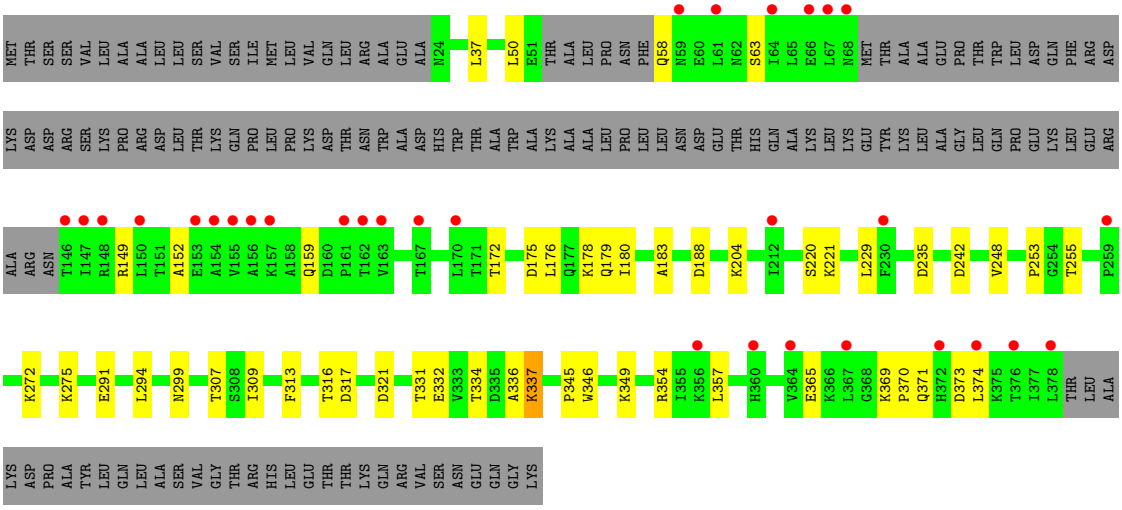
• Molecule 1: Variant surface glycoprotein



• Molecule 1: Variant surface glycoprotein

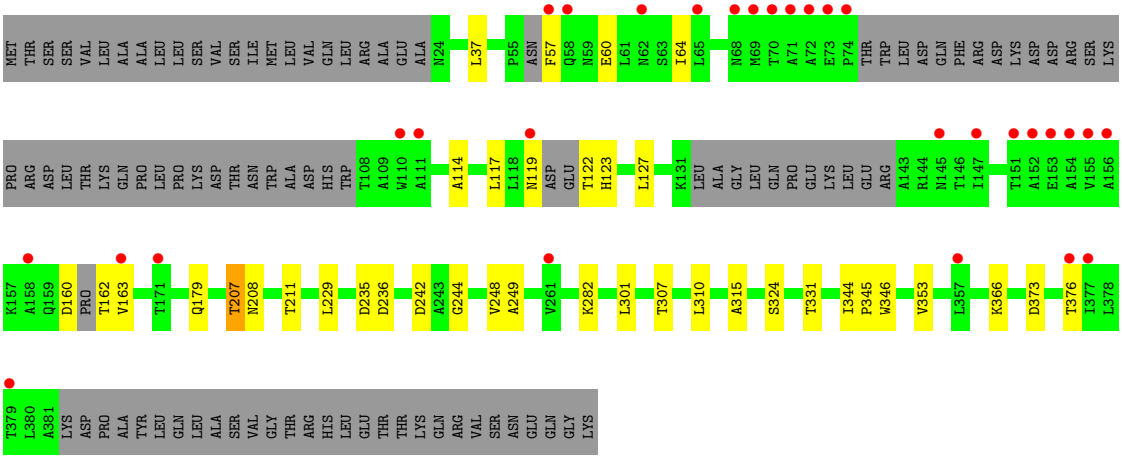


• Molecule 1: Variant surface glycoprotein



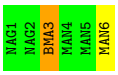
• Molecule 1: Variant surface glycoprotein

Chain R:



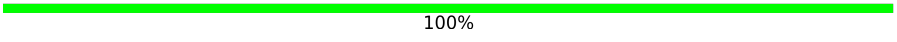
• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain Z:



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

Chain T:

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

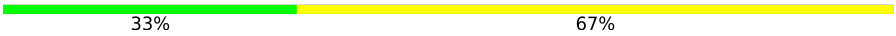
Chain U:

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

Chain V:

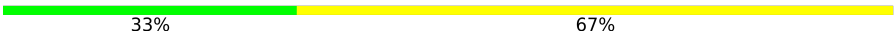
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



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

Chain Y:



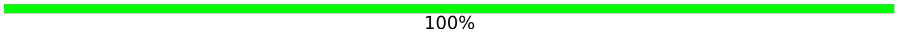
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

nose

Chain c:

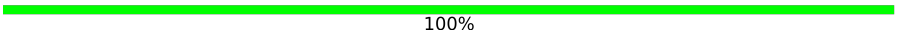


• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

• Molecule 7: alpha-D-mannopyranose-(1-3)-[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 b:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.88Å 210.77Å 133.75Å 90.00° 104.54° 90.00°	Depositor
Resolution (Å)	48.81 – 2.59 48.81 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.81-2.59) 98.9 (48.81-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.270 0.228 , 0.269	Depositor DCC
R_{free} test set	10865 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 58.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	43982	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: NAG, BMA, MAN, GLC

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	0.27	0/2793	0.50	0/3795
1	B	0.27	0/2747	0.50	0/3744
1	C	0.26	0/2765	0.49	0/3761
1	D	0.28	0/2359	0.51	0/3196
1	E	0.27	0/2069	0.49	0/2810
1	F	0.26	0/2066	0.49	0/2801
1	G	0.25	0/2748	0.48	0/3742
1	H	0.26	0/2081	0.50	0/2830
1	I	0.25	0/2489	0.49	0/3386
1	J	0.28	0/2784	0.51	0/3782
1	K	0.26	0/2742	0.50	0/3736
1	L	0.26	0/2701	0.48	0/3672
1	M	0.26	0/2103	0.50	0/2855
1	N	0.27	0/2655	0.50	0/3602
1	O	0.26	0/2196	0.50	0/2980
1	P	0.26	0/1901	0.49	0/2575
1	Q	0.25	0/1987	0.49	0/2693
1	R	0.26	0/2239	0.49	0/3042
All	All	0.26	0/43425	0.49	0/59002

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2749	0	2710	26	0
1	B	2704	0	2604	26	0
1	C	2721	0	2649	35	0
1	D	2332	0	2294	32	0
1	E	2046	0	1988	33	0
1	F	2044	0	1976	31	0
1	G	2704	0	2628	56	0
1	H	2057	0	1991	48	0
1	I	2461	0	2319	68	0
1	J	2741	0	2703	41	0
1	K	2698	0	2616	25	0
1	L	2660	0	2593	21	0
1	M	2079	0	2013	25	0
1	N	2618	0	2540	37	0
1	O	2172	0	2098	41	0
1	P	1882	0	1822	19	0
1	Q	1967	0	1916	30	0
1	R	2215	0	2143	17	0
2	S	72	0	61	1	0
2	Z	72	0	61	0	0
3	T	61	0	52	3	0
4	U	39	0	34	2	0
5	V	39	0	34	0	0
5	X	39	0	34	1	0
5	Y	39	0	34	2	0
6	W	61	0	52	2	0
6	c	61	0	52	0	0
7	a	61	0	52	0	0
7	b	61	0	52	0	0
8	A	11	0	10	0	0
8	B	11	0	10	0	0
8	C	11	0	10	0	0
8	D	11	0	10	0	0
8	E	11	0	10	0	0
8	F	11	0	10	0	0
8	H	11	0	10	0	0
8	I	11	0	10	0	0
8	J	11	0	10	0	0
8	K	11	0	10	0	0
8	L	11	0	10	0	0
8	M	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	N	11	0	10	0	0
8	O	11	0	10	0	0
8	P	11	0	10	0	0
8	Q	11	0	10	0	0
8	R	11	0	10	0	0
9	E	14	0	13	0	0
9	O	14	0	13	0	0
9	Q	14	0	13	0	0
9	R	14	0	13	0	0
10	A	53	0	0	2	0
10	B	43	0	0	0	0
10	C	28	0	0	0	0
10	D	19	0	0	0	0
10	E	4	0	0	0	0
10	F	12	0	0	0	0
10	J	51	0	0	0	0
10	K	13	0	0	0	0
10	L	15	0	0	0	0
10	M	20	0	0	0	0
10	N	19	0	0	0	0
10	P	2	0	0	0	0
10	R	5	0	0	0	0
All	All	43982	0	42343	575	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 7.

All (575) 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:J:52:THR:HG21	1:J:360:HIS:HE2	1.38	0.87
1:C:127:LEU:HB3	1:C:133:ALA:HB2	1.63	0.80
1:B:92:LEU:HD21	1:B:97:LEU:HG	1.63	0.79
1:G:64:ILE:HG22	1:G:378:LEU:HD23	1.70	0.73
1:M:162:THR:HA	1:M:165:GLU:HG2	1.71	0.73
1:D:376:THR:HG21	1:E:157:LYS:HD3	1.70	0.72
1:R:119:ASN:HB3	1:R:122:THR:HB	1.72	0.72
1:K:147:ILE:HG13	1:K:387:LEU:HD11	1.72	0.72
1:I:285:LEU:HG	1:I:357:LEU:HD11	1.73	0.71
1:J:272:LYS:HA	1:J:275:LYS:HE3	1.73	0.70
1:Q:334:THR:HG23	1:Q:336:ALA:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:285:LEU:HG	1:N:357:LEU:HD11	1.74	0.68
1:D:144:ARG:HG2	1:D:148:ARG:HD3	1.75	0.68
1:C:90:ARG:NH2	1:C:96:PRO:O	2.27	0.67
1:O:70:THR:HB	1:O:127:LEU:HD21	1.78	0.66
1:O:213:CYS:HA	1:O:220:SER:HB2	1.77	0.66
1:A:82:ASP:HA	1:A:95:GLN:HE22	1.60	0.66
1:E:245:LYS:HG2	1:E:252:ALA:HB2	1.78	0.66
1:H:303:ARG:NH2	1:H:338:GLY:O	2.29	0.66
1:I:300:LEU:HG	1:I:310:LEU:HD23	1.78	0.66
1:I:48:ALA:HB1	1:I:285:LEU:HD13	1.77	0.66
1:G:99:LYS:NZ	1:O:237:ARG:O	2.29	0.65
1:F:48:ALA:HB1	1:F:285:LEU:HG	1.76	0.65
1:Q:307:THR:HG22	1:Q:331:THR:HG22	1.79	0.65
1:A:101:THR:HG22	2:S:3:BMA:H4	1.78	0.65
1:C:52:THR:HG21	1:C:360:HIS:HE2	1.60	0.65
1:I:101:THR:HA	5:Y:3:BMA:H4	1.80	0.64
1:D:127:LEU:HB3	1:D:133:ALA:HB2	1.78	0.64
1:D:202:GLU:HB2	1:D:204:LYS:HD3	1.78	0.64
1:F:212:ILE:HD11	1:F:263:ALA:HB1	1.80	0.64
1:G:37:LEU:HD21	1:G:310:LEU:HD21	1.79	0.64
1:G:34:ARG:HD3	1:G:247:CYS:HB3	1.80	0.64
1:J:139:LYS:HZ2	1:J:142:ARG:HH21	1.46	0.64
1:O:209:ARG:HG3	1:O:212:ILE:HD11	1.80	0.64
1:O:201:PHE:HE2	1:O:212:ILE:HD13	1.63	0.63
1:C:98:PRO:HB2	1:C:101:THR:HB	1.80	0.63
1:P:36:ALA:HB1	1:P:297:VAL:HG12	1.81	0.63
1:N:249:ALA:HB1	1:O:313:PHE:HB3	1.80	0.63
1:D:116:PRO:O	1:D:122:THR:OG1	2.17	0.62
1:G:127:LEU:HD21	1:G:134:GLY:H	1.64	0.62
1:C:81:ARG:HG2	1:C:118:LEU:HD22	1.81	0.62
1:G:317:ASP:CG	1:G:318:CYS:H	2.03	0.62
1:R:179:GLN:HG2	1:R:353:VAL:HG23	1.80	0.62
1:M:146:THR:HG23	1:M:149:ARG:HH21	1.65	0.62
1:H:171:THR:HG21	1:H:356:LYS:HB3	1.82	0.62
1:H:255:THR:HB	1:H:269:MET:HB3	1.82	0.61
1:I:228:ALA:HA	1:I:328:VAL:HG11	1.81	0.61
1:I:248:VAL:HG12	1:I:249:ALA:H	1.65	0.61
1:E:255:THR:HB	1:E:269:MET:HB3	1.82	0.61
1:J:64:ILE:HG13	1:J:378:LEU:HD23	1.81	0.61
1:F:172:THR:HG23	1:F:175:ASP:H	1.66	0.61
1:H:43:LEU:HD11	1:H:293:ARG:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:PRO:O	1:B:163:VAL:N	2.34	0.61
1:J:301:LEU:HD23	1:J:310:LEU:HB2	1.81	0.60
1:M:339:THR:HG23	1:O:278:ASN:HD21	1.67	0.60
1:N:176:LEU:HD22	1:N:353:VAL:HG13	1.82	0.60
1:O:237:ARG:NE	1:O:258:ASN:OD1	2.35	0.60
1:A:303:ARG:NH2	1:A:338:GLY:O	2.35	0.60
1:N:266:THR:H	1:N:269:MET:HE3	1.67	0.60
1:R:207:THR:OG1	1:R:208:ASN:N	2.35	0.60
1:P:307:THR:HG22	1:P:331:THR:HG22	1.84	0.60
1:K:82:ASP:CG	1:K:84:ASP:H	2.04	0.59
1:F:334:THR:HG23	1:F:336:ALA:H	1.67	0.59
1:G:103:TRP:HZ2	6:W:3:BMA:H62	1.67	0.59
1:H:250:GLY:H	1:I:313:PHE:HE1	1.49	0.59
1:H:376:THR:HG21	1:I:157:LYS:HD3	1.84	0.59
1:M:299:ASN:HB3	1:O:35:ALA:HB1	1.82	0.59
1:B:81:ARG:NH2	1:B:118:LEU:O	2.34	0.59
1:L:285:LEU:HB3	1:L:357:LEU:HD11	1.83	0.59
1:I:193:ASP:HA	1:I:271:GLN:HG3	1.84	0.59
1:I:384:PRO:HA	1:I:387:LEU:HD12	1.85	0.59
1:I:80:PHE:CE2	1:I:110:TRP:HB3	2.37	0.59
1:G:24:ASN:HA	1:G:314:LEU:HD11	1.84	0.58
1:D:172:THR:HG23	1:D:175:ASP:H	1.69	0.58
1:B:127:LEU:HB3	1:B:133:ALA:HB2	1.86	0.58
1:C:285:LEU:HD22	1:C:357:LEU:HD11	1.84	0.58
1:F:327:CYS:SG	1:F:328:VAL:N	2.76	0.58
1:I:318:CYS:HA	1:I:325:GLY:HA3	1.86	0.58
1:O:176:LEU:HG	1:O:353:VAL:HG13	1.85	0.58
1:N:64:ILE:HG12	1:N:378:LEU:HD23	1.86	0.58
1:K:43:LEU:HD11	1:K:293:ARG:HD3	1.86	0.58
1:B:78:ASP:HA	1:B:81:ARG:HD2	1.86	0.58
1:H:259:PRO:HA	1:H:263:ALA:HA	1.85	0.58
1:L:43:LEU:HD11	1:L:293:ARG:HD3	1.86	0.57
1:A:179:GLN:HE22	1:A:349:LYS:HG2	1.69	0.57
1:R:207:THR:OG1	1:R:211:THR:OG1	2.22	0.57
1:C:148:ARG:HG2	4:U:1:NAG:H5	1.87	0.57
1:C:43:LEU:HD11	1:C:293:ARG:HD3	1.86	0.57
1:C:80:PHE:HA	1:C:107:TRP:HH2	1.70	0.57
1:A:127:LEU:HB3	1:A:133:ALA:HB2	1.85	0.57
1:D:72:ALA:HA	1:D:144:ARG:HE	1.69	0.56
1:I:232:VAL:HG23	1:I:327:CYS:HA	1.88	0.56
1:J:260:GLY:O	1:M:237:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:248:VAL:HG22	1:P:249:ALA:H	1.70	0.56
1:F:309:ILE:HG23	1:F:327:CYS:SG	2.46	0.56
1:I:361:GLU:O	1:I:365:GLU:HG2	2.06	0.56
1:J:48:ALA:HB1	1:J:285:LEU:HG	1.88	0.56
1:Q:365:GLU:O	1:Q:369:LYS:NZ	2.37	0.56
1:H:34:ARG:NH2	1:I:300:LEU:O	2.39	0.56
1:P:249:ALA:HB1	1:Q:313:PHE:HB3	1.88	0.56
1:D:272:LYS:HA	1:D:275:LYS:HD3	1.87	0.55
1:A:272:LYS:HA	1:A:275:LYS:HD2	1.87	0.55
1:E:275:LYS:HG2	1:F:335:ASP:HB2	1.87	0.55
1:Q:58:GLN:HB2	1:Q:371:GLN:HB2	1.88	0.55
1:B:257:TRP:CE2	1:B:259:PRO:HG3	2.42	0.55
1:G:210:GLN:HG2	1:G:319:SER:HB2	1.88	0.55
1:H:200:ALA:HB2	1:H:270:LEU:HD11	1.87	0.55
1:B:84:ASP:OD1	1:B:84:ASP:N	2.40	0.55
1:C:83:LYS:H	1:C:95:GLN:NE2	2.05	0.55
1:I:136:GLN:HG2	1:I:137:PRO:HD2	1.88	0.55
1:J:90:ARG:HE	1:J:95:GLN:HB3	1.72	0.55
1:M:42:GLU:OE2	1:M:293:ARG:NH1	2.30	0.55
1:C:149:ARG:NH1	1:C:153:GLU:OE2	2.39	0.55
1:I:80:PHE:HE2	1:I:110:TRP:HB3	1.71	0.55
1:L:158:ALA:HB2	1:L:374:LEU:HD11	1.89	0.55
1:E:200:ALA:HB3	1:E:265:PRO:HD2	1.89	0.54
1:F:42:GLU:OE2	1:F:293:ARG:NH2	2.37	0.54
1:B:43:LEU:HD11	1:B:293:ARG:HD3	1.89	0.54
1:G:168:ALA:HB1	1:M:337:LYS:HD3	1.88	0.54
1:G:316:THR:OG1	1:G:324:SER:HA	2.08	0.54
1:D:69:MET:C	1:D:71:ALA:H	2.11	0.54
1:E:209:ARG:HE	1:E:257:TRP:HZ3	1.56	0.54
1:Q:334:THR:HG22	1:Q:337:LYS:HG3	1.89	0.54
1:G:242:ASP:HB3	1:G:322:GLN:HG2	1.90	0.54
1:B:115:LEU:HA	1:B:118:LEU:HD13	1.90	0.54
1:K:143:ALA:HA	1:K:387:LEU:HD12	1.88	0.54
1:N:235:ASP:O	1:N:255:THR:OG1	2.23	0.54
1:O:242:ASP:OD2	1:O:322:GLN:NE2	2.39	0.54
1:C:89:PRO:HG3	1:C:115:LEU:HD11	1.91	0.53
1:L:172:THR:OG1	1:L:174:GLU:OE1	2.25	0.53
1:B:157:LYS:HD3	1:B:373:ASP:HB3	1.90	0.53
1:H:34:ARG:HH12	1:I:302:THR:HA	1.73	0.53
1:P:50:LEU:HB3	1:P:173:GLU:HB2	1.90	0.53
1:A:369:LYS:HD2	1:C:369:LYS:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:THR:HG23	1:K:175:ASP:H	1.73	0.53
1:K:309:ILE:HG22	1:K:327:CYS:HB2	1.90	0.53
1:N:101:THR:HG23	1:N:103:TRP:H	1.73	0.53
1:N:377:ILE:HA	1:N:380:LEU:HD12	1.89	0.53
1:C:101:THR:HG23	1:C:103:TRP:H	1.73	0.53
1:H:150:LEU:HB3	1:H:377:ILE:HG23	1.90	0.53
1:G:200:ALA:HB2	1:G:270:LEU:HD11	1.91	0.53
1:G:248:VAL:HG12	1:G:249:ALA:H	1.74	0.53
1:J:257:TRP:CE2	1:J:259:PRO:HG3	2.43	0.52
1:N:78:ASP:OD1	1:N:81:ARG:NH2	2.42	0.52
1:J:83:LYS:H	1:J:95:GLN:HE22	1.57	0.52
1:D:307:THR:HG22	1:D:331:THR:HG22	1.92	0.52
1:M:372:HIS:NE2	1:N:370:PRO:HG3	2.25	0.52
1:G:314:LEU:HD12	1:G:323:GLY:HA2	1.91	0.52
1:K:85:ASP:C	1:K:87:SER:H	2.12	0.52
1:E:206:SER:OG	1:E:207:THR:N	2.40	0.52
1:F:176:LEU:HD22	1:F:353:VAL:HG13	1.92	0.52
1:N:60:GLU:H	1:N:60:GLU:CD	2.12	0.52
1:P:367:LEU:O	1:P:371:GLN:HG2	2.10	0.52
1:Q:172:THR:HG23	1:Q:175:ASP:H	1.74	0.52
1:I:316:THR:HB	1:I:324:SER:HB3	1.90	0.52
1:O:224:ASN:OD1	1:O:224:ASN:N	2.42	0.52
1:Q:346:TRP:HA	1:Q:349:LYS:HG3	1.92	0.52
1:F:214:GLY:HA3	1:F:329:ALA:HB3	1.92	0.52
1:I:251:THR:HG22	1:I:252:ALA:H	1.75	0.52
1:Q:309:ILE:HG21	1:Q:313:PHE:HB2	1.91	0.52
1:R:248:VAL:HG12	1:R:249:ALA:H	1.74	0.52
1:J:249:ALA:HB1	1:K:313:PHE:CD1	2.45	0.52
1:E:369:LYS:NZ	1:E:373:ASP:OD2	2.42	0.52
1:J:139:LYS:NZ	1:J:142:ARG:HE	2.08	0.52
1:N:57:PHE:HA	1:N:371:GLN:NE2	2.23	0.51
1:G:242:ASP:OD1	1:G:242:ASP:N	2.42	0.51
1:M:278:ASN:HD21	1:N:339:THR:HG23	1.74	0.51
1:R:315:ALA:HB3	1:R:324:SER:HA	1.92	0.51
1:K:130:TYR:HA	1:K:382:LYS:HE3	1.92	0.51
1:F:243:ALA:HB1	1:F:326:MET:HG3	1.92	0.51
1:H:192:ASP:OD1	1:H:192:ASP:N	2.44	0.51
1:A:57:PHE:CE1	1:A:370:PRO:HB2	2.46	0.51
1:E:273:VAL:HA	1:E:276:LEU:HD12	1.93	0.51
1:F:315:ALA:HB3	1:F:324:SER:HA	1.93	0.51
1:K:144:ARG:O	1:K:148:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:PHE:HZ	1:K:163:VAL:HG11	1.76	0.51
1:E:242:ASP:OD1	1:E:243:ALA:N	2.42	0.50
1:J:66:GLU:O	1:J:70:THR:HG23	2.11	0.50
1:N:71:ALA:O	1:N:144:ARG:NH1	2.44	0.50
1:N:78:ASP:HA	1:N:81:ARG:HE	1.76	0.50
1:F:261:VAL:HG23	1:F:262:THR:HG23	1.94	0.50
1:I:95:GLN:C	1:I:97:LEU:H	2.15	0.50
1:I:375:LYS:O	1:I:379:THR:HG23	2.11	0.50
1:Q:316:THR:OG1	1:Q:317:ASP:OD1	2.29	0.50
1:L:64:ILE:HG22	1:L:151:THR:HG23	1.93	0.50
1:D:122:THR:O	1:D:126:LYS:HG3	2.11	0.50
1:K:255:THR:HB	1:K:269:MET:HB3	1.94	0.50
1:G:148:ARG:HG2	6:W:1:NAG:H5	1.93	0.50
1:I:225:ALA:HB2	1:I:346:TRP:CE3	2.46	0.50
1:B:114:ALA:HA	1:B:117:LEU:HD12	1.92	0.50
1:D:371:GLN:HG2	1:D:375:LYS:HE3	1.94	0.50
1:G:301:LEU:HD23	1:G:310:LEU:HB2	1.93	0.50
1:R:373:ASP:HA	1:R:376:THR:HG22	1.94	0.50
1:D:369:LYS:HB2	1:D:370:PRO:HD3	1.94	0.50
1:B:91:ASP:HB2	1:B:94:LYS:HB2	1.93	0.50
1:B:148:ARG:HD3	3:T:1:NAG:O4	2.12	0.50
1:D:66:GLU:HA	1:D:113:ALA:HB1	1.93	0.50
1:N:102:ASN:C	1:N:102:ASN:HD22	2.14	0.50
1:O:242:ASP:OD1	1:O:242:ASP:N	2.44	0.50
1:Q:248:VAL:HG11	1:Q:253:PRO:HD3	1.94	0.50
1:E:185:TYR:OH	1:E:274:ARG:HD2	2.12	0.50
1:E:212:ILE:HD11	1:E:263:ALA:HB1	1.94	0.50
1:I:64:ILE:HG22	1:I:151:THR:HG22	1.94	0.49
1:I:303:ARG:HD3	1:I:335:ASP:HA	1.94	0.49
1:G:64:ILE:HG13	1:G:65:LEU:N	2.27	0.49
1:H:176:LEU:HD23	1:H:285:LEU:HD13	1.94	0.49
1:I:43:LEU:HD11	1:I:293:ARG:HD3	1.93	0.49
1:Q:220:SER:OG	1:Q:221:LYS:N	2.45	0.49
1:F:166:SER:HB2	1:F:367:LEU:HD13	1.93	0.49
1:Q:317:ASP:OD1	1:Q:317:ASP:N	2.46	0.49
1:R:160:ASP:C	1:R:163:VAL:H	2.16	0.49
1:A:208:ASN:OD1	1:A:210:GLN:HG2	2.12	0.49
1:G:261:VAL:HG12	1:G:262:THR:HG23	1.94	0.49
1:M:303:ARG:NH1	1:M:334:THR:O	2.44	0.49
1:C:142:ARG:HD3	1:C:388:GLN:HA	1.94	0.49
1:G:25:ILE:HG13	1:G:325:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:ASN:HB2	1:G:246:ALA:HB1	1.93	0.49
1:D:141:GLU:O	1:D:143:ALA:N	2.46	0.49
1:E:239:ASN:HB2	1:E:243:ALA:HB3	1.94	0.49
1:R:235:ASP:HB3	1:R:244:GLY:HA3	1.94	0.49
1:A:82:ASP:HB3	1:A:90:ARG:HA	1.94	0.49
1:G:342:LYS:C	1:G:344:ILE:H	2.16	0.49
1:R:301:LEU:HD23	1:R:310:LEU:HB2	1.95	0.49
1:P:294:LEU:HD21	1:P:350:LEU:HB3	1.94	0.49
1:B:164:ALA:H	1:B:167:THR:HG23	1.77	0.49
1:D:69:MET:O	1:D:71:ALA:N	2.46	0.48
1:A:56:ASN:OD1	1:A:59:ASN:ND2	2.46	0.48
1:G:317:ASP:OD1	1:G:319:SER:N	2.46	0.48
1:H:210:GLN:HB3	1:H:319:SER:HB3	1.95	0.48
1:I:64:ILE:HG12	1:I:378:LEU:HD23	1.95	0.48
1:L:171:THR:HG22	1:L:172:THR:H	1.78	0.48
1:J:285:LEU:HD22	1:J:357:LEU:HD11	1.96	0.48
1:N:121:GLU:O	1:N:124:GLN:NE2	2.46	0.48
1:O:56:ASN:O	1:O:371:GLN:NE2	2.44	0.48
1:I:248:VAL:HG12	1:I:249:ALA:N	2.28	0.48
1:J:200:ALA:HB3	1:J:265:PRO:HD2	1.94	0.48
1:C:124:GLN:O	1:C:128:LYS:HD2	2.13	0.48
1:E:198:TYR:OH	1:E:224:ASN:ND2	2.43	0.48
1:J:237:ARG:HG3	1:J:258:ASN:HB2	1.94	0.48
1:O:294:LEU:HD22	1:O:347:MET:HE3	1.93	0.48
1:Q:332:GLU:N	1:Q:332:GLU:OE1	2.46	0.48
1:Q:183:ALA:HB2	1:Q:349:LYS:HB2	1.96	0.48
1:A:57:PHE:HE1	1:A:370:PRO:HB2	1.78	0.48
1:B:372:HIS:NE2	1:C:162:THR:HG21	2.29	0.48
1:G:226:MET:HE1	1:G:274:ARG:HD3	1.96	0.48
1:H:176:LEU:HG	1:H:353:VAL:HG13	1.96	0.48
1:N:146:THR:HG22	1:N:149:ARG:HH21	1.78	0.48
1:R:307:THR:HG22	1:R:331:THR:HG22	1.95	0.48
1:C:55:PRO:HD3	1:C:364:VAL:HG22	1.95	0.48
1:D:70:THR:HB	1:D:117:LEU:HD11	1.96	0.48
1:I:38:CYS:HA	1:I:41:ILE:HG12	1.96	0.48
1:O:317:ASP:OD1	1:O:317:ASP:N	2.47	0.48
1:Q:242:ASP:OD1	1:Q:242:ASP:N	2.45	0.48
1:H:209:ARG:NH1	1:H:326:MET:SD	2.87	0.47
1:I:214:GLY:HA3	1:I:329:ALA:HB3	1.95	0.47
1:I:309:ILE:HG13	1:I:328:VAL:O	2.14	0.47
1:G:317:ASP:O	1:G:318:CYS:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:25:ILE:HG13	1:O:314:LEU:HD12	1.96	0.47
1:D:70:THR:HG21	1:D:130:TYR:HD2	1.79	0.47
1:H:351:ASP:OD1	1:H:354:ARG:NH1	2.47	0.47
1:J:90:ARG:NH2	1:J:96:PRO:O	2.48	0.47
1:L:135:LEU:HD12	1:L:140:LEU:HD23	1.96	0.47
1:N:239:ASN:HB2	1:N:242:ASP:O	2.14	0.47
1:A:99:LYS:NZ	10:A:606:HOH:O	2.48	0.47
1:E:173:GLU:O	1:E:177:GLN:HG3	2.14	0.47
1:E:278:ASN:HD21	1:F:339:THR:HG23	1.79	0.47
1:N:229:LEU:HD13	1:N:273:VAL:HG12	1.96	0.47
1:P:365:GLU:HG3	1:P:366:LYS:HE2	1.97	0.47
1:C:80:PHE:HA	1:C:107:TRP:CH2	2.48	0.47
1:H:52:THR:HG21	1:H:360:HIS:CD2	2.49	0.47
1:H:184:VAL:HA	1:H:225:ALA:HB3	1.96	0.47
1:H:208:ASN:HA	1:H:259:PRO:HB2	1.96	0.47
1:J:90:ARG:NE	1:J:95:GLN:HB3	2.29	0.47
1:A:71:ALA:O	1:A:144:ARG:NE	2.47	0.47
1:G:319:SER:OG	1:G:320:GLY:N	2.47	0.47
1:H:344:ILE:HD11	1:H:347:MET:SD	2.55	0.47
1:K:360:HIS:O	1:K:364:VAL:HG13	2.15	0.47
1:Q:204:LYS:HE2	1:Q:221:LYS:HG2	1.96	0.47
1:Q:235:ASP:O	1:Q:255:THR:OG1	2.32	0.47
1:C:148:ARG:NH2	4:U:2:NAG:H83	2.30	0.47
1:B:111:ALA:O	1:B:115:LEU:N	2.43	0.47
1:F:105:ASP:OD1	1:F:105:ASP:N	2.45	0.47
1:H:214:GLY:HA3	1:H:329:ALA:HB3	1.97	0.47
1:J:339:THR:HG23	1:L:278:ASN:HD21	1.80	0.47
1:D:321:ASP:OD1	1:D:322:GLN:N	2.48	0.47
1:N:245:LYS:HE2	1:N:245:LYS:HB3	1.73	0.47
1:A:144:ARG:O	1:A:148:ARG:HG3	2.15	0.46
1:C:220:SER:OG	1:C:221:LYS:N	2.48	0.46
1:J:42:GLU:OE2	1:J:293:ARG:NH2	2.47	0.46
1:N:166:SER:HB3	1:N:363:ALA:HB1	1.97	0.46
1:Q:272:LYS:HA	1:Q:275:LYS:HE3	1.96	0.46
1:Q:345:PRO:O	1:Q:349:LYS:HG2	2.15	0.46
1:D:176:LEU:HG	1:D:353:VAL:HG13	1.96	0.46
1:H:202:GLU:OE1	1:H:204:LYS:HG2	2.16	0.46
1:I:195:PHE:CD1	1:I:271:GLN:HG2	2.50	0.46
1:N:100:ASP:OD1	1:N:100:ASP:N	2.49	0.46
1:L:73:GLU:HG3	1:L:144:ARG:CZ	2.46	0.46
1:M:153:GLU:HA	1:O:380:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:206:SER:OG	1:M:207:THR:N	2.48	0.46
1:D:48:ALA:HB1	1:D:285:LEU:HG	1.97	0.46
1:I:171:THR:OG1	1:I:172:THR:N	2.47	0.46
1:K:35:ALA:HB1	1:L:299:ASN:HB3	1.98	0.46
1:O:352:SER:O	1:O:356:LYS:HG2	2.14	0.46
1:F:158:ALA:HB2	1:F:374:LEU:HD11	1.97	0.46
1:I:184:VAL:HG13	1:I:226:MET:HB2	1.98	0.46
1:O:128:LYS:HG2	1:O:131:LYS:HD3	1.98	0.46
1:A:80:PHE:CE2	1:A:110:TRP:HB3	2.50	0.46
1:B:103:TRP:HE1	3:T:2:NAG:H3	1.81	0.46
1:C:80:PHE:CE1	1:C:110:TRP:HB3	2.51	0.46
1:I:207:THR:OG1	1:I:208:ASN:N	2.49	0.46
1:J:242:ASP:HB2	1:J:243:ALA:H	1.55	0.46
1:K:92:LEU:HD11	1:K:107:TRP:CD1	2.50	0.46
1:N:237:ARG:HA	1:N:237:ARG:HD2	1.79	0.46
1:A:25:ILE:HD12	1:A:312:SER:HB3	1.97	0.46
1:H:215:SER:O	1:H:307:THR:HG21	2.16	0.46
1:I:226:MET:HE1	1:I:274:ARG:HB3	1.98	0.46
1:J:123:HIS:C	1:J:125:ALA:H	2.19	0.46
1:J:132:LEU:HA	1:J:135:LEU:HD11	1.98	0.46
1:O:344:ILE:O	1:O:348:GLN:HG3	2.15	0.46
1:B:259:PRO:HA	1:B:263:ALA:HA	1.98	0.46
1:E:68:ASN:HA	1:E:151:THR:HG21	1.97	0.46
1:H:224:ASN:ND2	1:H:227:ASP:OD2	2.49	0.46
1:N:48:ALA:HB1	1:N:285:LEU:HD13	1.97	0.46
1:B:48:ALA:HB1	1:B:285:LEU:HG	1.97	0.46
1:F:301:LEU:HD23	1:F:310:LEU:HB2	1.98	0.46
1:H:208:ASN:ND2	1:H:210:GLN:OE1	2.41	0.46
1:I:191:PRO:HG2	1:I:195:PHE:CE2	2.51	0.46
1:L:119:ASN:OD1	1:L:121:GLU:N	2.49	0.46
1:I:239:ASN:ND2	1:I:320:GLY:O	2.44	0.46
1:J:100:ASP:OD1	1:J:100:ASP:N	2.46	0.46
1:J:313:PHE:CD1	1:L:249:ALA:HB1	2.51	0.45
1:P:366:LYS:HD3	1:P:366:LYS:HA	1.75	0.45
1:B:372:HIS:NE2	1:C:160:ASP:OD2	2.49	0.45
1:I:58:GLN:O	1:I:60:GLU:N	2.48	0.45
1:J:50:LEU:HB3	1:J:173:GLU:HB2	1.97	0.45
1:P:214:GLY:HA3	1:P:329:ALA:HB3	1.98	0.45
1:J:43:LEU:HD11	1:J:293:ARG:HD3	1.99	0.45
1:N:208:ASN:OD1	1:N:208:ASN:N	2.50	0.45
1:G:342:LYS:O	1:G:344:ILE:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:146:THR:OG1	1:K:387:LEU:HD13	2.16	0.45
1:C:172:THR:HG23	1:C:175:ASP:H	1.81	0.45
1:G:64:ILE:HD12	1:G:151:THR:HA	1.99	0.45
1:H:237:ARG:HD2	1:H:258:ASN:HB2	1.99	0.45
1:M:165:GLU:HG3	1:M:166:SER:N	2.31	0.45
1:N:342:LYS:HE2	1:N:342:LYS:HB2	1.78	0.45
1:Q:149:ARG:HA	1:Q:152:ALA:HB3	1.99	0.45
1:F:237:ARG:HD2	1:F:237:ARG:HA	1.70	0.45
1:H:215:SER:HB2	1:H:317:ASP:HB3	1.98	0.45
1:J:124:GLN:HA	1:J:127:LEU:HD12	1.99	0.45
1:J:372:HIS:O	1:J:376:THR:HG23	2.17	0.45
1:P:248:VAL:HG11	1:P:252:ALA:HA	1.97	0.45
3:T:3:BMA:H61	3:T:5:MAN:H2	1.39	0.45
1:E:221:LYS:HA	1:E:221:LYS:HD3	1.76	0.45
1:H:334:THR:OG1	1:H:335:ASP:N	2.50	0.45
1:I:350:LEU:O	1:I:353:VAL:HG22	2.17	0.45
1:O:214:GLY:HA3	1:O:329:ALA:HB3	1.99	0.45
1:I:32:LEU:HD12	1:I:33:HIS:N	2.32	0.45
1:L:375:LYS:HB2	1:L:375:LYS:HE3	1.76	0.45
1:D:213:CYS:O	1:D:220:SER:HB2	2.17	0.45
1:E:248:VAL:HG21	1:E:253:PRO:HD3	1.99	0.45
1:G:150:LEU:HB3	1:G:377:ILE:HG23	1.99	0.45
1:L:357:LEU:O	1:L:361:GLU:HG3	2.16	0.45
1:D:69:MET:C	1:D:71:ALA:N	2.70	0.44
1:G:60:GLU:O	1:G:64:ILE:HG23	2.17	0.44
1:H:201:PHE:C	1:H:203:GLY:H	2.21	0.44
1:I:132:LEU:HA	1:I:135:LEU:HD11	2.00	0.44
1:M:62:ASN:O	1:M:65:LEU:HG	2.16	0.44
1:Q:370:PRO:O	1:Q:374:LEU:HB2	2.16	0.44
1:C:84:ASP:OD1	1:C:85:ASP:N	2.50	0.44
1:G:100:ASP:OD1	1:G:100:ASP:N	2.49	0.44
1:G:275:LYS:HB2	1:H:335:ASP:HB2	1.99	0.44
1:H:243:ALA:HB2	1:H:322:GLN:HB3	1.99	0.44
1:H:249:ALA:HB1	1:I:313:PHE:CD1	2.51	0.44
1:M:58:GLN:O	1:M:61:LEU:N	2.49	0.44
1:M:372:HIS:CD2	1:N:157:LYS:HE3	2.52	0.44
1:H:358:GLN:OE1	1:H:362:ARG:NH2	2.51	0.44
1:O:334:THR:HG22	1:O:335:ASP:H	1.82	0.44
1:Q:178:LYS:HE2	1:Q:188:ASP:HB3	2.00	0.44
1:E:204:LYS:NZ	1:K:165:GLU:HG3	2.32	0.44
1:E:266:THR:HG22	1:E:269:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:345:PRO:O	1:F:348:GLN:HG3	2.16	0.44
1:K:82:ASP:CG	1:K:84:ASP:N	2.71	0.44
1:L:150:LEU:HB3	1:L:377:ILE:HG23	2.00	0.44
1:D:257:TRP:CE2	1:D:259:PRO:HG3	2.52	0.44
1:G:43:LEU:HD11	1:G:293:ARG:HD3	1.99	0.44
1:G:257:TRP:CD1	1:G:269:MET:HE1	2.52	0.44
1:K:142:ARG:NH2	1:K:389:LEU:O	2.51	0.44
1:N:172:THR:OG1	1:N:173:GLU:N	2.50	0.44
1:O:204:LYS:HB2	1:O:221:LYS:HG2	1.99	0.44
1:G:155:VAL:O	1:G:159:GLN:HB2	2.18	0.44
1:G:242:ASP:HB2	1:G:243:ALA:H	1.61	0.44
1:B:386:TYR:CE1	1:C:149:ARG:HG3	2.53	0.44
1:I:61:LEU:HD12	1:I:61:LEU:HA	1.82	0.44
1:O:50:LEU:C	1:O:52:THR:H	2.21	0.44
1:P:35:ALA:HB1	1:Q:299:ASN:HB3	1.99	0.44
1:P:48:ALA:HB1	1:P:285:LEU:HD21	1.99	0.44
1:G:249:ALA:HB1	1:H:313:PHE:CD1	2.53	0.44
1:H:278:ASN:HA	1:I:303:ARG:HH12	1.83	0.44
1:O:171:THR:HG22	1:O:172:THR:H	1.82	0.44
1:O:352:SER:HA	1:O:355:ILE:HG12	1.99	0.44
1:F:362:ARG:HE	1:F:362:ARG:HB2	1.46	0.44
1:J:50:LEU:HG	1:J:52:THR:HG22	2.00	0.44
1:J:149:ARG:O	1:J:153:GLU:HG3	2.17	0.44
1:J:366:LYS:C	1:J:368:GLY:H	2.22	0.44
1:N:275:LYS:HE2	1:O:335:ASP:HB2	2.00	0.44
1:C:373:ASP:O	1:C:377:ILE:HG12	2.18	0.43
1:E:161:PRO:O	1:E:164:ALA:N	2.50	0.43
1:E:214:GLY:HA3	1:E:329:ALA:HB3	1.99	0.43
1:J:69:MET:HE1	1:J:80:PHE:CE1	2.53	0.43
1:O:185:TYR:CG	1:O:191:PRO:HD2	2.53	0.43
1:Q:369:LYS:N	1:Q:370:PRO:HD2	2.32	0.43
1:A:249:ALA:HB1	1:B:313:PHE:CD1	2.53	0.43
1:G:337:LYS:NZ	1:M:168:ALA:O	2.42	0.43
1:E:56:ASN:O	1:E:59:ASN:N	2.51	0.43
1:F:349:LYS:HB2	1:F:349:LYS:HE3	1.82	0.43
1:J:139:LYS:HZ1	1:J:142:ARG:HE	1.65	0.43
1:I:251:THR:HG22	1:I:252:ALA:N	2.33	0.43
1:K:80:PHE:CZ	1:K:110:TRP:HB3	2.53	0.43
1:E:215:SER:HA	1:E:317:ASP:HA	2.01	0.43
1:K:85:ASP:HB3	1:K:88:LYS:H	1.83	0.43
1:P:285:LEU:HD23	1:P:285:LEU:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:ARG:HA	1:E:362:ARG:HD3	1.75	0.43
1:F:43:LEU:HD11	1:F:293:ARG:HD3	2.01	0.43
1:I:231:CYS:O	1:I:327:CYS:N	2.52	0.43
1:I:110:TRP:HE1	5:Y:1:NAG:H82	1.83	0.43
1:I:309:ILE:HD12	1:I:329:ALA:HB2	2.01	0.43
1:P:43:LEU:HD11	1:P:293:ARG:HD3	2.01	0.43
1:P:242:ASP:OD1	1:P:242:ASP:N	2.52	0.43
1:G:255:THR:HB	1:G:269:MET:HB3	2.01	0.43
1:G:308:SER:HB2	1:G:333:VAL:HG23	2.01	0.43
1:I:30:ASN:N	1:I:246:ALA:HB1	2.34	0.43
1:I:33:HIS:CD2	1:I:310:LEU:HG	2.54	0.43
1:M:144:ARG:HA	1:M:147:ILE:HD13	2.01	0.43
1:M:358:GLN:O	1:M:362:ARG:HG2	2.18	0.43
1:Q:294:LEU:HD23	1:Q:294:LEU:HA	1.78	0.43
1:G:318:CYS:SG	1:G:327:CYS:N	2.91	0.43
1:H:355:ILE:O	1:H:359:LYS:HG2	2.18	0.43
1:Q:176:LEU:O	1:Q:180:ILE:HG13	2.18	0.43
1:Q:291:GLU:HG2	1:Q:354:ARG:HE	1.82	0.43
1:G:255:THR:O	1:G:269:MET:HG2	2.19	0.42
1:I:171:THR:HG22	1:I:360:HIS:HB2	2.01	0.42
1:K:114:ALA:HA	1:K:117:LEU:HD12	2.01	0.42
1:O:221:LYS:HD2	1:O:221:LYS:HA	1.80	0.42
1:O:357:LEU:HD23	1:O:357:LEU:HA	1.87	0.42
1:R:64:ILE:HD13	1:R:64:ILE:HA	1.86	0.42
1:A:171:THR:HG22	1:A:172:THR:H	1.83	0.42
1:D:124:GLN:HA	1:D:127:LEU:HD12	2.01	0.42
1:F:236:ASP:N	1:F:239:ASN:OD1	2.47	0.42
1:P:248:VAL:HG22	1:P:249:ALA:N	2.34	0.42
1:E:56:ASN:OD1	1:E:57:PHE:N	2.53	0.42
1:I:173:GLU:C	1:I:175:ASP:H	2.23	0.42
1:O:205:ALA:HB1	1:O:263:ALA:O	2.20	0.42
1:G:333:VAL:HG12	1:G:338:GLY:HA3	2.01	0.42
1:I:95:GLN:O	1:I:97:LEU:N	2.47	0.42
1:N:146:THR:HG22	1:N:149:ARG:NH2	2.35	0.42
1:R:37:LEU:HD13	1:R:229:LEU:HA	2.01	0.42
1:C:169:ASP:HB3	1:C:359:LYS:HB3	2.02	0.42
1:G:143:ALA:HB1	1:G:387:LEU:HD13	2.00	0.42
1:I:53:ALA:HB1	1:I:364:VAL:HG21	2.01	0.42
1:I:172:THR:OG1	1:I:173:GLU:N	2.53	0.42
1:J:380:LEU:HD23	1:J:380:LEU:HA	1.90	0.42
1:M:285:LEU:HD23	1:M:285:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:380:LEU:HD22	1:O:386:TYR:CG	2.54	0.42
1:P:237:ARG:HG2	1:P:257:TRP:O	2.20	0.42
1:C:255:THR:O	1:C:269:MET:HG2	2.19	0.42
1:G:25:ILE:HD12	1:G:312:SER:HB3	2.01	0.42
1:G:185:TYR:CE2	1:G:190:GLU:HG3	2.55	0.42
1:H:166:SER:O	1:H:363:ALA:HB1	2.20	0.42
1:O:204:LYS:CB	1:O:221:LYS:HG2	2.49	0.42
1:Q:50:LEU:HD23	1:Q:50:LEU:HA	1.82	0.42
1:A:66:GLU:O	1:A:70:THR:HG23	2.19	0.42
1:C:385:ALA:O	1:C:389:LEU:HD13	2.20	0.42
1:F:360:HIS:O	1:F:364:VAL:HG23	2.20	0.42
1:I:180:ILE:HD11	1:I:353:VAL:HG11	2.01	0.42
1:M:214:GLY:HA3	1:M:329:ALA:HB3	2.02	0.42
1:N:61:LEU:HG	1:N:65:LEU:CD2	2.49	0.42
1:N:209:ARG:HB2	1:N:259:PRO:HG3	2.01	0.42
1:D:149:ARG:O	1:D:153:GLU:HG3	2.19	0.42
1:E:234:ALA:HB2	1:E:273:VAL:HG21	2.02	0.42
1:F:285:LEU:HD23	1:F:285:LEU:HA	1.84	0.42
1:I:30:ASN:H	1:I:246:ALA:HB1	1.84	0.42
1:L:42:GLU:OE2	1:L:293:ARG:NH2	2.51	0.42
1:O:153:GLU:O	1:O:157:LYS:HG3	2.19	0.42
1:A:135:LEU:HD12	1:A:135:LEU:HA	1.90	0.42
1:A:261:VAL:HG12	1:A:262:THR:HG23	2.00	0.42
1:D:108:THR:HG23	1:D:109:ALA:H	1.85	0.42
1:G:108:THR:O	1:G:112:LYS:HG2	2.20	0.42
1:H:248:VAL:HG12	1:H:276:LEU:HD21	2.02	0.42
1:L:294:LEU:HD11	1:L:350:LEU:HB3	2.02	0.42
1:O:61:LEU:HA	1:O:64:ILE:HD12	2.00	0.42
1:O:131:LYS:HA	1:O:131:LYS:HD2	1.63	0.42
1:E:54:LEU:HD23	1:E:364:VAL:HB	2.01	0.41
1:G:151:THR:O	1:G:155:VAL:HG13	2.20	0.41
1:H:366:LYS:HD3	1:H:366:LYS:HA	1.84	0.41
1:O:176:LEU:HD23	1:O:285:LEU:HD13	2.01	0.41
1:R:344:ILE:HG22	1:R:345:PRO:O	2.20	0.41
1:H:240:GLY:N	1:H:242:ASP:OD1	2.52	0.41
1:L:54:LEU:HA	1:L:54:LEU:HD23	1.81	0.41
1:C:200:ALA:HB3	1:C:265:PRO:HD2	2.02	0.41
1:F:282:LYS:HE3	1:F:282:LYS:HB2	1.92	0.41
1:R:114:ALA:O	1:R:117:LEU:N	2.54	0.41
1:R:123:HIS:O	1:R:127:LEU:HD22	2.20	0.41
5:X:2:NAG:H4	5:X:3:BMA:H2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:SER:OG	1:C:207:THR:N	2.54	0.41
1:D:206:SER:O	1:D:208:ASN:N	2.53	0.41
1:I:355:ILE:O	1:I:359:LYS:HG3	2.21	0.41
1:J:366:LYS:O	1:J:367:LEU:HB2	2.20	0.41
1:P:177:GLN:C	1:P:180:ILE:H	2.23	0.41
1:B:163:VAL:HG12	1:B:164:ALA:N	2.35	0.41
1:B:176:LEU:HD22	1:B:353:VAL:HG13	2.02	0.41
1:E:180:ILE:O	1:E:184:VAL:HG23	2.20	0.41
1:F:30:ASN:OD1	1:F:312:SER:HB2	2.21	0.41
1:G:103:TRP:O	1:G:107:TRP:HB2	2.20	0.41
1:Q:37:LEU:HD13	1:Q:229:LEU:HA	2.03	0.41
1:D:362:ARG:HA	1:D:362:ARG:HD3	1.69	0.41
1:H:231:CYS:HB2	1:H:328:VAL:HG22	2.02	0.41
1:H:249:ALA:HB1	1:I:313:PHE:HD1	1.86	0.41
1:I:176:LEU:O	1:I:180:ILE:HD12	2.20	0.41
1:K:90:ARG:NH2	1:K:96:PRO:O	2.53	0.41
1:L:55:PRO:HD3	1:L:364:VAL:HG23	2.03	0.41
1:O:228:ALA:O	1:O:232:VAL:HG23	2.20	0.41
1:A:56:ASN:O	1:A:60:GLU:HG2	2.20	0.41
1:E:259:PRO:HA	1:E:263:ALA:HA	2.02	0.41
1:G:294:LEU:HD21	1:G:350:LEU:HD23	2.03	0.41
1:G:302:THR:N	1:G:309:ILE:O	2.53	0.41
1:K:286:SER:O	1:K:290:ILE:HG12	2.20	0.41
1:A:155:VAL:O	1:A:159:GLN:HG3	2.20	0.41
1:C:72:ALA:HA	1:C:144:ARG:HD3	2.03	0.41
1:C:176:LEU:HD13	1:C:357:LEU:HD21	2.03	0.41
1:F:209:ARG:HD3	1:F:319:SER:C	2.41	0.41
1:G:54:LEU:CD2	1:G:56:ASN:HB2	2.50	0.41
1:G:195:PHE:HB2	1:G:267:GLY:HA3	2.03	0.41
1:G:242:ASP:HB3	1:G:322:GLN:CG	2.49	0.41
1:H:320:GLY:HA2	1:H:326:MET:SD	2.61	0.41
1:I:115:LEU:HB3	1:I:116:PRO:HD3	2.02	0.41
1:I:257:TRP:HB2	1:I:266:THR:HB	2.02	0.41
1:J:285:LEU:HD23	1:J:285:LEU:HA	1.94	0.41
1:L:389:LEU:HD12	1:L:389:LEU:HA	1.88	0.41
1:M:360:HIS:O	1:M:364:VAL:HG13	2.21	0.41
1:O:212:ILE:H	1:O:212:ILE:HG13	1.61	0.41
1:C:101:THR:C	1:C:103:TRP:H	2.24	0.41
1:D:71:ALA:HB2	1:D:132:LEU:HD22	2.03	0.41
1:E:209:ARG:NH1	1:E:320:GLY:HA3	2.36	0.41
1:J:143:ALA:HA	1:J:387:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:160:ASP:OD1	1:M:162:THR:OG1	2.31	0.41
1:A:366:LYS:NZ	10:A:610:HOH:O	2.52	0.40
1:F:285:LEU:HD22	1:F:290:ILE:HD11	2.03	0.40
1:H:45:GLY:C	1:H:46:LYS:HD2	2.41	0.40
1:H:64:ILE:HG22	1:H:151:THR:HG23	2.03	0.40
1:I:195:PHE:HD2	1:I:198:TYR:CD1	2.39	0.40
1:J:140:LEU:O	1:J:144:ARG:HB2	2.20	0.40
1:K:314:LEU:HD23	1:K:314:LEU:HA	1.93	0.40
1:M:342:LYS:HB3	1:M:342:LYS:HE2	1.93	0.40
1:N:364:VAL:HA	1:N:367:LEU:HD23	2.03	0.40
1:O:235:ASP:OD1	1:O:253:PRO:HG2	2.21	0.40
1:D:313:PHE:CD1	1:F:249:ALA:HB1	2.57	0.40
1:I:32:LEU:HD13	1:I:300:LEU:HD21	2.03	0.40
1:I:316:THR:HG22	1:I:317:ASP:HB3	2.03	0.40
1:J:176:LEU:HD22	1:J:353:VAL:HG13	2.04	0.40
1:A:214:GLY:HA3	1:A:329:ALA:HB3	2.03	0.40
1:H:245:LYS:HE2	1:H:249:ALA:O	2.21	0.40
1:L:67:LEU:HD13	1:L:130:TYR:CD1	2.57	0.40
1:M:210:GLN:H	1:M:210:GLN:HG2	1.52	0.40
1:N:285:LEU:HD12	1:N:285:LEU:HA	1.87	0.40
1:B:123:HIS:O	1:B:127:LEU:HB2	2.21	0.40
1:G:227:ASP:OD1	1:G:227:ASP:N	2.54	0.40
1:H:236:ASP:OD1	1:H:236:ASP:N	2.53	0.40
1:I:40:ILE:HG21	1:I:346:TRP:HZ3	1.86	0.40
1:I:67:LEU:HD23	1:I:67:LEU:HA	1.85	0.40
1:N:265:PRO:HA	1:N:269:MET:HE3	2.02	0.40
1:N:266:THR:H	1:N:269:MET:CE	2.33	0.40
1:R:60:GLU:H	1:R:60:GLU:CD	2.24	0.40
1:B:301:LEU:HD23	1:B:310:LEU:HB2	2.03	0.40
1:D:249:ALA:HB1	1:E:313:PHE:CD1	2.56	0.40
1:J:214:GLY:HA3	1:J:329:ALA:HB3	2.03	0.40

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	364/410 (89%)	351 (96%)	12 (3%)	1 (0%)	41	64
1	B	364/410 (89%)	340 (93%)	21 (6%)	3 (1%)	19	39
1	C	364/410 (89%)	341 (94%)	23 (6%)	0	100	100
1	D	313/410 (76%)	297 (95%)	15 (5%)	1 (0%)	41	64
1	E	281/410 (68%)	254 (90%)	26 (9%)	1 (0%)	34	57
1	F	274/410 (67%)	253 (92%)	21 (8%)	0	100	100
1	G	363/410 (88%)	326 (90%)	33 (9%)	4 (1%)	14	30
1	H	283/410 (69%)	255 (90%)	23 (8%)	5 (2%)	8	16
1	I	323/410 (79%)	287 (89%)	32 (10%)	4 (1%)	13	27
1	J	364/410 (89%)	349 (96%)	14 (4%)	1 (0%)	41	64
1	K	363/410 (88%)	345 (95%)	17 (5%)	1 (0%)	41	64
1	L	354/410 (86%)	340 (96%)	13 (4%)	1 (0%)	41	64
1	M	281/410 (68%)	268 (95%)	13 (5%)	0	100	100
1	N	347/410 (85%)	329 (95%)	18 (5%)	0	100	100
1	O	293/410 (72%)	265 (90%)	28 (10%)	0	100	100
1	P	253/410 (62%)	237 (94%)	16 (6%)	0	100	100
1	Q	266/410 (65%)	246 (92%)	19 (7%)	1 (0%)	34	57
1	R	300/410 (73%)	282 (94%)	16 (5%)	2 (1%)	22	43
All	All	5750/7380 (78%)	5365 (93%)	360 (6%)	25 (0%)	34	57

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	162	THR
1	D	70	THR
1	E	208	ASN
1	G	134	GLY
1	G	318	CYS
1	Q	159	GLN
1	G	315	ALA
1	R	162	THR
1	H	68	ASN
1	I	301	LEU
1	K	135	LEU

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Mol	Chain	Res	Type
1	L	207	THR
1	A	207	THR
1	H	207	THR
1	H	316	THR
1	B	207	THR
1	G	317	ASP
1	I	243	ALA
1	J	207	THR
1	B	160	ASP
1	H	242	ASP
1	I	97	LEU
1	R	207	THR
1	H	252	ALA
1	I	96	PRO

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	288/330 (87%)	275 (96%)	13 (4%)	27	52
1	B	278/330 (84%)	267 (96%)	11 (4%)	31	57
1	C	281/330 (85%)	272 (97%)	9 (3%)	39	65
1	D	237/330 (72%)	226 (95%)	11 (5%)	27	51
1	E	211/330 (64%)	201 (95%)	10 (5%)	26	50
1	F	212/330 (64%)	203 (96%)	9 (4%)	30	55
1	G	280/330 (85%)	265 (95%)	15 (5%)	22	44
1	H	211/330 (64%)	200 (95%)	11 (5%)	23	46
1	I	243/330 (74%)	218 (90%)	25 (10%)	7	13
1	J	287/330 (87%)	283 (99%)	4 (1%)	67	85
1	K	277/330 (84%)	268 (97%)	9 (3%)	39	65
1	L	275/330 (83%)	270 (98%)	5 (2%)	59	80
1	M	215/330 (65%)	210 (98%)	5 (2%)	50	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	269/330 (82%)	256 (95%)	13 (5%)	25 49
1	O	222/330 (67%)	205 (92%)	17 (8%)	13 25
1	P	196/330 (59%)	188 (96%)	8 (4%)	30 56
1	Q	205/330 (62%)	199 (97%)	6 (3%)	42 68
1	R	223/330 (68%)	217 (97%)	6 (3%)	44 71
All	All	4410/5940 (74%)	4223 (96%)	187 (4%)	30 55

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	81	ARG
1	A	108	THR
1	A	120	ASP
1	A	124	GLN
1	A	171	THR
1	A	172	THR
1	A	179	GLN
1	A	237	ARG
1	A	238	THR
1	A	242	ASP
1	A	286	SER
1	A	362	ARG
1	B	57	PHE
1	B	75	THR
1	B	84	ASP
1	B	92	LEU
1	B	105	ASP
1	B	115	LEU
1	B	162	THR
1	B	242	ASP
1	B	367	LEU
1	B	388	GLN
1	B	389	LEU
1	C	107	TRP
1	C	128	LYS
1	C	135	LEU
1	C	189	THR
1	C	242	ASP
1	C	282	LYS

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Mol	Chain	Res	Type
1	C	286	SER
1	C	358	GLN
1	C	389	LEU
1	D	50	LEU
1	D	108	THR
1	D	126	LYS
1	D	132	LEU
1	D	169	ASP
1	D	242	ASP
1	D	282	LYS
1	D	305	SER
1	D	362	ARG
1	D	367	LEU
1	D	380	LEU
1	E	27	THR
1	E	52	THR
1	E	63	SER
1	E	188	ASP
1	E	269	MET
1	E	276	LEU
1	E	280	HIS
1	E	305	SER
1	E	365	GLU
1	E	371	GLN
1	F	106	HIS
1	F	210	GLN
1	F	237	ARG
1	F	238	THR
1	F	242	ASP
1	F	251	THR
1	F	286	SER
1	F	327	CYS
1	F	376	THR
1	G	57	PHE
1	G	120	ASP
1	G	127	LEU
1	G	142	ARG
1	G	199	THR
1	G	226	MET
1	G	236	ASP
1	G	238	THR
1	G	242	ASP

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Mol	Chain	Res	Type
1	G	264	THR
1	G	282	LYS
1	G	327	CYS
1	G	328	VAL
1	G	331	THR
1	G	333	VAL
1	H	32	LEU
1	H	46	LYS
1	H	50	LEU
1	H	188	ASP
1	H	209	ARG
1	H	211	THR
1	H	223	THR
1	H	286	SER
1	H	331	THR
1	H	341	THR
1	H	359	LYS
1	I	40	ILE
1	I	41	ILE
1	I	51	GLU
1	I	61	LEU
1	I	64	ILE
1	I	106	HIS
1	I	108	THR
1	I	136	GLN
1	I	140	LEU
1	I	172	THR
1	I	196	ASN
1	I	231	CYS
1	I	232	VAL
1	I	235	ASP
1	I	239	ASN
1	I	255	THR
1	I	280	HIS
1	I	286	SER
1	I	314	LEU
1	I	317	ASP
1	I	324	SER
1	I	327	CYS
1	I	328	VAL
1	I	350	LEU
1	I	371	GLN

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Mol	Chain	Res	Type
1	J	84	ASP
1	J	238	THR
1	J	242	ASP
1	J	389	LEU
1	K	86	ARG
1	K	120	ASP
1	K	142	ARG
1	K	206	SER
1	K	248	VAL
1	K	282	LYS
1	K	286	SER
1	K	309	ILE
1	K	316	THR
1	L	171	THR
1	L	172	THR
1	L	242	ASP
1	L	286	SER
1	L	388	GLN
1	M	65	LEU
1	M	317	ASP
1	M	362	ARG
1	M	383	ASP
1	M	387	LEU
1	N	83	LYS
1	N	100	ASP
1	N	102	ASN
1	N	106	HIS
1	N	107	TRP
1	N	122	THR
1	N	127	LEU
1	N	179	GLN
1	N	217	VAL
1	N	229	LEU
1	N	242	ASP
1	N	251	THR
1	N	367	LEU
1	O	67	LEU
1	O	69	MET
1	O	127	LEU
1	O	128	LYS
1	O	129	GLU
1	O	131	LYS

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Mol	Chain	Res	Type
1	O	171	THR
1	O	179	GLN
1	O	207	THR
1	O	237	ARG
1	O	266	THR
1	O	321	ASP
1	O	341	THR
1	O	360	HIS
1	O	367	LEU
1	O	379	THR
1	O	380	LEU
1	P	192	ASP
1	P	223	THR
1	P	231	CYS
1	P	242	ASP
1	P	322	GLN
1	P	337	LYS
1	P	348	GLN
1	P	367	LEU
1	Q	63	SER
1	Q	179	GLN
1	Q	321	ASP
1	Q	337	LYS
1	Q	357	LEU
1	Q	373	ASP
1	R	57	PHE
1	R	236	ASP
1	R	242	ASP
1	R	282	LYS
1	R	346	TRP
1	R	366	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	196	ASN
1	I	136	GLN
1	N	106	HIS
1	N	371	GLN
1	O	278	ASN
1	P	182	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

49 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	S	1	1,2	14,14,15	0.43	0	17,19,21	0.59	0
2	NAG	S	2	2	14,14,15	0.36	0	17,19,21	0.58	0
2	BMA	S	3	2	11,11,12	0.39	0	15,15,17	0.78	1 (6%)
2	MAN	S	4	2	11,11,12	0.21	0	15,15,17	0.59	0
2	MAN	S	5	2	11,11,12	0.40	0	15,15,17	0.69	0
2	MAN	S	6	2	11,11,12	0.63	0	15,15,17	0.77	1 (6%)
3	NAG	T	1	1,3	14,14,15	0.53	0	17,19,21	1.03	2 (11%)
3	NAG	T	2	3	14,14,15	0.40	0	17,19,21	0.91	1 (5%)
3	BMA	T	3	3	11,11,12	0.25	0	15,15,17	0.87	1 (6%)
3	MAN	T	4	3	11,11,12	0.41	0	15,15,17	0.66	0
3	MAN	T	5	3	11,11,12	0.37	0	15,15,17	0.62	0
4	NAG	U	1	1,4	14,14,15	0.51	0	17,19,21	0.82	1 (5%)
4	NAG	U	2	4	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
4	BMA	U	3	4	11,11,12	0.28	0	15,15,17	0.69	0
5	NAG	V	1	5,1	14,14,15	0.34	0	17,19,21	0.56	0
5	NAG	V	2	5	14,14,15	0.42	0	17,19,21	0.53	0
5	BMA	V	3	5	11,11,12	0.29	0	15,15,17	0.63	0
6	NAG	W	1	1,6	14,14,15	0.57	0	17,19,21	1.07	2 (11%)
6	NAG	W	2	6	14,14,15	0.40	0	17,19,21	0.77	0
6	BMA	W	3	6	11,11,12	0.35	0	15,15,17	0.71	0
6	MAN	W	4	6	11,11,12	0.32	0	15,15,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	W	5	6	11,11,12	0.39	0	15,15,17	0.68	0
5	NAG	X	1	5,1	14,14,15	0.37	0	17,19,21	0.58	0
5	NAG	X	2	5	14,14,15	0.35	0	17,19,21	0.65	0
5	BMA	X	3	5	11,11,12	0.29	0	15,15,17	0.60	0
5	NAG	Y	1	5,1	14,14,15	0.38	0	17,19,21	0.62	0
5	NAG	Y	2	5	14,14,15	0.35	0	17,19,21	0.66	0
5	BMA	Y	3	5	11,11,12	0.29	0	15,15,17	0.64	0
2	NAG	Z	1	1,2	14,14,15	0.36	0	17,19,21	0.67	0
2	NAG	Z	2	2	14,14,15	0.34	0	17,19,21	0.58	0
2	BMA	Z	3	2	11,11,12	0.37	0	15,15,17	0.66	0
2	MAN	Z	4	2	11,11,12	0.30	0	15,15,17	0.63	0
2	MAN	Z	5	2	11,11,12	0.33	0	15,15,17	0.62	0
2	MAN	Z	6	2	11,11,12	0.29	0	15,15,17	0.64	0
7	NAG	a	1	1,7	14,14,15	0.34	0	17,19,21	0.65	0
7	NAG	a	2	7	14,14,15	0.30	0	17,19,21	0.60	0
7	BMA	a	3	7	11,11,12	0.26	0	15,15,17	0.83	0
7	MAN	a	4	7	11,11,12	0.25	0	15,15,17	0.62	0
7	MAN	a	5	7	11,11,12	1.51	2 (18%)	15,15,17	0.89	1 (6%)
7	NAG	b	1	1,7	14,14,15	0.33	0	17,19,21	0.61	0
7	NAG	b	2	7	14,14,15	0.30	0	17,19,21	0.60	0
7	BMA	b	3	7	11,11,12	0.23	0	15,15,17	0.63	0
7	MAN	b	4	7	11,11,12	0.39	0	15,15,17	0.68	0
7	MAN	b	5	7	11,11,12	0.22	0	15,15,17	0.64	0
6	NAG	c	1	1,6	14,14,15	0.53	0	17,19,21	0.87	0
6	NAG	c	2	6	14,14,15	0.54	0	17,19,21	0.69	0
6	BMA	c	3	6	11,11,12	0.48	0	15,15,17	0.78	0
6	MAN	c	4	6	11,11,12	0.39	0	15,15,17	0.69	0
6	MAN	c	5	6	11,11,12	0.27	0	15,15,17	0.64	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	S	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	S	2	2	-	2/6/23/26	0/1/1/1
2	BMA	S	3	2	-	0/2/19/22	0/1/1/1
2	MAN	S	4	2	-	0/2/19/22	0/1/1/1
2	MAN	S	5	2	-	0/2/19/22	0/1/1/1
2	MAN	S	6	2	-	0/2/19/22	0/1/1/1
3	NAG	T	1	1,3	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	BMA	T	3	3	-	0/2/19/22	0/1/1/1
3	MAN	T	4	3	-	1/2/19/22	0/1/1/1
3	MAN	T	5	3	-	2/2/19/22	0/1/1/1
4	NAG	U	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1
4	BMA	U	3	4	-	0/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	BMA	V	3	5	-	1/2/19/22	0/1/1/1
6	NAG	W	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	W	2	6	-	3/6/23/26	0/1/1/1
6	BMA	W	3	6	-	2/2/19/22	0/1/1/1
6	MAN	W	4	6	-	0/2/19/22	0/1/1/1
6	MAN	W	5	6	-	0/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	3/6/23/26	0/1/1/1
5	BMA	X	3	5	-	0/2/19/22	0/1/1/1
5	NAG	Y	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	0/2/19/22	0/1/1/1
2	NAG	Z	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	0/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	0/2/19/22	0/1/1/1
2	MAN	Z	4	2	-	0/2/19/22	0/1/1/1
2	MAN	Z	5	2	-	1/2/19/22	0/1/1/1
2	MAN	Z	6	2	-	0/2/19/22	0/1/1/1
7	NAG	a	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
7	BMA	a	3	7	-	2/2/19/22	0/1/1/1
7	MAN	a	4	7	-	0/2/19/22	0/1/1/1
7	MAN	a	5	7	-	1/2/19/22	0/1/1/1
7	NAG	b	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
7	BMA	b	3	7	-	0/2/19/22	0/1/1/1
7	MAN	b	4	7	-	0/2/19/22	0/1/1/1
7	MAN	b	5	7	-	0/2/19/22	0/1/1/1
6	NAG	c	1	1,6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	c	2	6	-	4/6/23/26	0/1/1/1
6	BMA	c	3	6	-	2/2/19/22	0/1/1/1
6	MAN	c	4	6	-	0/2/19/22	0/1/1/1
6	MAN	c	5	6	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	5	MAN	O5-C1	4.06	1.50	1.43
7	a	5	MAN	C1-C2	2.71	1.58	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	1	NAG	O5-C1-C2	-2.43	107.45	111.29
3	T	2	NAG	O5-C1-C2	-2.42	107.47	111.29
3	T	1	NAG	C3-C4-C5	2.35	114.43	110.24
7	a	5	MAN	C1-C2-C3	2.35	112.55	109.67
4	U	2	NAG	O5-C1-C2	-2.33	107.60	111.29
3	T	1	NAG	O5-C1-C2	-2.27	107.71	111.29
4	U	1	NAG	O5-C1-C2	-2.06	108.03	111.29
2	S	3	BMA	C1-C2-C3	2.06	112.19	109.67
3	T	3	BMA	C1-C2-C3	2.05	112.18	109.67
2	S	6	MAN	C1-C2-C3	2.02	112.15	109.67
6	W	1	NAG	C3-C4-C5	2.02	113.84	110.24

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	1	NAG	C8-C7-N2-C2
5	Y	1	NAG	O7-C7-N2-C2
6	W	1	NAG	C1-C2-N2-C7
6	W	1	NAG	C8-C7-N2-C2
6	W	1	NAG	O7-C7-N2-C2
6	W	2	NAG	C8-C7-N2-C2
6	W	2	NAG	O7-C7-N2-C2
6	W	3	BMA	C4-C5-C6-O6
6	c	5	MAN	C4-C5-C6-O6
6	c	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	b	1	NAG	C8-C7-N2-C2
3	T	5	MAN	C4-C5-C6-O6
6	W	3	BMA	O5-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
2	S	2	NAG	C8-C7-N2-C2
2	S	2	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
6	c	2	NAG	C8-C7-N2-C2
7	b	1	NAG	O7-C7-N2-C2
6	c	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
6	c	2	NAG	O7-C7-N2-C2
7	a	2	NAG	C8-C7-N2-C2
7	a	2	NAG	O7-C7-N2-C2
7	a	3	BMA	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	T	4	MAN	O5-C5-C6-O6
3	T	5	MAN	O5-C5-C6-O6
5	V	1	NAG	C8-C7-N2-C2
7	a	3	BMA	O5-C5-C6-O6
5	V	1	NAG	O7-C7-N2-C2
2	Z	1	NAG	C8-C7-N2-C2
3	T	1	NAG	C4-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
2	Z	5	MAN	O5-C5-C6-O6
7	a	5	MAN	O5-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
6	c	3	BMA	C4-C5-C6-O6
6	c	1	NAG	C8-C7-N2-C2
2	Z	1	NAG	O7-C7-N2-C2
6	c	3	BMA	O5-C5-C6-O6
6	c	1	NAG	O7-C7-N2-C2
6	W	1	NAG	C4-C5-C6-O6
6	c	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C3-C2-N2-C7
5	X	2	NAG	C3-C2-N2-C7
5	X	2	NAG	C1-C2-N2-C7

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	T	1	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
5	V	2	NAG	C1-C2-N2-C7

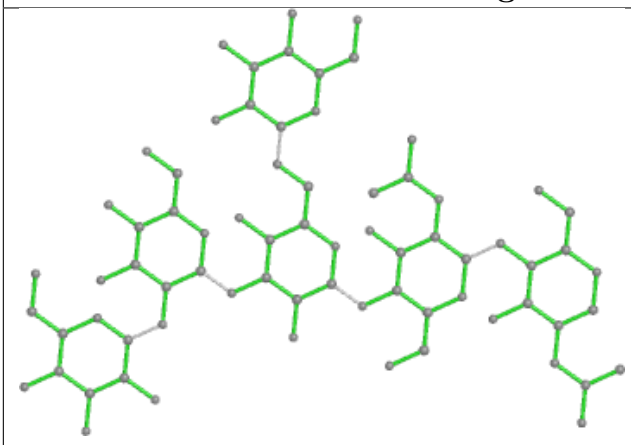
There are no ring outliers.

13 monomers are involved in 11 short contacts:

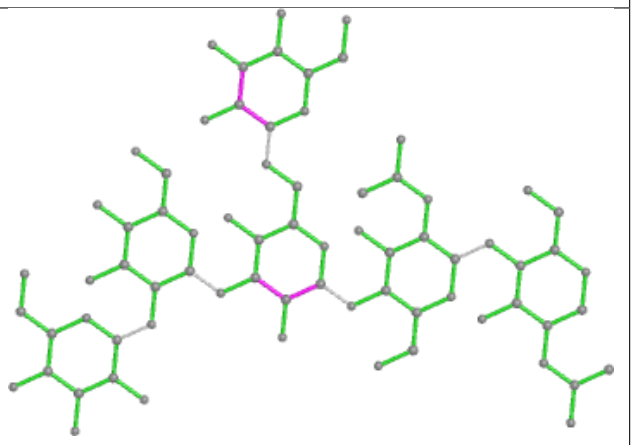
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	X	2	NAG	1	0
4	U	1	NAG	1	0
5	Y	1	NAG	1	0
4	U	2	NAG	1	0
5	X	3	BMA	1	0
6	W	1	NAG	1	0
5	Y	3	BMA	1	0
3	T	1	NAG	1	0
3	T	5	MAN	1	0
3	T	3	BMA	1	0
6	W	3	BMA	1	0
2	S	3	BMA	1	0
3	T	2	NAG	1	0

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

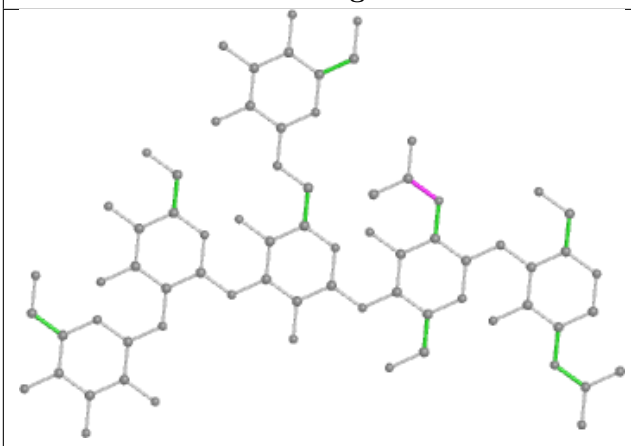
Oligosaccharide Chain S



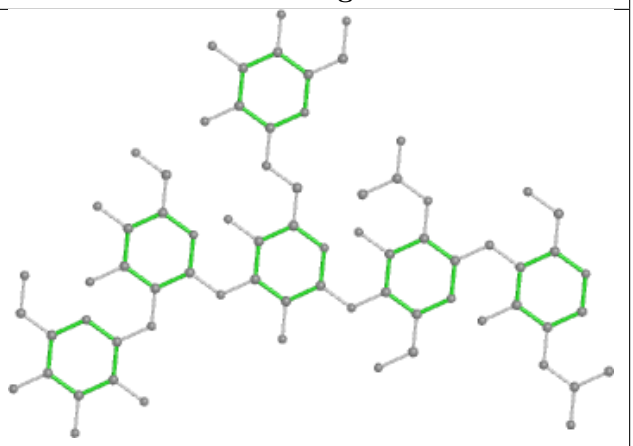
Bond lengths



Bond angles

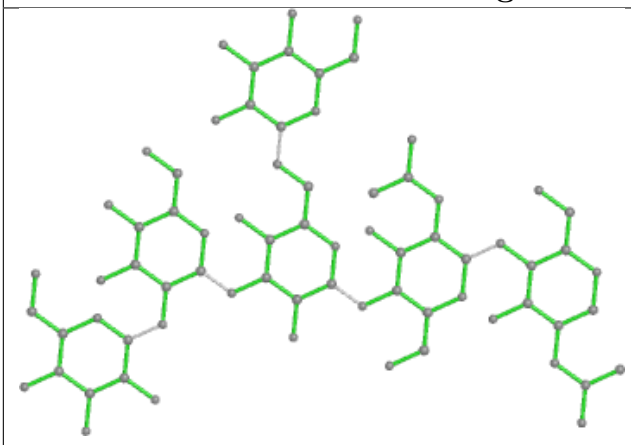


Torsions

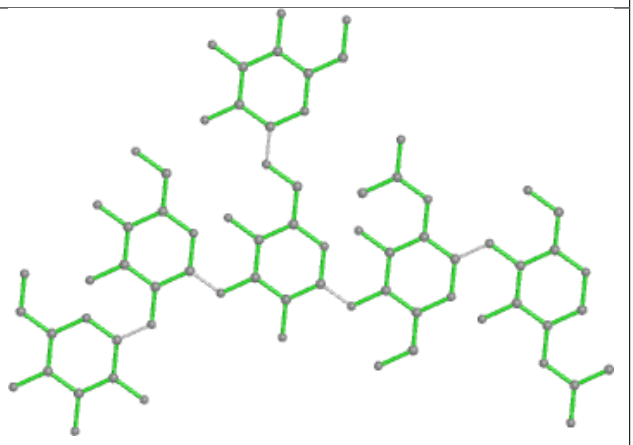


Rings

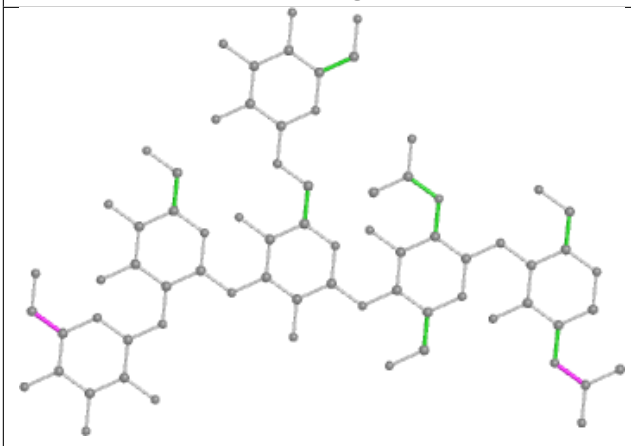
Oligosaccharide Chain Z



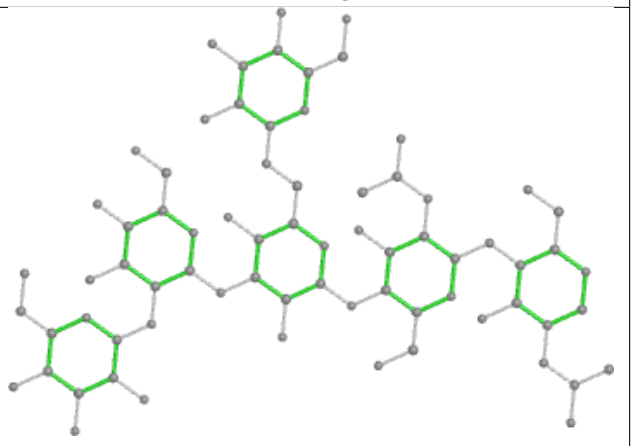
Bond lengths



Bond angles

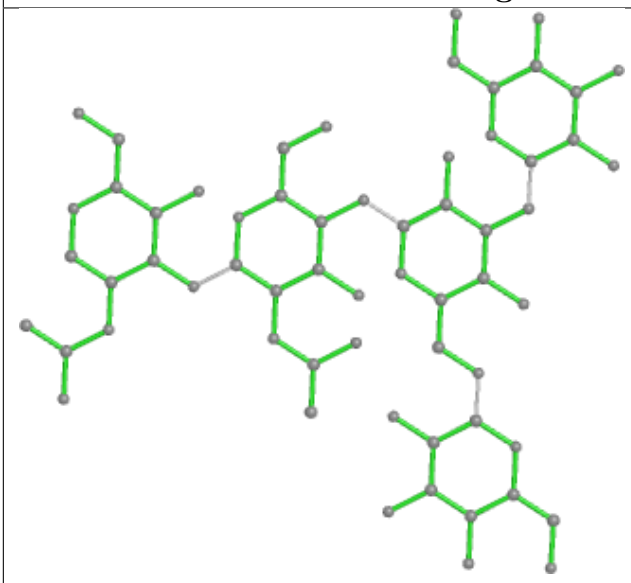


Torsions

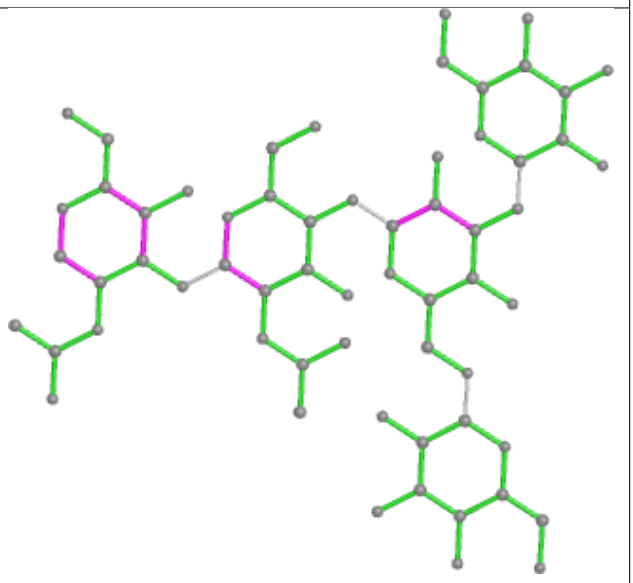


Rings

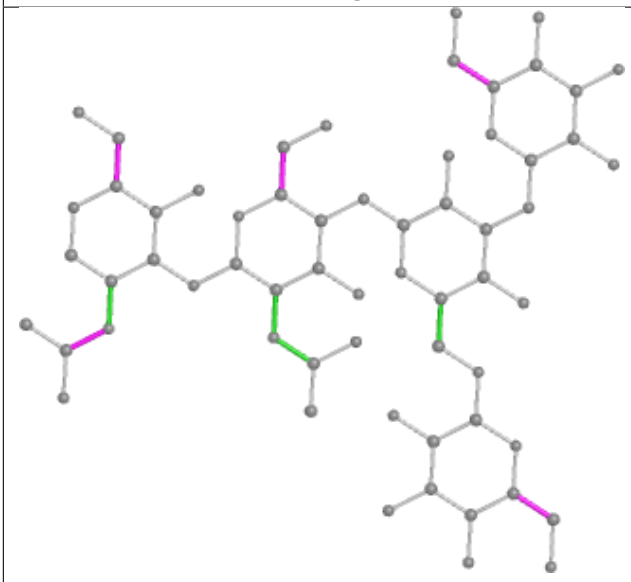
Oligosaccharide Chain T



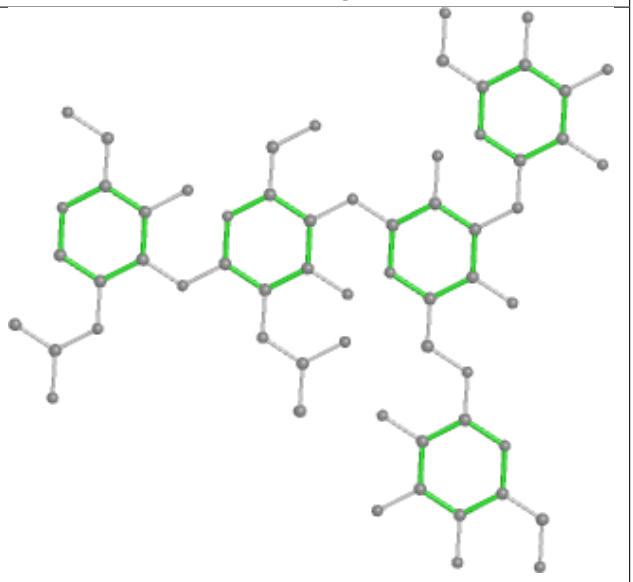
Bond lengths



Bond angles

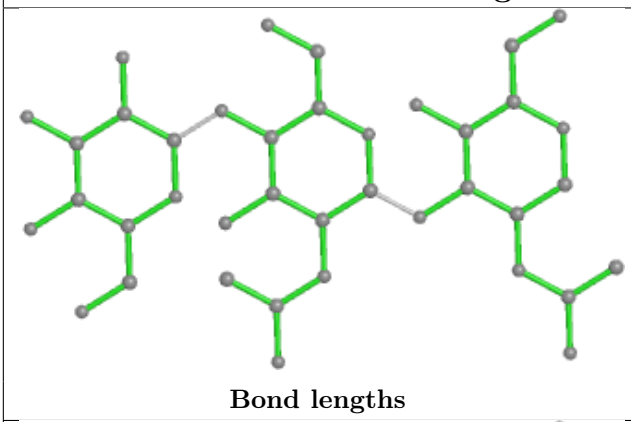


Torsions

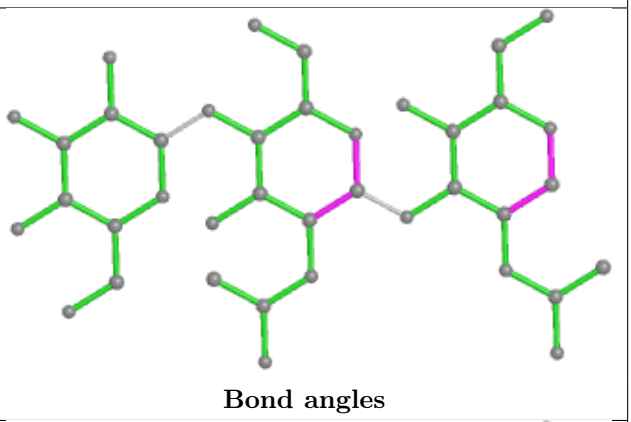


Rings

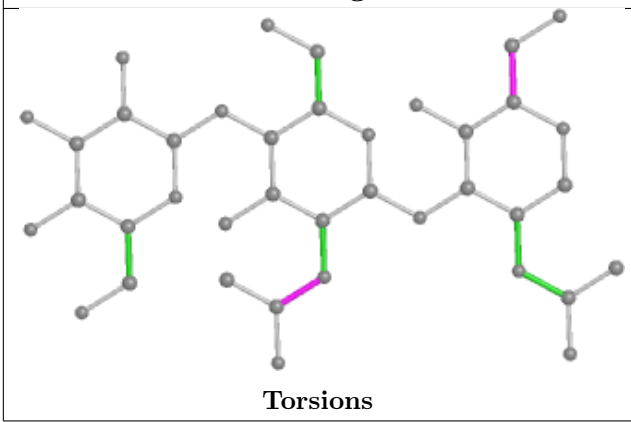
Oligosaccharide Chain U



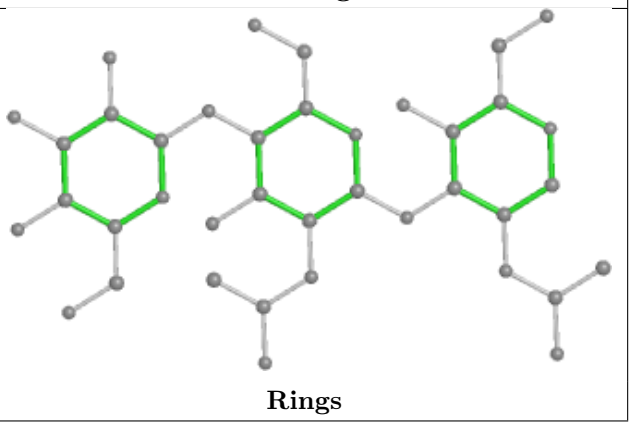
Bond lengths



Bond angles

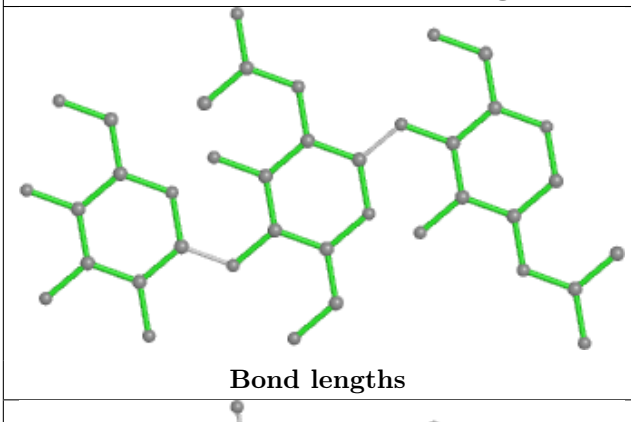


Torsions

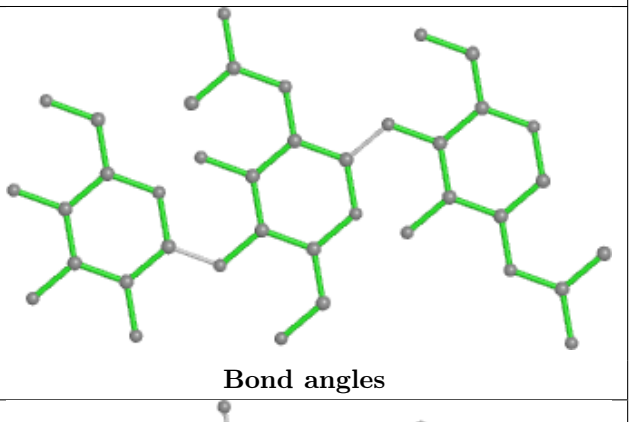


Rings

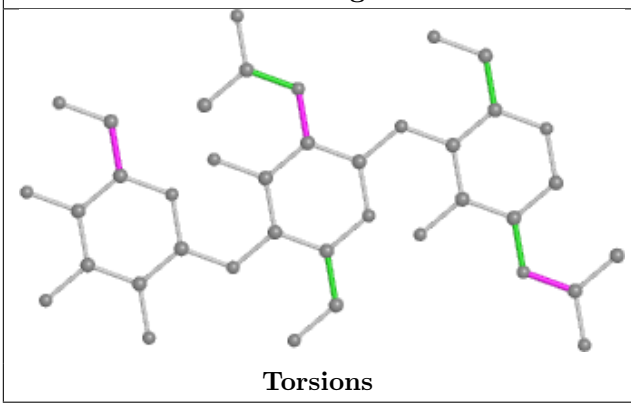
Oligosaccharide Chain V



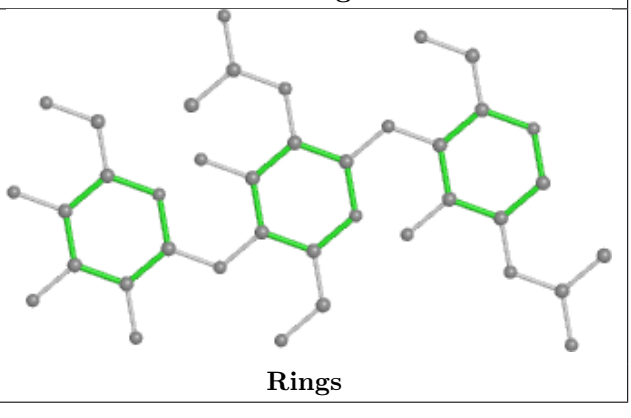
Bond lengths



Bond angles

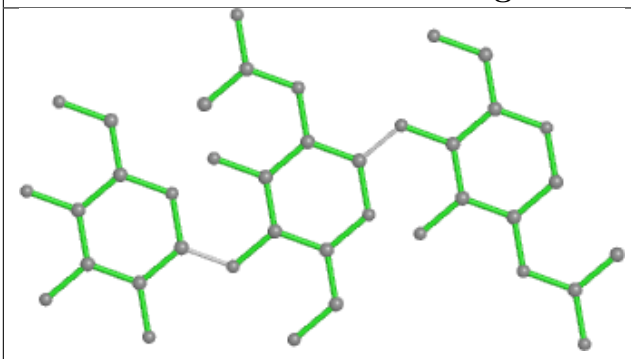


Torsions

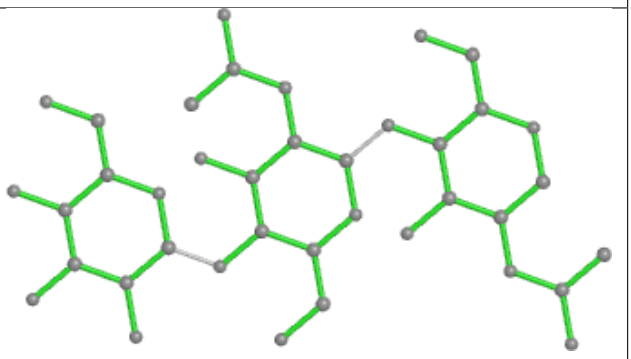


Rings

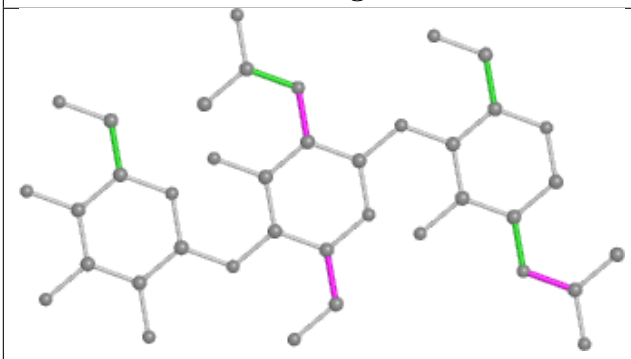
Oligosaccharide Chain X



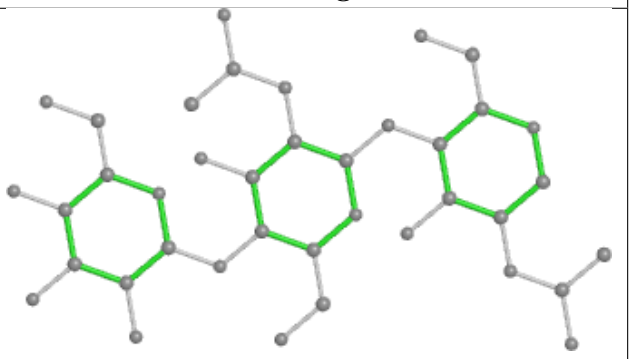
Bond lengths



Bond angles

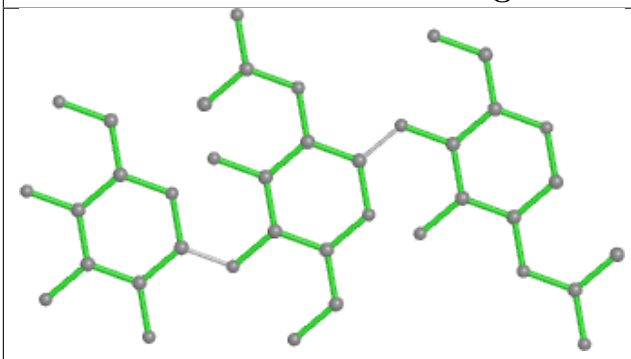


Torsions

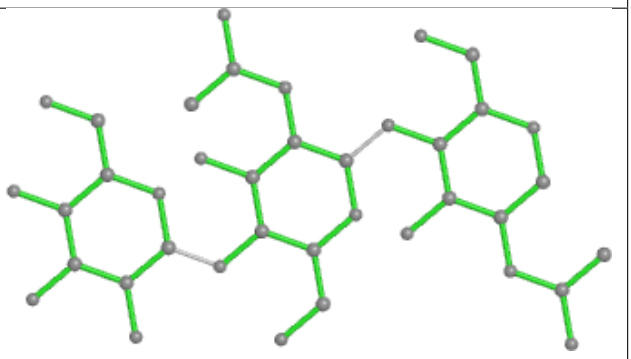


Rings

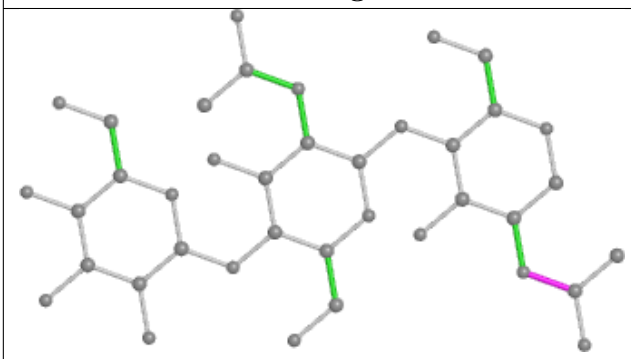
Oligosaccharide Chain Y



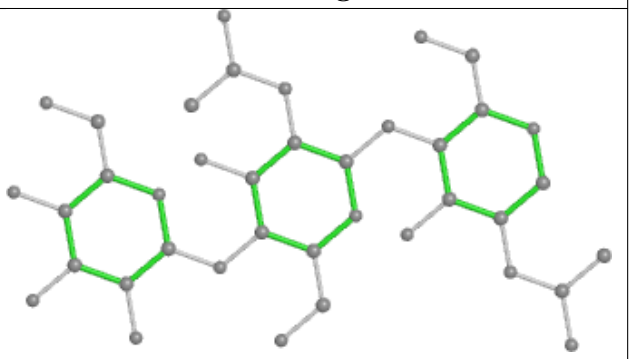
Bond lengths



Bond angles

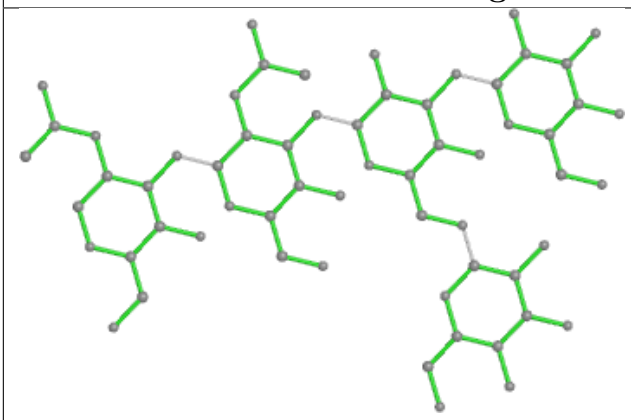


Torsions

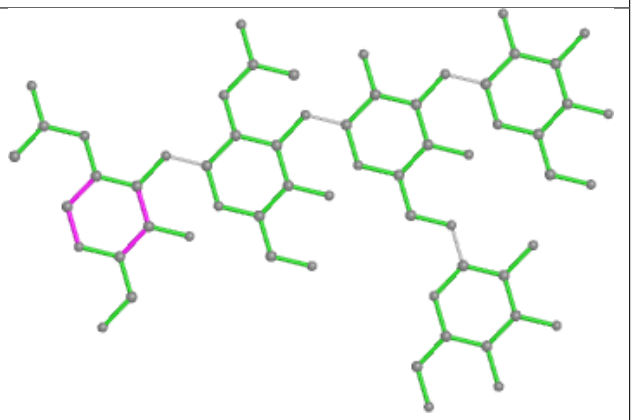


Rings

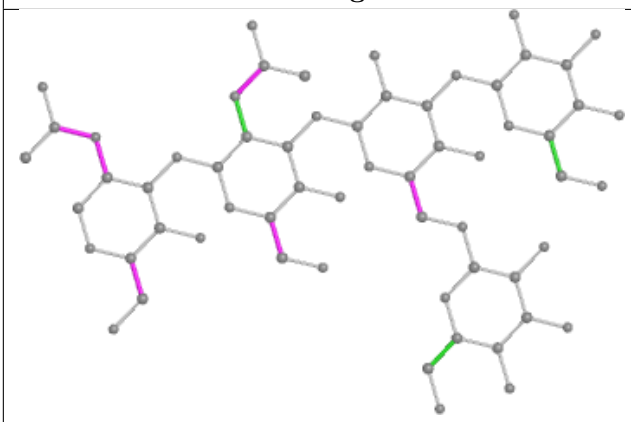
Oligosaccharide Chain W



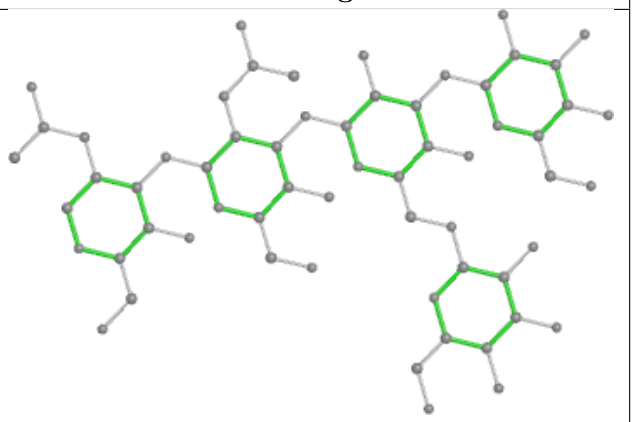
Bond lengths



Bond angles

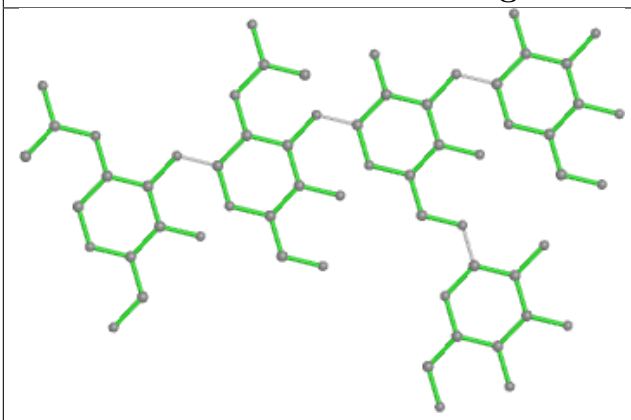


Torsions

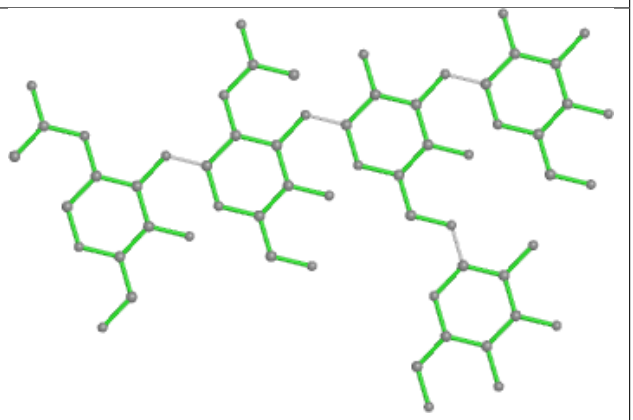


Rings

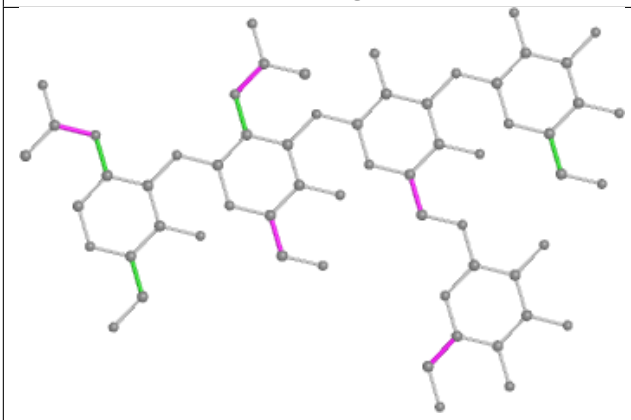
Oligosaccharide Chain c



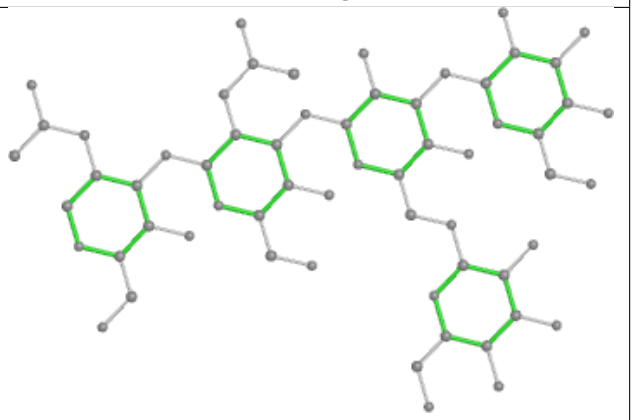
Bond lengths



Bond angles

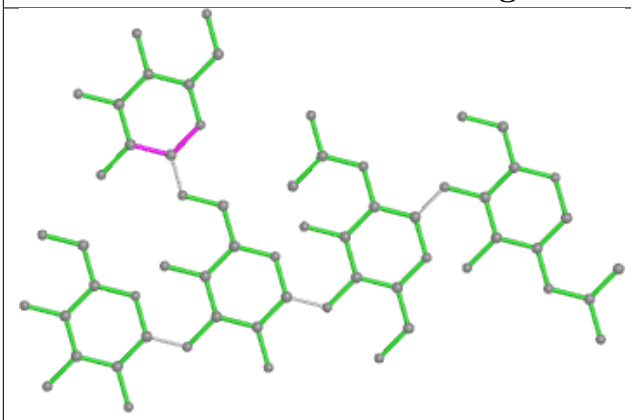


Torsions

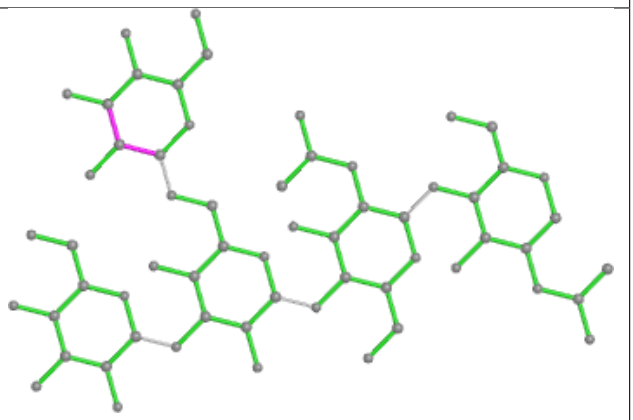


Rings

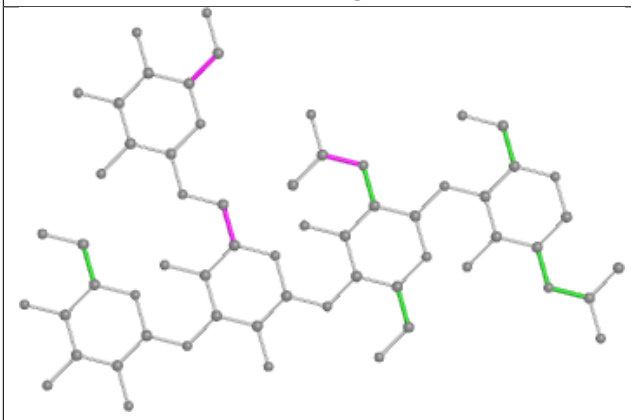
Oligosaccharide Chain a



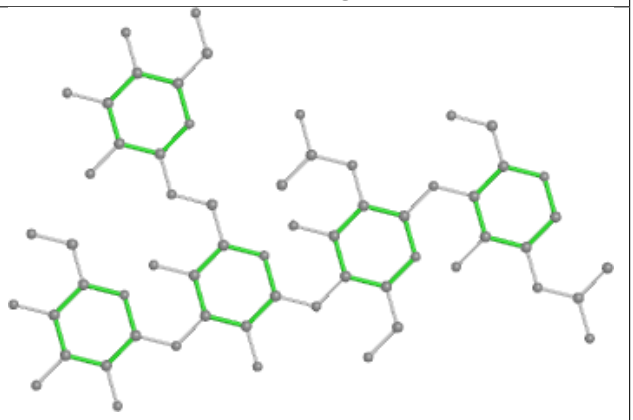
Bond lengths



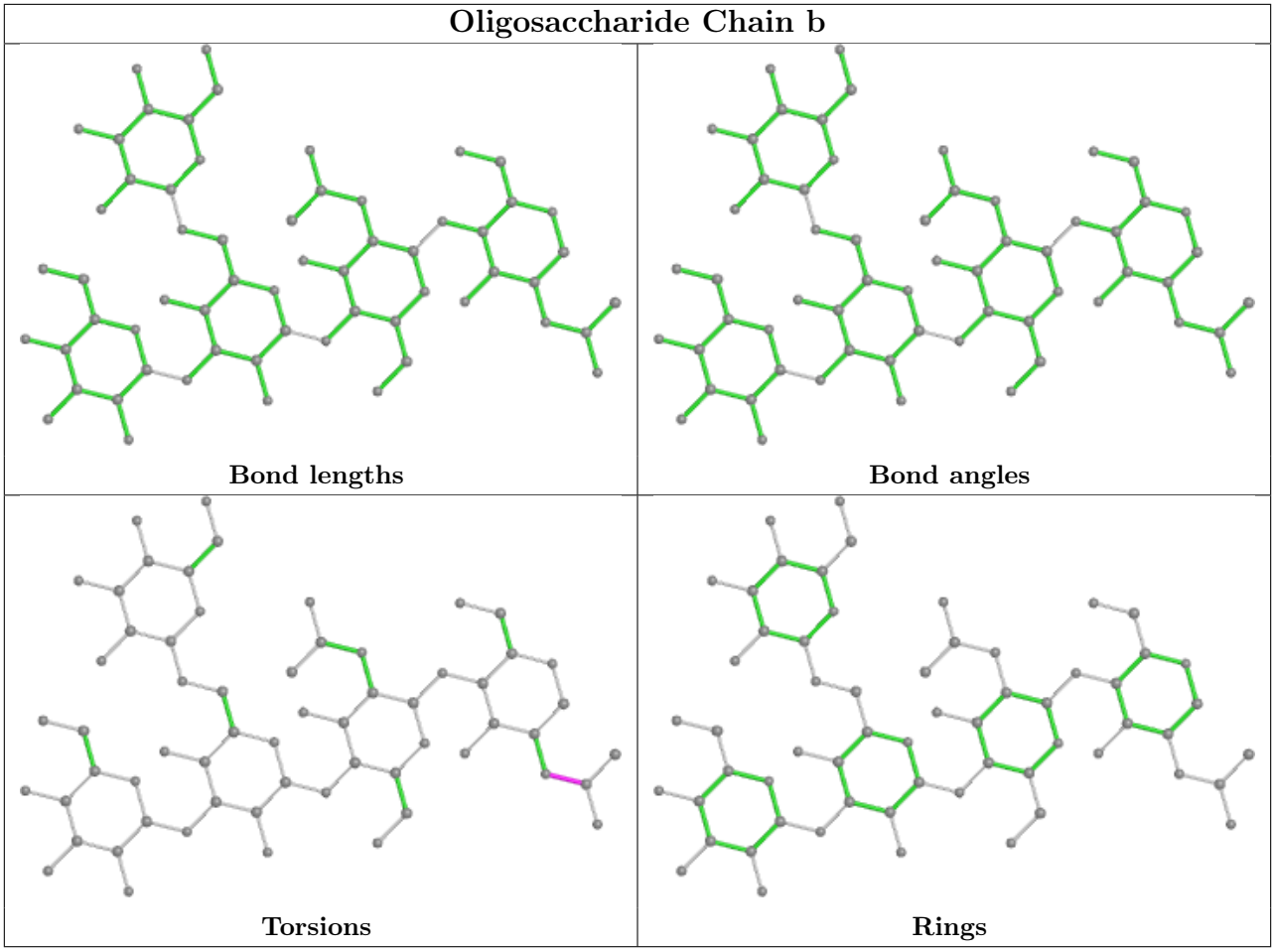
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

21 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	NAG	R	501	1	14,14,15	0.30	0	17,19,21	0.55	0
8	GLC	J	501	1	11,11,12	0.83	0	15,15,17	0.61	0
8	GLC	D	501	1	11,11,12	0.79	0	15,15,17	0.62	0
8	GLC	P	501	1	11,11,12	0.83	0	15,15,17	0.64	0
8	GLC	R	502	1	11,11,12	0.83	0	15,15,17	0.61	0
8	GLC	L	501	1	11,11,12	0.76	0	15,15,17	0.59	0
8	GLC	O	501	1	11,11,12	0.80	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GLC	F	501	1	11,11,12	0.72	0	15,15,17	0.68	0
8	GLC	C	501	1	11,11,12	0.73	0	15,15,17	0.60	0
8	GLC	H	501	1	11,11,12	0.79	0	15,15,17	0.75	0
9	NAG	E	502	1	14,14,15	0.50	0	17,19,21	0.57	0
8	GLC	I	501	1	11,11,12	0.82	0	15,15,17	0.63	0
8	GLC	E	501	1	11,11,12	0.80	0	15,15,17	0.61	0
8	GLC	N	501	1	11,11,12	0.74	0	15,15,17	0.62	0
8	GLC	B	501	1	11,11,12	0.74	0	15,15,17	0.62	0
8	GLC	Q	502	1	11,11,12	0.82	0	15,15,17	0.57	0
9	NAG	O	502	1	14,14,15	0.28	0	17,19,21	0.60	0
9	NAG	Q	501	1	14,14,15	0.36	0	17,19,21	0.56	0
8	GLC	K	501	1	11,11,12	0.83	0	15,15,17	0.61	0
8	GLC	A	501	1	11,11,12	0.78	0	15,15,17	0.62	0
8	GLC	M	501	1	11,11,12	0.80	0	15,15,17	0.61	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
9	NAG	R	501	1	-	3/6/23/26	0/1/1/1
8	GLC	J	501	1	-	0/2/19/22	0/1/1/1
8	GLC	D	501	1	-	0/2/19/22	0/1/1/1
8	GLC	P	501	1	-	0/2/19/22	0/1/1/1
8	GLC	R	502	1	-	0/2/19/22	0/1/1/1
8	GLC	L	501	1	-	0/2/19/22	0/1/1/1
8	GLC	O	501	1	-	0/2/19/22	0/1/1/1
8	GLC	F	501	1	-	0/2/19/22	0/1/1/1
8	GLC	C	501	1	-	0/2/19/22	0/1/1/1
8	GLC	H	501	1	-	1/2/19/22	0/1/1/1
9	NAG	E	502	1	-	0/6/23/26	0/1/1/1
8	GLC	I	501	1	-	0/2/19/22	0/1/1/1
8	GLC	E	501	1	-	0/2/19/22	0/1/1/1
8	GLC	N	501	1	-	0/2/19/22	0/1/1/1
8	GLC	B	501	1	-	0/2/19/22	0/1/1/1
8	GLC	Q	502	1	-	0/2/19/22	0/1/1/1
9	NAG	O	502	1	-	3/6/23/26	0/1/1/1
9	NAG	Q	501	1	-	2/6/23/26	0/1/1/1
8	GLC	K	501	1	-	0/2/19/22	0/1/1/1
8	GLC	A	501	1	-	0/2/19/22	0/1/1/1
8	GLC	M	501	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

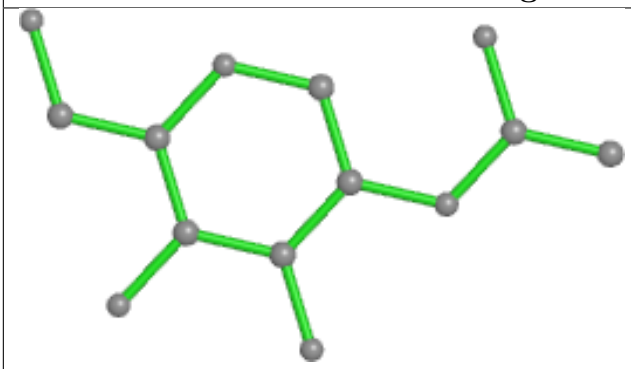
Mol	Chain	Res	Type	Atoms
9	O	502	NAG	C3-C2-N2-C7
9	O	502	NAG	C8-C7-N2-C2
9	O	502	NAG	O7-C7-N2-C2
9	R	501	NAG	C8-C7-N2-C2
9	R	501	NAG	O7-C7-N2-C2
9	R	501	NAG	O5-C5-C6-O6
8	H	501	GLC	O5-C5-C6-O6
9	Q	501	NAG	C1-C2-N2-C7
9	Q	501	NAG	C3-C2-N2-C7

There are no ring outliers.

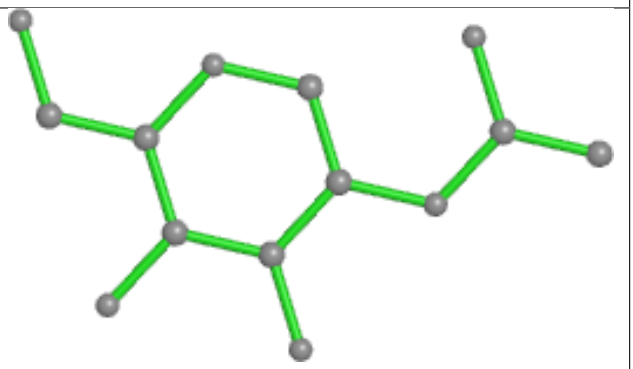
No monomer is involved in short contacts.

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.

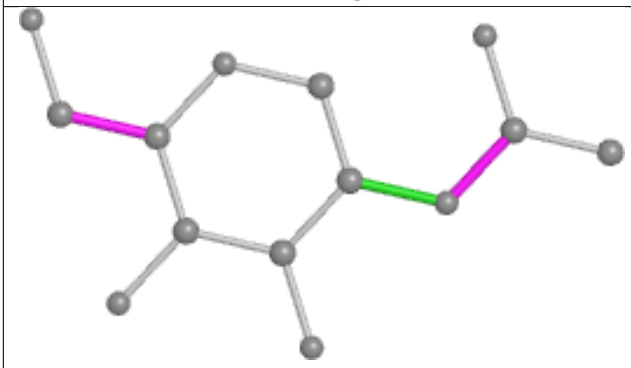
Ligand NAG R 501



Bond lengths



Bond angles



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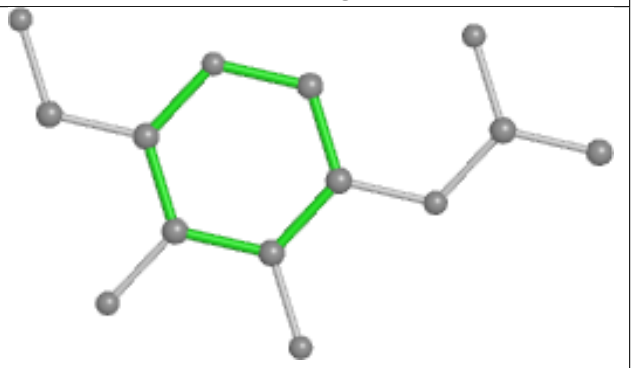
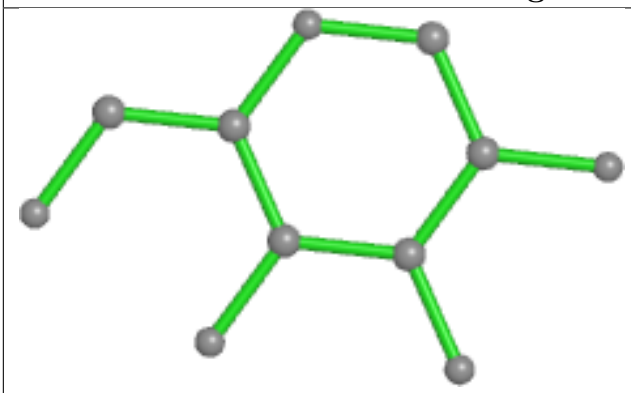


Rings

Ligand GLC J 501



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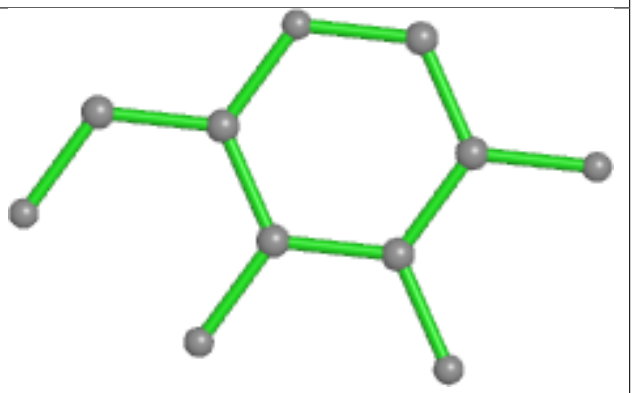

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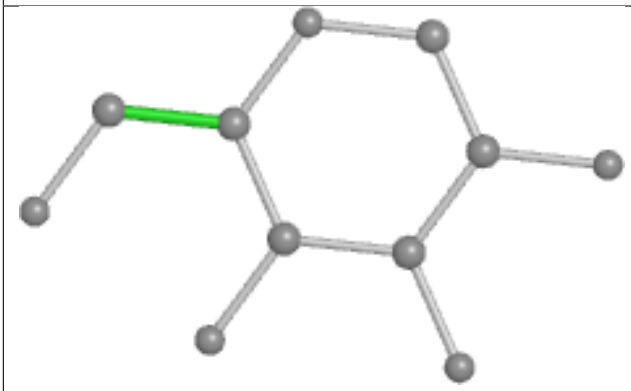

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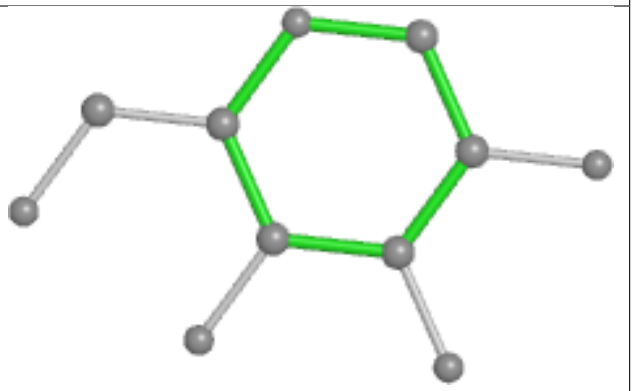
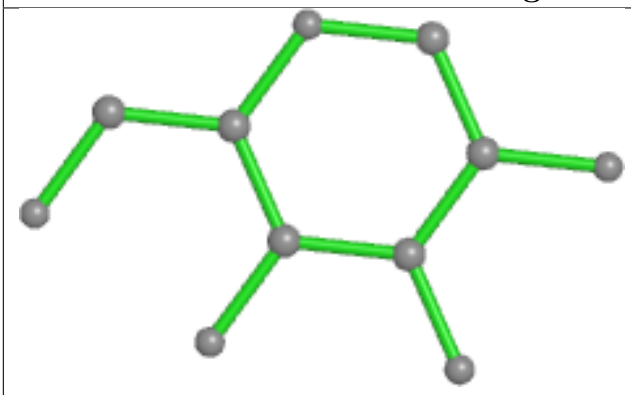


Rings

Ligand GLC D 501



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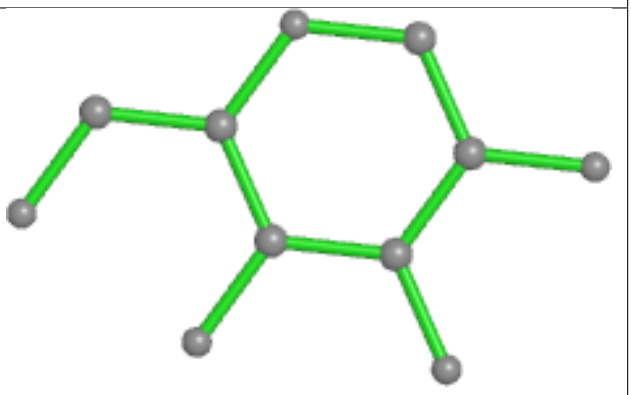

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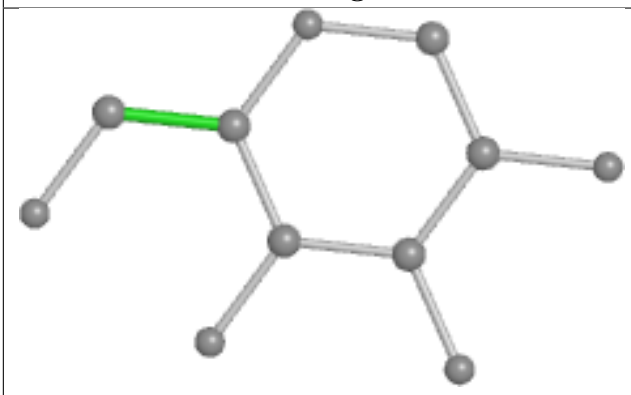

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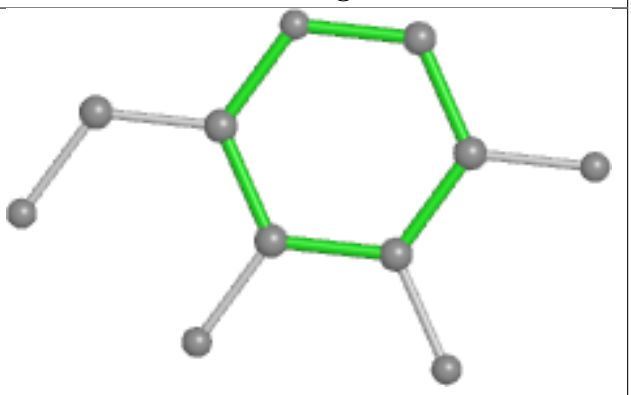
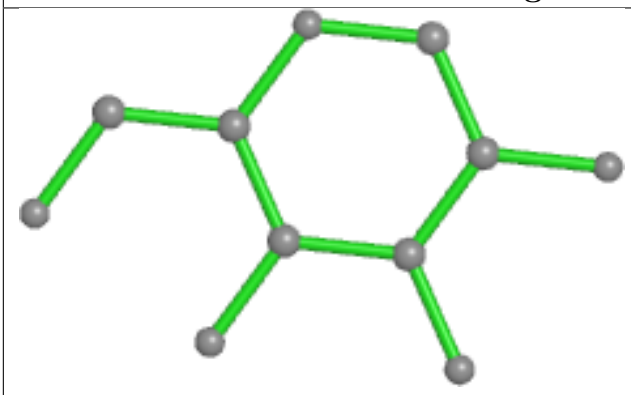


Rings

Ligand GLC P 501



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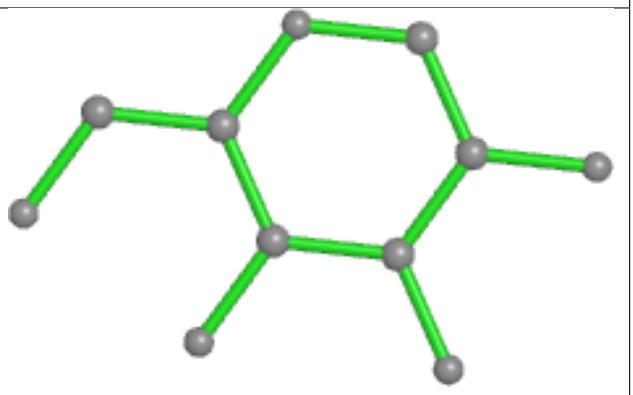

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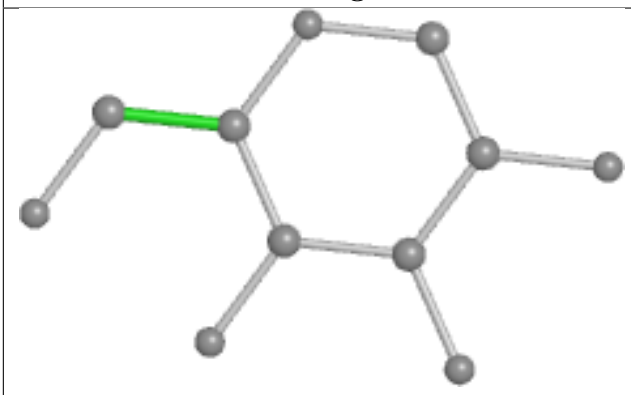

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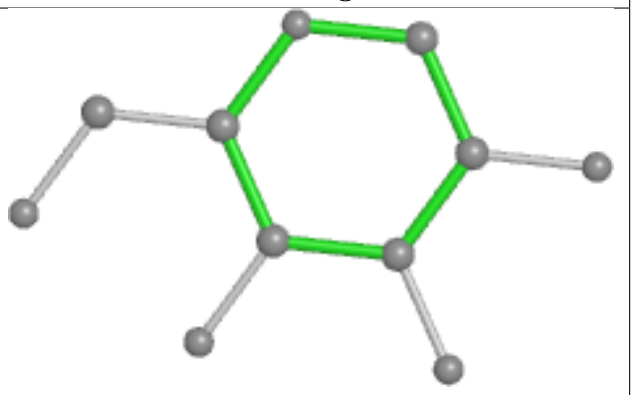
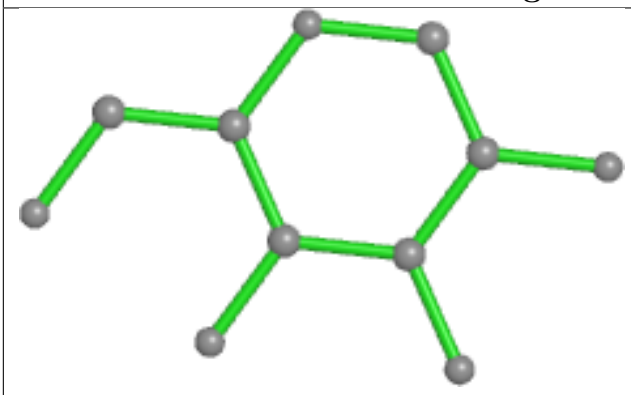


Rings

Ligand GLC R 502



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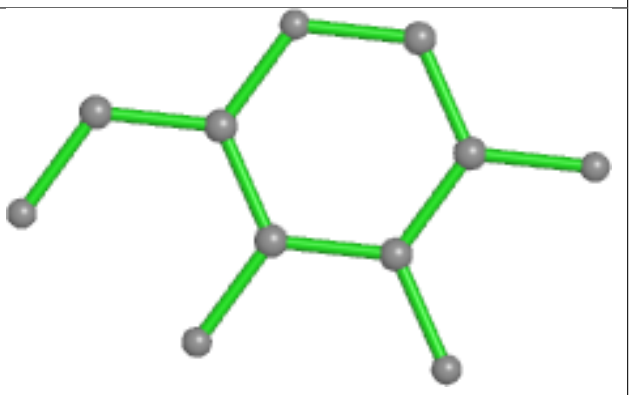

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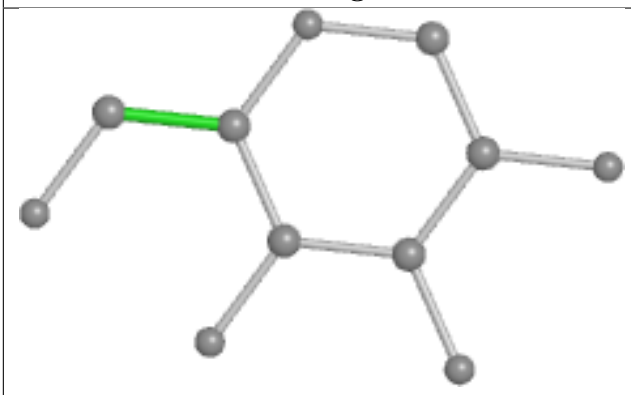

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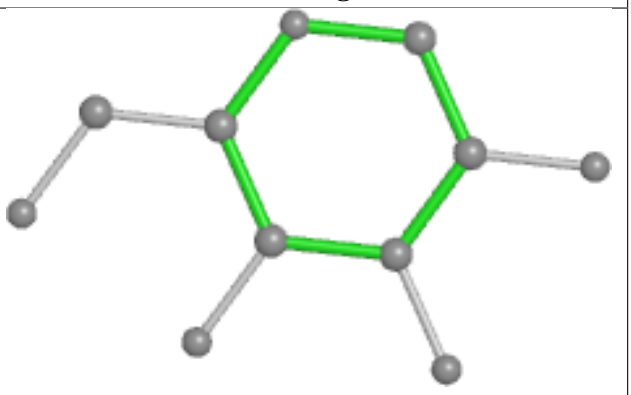

Rings

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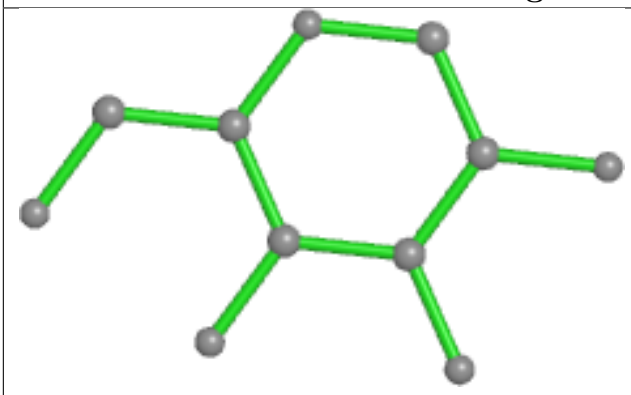

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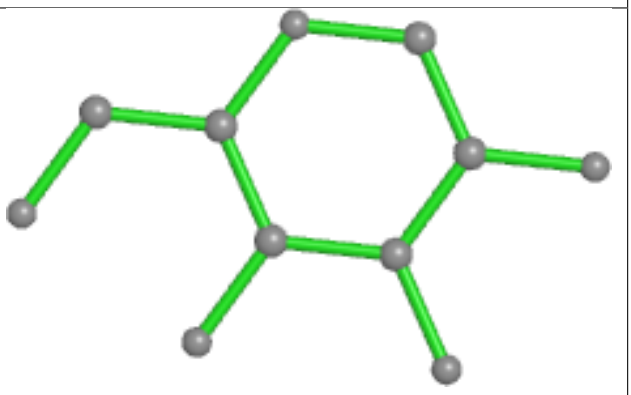

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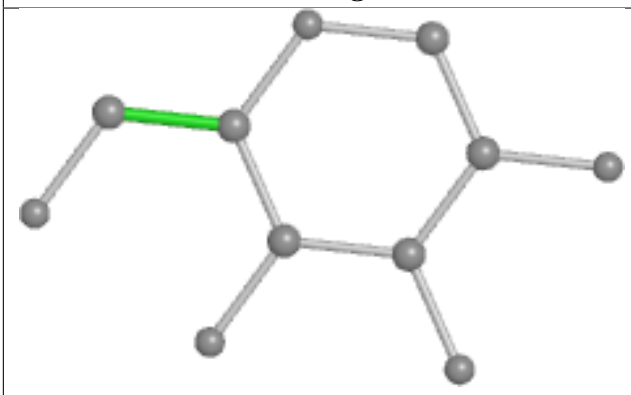

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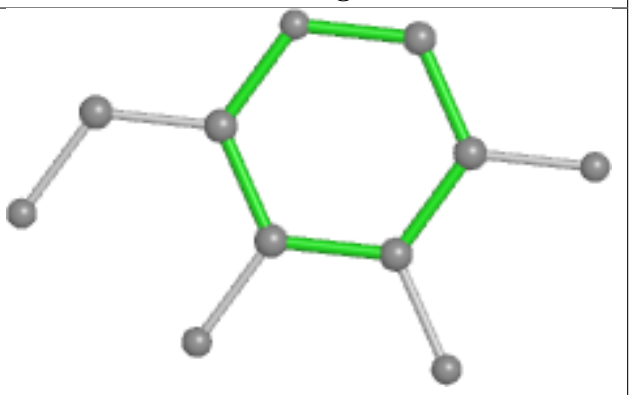

Rings

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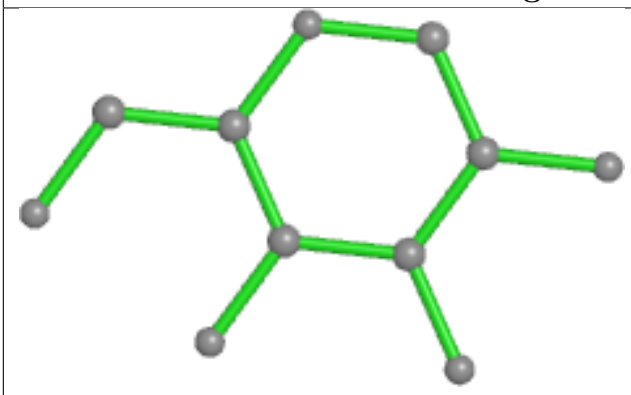

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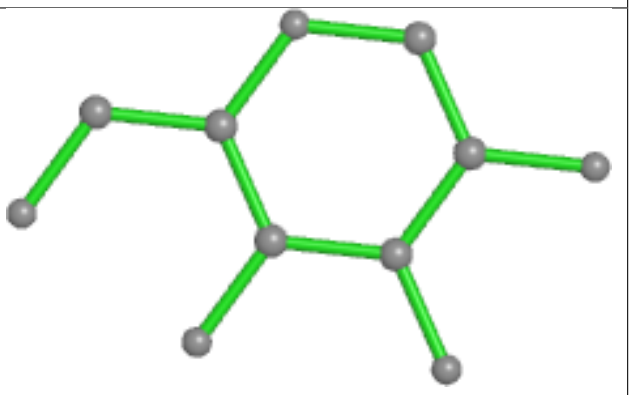

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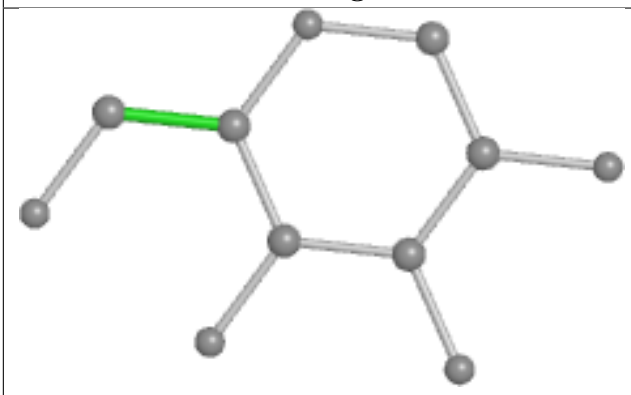

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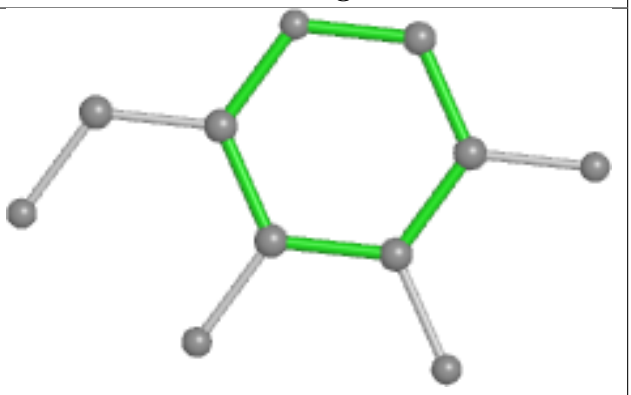

Rings

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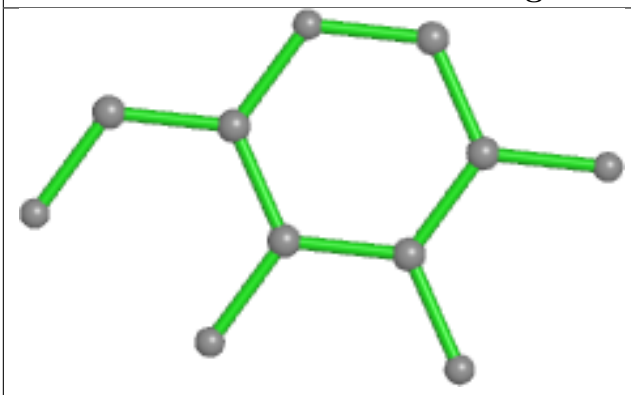

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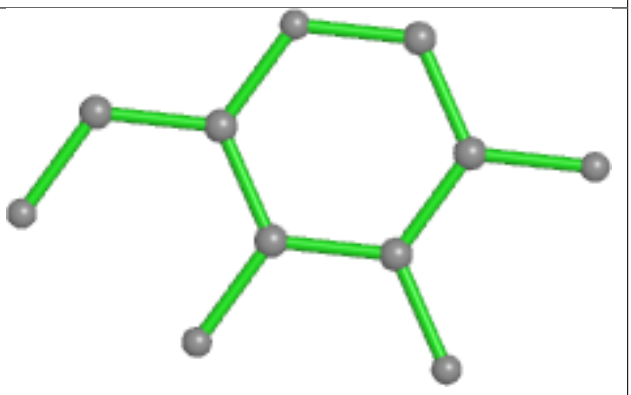

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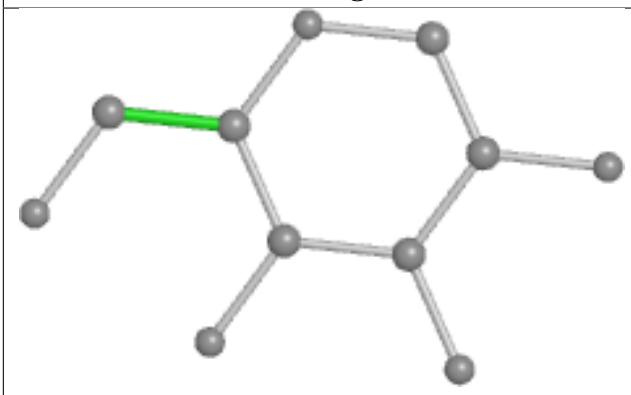

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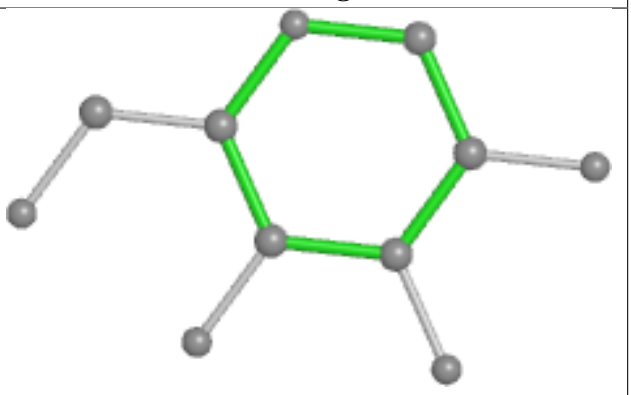
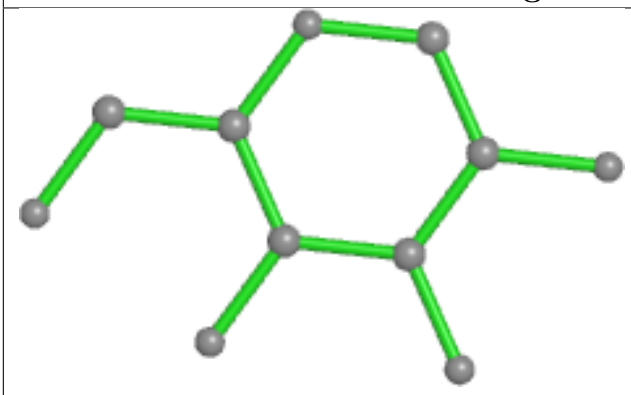


Rings

Ligand GLC C 501



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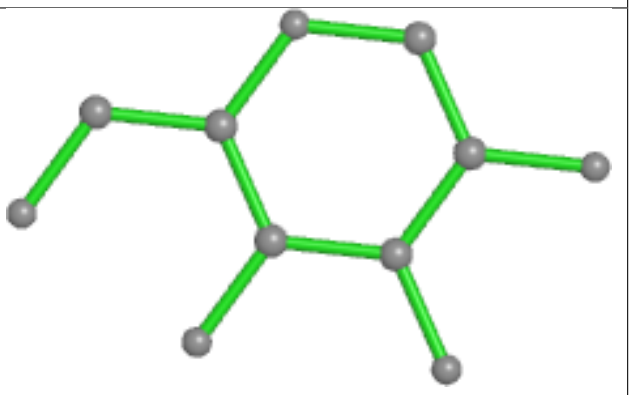

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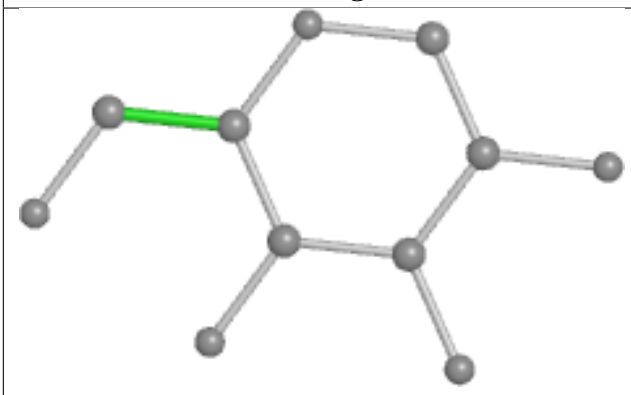

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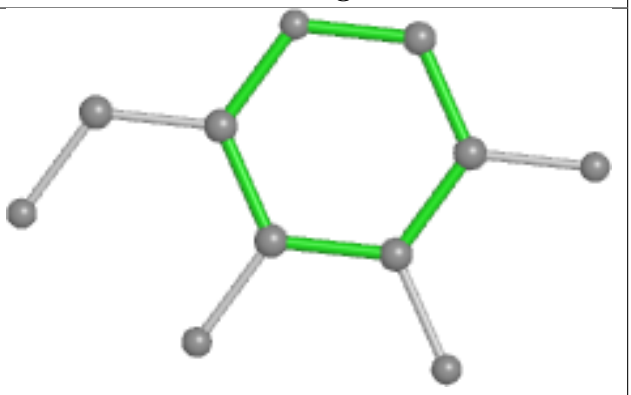
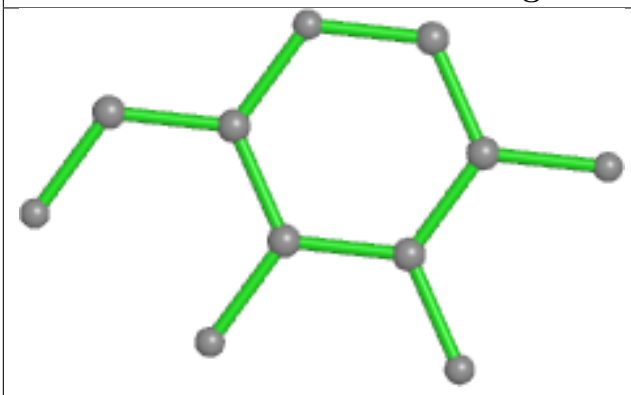


Rings

Ligand GLC H 501



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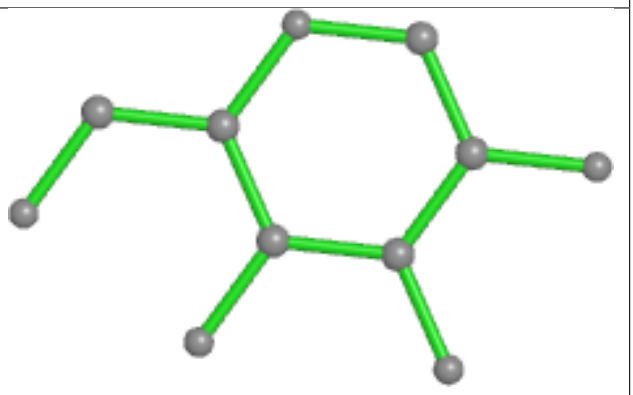

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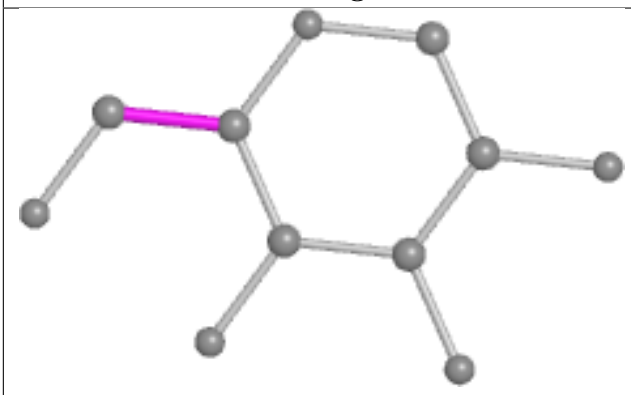

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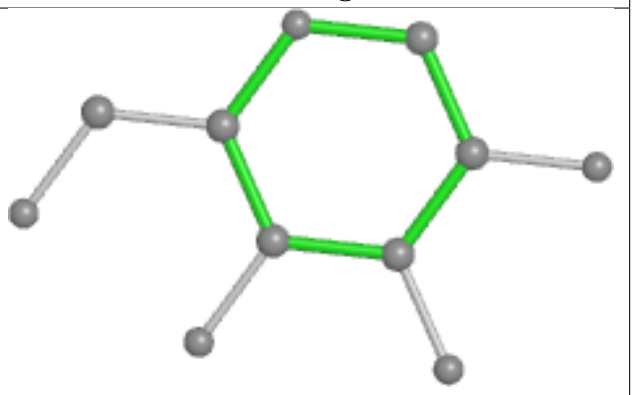
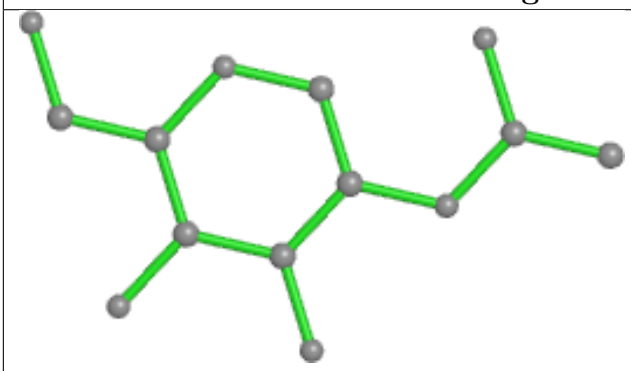


Rings

Ligand NAG E 502



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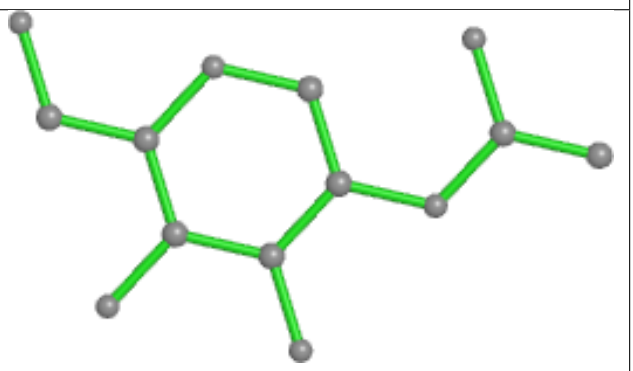

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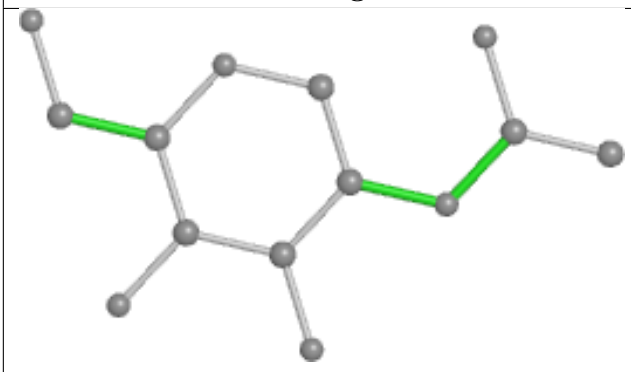

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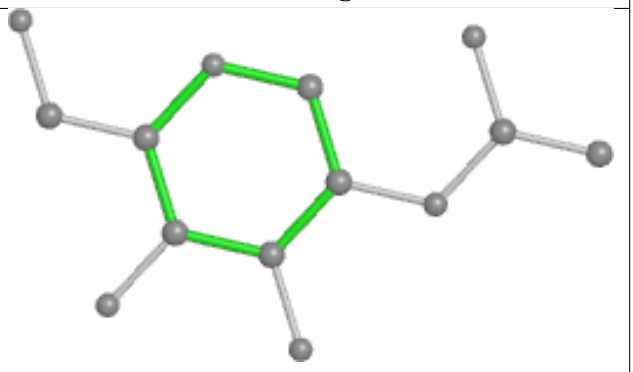
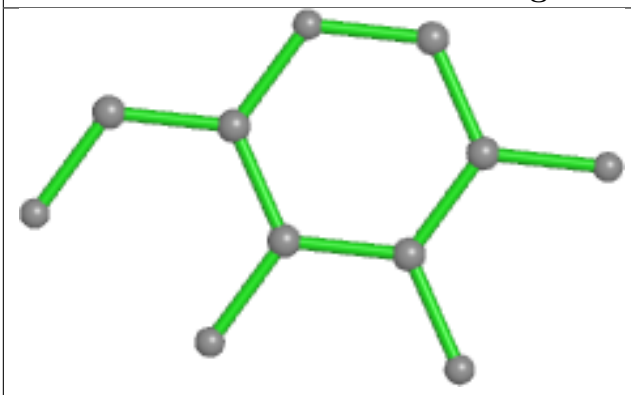


Rings

Ligand GLC I 501



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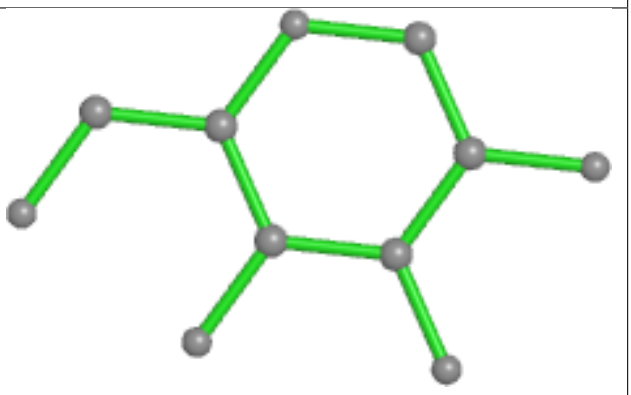

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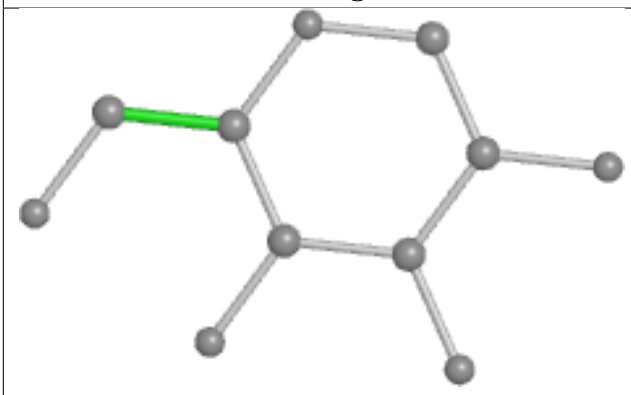

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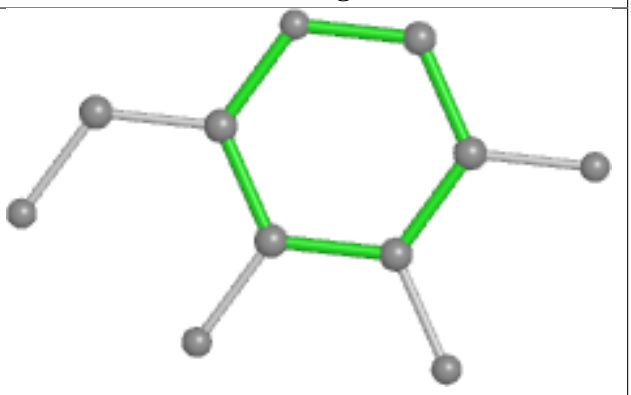
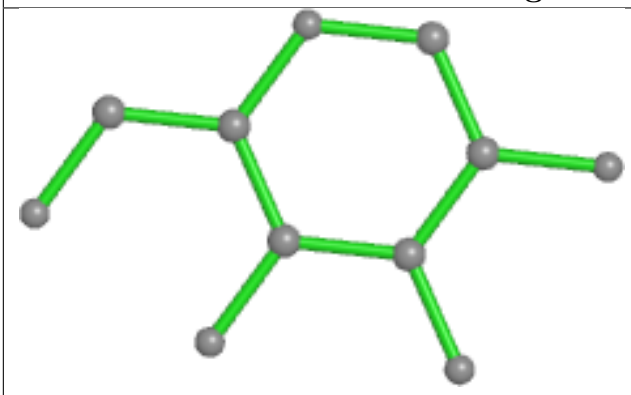


Rings

Ligand GLC E 501



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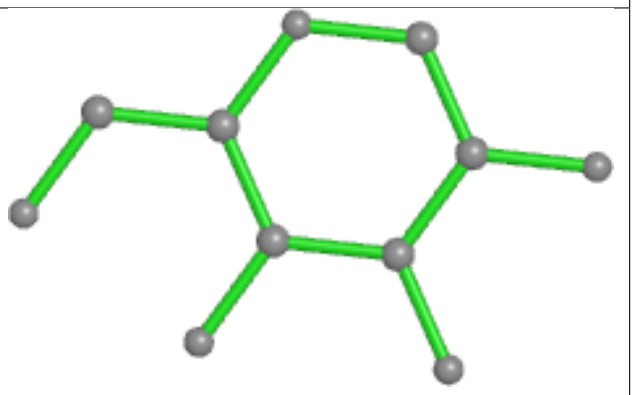
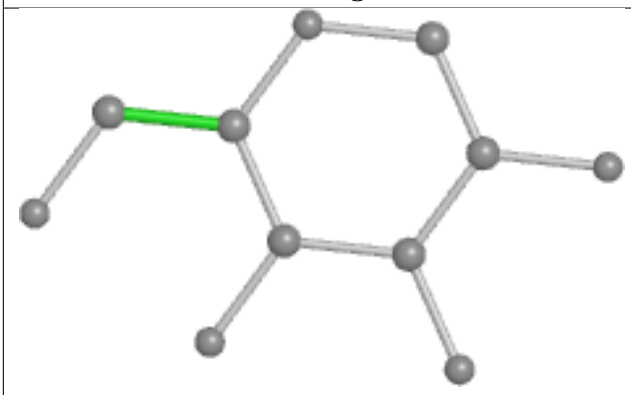


Bond angles



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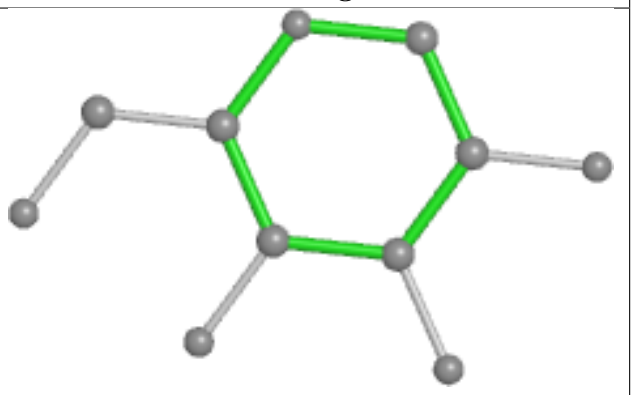
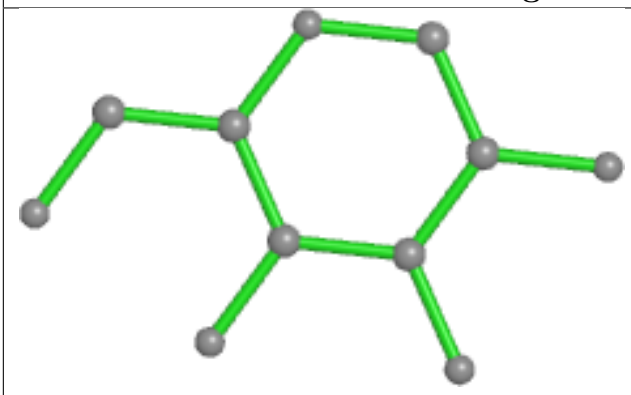


Rings

Ligand GLC N 501



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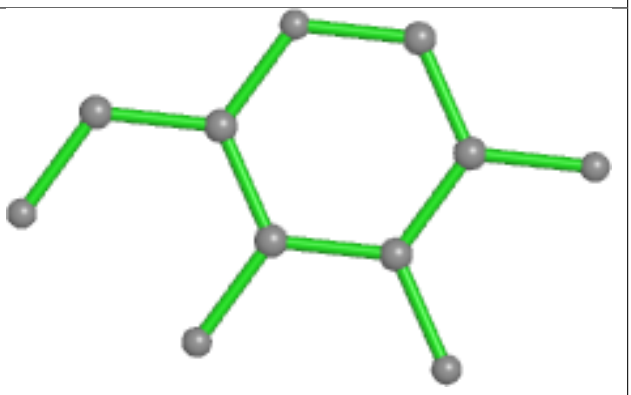
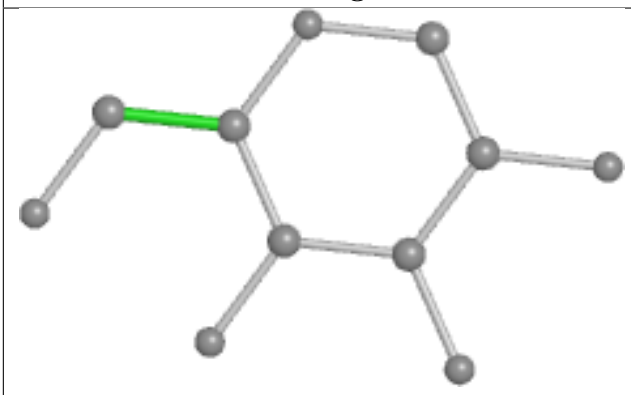
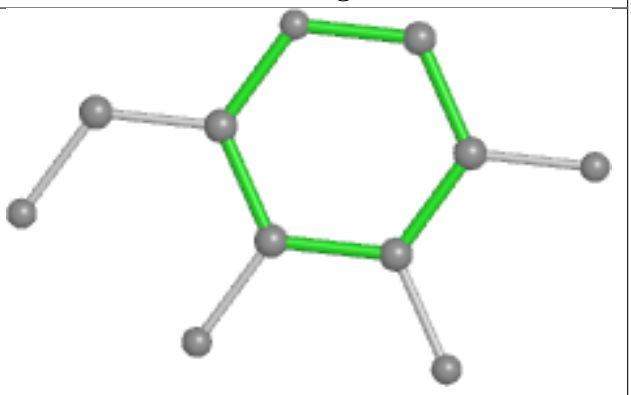


Bond angles

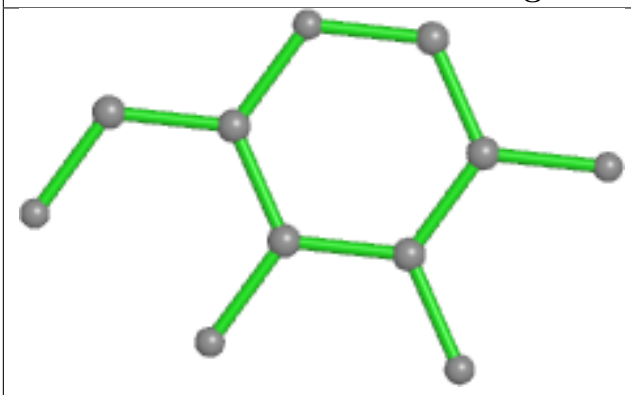


Torsions

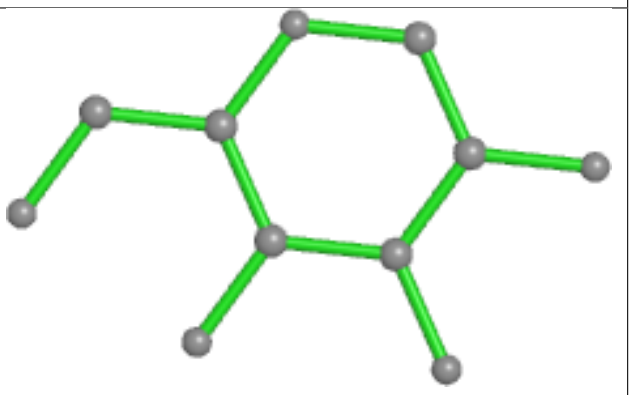


Rings

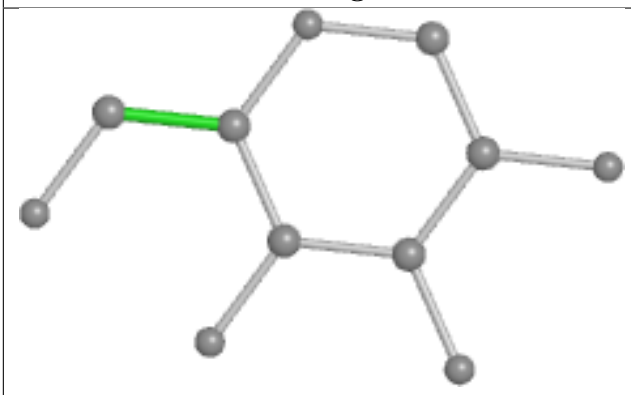
Ligand GLC B 501



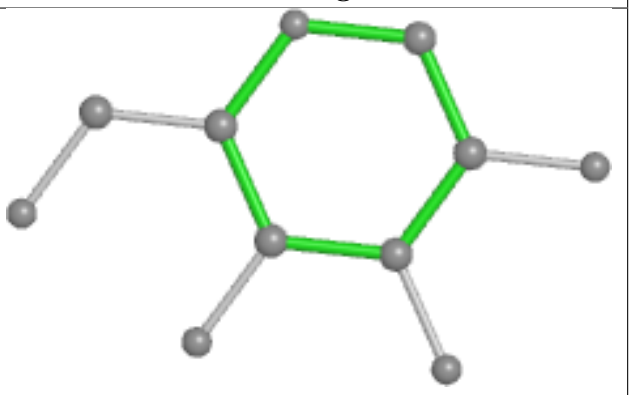
Bond lengths



Bond angles

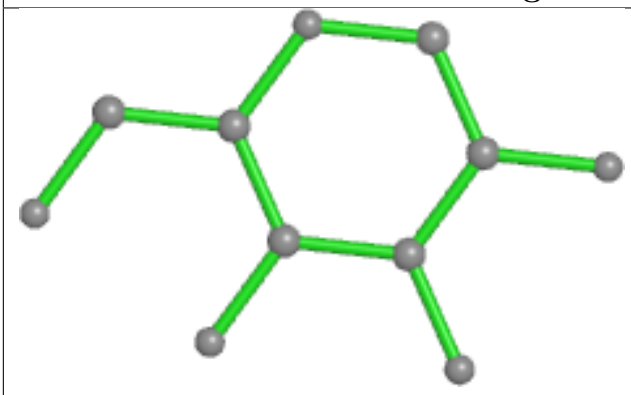


Torsions

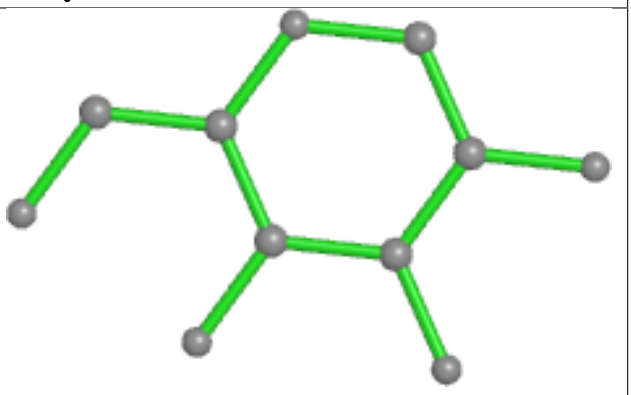


Rings

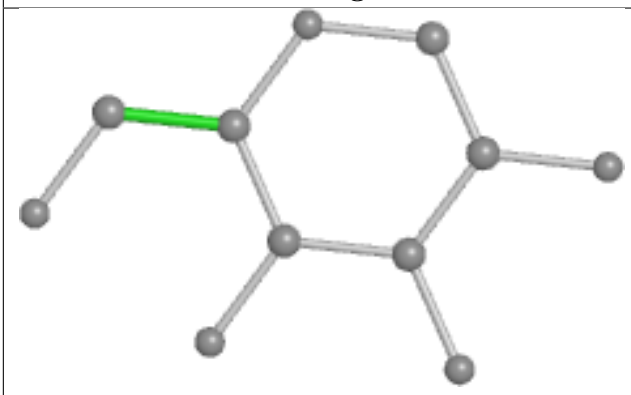
Ligand GLC Q 502



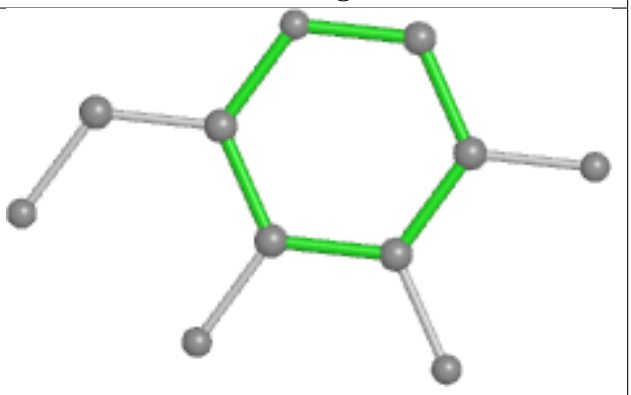
Bond lengths



Bond angles

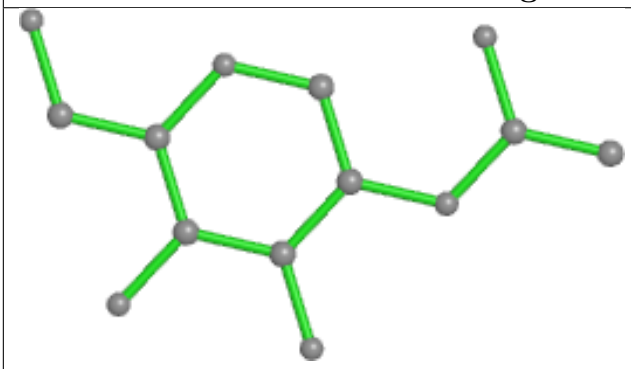


Torsions

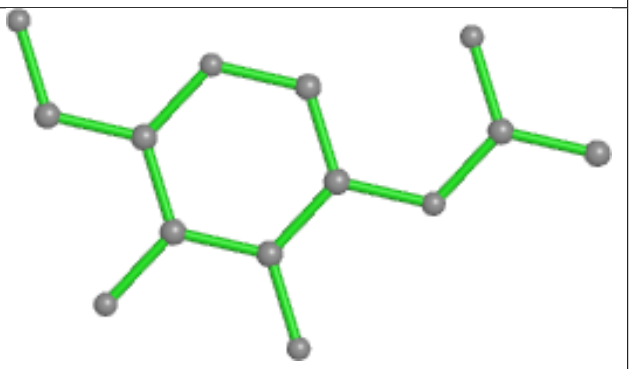


Rings

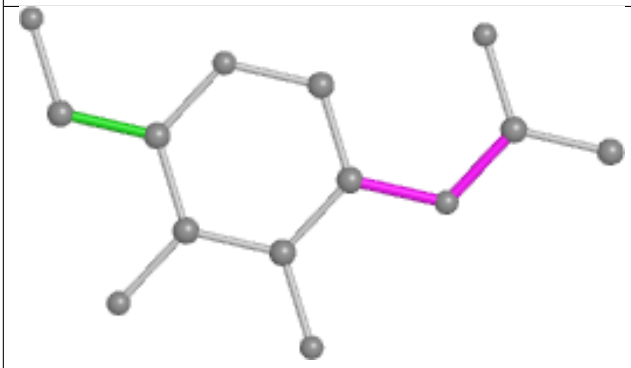
Ligand NAG O 502



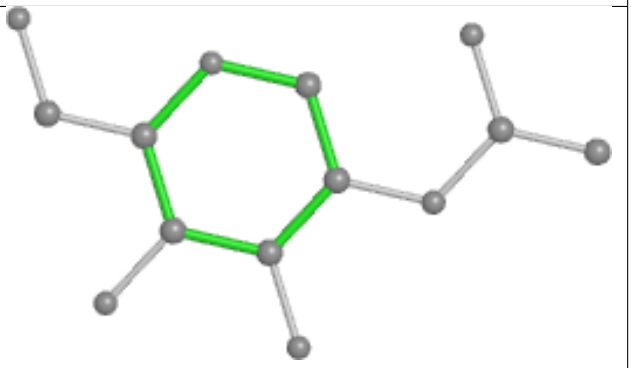
Bond lengths



Bond angles

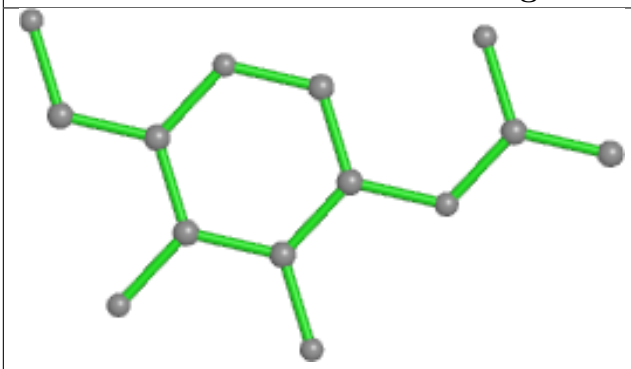


Torsions

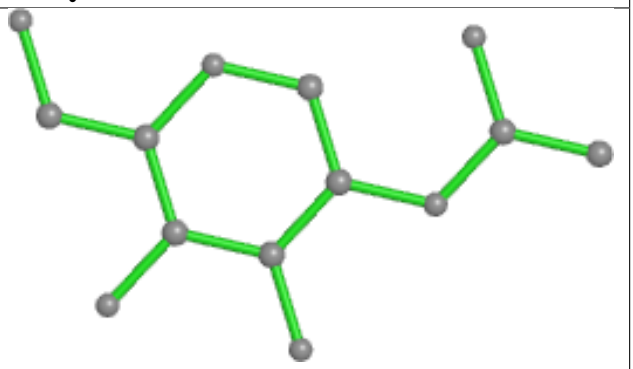


Rings

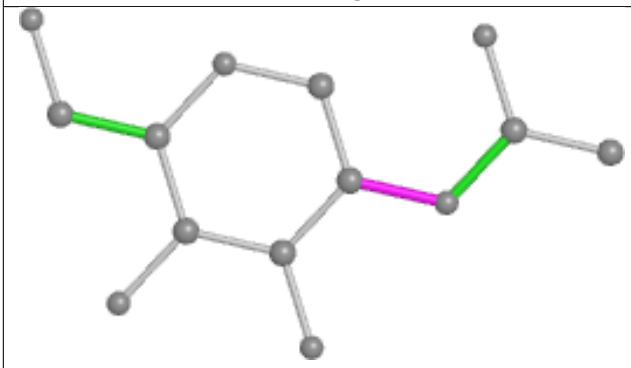
Ligand NAG Q 501



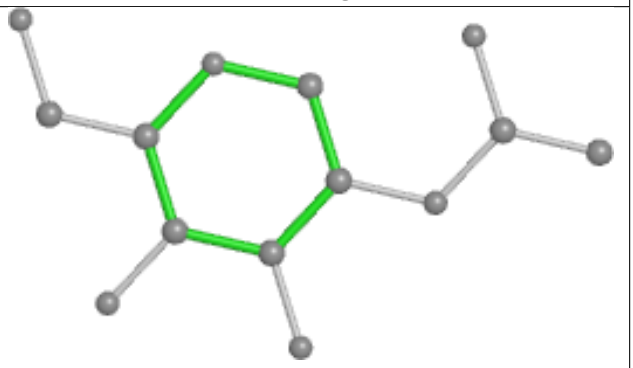
Bond lengths



Bond angles

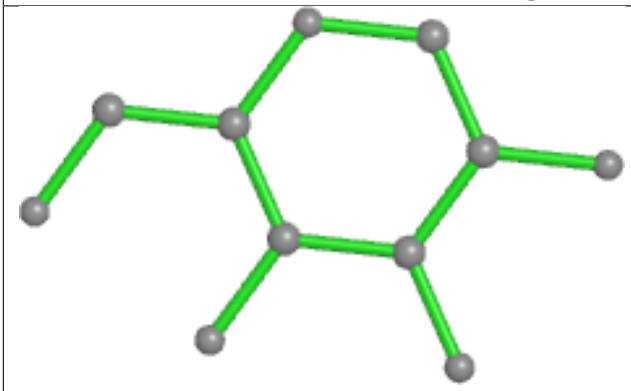


Torsions

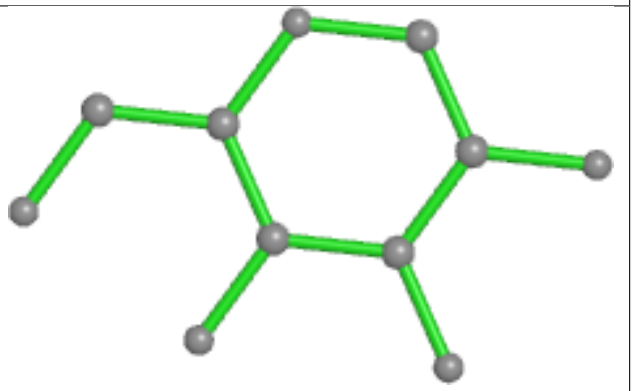


Rings

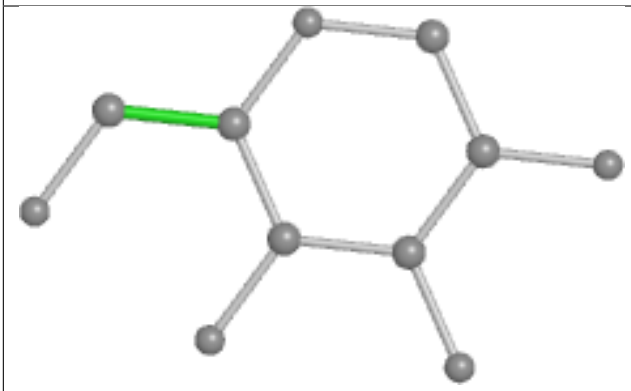
Ligand GLC K 501



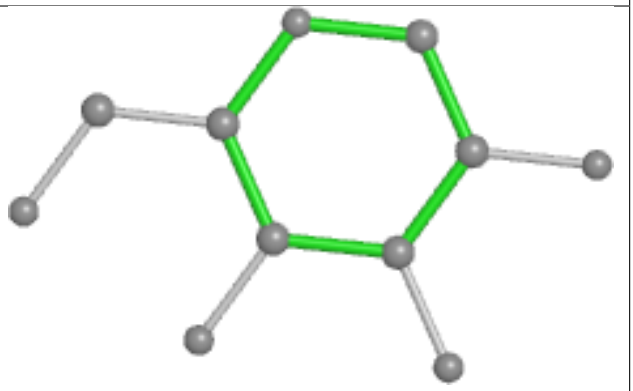
Bond lengths



Bond angles

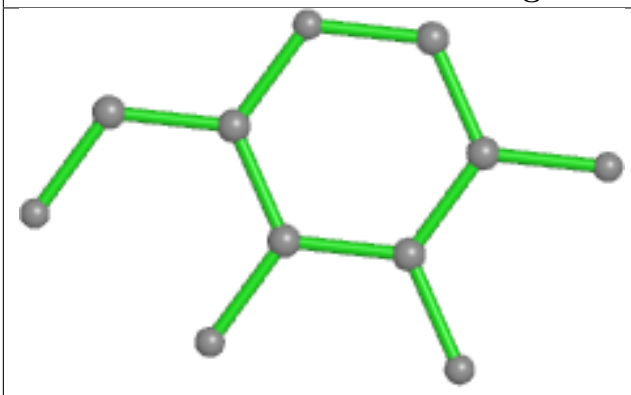


Torsions

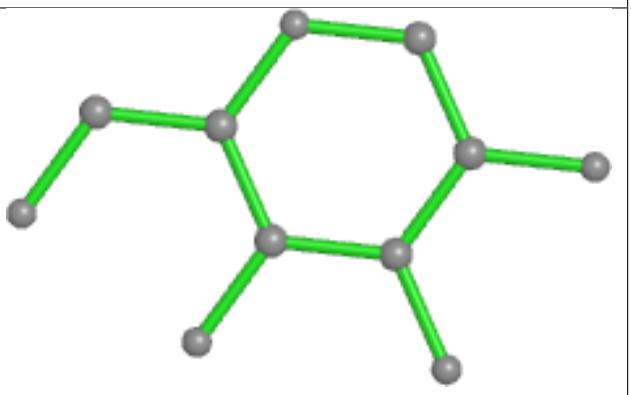


Rings

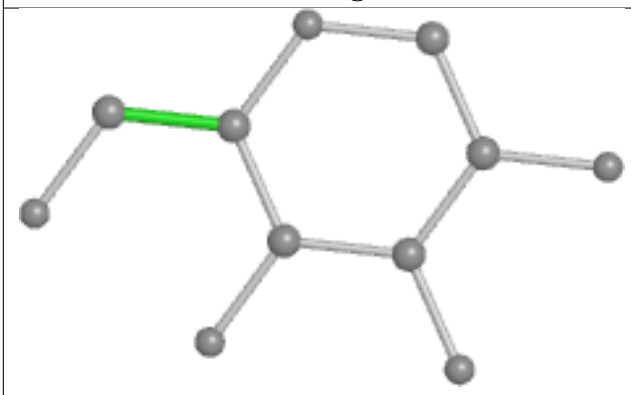
Ligand GLC A 501



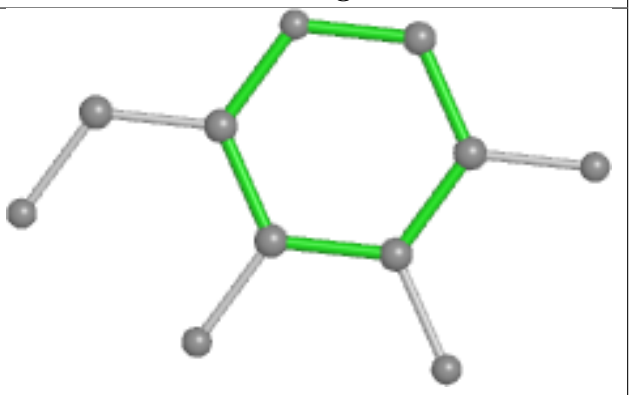
Bond lengths



Bond angles

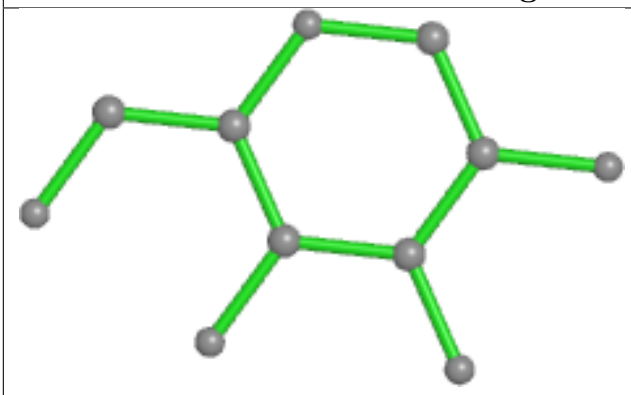


Torsions

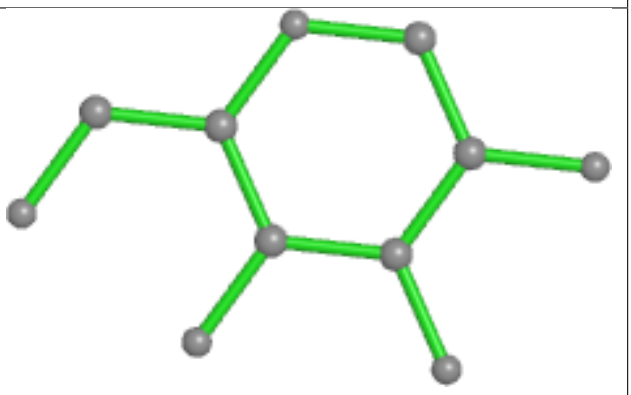


Rings

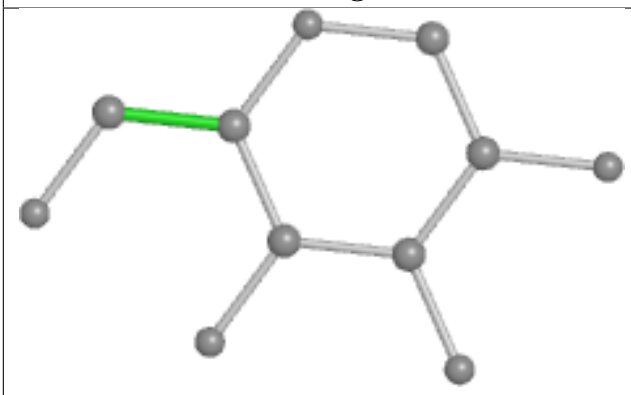
Ligand GLC M 501



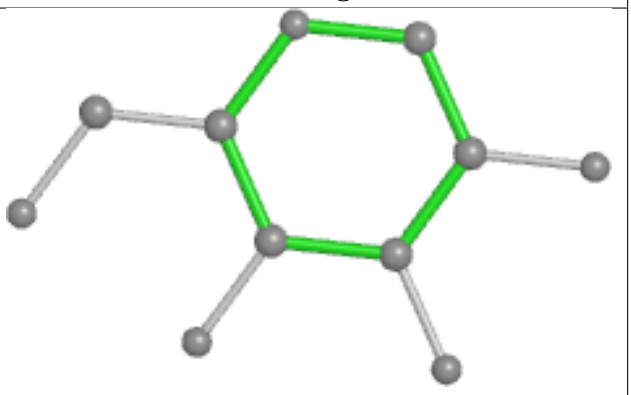
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	366/410 (89%)	0.10	1 (0%) 94 93	44, 61, 99, 114	0
1	B	366/410 (89%)	0.25	9 (2%) 57 51	45, 67, 132, 155	0
1	C	366/410 (89%)	0.31	14 (3%) 40 33	46, 72, 143, 173	0
1	D	321/410 (78%)	0.51	33 (10%) 6 4	51, 72, 141, 161	0
1	E	285/410 (69%)	0.51	17 (5%) 21 16	61, 98, 140, 148	0
1	F	282/410 (68%)	0.47	28 (9%) 7 5	58, 86, 152, 181	0
1	G	365/410 (89%)	0.59	26 (7%) 16 11	77, 106, 141, 153	0
1	H	287/410 (70%)	0.79	37 (12%) 3 2	96, 123, 148, 155	0
1	I	343/410 (83%)	1.26	87 (25%) 0 0	90, 136, 167, 185	0
1	J	366/410 (89%)	0.15	10 (2%) 54 48	44, 60, 118, 128	0
1	K	365/410 (89%)	0.29	17 (4%) 31 25	55, 83, 132, 143	0
1	L	358/410 (87%)	0.17	14 (3%) 39 32	52, 74, 138, 163	0
1	M	287/410 (70%)	0.36	20 (6%) 16 12	52, 71, 157, 166	0
1	N	353/410 (86%)	0.58	48 (13%) 3 1	55, 91, 154, 172	0
1	O	301/410 (73%)	0.72	42 (13%) 2 1	79, 125, 153, 178	0
1	P	261/410 (63%)	0.41	17 (6%) 18 14	67, 90, 144, 160	0
1	Q	272/410 (66%)	0.64	31 (11%) 5 3	73, 100, 162, 169	0
1	R	310/410 (75%)	0.53	30 (9%) 7 5	62, 82, 160, 171	0
All	All	5854/7380 (79%)	0.47	481 (8%) 11 8	44, 91, 151, 185	0

All (481) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	137	PRO	7.5
1	D	154	ALA	6.9
1	E	381	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
1	Q	154	ALA	6.5
1	R	152	ALA	5.7
1	N	57	PHE	5.7
1	M	150	LEU	5.5
1	Q	157	LYS	5.4
1	D	158	ALA	5.4
1	F	67	LEU	5.4
1	R	151	THR	5.2
1	D	152	ALA	5.2
1	N	143	ALA	5.2
1	R	69	MET	5.2
1	I	65	LEU	5.2
1	Q	163	VAL	5.2
1	P	69	MET	5.2
1	C	82	ASP	5.1
1	R	110	TRP	5.0
1	M	149	ARG	4.9
1	I	117	LEU	4.9
1	R	158	ALA	4.9
1	I	270	LEU	4.8
1	P	62	ASN	4.8
1	D	118	LEU	4.8
1	H	163	VAL	4.8
1	Q	147	ILE	4.8
1	M	67	LEU	4.7
1	O	386	TYR	4.7
1	D	67	LEU	4.7
1	N	92	LEU	4.7
1	D	73	GLU	4.6
1	N	126	LYS	4.6
1	P	64	ILE	4.6
1	I	96	PRO	4.5
1	I	77	LEU	4.5
1	I	41	ILE	4.5
1	I	301	LEU	4.5
1	G	252	ALA	4.5
1	N	262	THR	4.4
1	O	263	ALA	4.4
1	G	84	ASP	4.4
1	C	117	LEU	4.4
1	D	147	ILE	4.4
1	F	379	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	R	154	ALA	4.4
1	E	261	VAL	4.4
1	P	376	THR	4.4
1	N	93	THR	4.3
1	R	65	LEU	4.3
1	F	107	TRP	4.3
1	M	152	ALA	4.3
1	O	381	ALA	4.2
1	H	237	ARG	4.2
1	I	98	PRO	4.2
1	D	68	ASN	4.2
1	I	241	ALA	4.1
1	M	145	ASN	4.1
1	H	230	PHE	4.1
1	Q	59	ASN	4.1
1	I	71	ALA	4.1
1	I	114	ALA	4.1
1	I	314	LEU	4.0
1	K	92	LEU	4.0
1	R	70	THR	4.0
1	D	143	ALA	4.0
1	Q	167	THR	4.0
1	I	80	PHE	4.0
1	F	69	MET	4.0
1	N	113	ALA	4.0
1	N	150	LEU	4.0
1	I	73	GLU	4.0
1	I	277	CYS	4.0
1	O	171	THR	3.9
1	H	385	ALA	3.9
1	O	130	TYR	3.9
1	H	171	THR	3.9
1	I	129	GLU	3.9
1	O	380	LEU	3.9
1	R	72	ALA	3.9
1	N	97	LEU	3.9
1	I	86	ARG	3.9
1	G	325	GLY	3.9
1	I	333	VAL	3.9
1	N	96	PRO	3.9
1	D	155	VAL	3.9
1	J	117	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	211	THR	3.8
1	N	261	VAL	3.8
1	N	130	TYR	3.8
1	I	89	PRO	3.8
1	H	54	LEU	3.8
1	R	156	ALA	3.8
1	I	196	ASN	3.8
1	R	58	GLN	3.8
1	F	105	ASP	3.7
1	N	134	GLY	3.7
1	F	56	ASN	3.7
1	L	92	LEU	3.7
1	H	68	ASN	3.7
1	D	159	GLN	3.7
1	I	276	LEU	3.7
1	I	55	PRO	3.6
1	O	198	TYR	3.6
1	R	163	VAL	3.6
1	P	170	LEU	3.6
1	M	379	THR	3.6
1	P	67	LEU	3.6
1	N	163	VAL	3.6
1	D	114	ALA	3.6
1	L	114	ALA	3.6
1	N	122	THR	3.6
1	I	180	ILE	3.6
1	I	195	PHE	3.6
1	P	55	PRO	3.6
1	I	97	LEU	3.6
1	O	156	ALA	3.6
1	D	138	GLU	3.5
1	D	115	LEU	3.5
1	Q	374	LEU	3.5
1	F	164	ALA	3.5
1	N	144	ARG	3.5
1	N	367	LEU	3.5
1	I	128	LYS	3.5
1	F	110	TRP	3.5
1	O	65	LEU	3.5
1	P	380	LEU	3.5
1	I	186	SER	3.5
1	O	155	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	N	76	TRP	3.5
1	C	84	ASP	3.5
1	I	338	GLY	3.5
1	D	141	GLU	3.4
1	K	121	GLU	3.4
1	D	71	ALA	3.4
1	R	57	PHE	3.4
1	E	382	LYS	3.4
1	C	53	ALA	3.4
1	I	176	LEU	3.4
1	F	380	LEU	3.4
1	Q	67	LEU	3.4
1	F	374	LEU	3.4
1	I	64	ILE	3.4
1	Q	64	ILE	3.4
1	I	113	ALA	3.3
1	R	377	ILE	3.3
1	O	237	ARG	3.3
1	N	123	HIS	3.3
1	N	159	GLN	3.3
1	N	88	LYS	3.3
1	I	346	TRP	3.3
1	L	93	THR	3.3
1	O	152	ALA	3.3
1	F	157	LYS	3.3
1	M	59	ASN	3.2
1	N	119	ASN	3.2
1	Q	153	GLU	3.2
1	I	76	TRP	3.2
1	I	126	LYS	3.2
1	G	233	CYS	3.2
1	F	155	VAL	3.2
1	R	71	ALA	3.2
1	K	377	ILE	3.2
1	M	386	TYR	3.2
1	N	151	THR	3.2
1	R	111	ALA	3.2
1	L	84	ASP	3.2
1	F	153	GLU	3.2
1	Q	68	ASN	3.2
1	O	377	ILE	3.2
1	L	123	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	Q	148	ARG	3.2
1	H	313	PHE	3.1
1	G	313	PHE	3.1
1	K	93	THR	3.1
1	N	115	LEU	3.1
1	O	223	THR	3.1
1	Q	376	THR	3.1
1	H	259	PRO	3.1
1	D	72	ALA	3.1
1	J	115	LEU	3.1
1	O	170	LEU	3.1
1	P	374	LEU	3.1
1	Q	367	LEU	3.1
1	P	377	ILE	3.1
1	F	154	ALA	3.1
1	H	65	LEU	3.1
1	M	62	ASN	3.1
1	I	69	MET	3.1
1	N	242	ASP	3.1
1	J	87	SER	3.1
1	I	79	GLN	3.1
1	K	97	LEU	3.1
1	M	158	ALA	3.1
1	H	64	ILE	3.0
1	H	62	ASN	3.0
1	E	150	LEU	3.0
1	N	315	ALA	3.0
1	O	344	ILE	3.0
1	F	365	GLU	3.0
1	D	124	GLN	3.0
1	D	132	LEU	3.0
1	G	82	ASP	3.0
1	N	90	ARG	3.0
1	N	142	ARG	3.0
1	Q	259	PRO	3.0
1	M	69	MET	3.0
1	J	119	ASN	3.0
1	P	199	THR	3.0
1	N	106	HIS	3.0
1	I	110	TRP	3.0
1	I	223	THR	3.0
1	N	71	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	82	ASP	2.9
1	I	307	THR	2.9
1	J	86	ARG	2.9
1	G	250	GLY	2.9
1	R	73	GLU	2.9
1	F	163	VAL	2.9
1	H	261	VAL	2.9
1	E	63	SER	2.9
1	F	381	ALA	2.9
1	H	161	PRO	2.9
1	J	89	PRO	2.9
1	M	155	VAL	2.9
1	O	154	ALA	2.9
1	I	178	LYS	2.9
1	D	70	THR	2.9
1	G	241	ALA	2.9
1	H	262	THR	2.9
1	H	159	GLN	2.9
1	I	313	PHE	2.9
1	N	64	ILE	2.9
1	E	170	LEU	2.9
1	I	156	ALA	2.9
1	I	267	GLY	2.8
1	F	376	THR	2.8
1	C	107	TRP	2.8
1	G	321	ASP	2.8
1	H	206	SER	2.8
1	R	145	ASN	2.8
1	I	342	LYS	2.8
1	K	131	LYS	2.8
1	B	122	THR	2.8
1	I	175	ASP	2.8
1	I	45	GLY	2.8
1	C	137	PRO	2.8
1	D	380	LEU	2.8
1	I	127	LEU	2.8
1	I	320	GLY	2.8
1	R	119	ASN	2.8
1	E	377	ILE	2.8
1	C	93	THR	2.8
1	F	152	ALA	2.8
1	N	132	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	O	350	LEU	2.8
1	Q	61	LEU	2.8
1	I	179	GLN	2.8
1	E	152	ALA	2.8
1	G	240	GLY	2.8
1	G	251	THR	2.8
1	R	376	THR	2.8
1	H	166	SER	2.8
1	R	155	VAL	2.7
1	O	167	THR	2.7
1	G	54	LEU	2.7
1	N	56	ASN	2.7
1	N	135	LEU	2.7
1	H	155	VAL	2.7
1	E	255	THR	2.7
1	M	68	ASN	2.7
1	K	87	SER	2.7
1	N	62	ASN	2.7
1	C	164	ALA	2.7
1	I	72	ALA	2.7
1	I	111	ALA	2.7
1	E	384	PRO	2.7
1	I	257	TRP	2.7
1	H	273	VAL	2.7
1	O	151	THR	2.7
1	P	60	GLU	2.7
1	I	104	ALA	2.6
1	F	106	HIS	2.6
1	I	285	LEU	2.6
1	K	117	LEU	2.6
1	K	56	ASN	2.6
1	R	68	ASN	2.6
1	Q	66	GLU	2.6
1	Q	162	THR	2.6
1	L	83	LYS	2.6
1	F	70	THR	2.6
1	D	140	LEU	2.6
1	Q	378	LEU	2.6
1	H	297	VAL	2.6
1	M	61	LEU	2.6
1	O	150	LEU	2.6
1	J	85	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	60	GLU	2.6
1	L	85	ASP	2.6
1	C	127	LEU	2.5
1	J	83	LYS	2.5
1	M	380	LEU	2.5
1	O	127	LEU	2.5
1	I	309	ILE	2.5
1	Q	212	ILE	2.5
1	Q	230	PHE	2.5
1	G	59	ASN	2.5
1	K	133	ALA	2.5
1	P	375	LYS	2.5
1	O	199	THR	2.5
1	I	231	CYS	2.5
1	N	237	ARG	2.5
1	I	250	GLY	2.5
1	O	139	LYS	2.5
1	C	114	ALA	2.5
1	I	266	THR	2.5
1	C	85	ASP	2.5
1	K	82	ASP	2.5
1	O	164	ALA	2.5
1	I	130	TYR	2.5
1	K	120	ASP	2.5
1	Q	170	LEU	2.5
1	H	239	ASN	2.5
1	D	113	ALA	2.5
1	I	192	ASP	2.5
1	L	103	TRP	2.5
1	I	208	ASN	2.5
1	F	336	ALA	2.5
1	N	114	ALA	2.5
1	Q	372	HIS	2.5
1	R	261	VAL	2.5
1	I	120	ASP	2.5
1	O	161	PRO	2.5
1	O	384	PRO	2.5
1	R	62	ASN	2.5
1	G	261	VAL	2.4
1	B	103	TRP	2.4
1	C	105	ASP	2.4
1	Q	356	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	248	VAL	2.4
1	I	256	GLY	2.4
1	H	238	THR	2.4
1	I	155	VAL	2.4
1	B	84	ASP	2.4
1	E	40	ILE	2.4
1	I	290	ILE	2.4
1	M	56	ASN	2.4
1	E	146	THR	2.4
1	I	81	ARG	2.4
1	O	137	PRO	2.4
1	D	153	GLU	2.4
1	N	121	GLU	2.4
1	P	66	GLU	2.4
1	O	268	THR	2.4
1	D	150	LEU	2.4
1	E	148	ARG	2.4
1	G	333	VAL	2.4
1	N	147	ILE	2.4
1	M	154	ALA	2.4
1	N	133	ALA	2.4
1	I	171	THR	2.4
1	L	118	LEU	2.4
1	M	374	LEU	2.4
1	H	386	TYR	2.4
1	H	194	ASP	2.4
1	F	109	ALA	2.4
1	G	207	THR	2.4
1	Q	360	HIS	2.3
1	D	156	ALA	2.3
1	G	154	ALA	2.3
1	I	75	THR	2.3
1	N	146	THR	2.3
1	O	366	LYS	2.3
1	I	90	ARG	2.3
1	I	116	PRO	2.3
1	D	69	MET	2.3
1	G	83	LYS	2.3
1	B	362	ARG	2.3
1	J	124	GLN	2.3
1	D	157	LYS	2.3
1	I	325	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	341	THR	2.3
1	I	54	LEU	2.3
1	O	69	MET	2.3
1	I	355	ILE	2.3
1	R	147	ILE	2.3
1	F	68	ASN	2.3
1	N	125	ALA	2.3
1	P	379	THR	2.3
1	E	160	ASP	2.3
1	H	61	LEU	2.3
1	I	194	ASP	2.3
1	I	345	PRO	2.3
1	M	376	THR	2.3
1	R	171	THR	2.3
1	H	378	LEU	2.3
1	A	130	TYR	2.3
1	H	66	GLU	2.3
1	Q	150	LEU	2.3
1	I	272	LYS	2.2
1	I	37	LEU	2.2
1	R	357	LEU	2.2
1	K	102	ASN	2.2
1	O	138	GLU	2.2
1	B	315	ALA	2.2
1	D	110	TRP	2.2
1	F	170	LEU	2.2
1	I	74	PRO	2.2
1	N	79	GLN	2.2
1	I	310	LEU	2.2
1	E	51	GLU	2.2
1	H	56	ASN	2.2
1	I	28	GLY	2.2
1	N	131	LYS	2.2
1	F	362	ARG	2.2
1	G	328	VAL	2.2
1	I	328	VAL	2.2
1	O	362	ARG	2.2
1	B	164	ALA	2.2
1	G	249	ALA	2.2
1	L	71	ALA	2.2
1	Q	146	THR	2.2
1	O	159	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	89	PRO	2.2
1	O	176	LEU	2.2
1	N	107	TRP	2.2
1	O	142	ARG	2.2
1	Q	155	VAL	2.2
1	O	361	GLU	2.2
1	J	84	ASP	2.2
1	Q	161	PRO	2.2
1	C	102	ASN	2.2
1	R	379	THR	2.2
1	K	85	ASP	2.1
1	K	103	TRP	2.1
1	D	119	ASN	2.1
1	H	212	ILE	2.1
1	B	357	LEU	2.1
1	K	142	ARG	2.1
1	N	362	ARG	2.1
1	H	53	ALA	2.1
1	I	122	THR	2.1
1	H	180	ILE	2.1
1	G	314	LEU	2.1
1	E	166	SER	2.1
1	F	327	CYS	2.1
1	G	162	THR	2.1
1	H	384	PRO	2.1
1	H	170	LEU	2.1
1	P	378	LEU	2.1
1	P	372	HIS	2.1
1	O	53	ALA	2.1
1	Q	156	ALA	2.1
1	D	151	THR	2.1
1	E	280	HIS	2.1
1	H	160	ASP	2.1
1	I	78	ASP	2.1
1	L	115	LEU	2.1
1	I	70	THR	2.1
1	N	80	PHE	2.1
1	H	58	GLN	2.1
1	B	117	LEU	2.1
1	I	380	LEU	2.1
1	R	153	GLU	2.1
1	H	263	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	89	PRO	2.0
1	O	52	THR	2.0
1	Q	364	VAL	2.0
1	O	147	ILE	2.0
1	F	65	LEU	2.0
1	I	323	GLY	2.0
1	G	206	SER	2.0
1	D	64	ILE	2.0
1	L	54	LEU	2.0
1	L	77	LEU	2.0
1	L	121	GLU	2.0
1	G	136	GLN	2.0
1	C	80	PHE	2.0
1	O	169	ASP	2.0
1	O	49	LYS	2.0
1	R	74	PRO	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	BMA	U	3	11/12	0.37	0.22	112,134,140,145	0
5	BMA	V	3	11/12	0.55	0.23	141,154,162,163	0
5	BMA	Y	3	11/12	0.59	0.28	140,148,153,154	0
5	BMA	X	3	11/12	0.62	0.35	158,166,170,173	0
4	NAG	U	2	14/15	0.66	0.22	91,117,137,142	0
6	MAN	c	5	11/12	0.68	0.20	139,144,149,149	0
5	NAG	V	1	14/15	0.72	0.44	134,157,160,162	0
6	MAN	W	4	11/12	0.73	0.26	95,102,110,113	0
5	NAG	V	2	14/15	0.73	0.41	144,157,161,162	0
7	MAN	b	4	11/12	0.75	0.21	132,141,146,148	0
7	BMA	a	3	11/12	0.78	0.16	122,127,134,137	0
5	NAG	X	2	14/15	0.80	0.37	151,160,163,163	0

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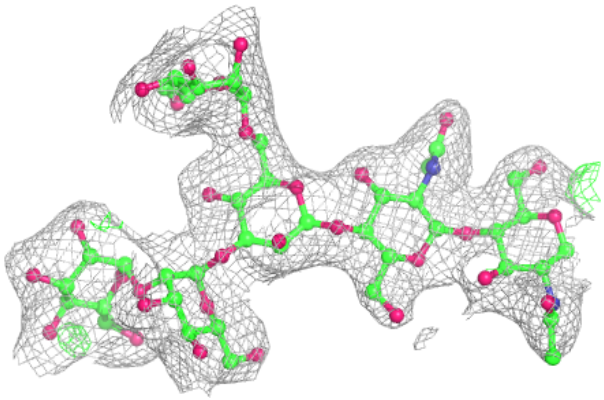
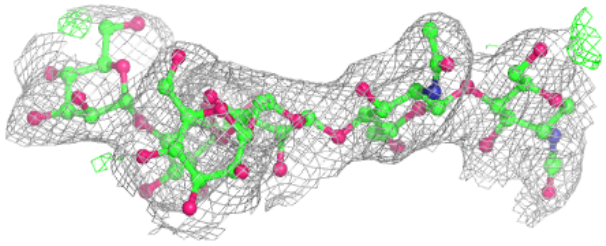
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	U	1	14/15	0.80	0.20	78,104,117,119	0
5	NAG	X	1	14/15	0.80	0.41	149,154,160,161	0
7	MAN	a	4	11/12	0.80	0.18	124,134,137,138	0
7	BMA	b	3	11/12	0.80	0.22	135,139,140,141	0
6	NAG	W	2	14/15	0.80	0.26	81,93,101,102	0
3	MAN	T	5	11/12	0.81	0.46	122,128,133,134	0
5	NAG	Y	1	14/15	0.81	0.18	113,124,130,130	0
6	NAG	c	1	14/15	0.82	0.21	132,137,141,144	0
3	MAN	T	4	11/12	0.83	0.18	119,125,130,132	0
6	NAG	W	1	14/15	0.84	0.22	77,84,97,97	0
2	MAN	Z	5	11/12	0.85	0.16	102,102,102,102	0
5	NAG	Y	2	14/15	0.85	0.49	123,136,142,148	0
6	MAN	c	4	11/12	0.86	0.21	142,146,150,151	0
7	MAN	a	5	11/12	0.86	0.14	126,131,132,133	0
6	NAG	c	2	14/15	0.86	0.34	129,138,151,157	0
6	BMA	c	3	11/12	0.86	0.21	137,141,145,147	0
3	BMA	T	3	11/12	0.87	0.15	111,118,126,127	0
3	NAG	T	1	14/15	0.87	0.18	91,97,106,108	0
7	NAG	b	2	14/15	0.87	0.15	113,124,135,144	0
7	NAG	a	2	14/15	0.87	0.21	104,113,123,129	0
3	NAG	T	2	14/15	0.87	0.20	87,101,109,121	0
2	MAN	S	5	11/12	0.88	0.15	103,109,117,121	0
6	BMA	W	3	11/12	0.88	0.17	95,99,103,104	0
2	BMA	S	3	11/12	0.88	0.13	73,87,92,93	0
2	NAG	Z	2	14/15	0.91	0.17	67,83,89,90	0
7	NAG	a	1	14/15	0.91	0.15	92,104,110,113	0
7	NAG	b	1	14/15	0.91	0.11	101,113,122,123	0
2	MAN	Z	6	11/12	0.93	0.13	78,79,86,92	0
6	MAN	W	5	11/12	0.93	0.20	93,98,106,108	0
2	MAN	Z	4	11/12	0.93	0.13	77,86,98,99	0
2	MAN	S	6	11/12	0.93	0.09	83,88,99,99	0
7	MAN	b	5	11/12	0.93	0.44	132,134,139,143	0
2	MAN	S	4	11/12	0.94	0.14	77,90,95,101	0
2	BMA	Z	3	11/12	0.94	0.12	74,83,86,93	0
2	NAG	Z	1	14/15	0.94	0.15	75,84,87,91	0
2	NAG	S	2	14/15	0.95	0.13	58,78,84,86	0
2	NAG	S	1	14/15	0.96	0.14	69,75,82,85	0

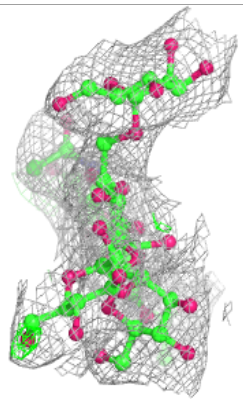
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain S:

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

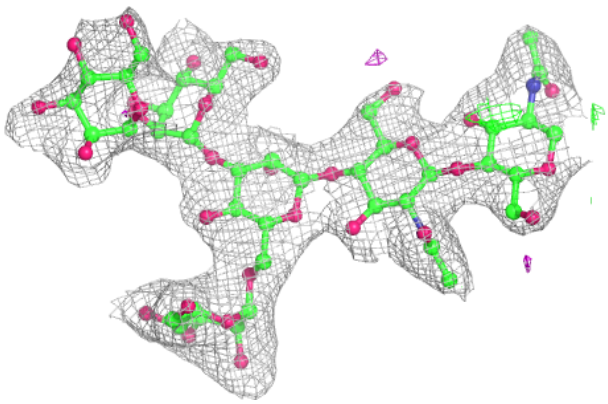


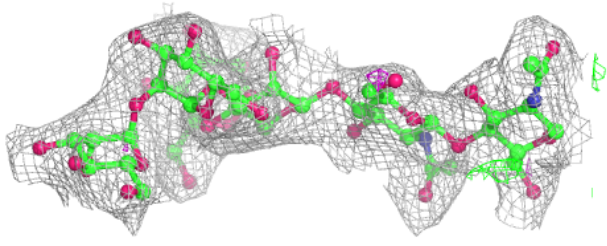


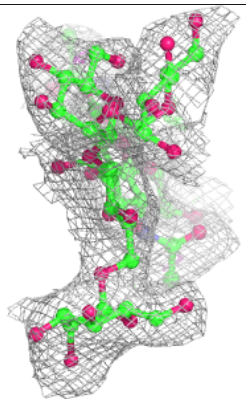


Electron density around Chain Z:

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

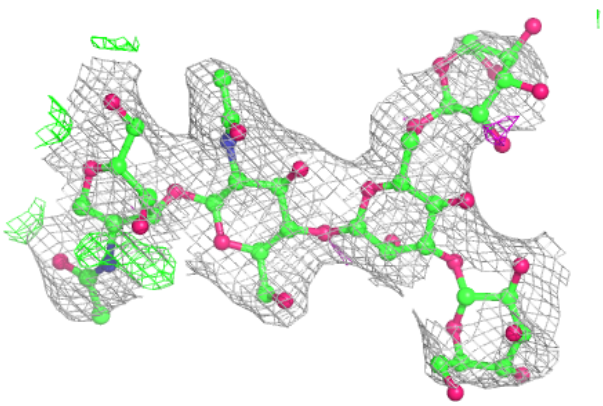


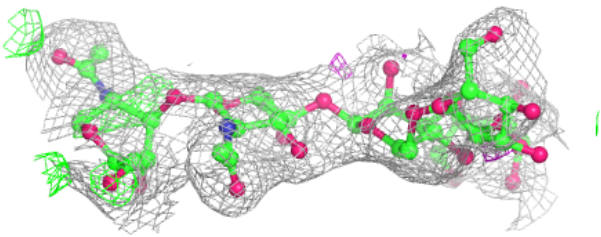


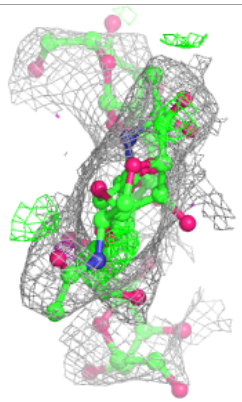


Electron density around Chain T:

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

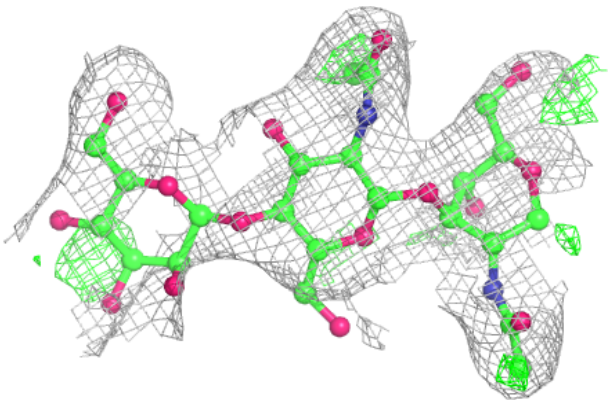


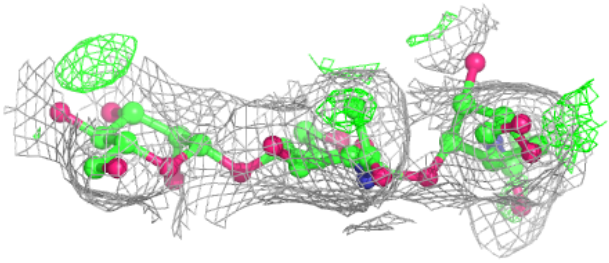




Electron density around Chain U:

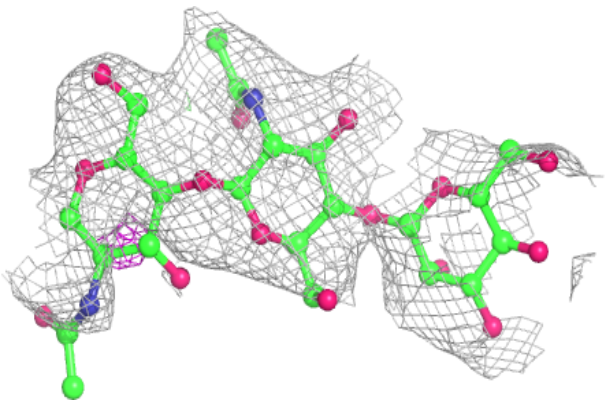
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

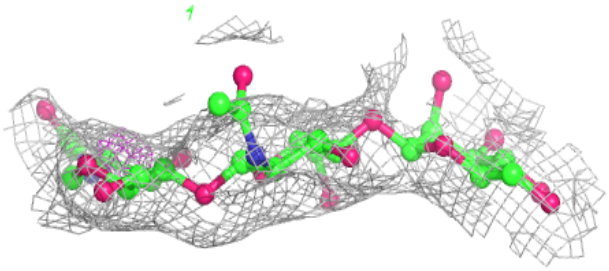


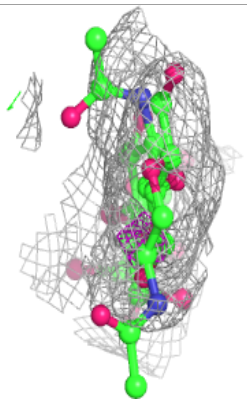


Electron density around Chain V:

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

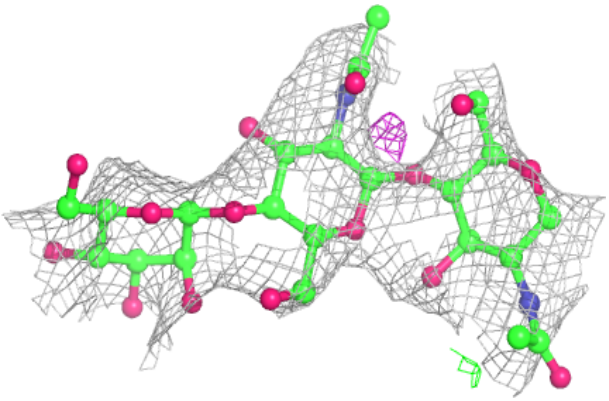


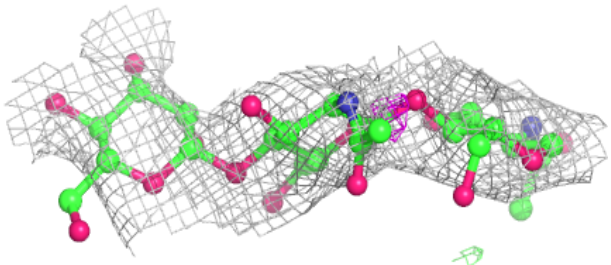


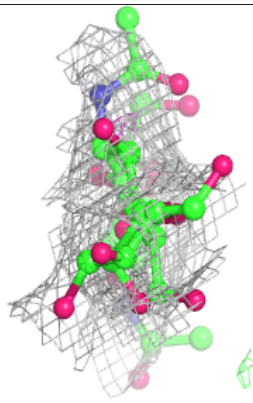


Electron density around Chain X:

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

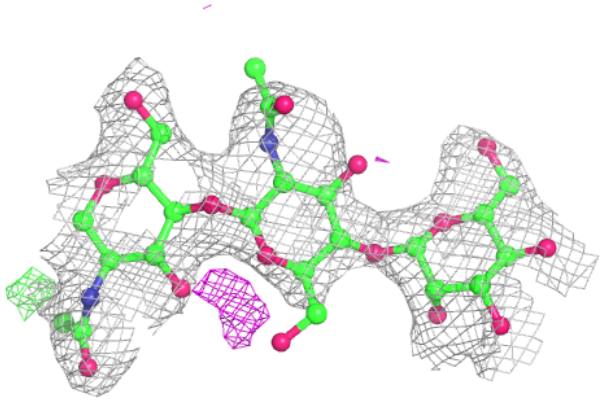


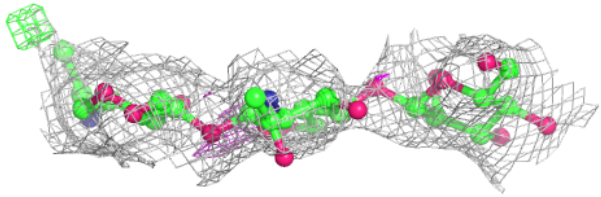


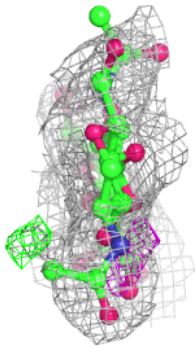


Electron density around Chain Y:

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

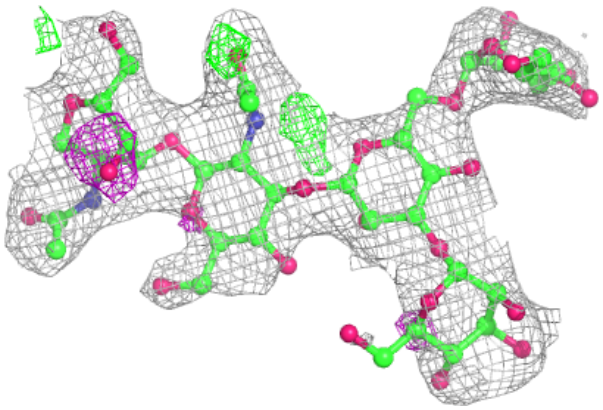


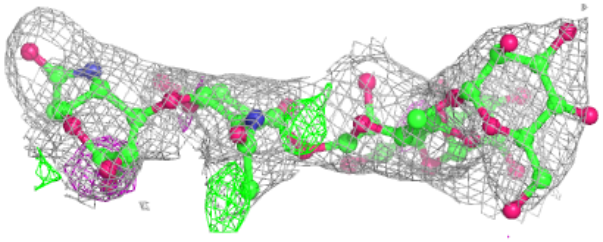


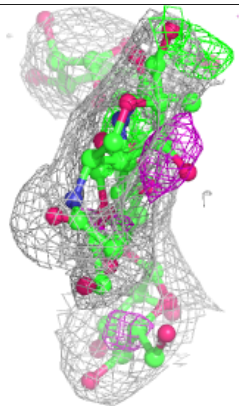


Electron density around Chain W:

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

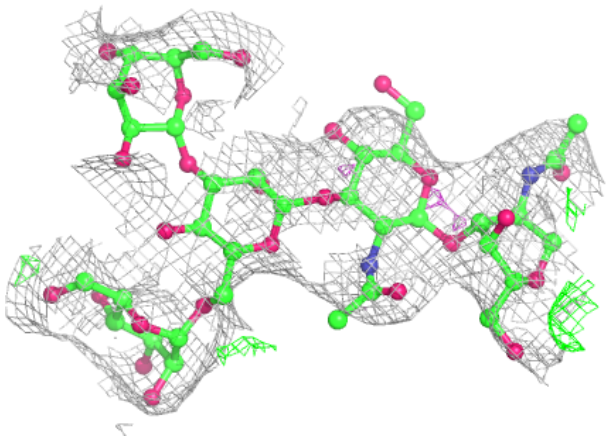


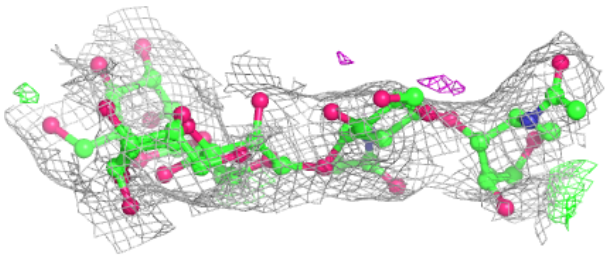


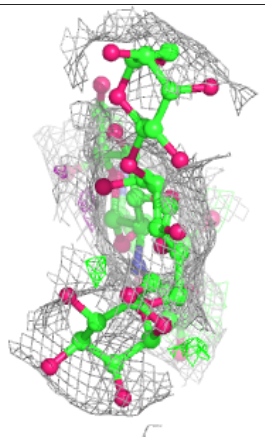


Electron density around Chain c:

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

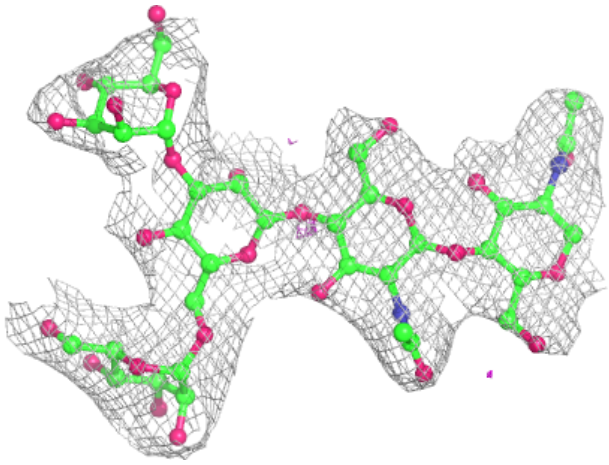


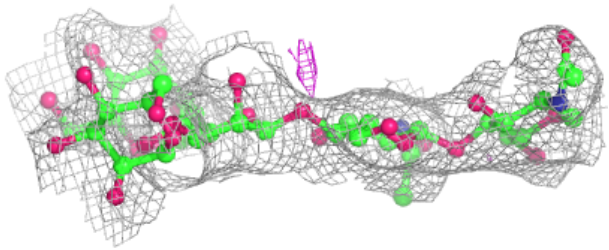


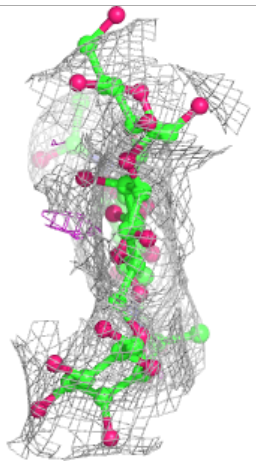


Electron density around Chain a:

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

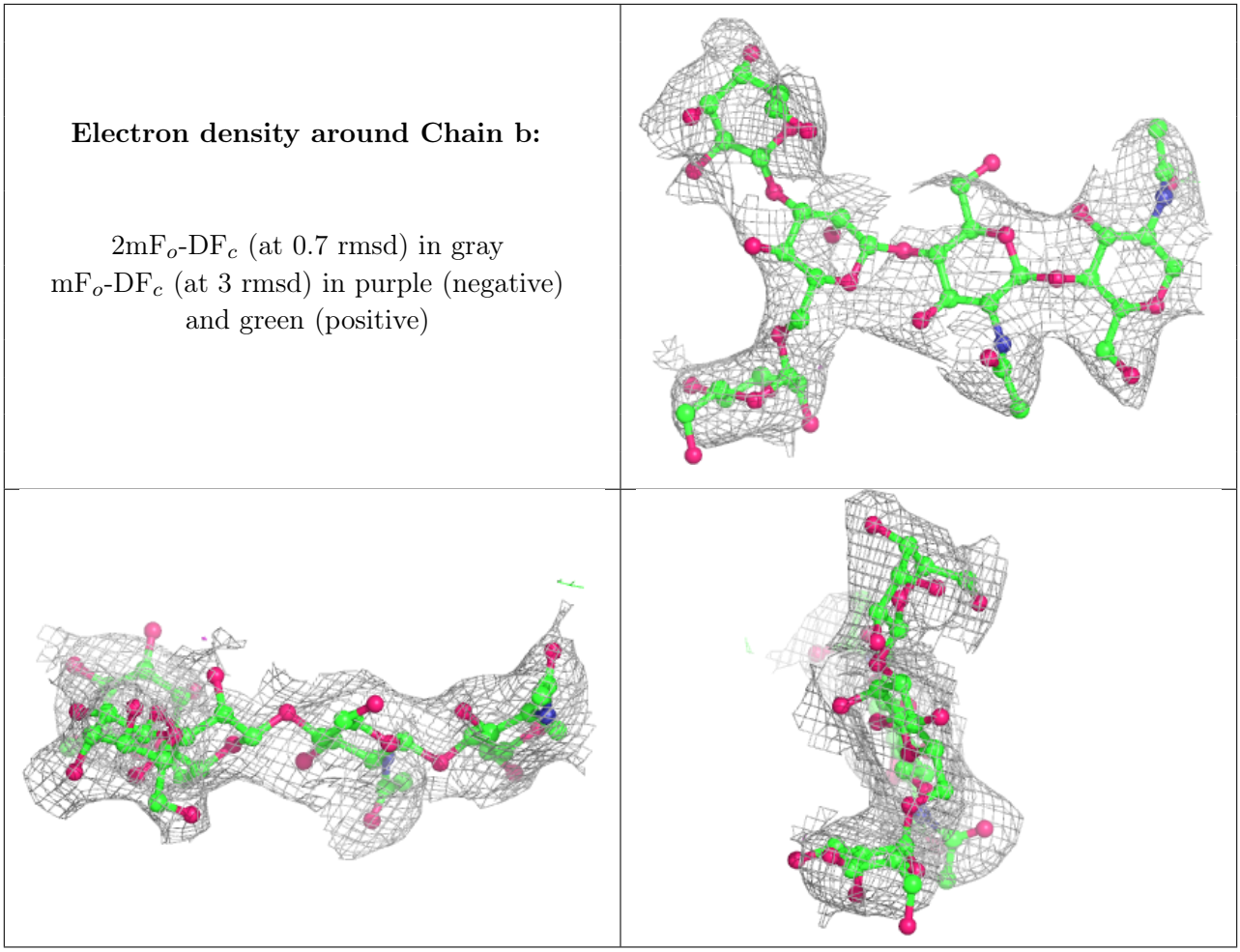






Electron density around Chain b:

$2mF_o$-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
9	NAG	E	502	14/15	0.54	0.37	127,138,144,147	0
9	NAG	Q	501	14/15	0.56	0.39	152,161,166,168	0
8	GLC	I	501	11/12	0.60	0.34	156,161,168,168	0
9	NAG	R	501	14/15	0.70	0.38	160,164,169,172	0
9	NAG	O	502	14/15	0.77	0.21	120,140,144,144	0
8	GLC	O	501	11/12	0.86	0.18	103,115,118,122	0
8	GLC	Q	502	11/12	0.88	0.19	96,103,107,109	0
8	GLC	H	501	11/12	0.89	0.15	123,133,140,141	0
8	GLC	F	501	11/12	0.91	0.14	90,100,105,105	0
8	GLC	R	502	11/12	0.92	0.17	81,91,98,103	0
8	GLC	L	501	11/12	0.94	0.14	67,72,78,83	0

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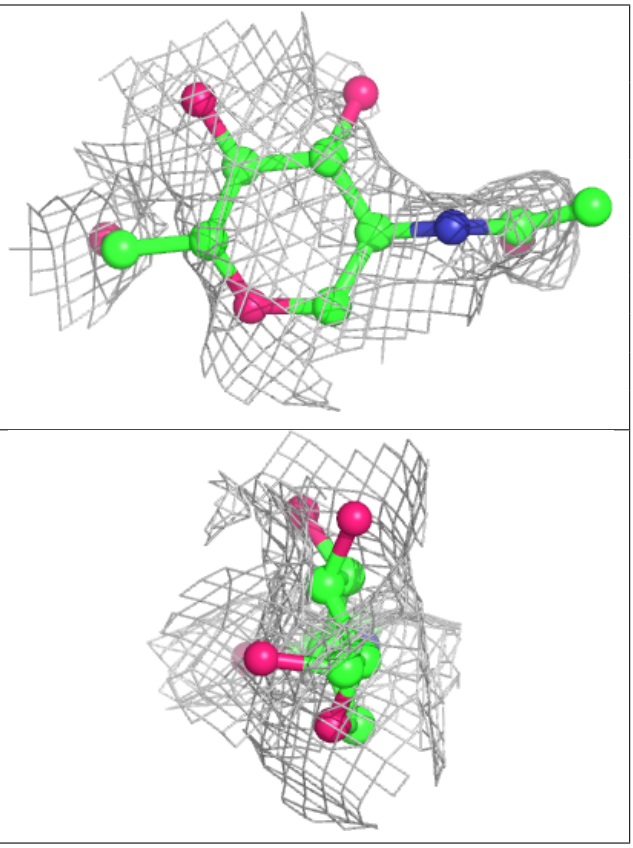
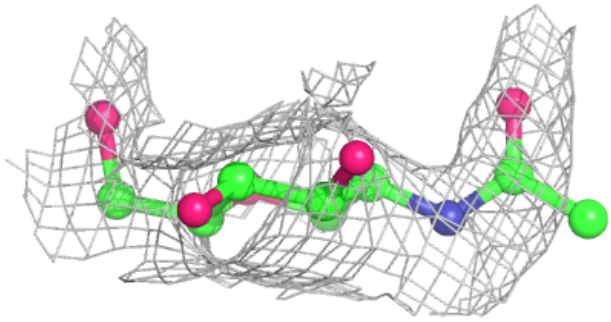
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	GLC	N	501	11/12	0.94	0.12	84,86,92,93	0
8	GLC	E	501	11/12	0.94	0.11	90,93,98,104	0
8	GLC	P	501	11/12	0.95	0.12	83,90,94,96	0
8	GLC	K	501	11/12	0.96	0.10	65,74,78,78	0
8	GLC	A	501	11/12	0.96	0.11	49,59,71,71	0
8	GLC	M	501	11/12	0.96	0.15	74,80,86,94	0
8	GLC	D	501	11/12	0.96	0.12	73,79,83,84	0
8	GLC	C	501	11/12	0.97	0.16	58,61,65,68	0
8	GLC	B	501	11/12	0.97	0.12	54,59,66,71	0
8	GLC	J	501	11/12	0.97	0.11	56,60,66,68	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 NAG E 502:

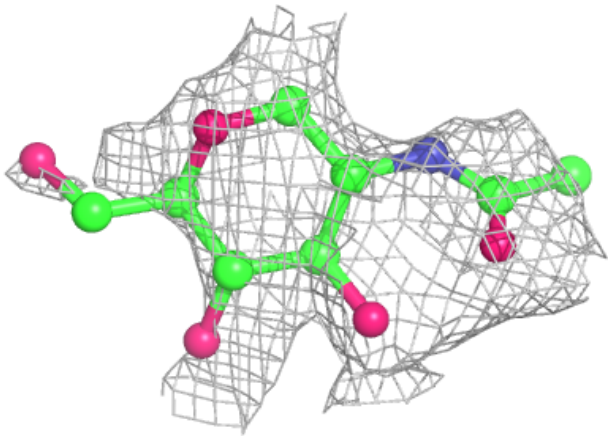
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

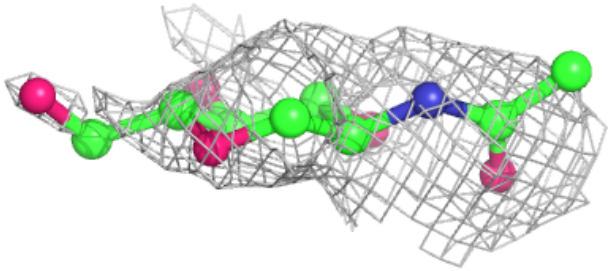


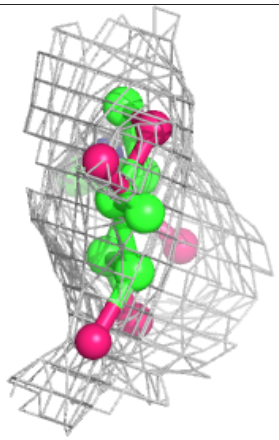


Electron density around NAG Q 501:

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

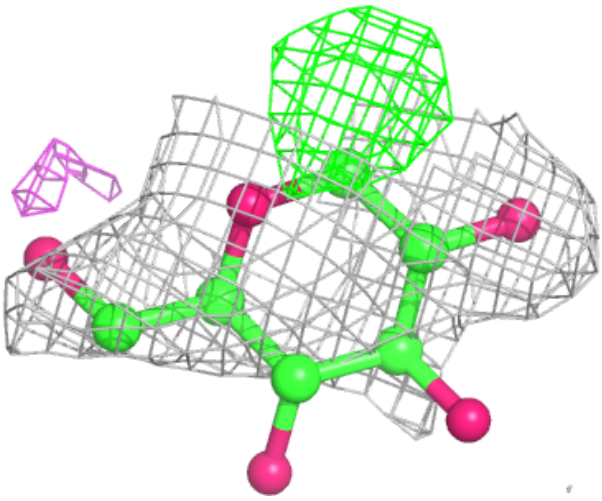


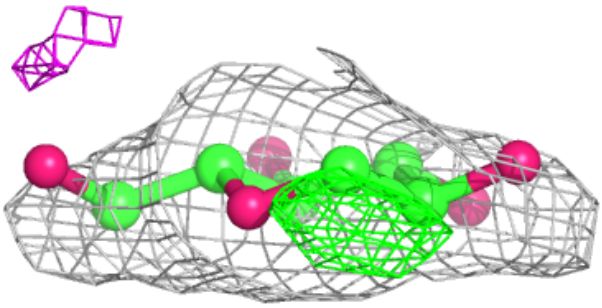


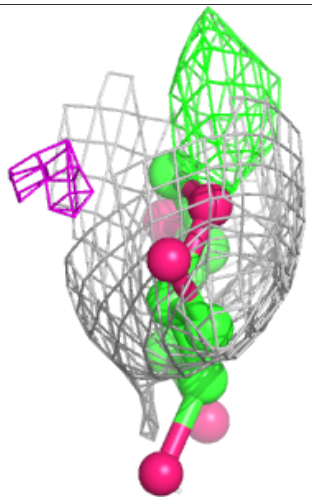


Electron density around GLC I 501:

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

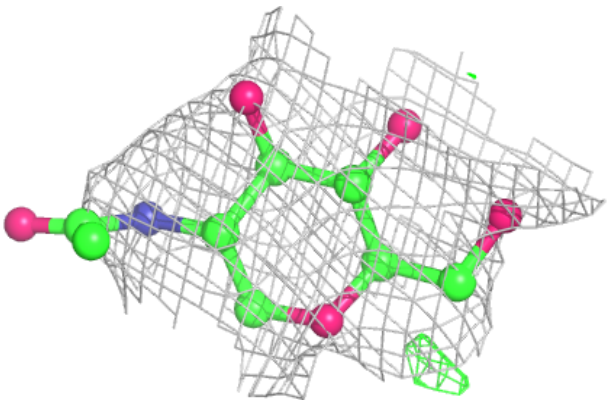


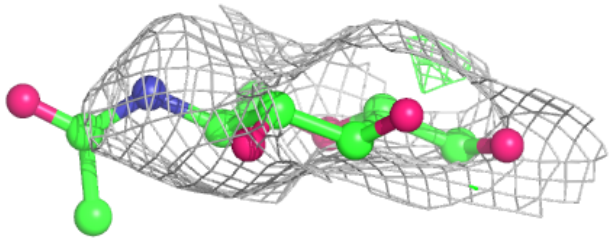


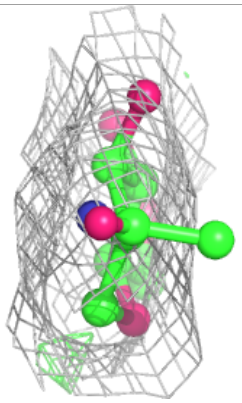


Electron density around NAG R 501:

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

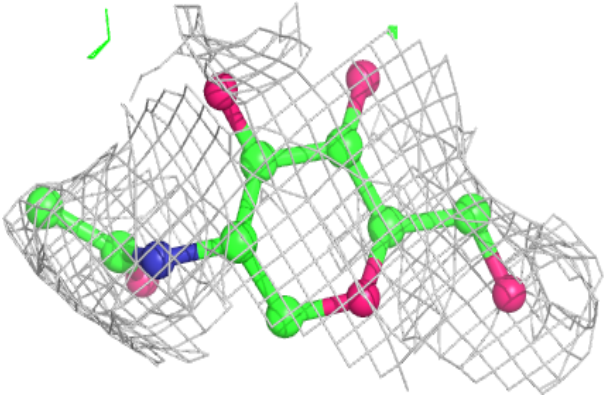


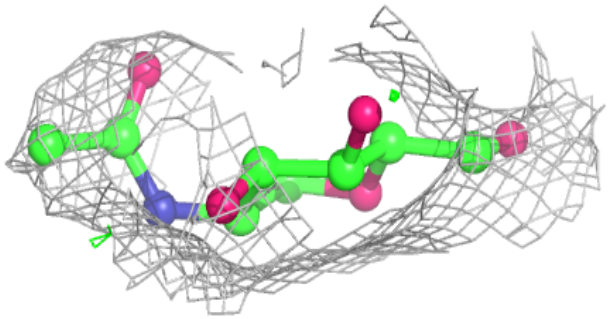


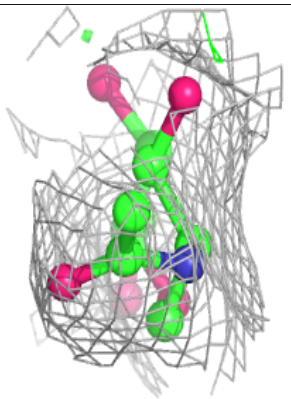


Electron density around NAG O 502:

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

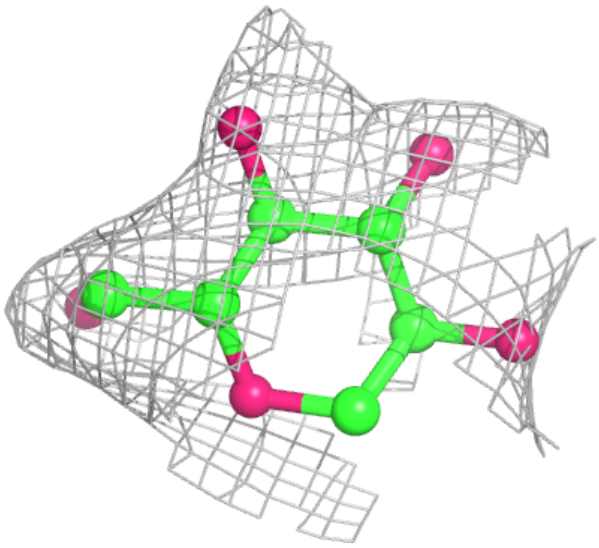


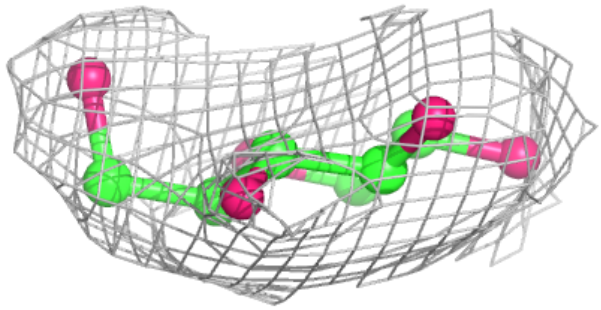


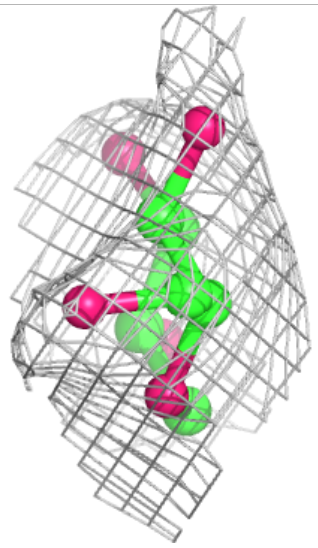


Electron density around GLC O 501:

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

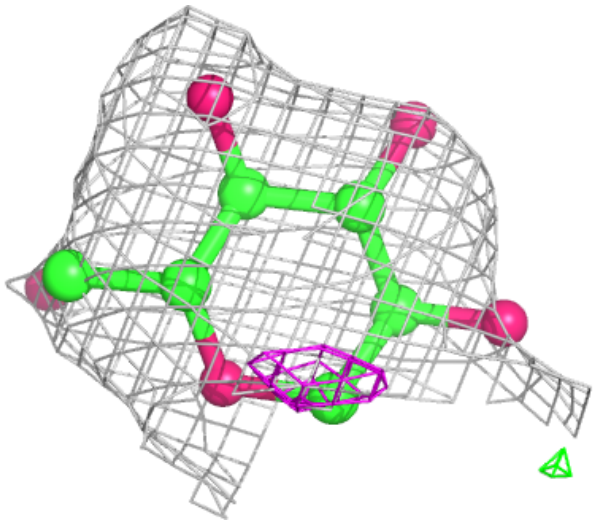


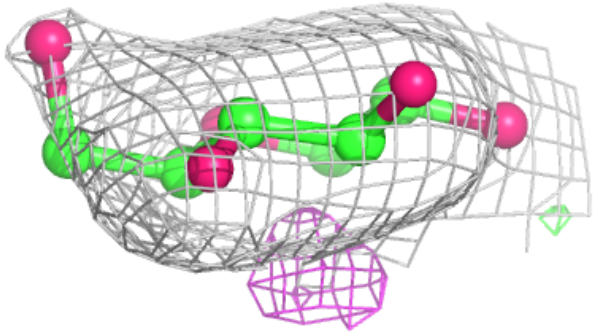


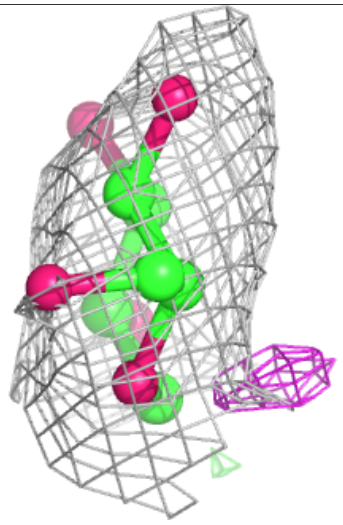


Electron density around GLC Q 502:

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

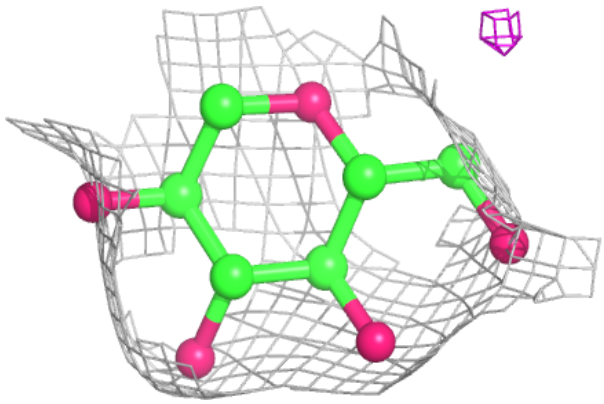


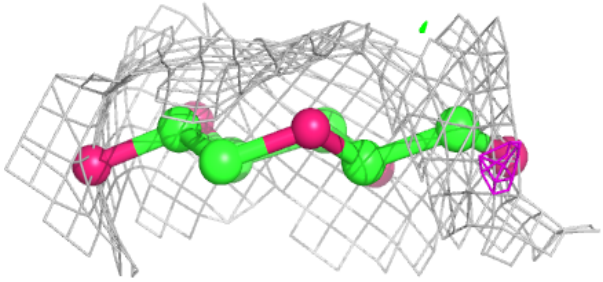


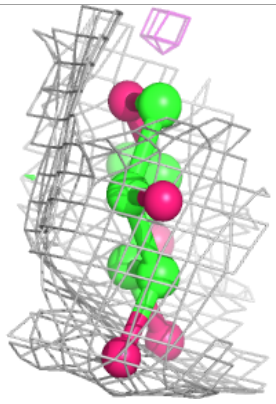


Electron density around GLC H 501:

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

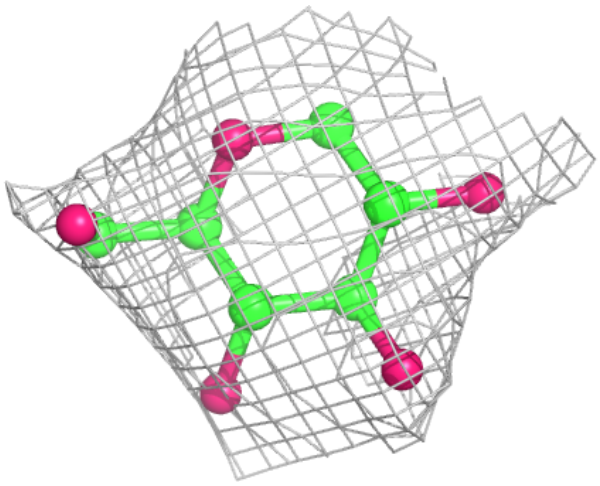


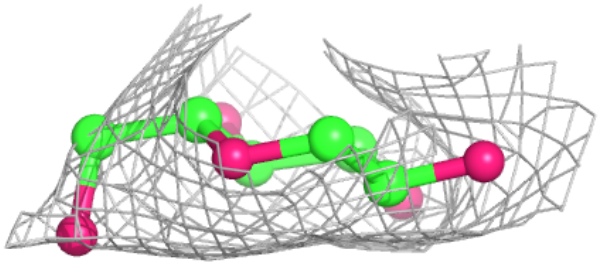


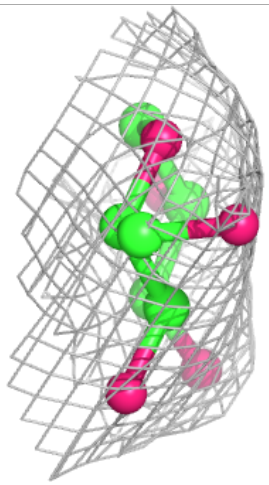


Electron density around GLC F 501:

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

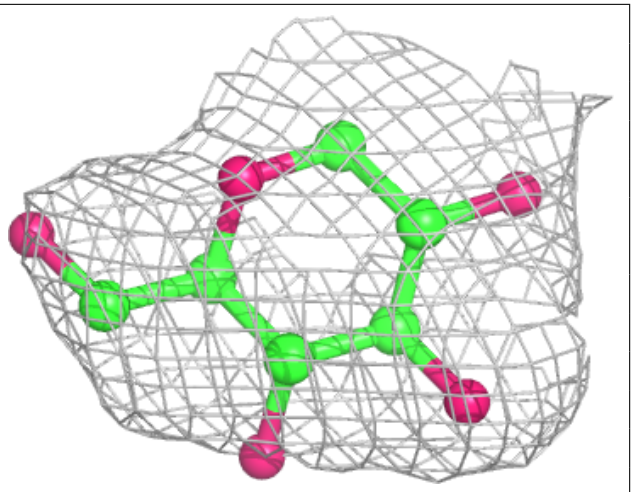


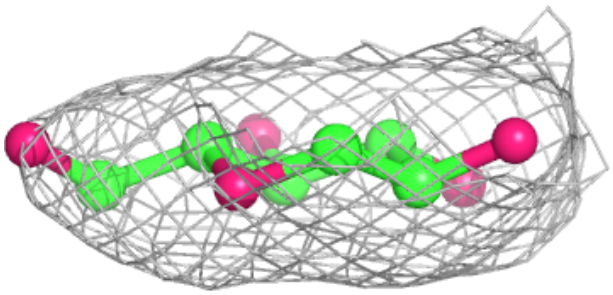


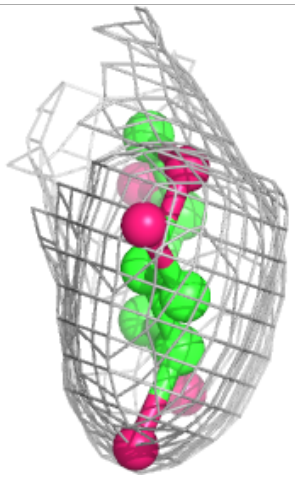


Electron density around GLC R 502:

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

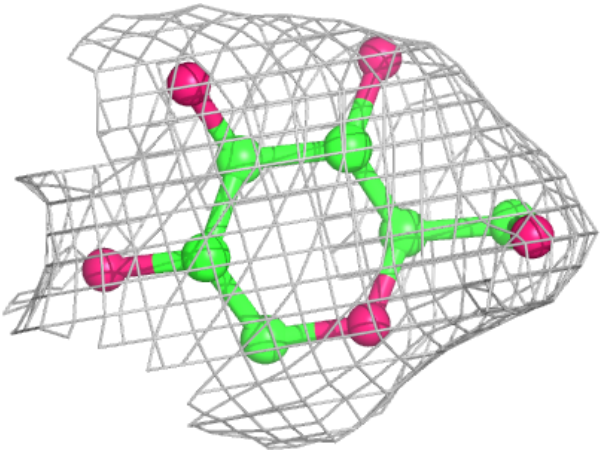


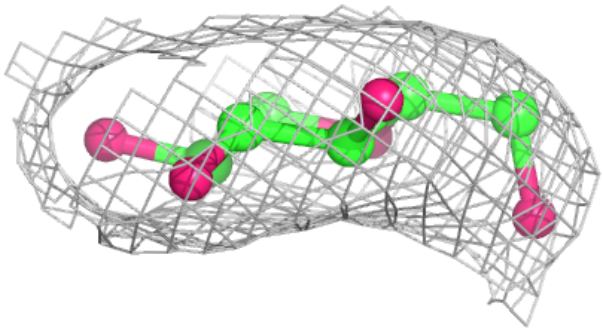


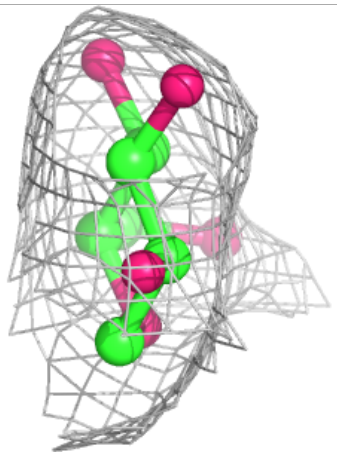


Electron density around GLC L 501:

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

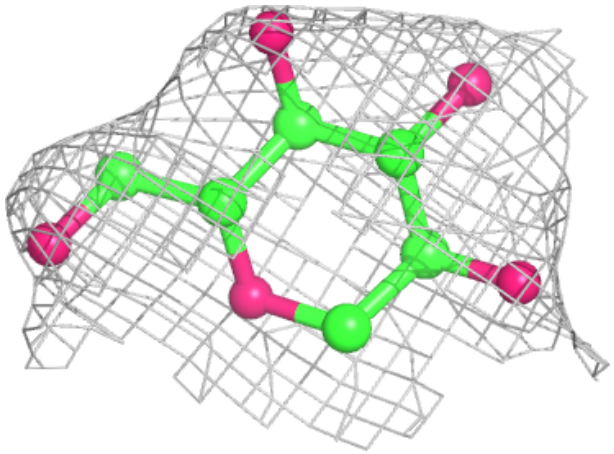


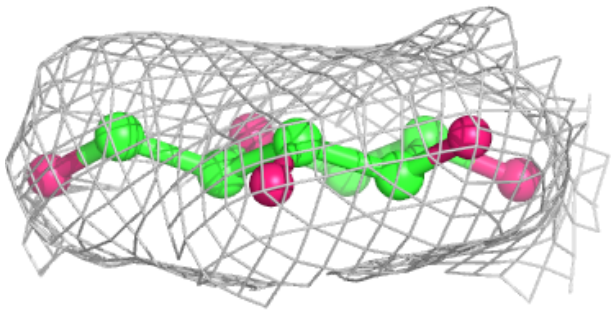


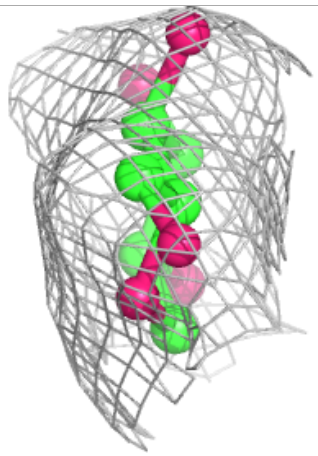


Electron density around GLC N 501:

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

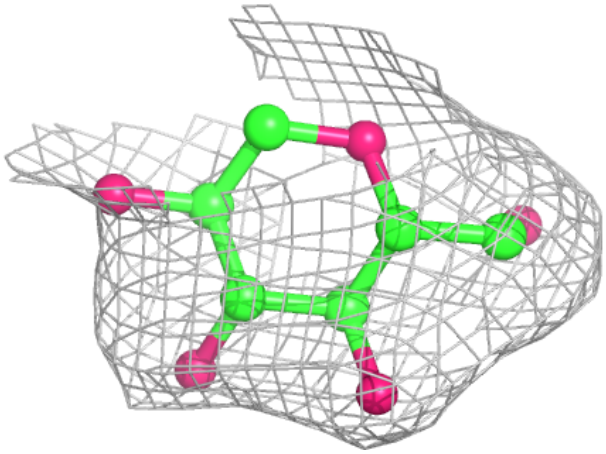


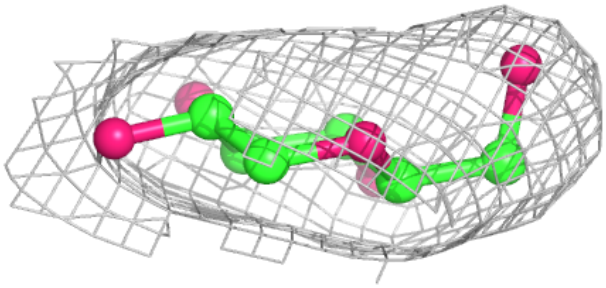


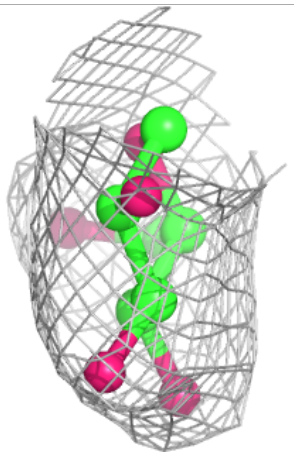


Electron density around GLC E 501:

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

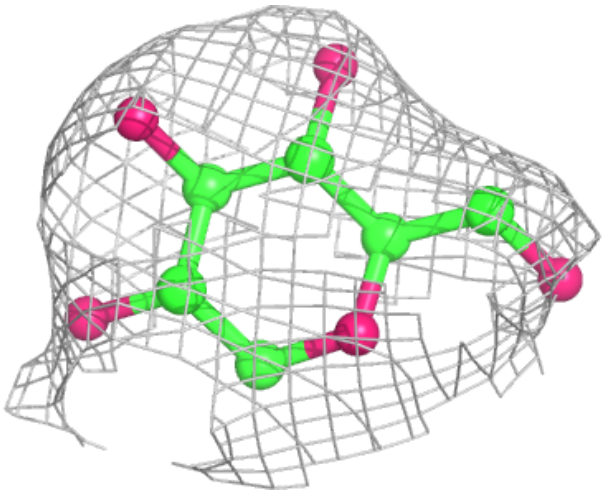


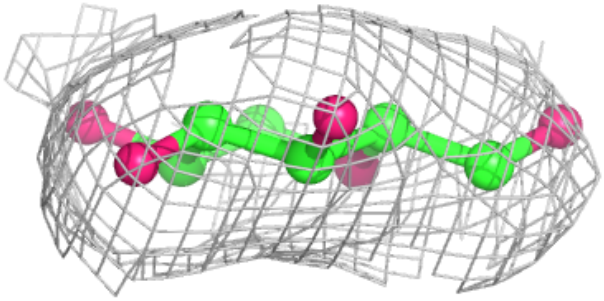


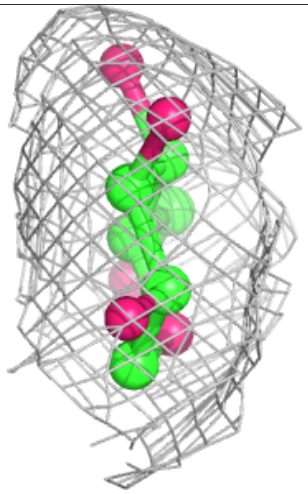


Electron density around GLC P 501:

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

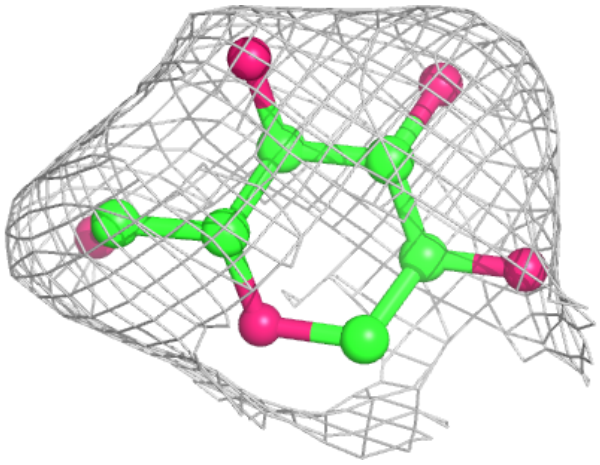


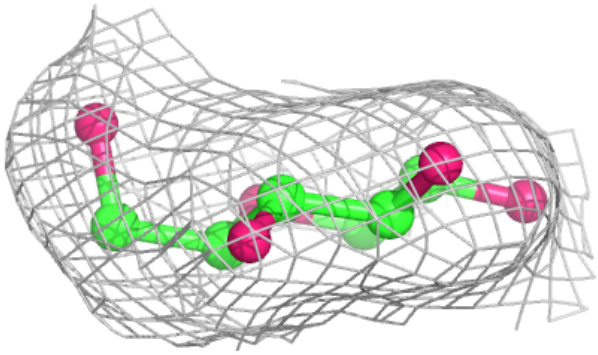


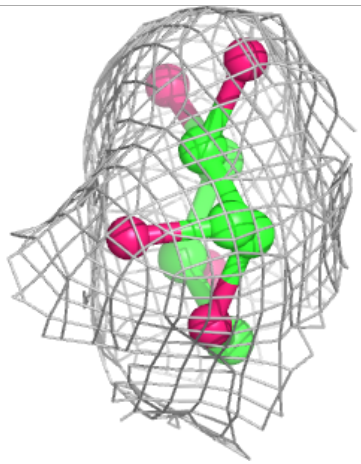


Electron density around GLC K 501:

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

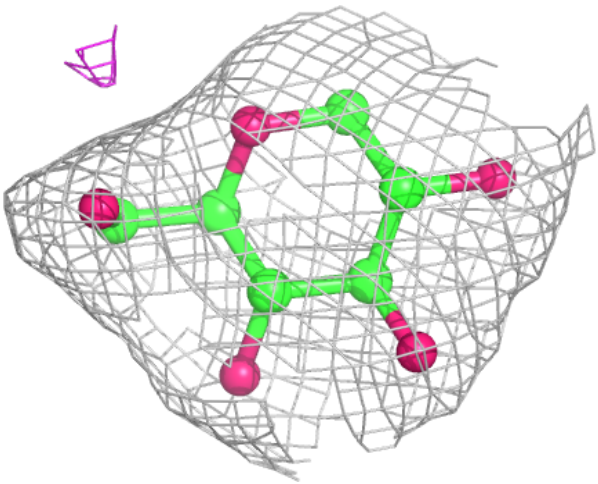


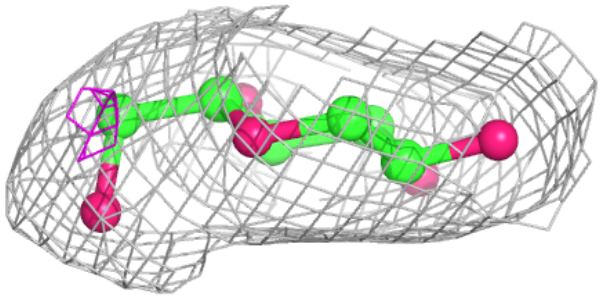


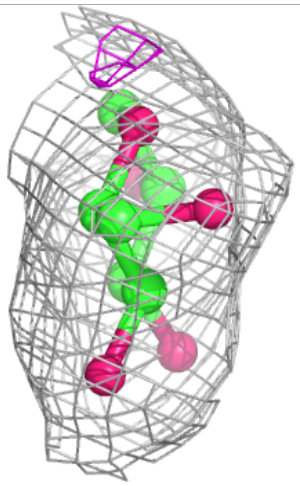


Electron density around GLC A 501:

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

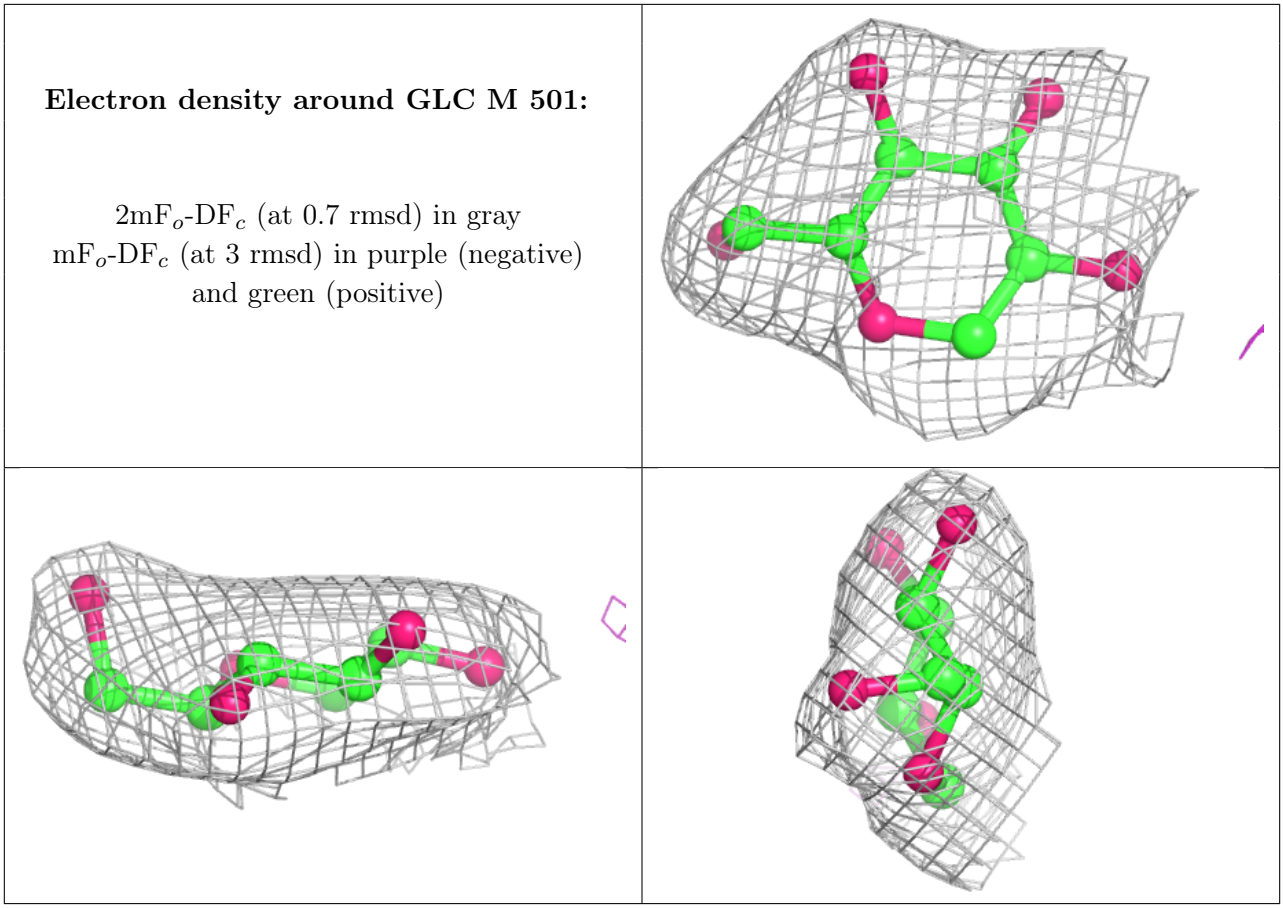






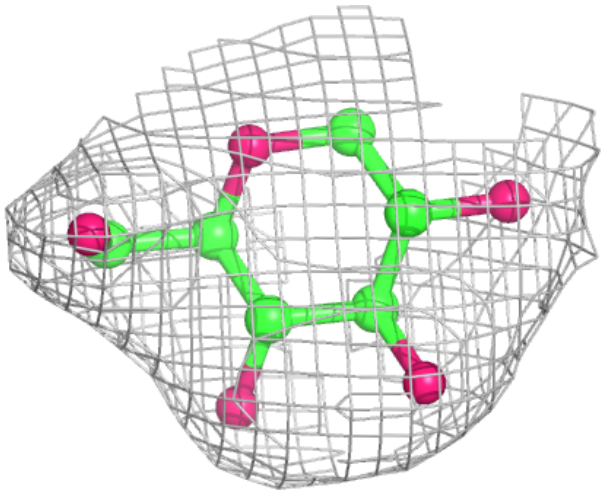
Electron density around GLC M 501:

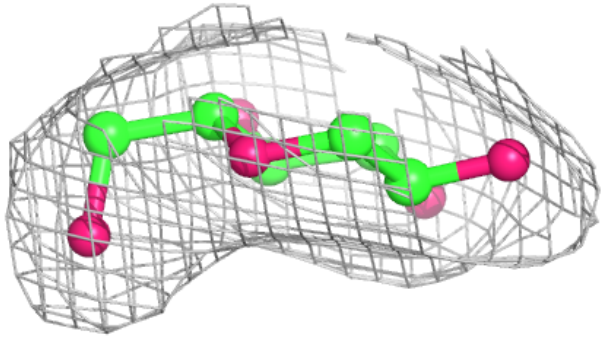
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

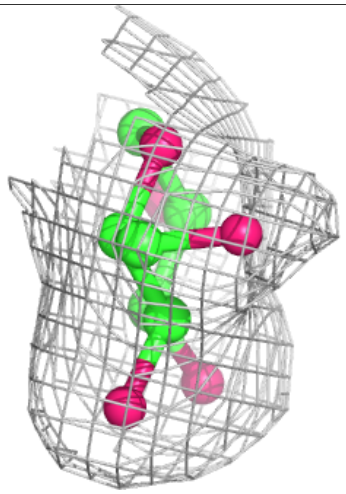


Electron density around GLC D 501:

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

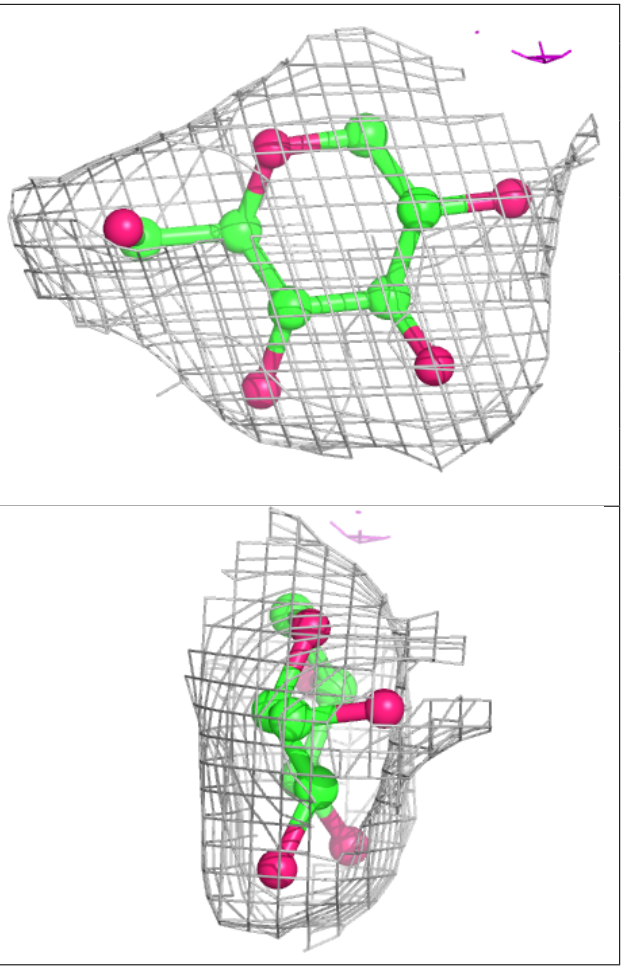






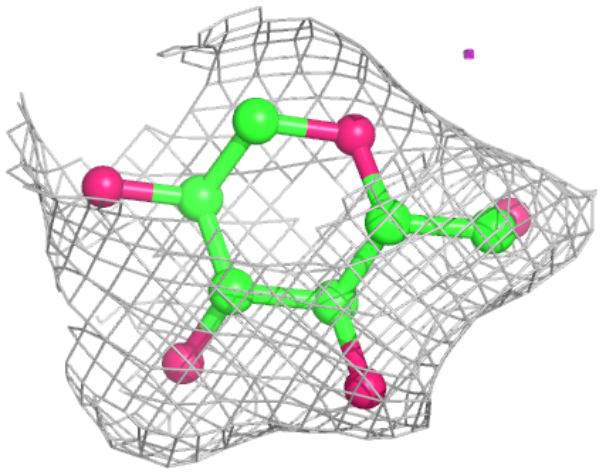
Electron density around GLC C 501:

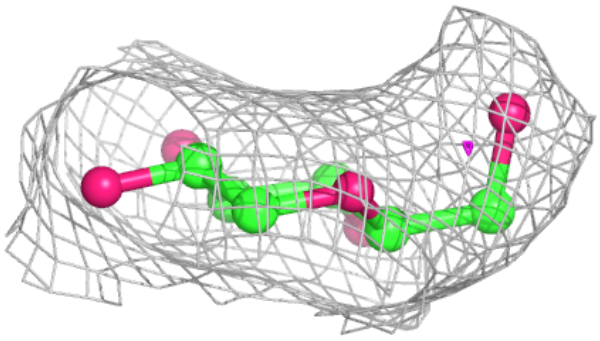
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

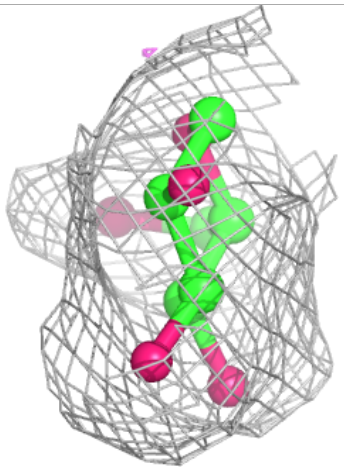


Electron density around GLC B 501:

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

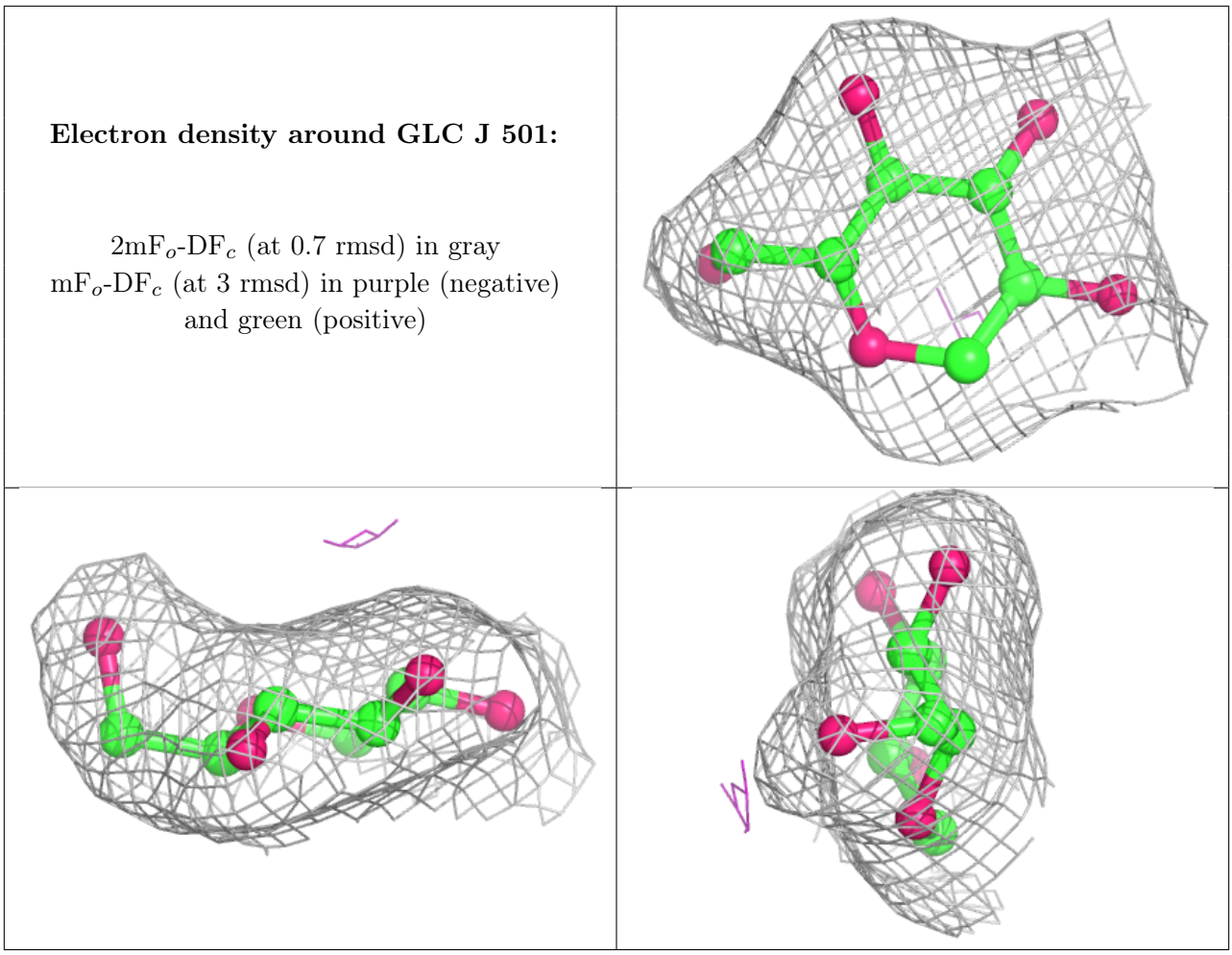






Electron density around GLC J 501:

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



6.5 Other polymers

There are no such residues in this entry.