Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2023 – 01:44 PM EST

PDB ID	:	8D3T
Title	:	Crystal structure of GalS1 from Populus trichocarpas
Authors	:	Pereira, J.H.; Prabhakar, P.K.; Urbanowicz, B.R.; Adams, P.D.
Deposited on	:	2022-06-01
Resolution	:	2.37 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 (i) symbol.

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

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

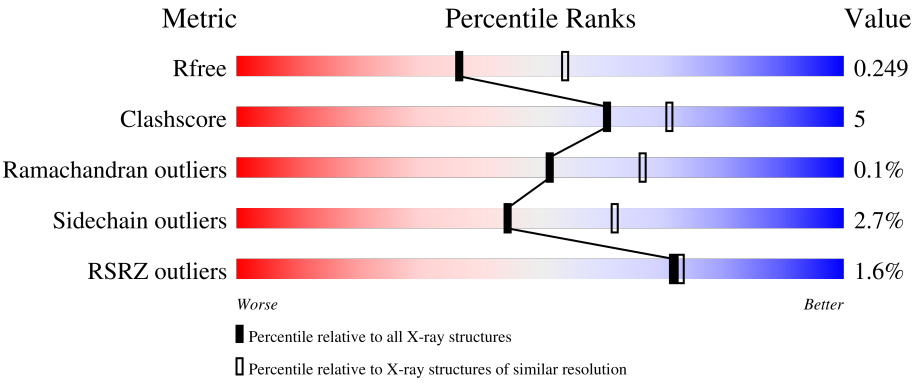
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	424	3% 82% 10% 7%
1	B	424	% 83% 10% 7%
1	C	424	% 83% 9% 7%
1	D	424	2% 81% 11% 8%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	G	2	100%
2	I	2	50% 50%
2	K	2	50% 50%
3	F	7	71% 29%
3	H	7	43% 43% 14%
3	J	7	43% 43% 14%
4	L	7	14% 29% 57%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	501	-	-	-	X
5	NAG	C	501	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27020 atoms, of which 12810 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 Galactan synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	393	Total	C	H	N	O	S	0	0	0
			6279	2076	3048	554	588	13			
1	B	394	Total	C	H	N	O	S	0	0	0
			6291	2080	3052	555	591	13			
1	C	394	Total	C	H	N	O	S	0	0	0
			6292	2080	3053	555	591	13			
1	D	392	Total	C	H	N	O	S	0	0	0
			6265	2071	3041	553	587	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A2K2AMS7
B	1	GLY	-	expression tag	UNP A0A2K2AMS7
C	1	GLY	-	expression tag	UNP A0A2K2AMS7
D	1	GLY	-	expression tag	UNP A0A2K2AMS7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	G	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	I	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

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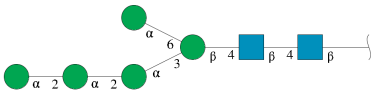
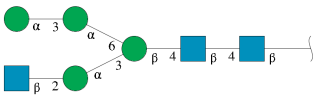
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



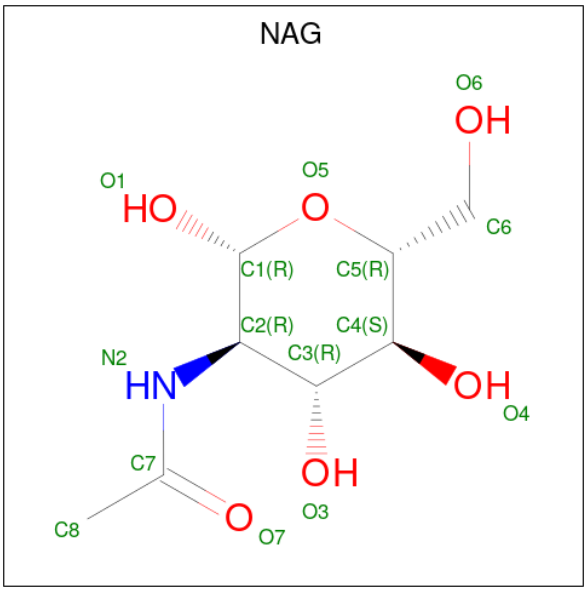
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			
3	H	7	Total	C	H	N	O	0	0	0
			152	46	69	2	35			
3	J	7	Total	C	H	N	O	0	0	0
			153	46	70	2	35			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
4	L	7	Total	C	H	N	O	0	0	0
			159	48	73	3	35			

- Molecule 5 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
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	C	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
5	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 6 is water.

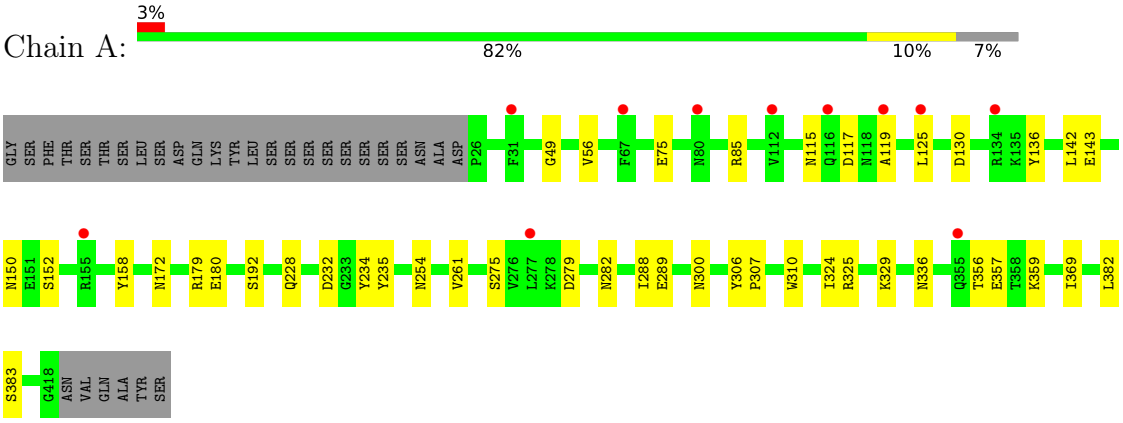
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	141	Total	O	0	0
			141	141		
6	B	145	Total	O	0	0
			145	145		
6	C	171	Total	O	0	0
			171	171		
6	D	121	Total	O	0	0
			121	121		

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.

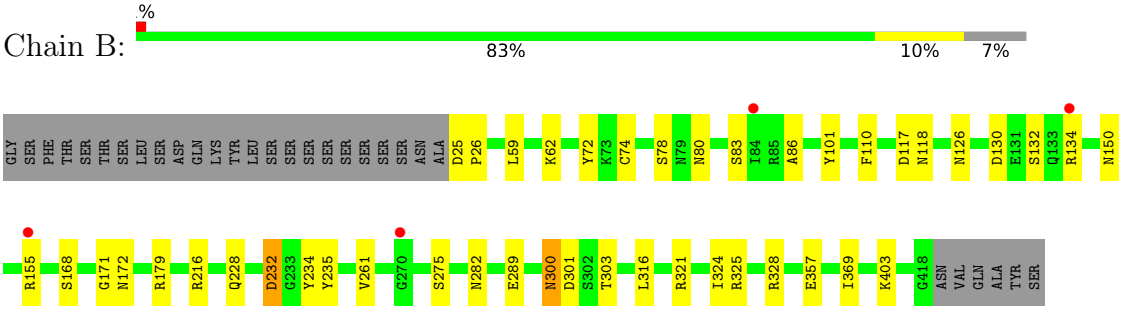
• Molecule 1: Galactan synthase

Chain A:



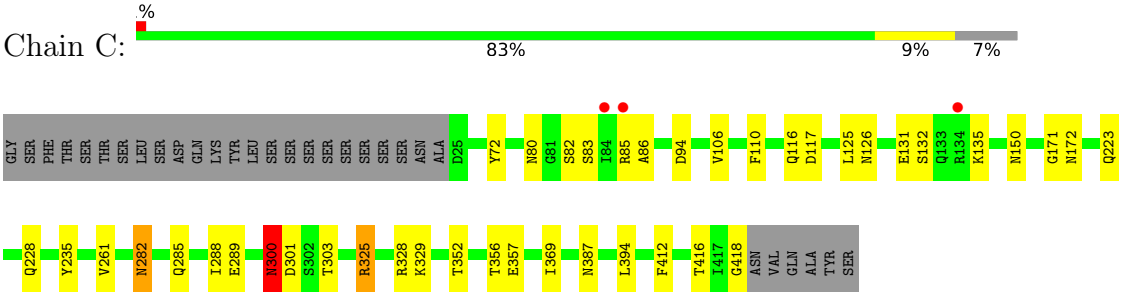
• Molecule 1: Galactan synthase

Chain B:



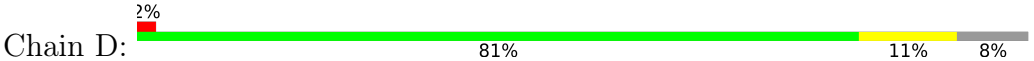
• Molecule 1: Galactan synthase

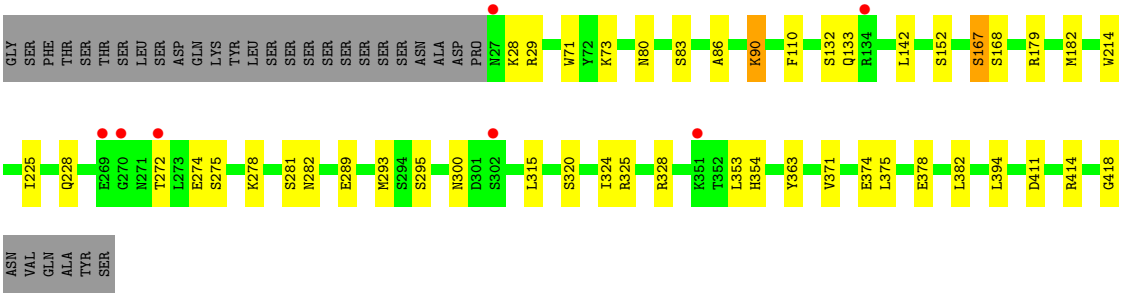
Chain C:



• Molecule 1: Galactan synthase

Chain D:



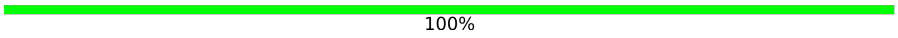


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

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

Chain G:



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

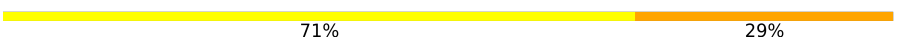
Chain I:

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

Chain K:

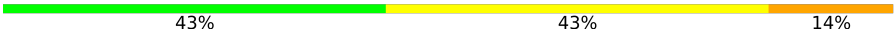
• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

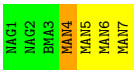
Chain F:



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

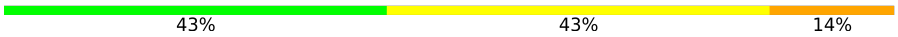
Chain H:

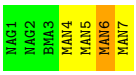




• Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:





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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.40Å 83.42Å 94.69Å 76.16° 69.67° 88.57°	Depositor
Resolution (Å)	80.84 – 2.37 80.83 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.2 (80.84-2.37) 98.2 (80.83-2.37)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.252 0.191 , 0.249	Depositor DCC
R_{free} test set	4011 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.007 for h,-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	27020	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: MAN, BMA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.28	0/3333	0.52	0/4525
1	B	0.26	0/3341	0.51	0/4537
1	C	0.27	0/3341	0.51	0/4537
1	D	0.26	0/3325	0.50	0/4514
All	All	0.27	0/13340	0.51	0/18113

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	3231	3048	3048	29	0
1	B	3239	3052	3054	27	0
1	C	3239	3053	3052	27	0
1	D	3224	3041	3042	30	0
2	E	28	25	25	2	0
2	G	28	25	25	0	0
2	I	28	25	25	1	0
2	K	28	25	25	0	0
3	F	83	70	70	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	83	69	70	2	0
3	J	83	70	70	1	0
4	L	86	73	73	3	0
5	A	56	52	52	5	0
5	B	70	65	65	12	0
5	C	70	65	65	9	0
5	D	56	52	52	0	0
6	A	141	0	0	1	0
6	B	145	0	0	0	0
6	C	171	0	0	3	0
6	D	121	0	0	4	0
All	All	14210	12810	12813	120	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 5.

All (120) 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:A:115:ASN:O	1:A:115:ASN:OD1	1.73	1.06
1:C:171:GLY:HA2	5:C:502:NAG:H82	1.64	0.80
1:B:117:ASP:OD2	5:B:501:NAG:H83	1.83	0.79
5:A:503:NAG:HO6	3:F:4:MAN:HO4	1.26	0.75
5:C:503:NAG:H3	5:C:503:NAG:H83	1.70	0.72
1:D:374:GLU:O	6:D:601:HOH:O	2.09	0.71
1:A:357:GLU:OE1	1:A:357:GLU:N	2.20	0.69
1:A:234:TYR:OH	1:B:130:ASP:OD2	2.10	0.68
1:C:301:ASP:OD1	1:C:303:THR:HG22	1.95	0.67
1:A:150:ASN:OD1	1:A:152:SER:OG	2.10	0.67
1:C:86:ALA:HB2	1:C:110:PHE:CE2	2.29	0.67
1:B:150:ASN:HD21	5:B:505:NAG:C1	2.09	0.66
1:D:282:ASN:OD1	6:D:602:HOH:O	2.13	0.66
1:D:73:LYS:NZ	1:D:133:GLN:OE1	2.29	0.64
1:B:80:ASN:HD21	5:B:501:NAG:C1	2.11	0.63
1:D:378:GLU:OE2	6:D:603:HOH:O	2.15	0.63
1:B:117:ASP:OD2	5:B:501:NAG:C8	2.47	0.62
1:C:418:GLY:O	6:C:601:HOH:O	2.16	0.60
1:A:75:GLU:OE2	1:A:85:ARG:HG2	2.01	0.60
1:B:321:ARG:HB3	1:B:324:ILE:HD13	1.84	0.59
1:C:261:VAL:HG23	1:C:369:ILE:HD12	1.83	0.59
1:A:192:SER:N	6:A:603:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:O	1:A:115:ASN:CG	2.41	0.59
1:B:86:ALA:HB2	1:B:110:PHE:CE2	2.38	0.58
1:A:228:GLN:NE2	1:A:232:ASP:OD1	2.35	0.58
1:B:86:ALA:HB2	1:B:110:PHE:CZ	2.38	0.57
1:C:171:GLY:CA	5:C:502:NAG:H82	2.35	0.56
1:A:49:GLY:HA3	3:F:1:NAG:H83	1.88	0.56
1:C:80:ASN:HB3	5:C:501:NAG:N2	2.21	0.56
1:C:116:GLN:N	6:C:602:HOH:O	2.38	0.56
1:A:130:ASP:OD2	1:B:234:TYR:OH	2.12	0.55
1:A:117:ASP:OD2	1:A:119:ALA:HB3	2.05	0.55
1:D:353:LEU:HD12	1:D:354:HIS:N	2.21	0.55
2:I:2:NAG:H82	3:J:6:MAN:O4	2.07	0.54
1:A:289:GLU:HG3	1:A:357:GLU:HG3	1.90	0.53
1:B:74:CYS:HB2	1:B:86:ALA:HB3	1.89	0.53
1:B:261:VAL:HG23	1:B:369:ILE:HD13	1.89	0.53
4:L:2:NAG:H61	4:L:3:BMA:C1	2.38	0.53
1:B:316:LEU:HD11	1:B:403:LYS:HD2	1.90	0.53
5:B:503:NAG:HO6	3:H:4:MAN:HO4	1.54	0.53
5:B:501:NAG:O7	5:B:501:NAG:O3	2.27	0.53
1:D:272:THR:HG22	1:D:274:GLU:N	2.24	0.52
1:C:412:PHE:O	1:C:416:THR:HG23	2.10	0.52
1:A:300:ASN:OD1	5:A:504:NAG:H2	2.10	0.51
1:B:117:ASP:OD1	1:B:118:ASN:N	2.43	0.51
1:C:80:ASN:HB3	5:C:501:NAG:HN2	1.75	0.51
1:D:278:LYS:HD2	1:D:278:LYS:C	2.31	0.51
1:D:325:ARG:O	1:D:325:ARG:HG3	2.09	0.51
5:A:502:NAG:H62	1:C:394:LEU:HD12	1.93	0.51
1:C:82:SER:OG	5:C:501:NAG:H83	2.09	0.51
1:B:321:ARG:NH2	1:B:324:ILE:HG21	2.25	0.51
1:C:228:GLN:HG3	1:C:235:TYR:OH	2.10	0.51
1:B:301:ASP:CG	1:B:303:THR:HG22	2.32	0.51
1:C:106:VAL:HG11	1:C:125:LEU:HD11	1.92	0.50
1:B:80:ASN:ND2	5:B:501:NAG:C1	2.74	0.50
1:B:228:GLN:HE22	1:B:232:ASP:CG	2.14	0.50
1:D:289:GLU:OE2	1:D:328:ARG:HD3	2.11	0.50
1:D:167:SER:OG	1:D:168:SER:N	2.45	0.50
1:D:281:SER:O	4:L:5:NAG:H83	2.12	0.49
1:C:117:ASP:OD1	5:C:501:NAG:O6	2.30	0.49
1:D:278:LYS:HD2	1:D:278:LYS:O	2.12	0.49
1:A:336:ASN:OD1	3:F:2:NAG:H61	2.13	0.49
1:C:289:GLU:OE2	1:C:328:ARG:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:6:MAN:O4	4:L:7:MAN:H3	2.13	0.49
1:B:150:ASN:ND2	5:B:505:NAG:C1	2.75	0.48
1:D:132:SER:OG	1:D:132:SER:O	2.28	0.48
1:A:356:THR:N	1:A:357:GLU:OE1	2.46	0.48
1:B:289:GLU:OE2	1:B:328:ARG:HD2	2.14	0.48
1:D:411:ASP:OD1	1:D:414:ARG:NH2	2.47	0.48
1:B:171:GLY:HA3	5:B:502:NAG:H82	1.96	0.47
1:C:223:GLN:OE1	1:D:29:ARG:NH1	2.41	0.47
1:D:272:THR:HG22	1:D:274:GLU:H	1.80	0.47
1:D:382:LEU:HD12	1:D:382:LEU:H	1.79	0.47
1:A:288:ILE:N	1:A:329:LYS:O	2.47	0.46
1:B:300:ASN:OD1	5:B:504:NAG:C1	2.63	0.46
1:C:356:THR:N	1:C:357:GLU:OE1	2.49	0.46
1:D:142:LEU:C	1:D:142:LEU:HD12	2.36	0.46
5:C:503:NAG:H3	5:C:503:NAG:C8	2.42	0.46
1:A:279:ASP:OD2	1:A:359:LYS:NZ	2.46	0.46
1:C:300:ASN:OD1	5:C:504:NAG:H2	2.15	0.46
1:C:325:ARG:O	1:C:325:ARG:HG3	2.15	0.45
1:C:288:ILE:N	1:C:329:LYS:O	2.47	0.45
1:D:182:MET:HE2	1:D:214:TRP:CG	2.52	0.45
1:D:418:GLY:O	6:D:604:HOH:O	2.20	0.44
5:B:503:NAG:O6	3:H:4:MAN:O4	2.17	0.44
1:C:86:ALA:HB2	1:C:110:PHE:CZ	2.52	0.44
1:D:80:ASN:OD1	1:D:80:ASN:C	2.56	0.44
5:B:502:NAG:H62	1:D:394:LEU:HD12	1.99	0.44
1:C:282:ASN:O	1:C:282:ASN:CG	2.56	0.44
1:D:225:ILE:O	1:D:228:GLN:HG3	2.18	0.43
1:B:25:ASP:HB3	1:B:26:PRO:HD3	2.01	0.43
1:A:254:ASN:OD1	2:E:1:NAG:C2	2.67	0.43
1:A:158:TYR:H	2:E:1:NAG:H83	1.83	0.43
1:A:261:VAL:HG23	1:A:369:ILE:HD12	2.00	0.43
1:C:72:TYR:HA	1:C:126:ASN:O	2.19	0.43
1:D:324:ILE:N	1:D:324:ILE:HD13	2.34	0.42
1:D:293:MET:SD	1:D:363:TYR:HD2	2.42	0.42
1:A:228:GLN:HG3	1:A:235:TYR:OH	2.20	0.42
1:C:94:ASP:OD1	1:C:94:ASP:C	2.58	0.42
1:D:295:SER:HA	1:D:315:LEU:HD13	2.01	0.42
1:B:132:SER:O	1:B:134:ARG:N	2.47	0.42
1:A:382:LEU:HD22	1:A:382:LEU:H	1.85	0.41
1:D:71:TRP:CD2	1:D:90:LYS:HE3	2.55	0.41
1:A:282:ASN:OD1	5:A:503:NAG:C2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:N	1:A:324:ILE:HD13	2.35	0.41
1:B:228:GLN:HG3	1:B:235:TYR:OH	2.20	0.41
1:B:357:GLU:OE1	1:B:357:GLU:N	2.40	0.41
1:C:261:VAL:HG22	6:C:704:HOH:O	2.20	0.41
1:D:86:ALA:HB2	1:D:110:PHE:CE2	2.56	0.41
1:A:136:TYR:CD1	1:A:136:TYR:N	2.89	0.41
5:A:503:NAG:O6	3:F:4:MAN:O4	2.02	0.41
1:B:72:TYR:HA	1:B:126:ASN:O	2.21	0.41
1:C:285:GLN:HG3	1:C:352:THR:HG23	2.03	0.41
1:A:56:VAL:HG21	1:A:125:LEU:HD22	2.03	0.41
1:D:371:VAL:HG11	1:D:375:LEU:HD23	2.03	0.41
1:D:86:ALA:HB2	1:D:110:PHE:CZ	2.56	0.40
1:A:306:TYR:N	1:A:307:PRO:CD	2.85	0.40
1:B:59:LEU:HB3	1:B:101:TYR:HB3	2.02	0.40
1:A:142:LEU:HD12	1:A:143:GLU:N	2.36	0.40
1:A:180:GLU:HG2	1:A:310:TRP:CD2	2.56	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	391/424 (92%)	376 (96%)	15 (4%)	0	100	100
1	B	392/424 (92%)	376 (96%)	15 (4%)	1 (0%)	41	53
1	C	392/424 (92%)	384 (98%)	7 (2%)	1 (0%)	41	53
1	D	390/424 (92%)	374 (96%)	16 (4%)	0	100	100
All	All	1565/1696 (92%)	1510 (96%)	53 (3%)	2 (0%)	51	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	300	ASN
1	B	282	ASN

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	337/365 (92%)	332 (98%)	5 (2%)	65	79
1	B	338/365 (93%)	326 (96%)	12 (4%)	35	51
1	C	338/365 (93%)	327 (97%)	11 (3%)	38	55
1	D	336/365 (92%)	327 (97%)	9 (3%)	44	62
All	All	1349/1460 (92%)	1312 (97%)	37 (3%)	44	62

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	179	ARG
1	A	275	SER
1	A	325	ARG
1	A	383	SER
1	B	62	LYS
1	B	78	SER
1	B	83	SER
1	B	155	ARG
1	B	168	SER
1	B	172	ASN
1	B	179	ARG
1	B	216	ARG
1	B	232	ASP
1	B	275	SER
1	B	300	ASN
1	B	325	ARG
1	C	83	SER
1	C	85	ARG
1	C	131	GLU

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Mol	Chain	Res	Type
1	C	132	SER
1	C	135	LYS
1	C	150	ASN
1	C	172	ASN
1	C	282	ASN
1	C	300	ASN
1	C	325	ARG
1	C	387	ASN
1	D	28	LYS
1	D	83	SER
1	D	90	LYS
1	D	152	SER
1	D	167	SER
1	D	179	ARG
1	D	275	SER
1	D	300	ASN
1	D	320	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	115	ASN
1	B	237	ASN
1	C	159	GLN
1	D	237	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2,1	14,14,15	0.43	0	17,19,21	0.73	0
2	NAG	E	2	2	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	F	1	3,1	14,14,15	0.35	0	17,19,21	0.42	0
3	NAG	F	2	3	14,14,15	0.63	1 (7%)	17,19,21	0.47	0
3	BMA	F	3	3	11,11,12	0.77	0	15,15,17	1.10	1 (6%)
3	MAN	F	4	3	11,11,12	0.70	0	15,15,17	1.16	1 (6%)
3	MAN	F	5	3	11,11,12	1.01	1 (9%)	15,15,17	1.27	1 (6%)
3	MAN	F	6	3	11,11,12	0.63	0	15,15,17	1.13	2 (13%)
3	MAN	F	7	3	11,11,12	0.66	0	15,15,17	0.95	2 (13%)
2	NAG	G	1	2,1	14,14,15	0.54	0	17,19,21	0.50	0
2	NAG	G	2	2	14,14,15	0.23	0	17,19,21	0.36	0
3	NAG	H	1	3,1	14,14,15	0.32	0	17,19,21	0.40	0
3	NAG	H	2	3	14,14,15	0.19	0	17,19,21	0.39	0
3	BMA	H	3	3	11,11,12	0.45	0	15,15,17	0.97	0
3	MAN	H	4	3	11,11,12	0.80	1 (9%)	15,15,17	1.14	1 (6%)
3	MAN	H	5	3	11,11,12	0.94	1 (9%)	15,15,17	1.17	1 (6%)
3	MAN	H	6	3	11,11,12	0.59	0	15,15,17	1.31	2 (13%)
3	MAN	H	7	3	11,11,12	0.61	0	15,15,17	1.21	2 (13%)
2	NAG	I	1	2,1	14,14,15	0.62	0	17,19,21	0.69	0
2	NAG	I	2	2	14,14,15	0.29	0	17,19,21	0.55	0
3	NAG	J	1	3,1	14,14,15	0.48	0	17,19,21	0.61	0
3	NAG	J	2	3	14,14,15	0.36	0	17,19,21	0.44	0
3	BMA	J	3	3	11,11,12	0.50	0	15,15,17	0.98	0
3	MAN	J	4	3	11,11,12	0.58	0	15,15,17	1.43	2 (13%)
3	MAN	J	5	3	11,11,12	0.80	0	15,15,17	1.31	2 (13%)
3	MAN	J	6	3	11,11,12	0.65	0	15,15,17	1.24	2 (13%)
3	MAN	J	7	3	11,11,12	0.93	1 (9%)	15,15,17	2.13	4 (26%)
2	NAG	K	1	2,1	14,14,15	0.20	0	17,19,21	0.68	1 (5%)
2	NAG	K	2	2	14,14,15	0.45	0	17,19,21	0.47	0
4	NAG	L	1	4,1	14,14,15	0.38	0	17,19,21	0.58	0
4	NAG	L	2	4	14,14,15	0.58	0	17,19,21	0.56	0
4	BMA	L	3	4	11,11,12	0.99	0	15,15,17	1.80	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	MAN	L	4	4	11,11,12	1.42	2 (18%)	15,15,17	1.88	3 (20%)
4	NAG	L	5	4	14,14,15	0.69	1 (7%)	17,19,21	0.57	0
4	MAN	L	6	4	11,11,12	1.03	1 (9%)	15,15,17	1.26	2 (13%)
4	MAN	L	7	4	11,11,12	1.32	1 (9%)	15,15,17	1.79	2 (13%)

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

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	7	MAN	C1-C2	3.93	1.61	1.52
4	L	4	MAN	O5-C1	-3.14	1.38	1.43
4	L	4	MAN	C2-C3	2.83	1.56	1.52
3	F	5	MAN	O5-C1	-2.72	1.39	1.43
3	J	7	MAN	C1-C2	2.63	1.58	1.52
3	H	5	MAN	O5-C1	-2.62	1.39	1.43
4	L	5	NAG	C1-C2	2.34	1.55	1.52
3	F	2	NAG	O5-C1	-2.20	1.40	1.43
3	H	4	MAN	O5-C1	-2.11	1.40	1.43
4	L	6	MAN	C1-C2	2.09	1.57	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	7	MAN	C1-O5-C5	6.28	120.70	112.19
4	L	3	BMA	C1-O5-C5	5.93	120.22	112.19
4	L	4	MAN	O2-C2-C1	5.13	119.66	109.15
4	L	7	MAN	C1-C2-C3	4.98	115.79	109.67
3	J	4	MAN	C1-O5-C5	4.15	117.82	112.19
3	H	6	MAN	C1-O5-C5	3.73	117.25	112.19
3	J	5	MAN	O2-C2-C3	-3.55	103.04	110.14
4	L	7	MAN	O2-C2-C3	-3.45	103.23	110.14
4	L	4	MAN	O2-C2-C3	-3.44	103.25	110.14
3	H	7	MAN	C1-O5-C5	3.41	116.81	112.19
3	F	5	MAN	O2-C2-C3	-3.36	103.41	110.14
3	F	4	MAN	O2-C2-C3	-3.32	103.48	110.14
3	H	5	MAN	O2-C2-C3	-3.17	103.80	110.14
4	L	6	MAN	C1-C2-C3	3.16	113.55	109.67
3	J	6	MAN	C1-O5-C5	2.96	116.20	112.19
3	H	4	MAN	O2-C2-C3	-2.89	104.35	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	7	MAN	O5-C1-C2	2.88	115.21	110.77
3	F	6	MAN	C1-O5-C5	2.84	116.03	112.19
3	J	7	MAN	O2-C2-C3	-2.80	104.53	110.14
3	J	7	MAN	C1-C2-C3	2.58	112.83	109.67
3	F	3	BMA	C1-C2-C3	2.48	112.71	109.67
4	L	6	MAN	O2-C2-C3	-2.40	105.33	110.14
3	J	4	MAN	O2-C2-C3	-2.38	105.38	110.14
3	J	6	MAN	O2-C2-C3	-2.34	105.46	110.14
2	K	1	NAG	C1-O5-C5	2.25	115.24	112.19
3	F	6	MAN	O2-C2-C3	-2.22	105.70	110.14
4	L	4	MAN	O5-C1-C2	2.21	114.18	110.77
3	F	7	MAN	C1-O5-C5	2.20	115.18	112.19
3	J	5	MAN	C1-O5-C5	2.20	115.17	112.19
3	H	6	MAN	O2-C2-C3	-2.13	105.87	110.14
3	H	7	MAN	O2-C2-C3	-2.13	105.87	110.14
3	F	7	MAN	O2-C2-C3	-2.10	105.93	110.14

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	5	NAG	C3-C2-N2-C7
3	H	4	MAN	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	J	4	MAN	C4-C5-C6-O6
4	L	4	MAN	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	H	4	MAN	O5-C5-C6-O6
3	J	4	MAN	O5-C5-C6-O6
3	F	6	MAN	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	F	6	MAN	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6
2	K	1	NAG	C4-C5-C6-O6
4	L	3	BMA	O5-C5-C6-O6
4	L	6	MAN	O5-C5-C6-O6
4	L	5	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	L	4	MAN	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
2	K	1	NAG	C3-C2-N2-C7
3	F	4	MAN	C4-C5-C6-O6
2	K	1	NAG	C1-C2-N2-C7

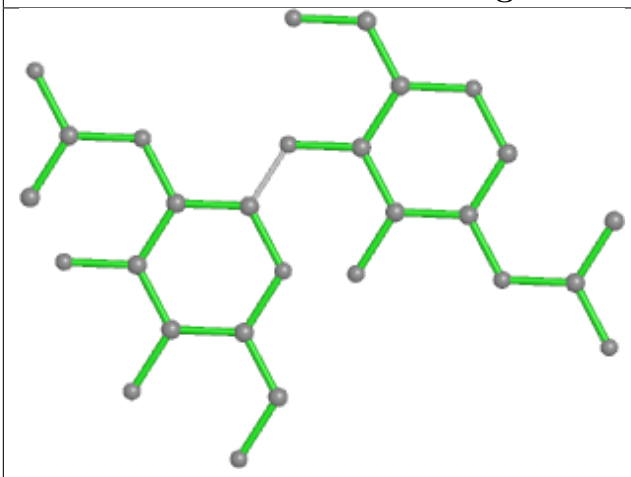
There are no ring outliers.

12 monomers are involved in 12 short contacts:

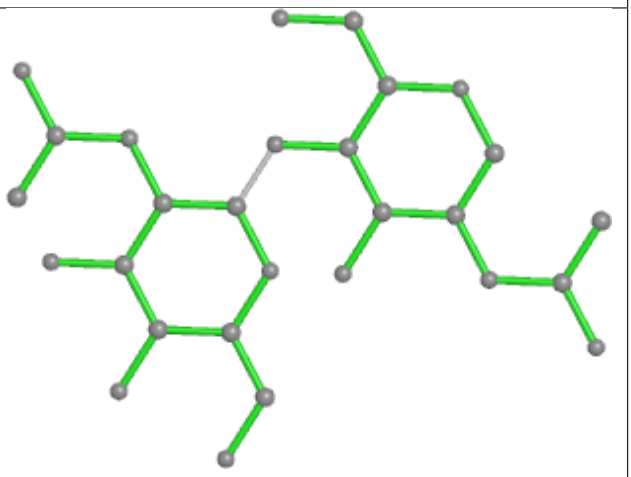
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
2	E	1	NAG	2	0
3	F	2	NAG	1	0
4	L	2	NAG	1	0
3	J	6	MAN	1	0
3	H	4	MAN	2	0
3	F	4	MAN	2	0
4	L	5	NAG	1	0
2	I	2	NAG	1	0
4	L	3	BMA	1	0
4	L	6	MAN	1	0
4	L	7	MAN	1	0

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

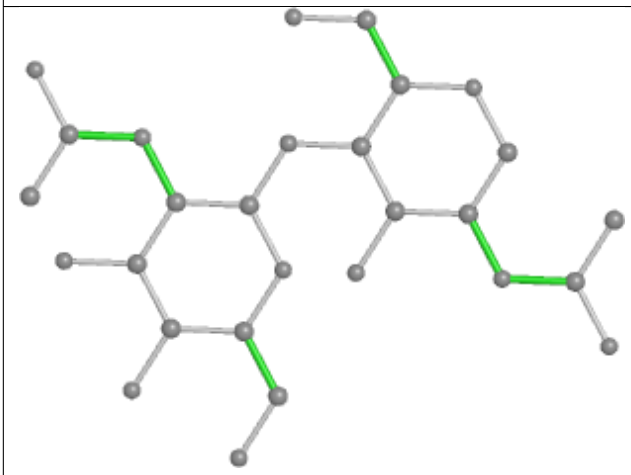
Oligosaccharide Chain E



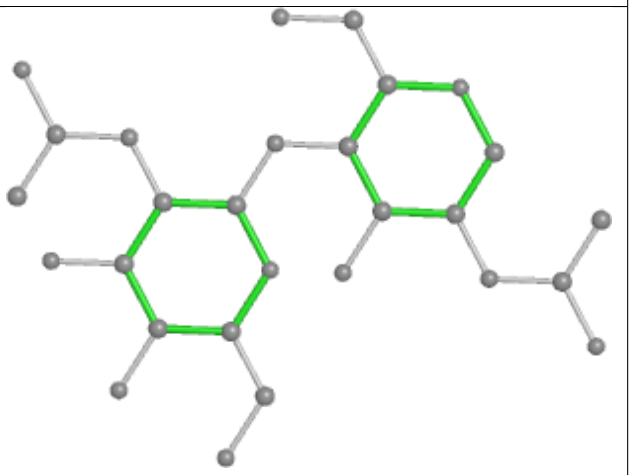
Bond lengths



Bond angles

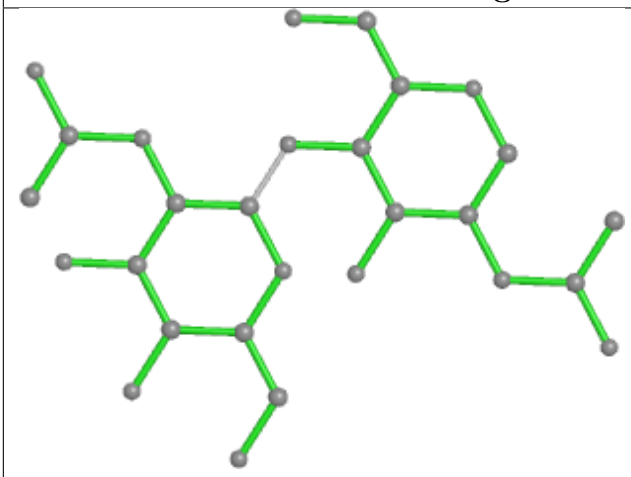


Torsions

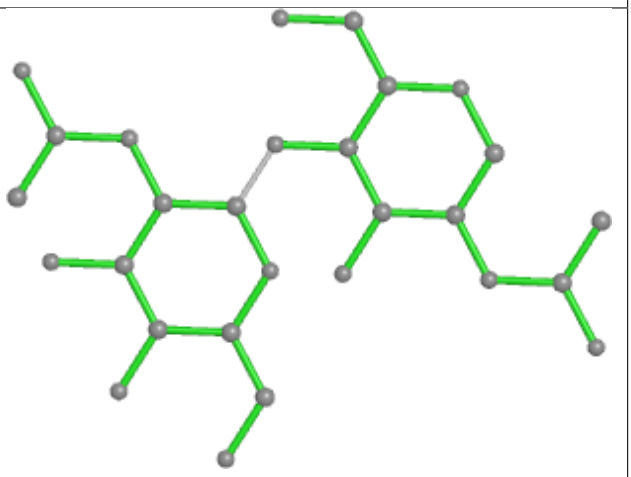


Rings

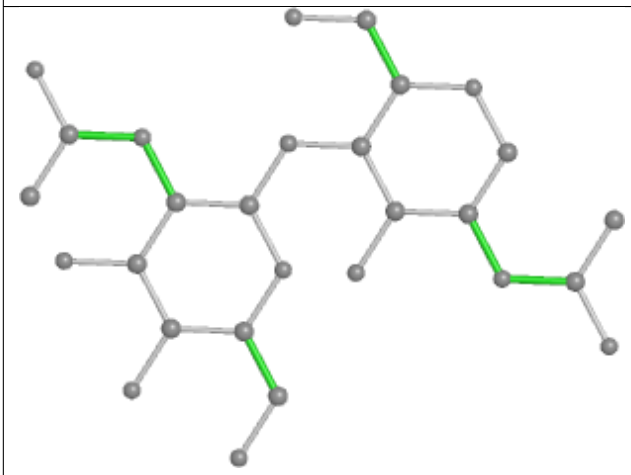
Oligosaccharide Chain G



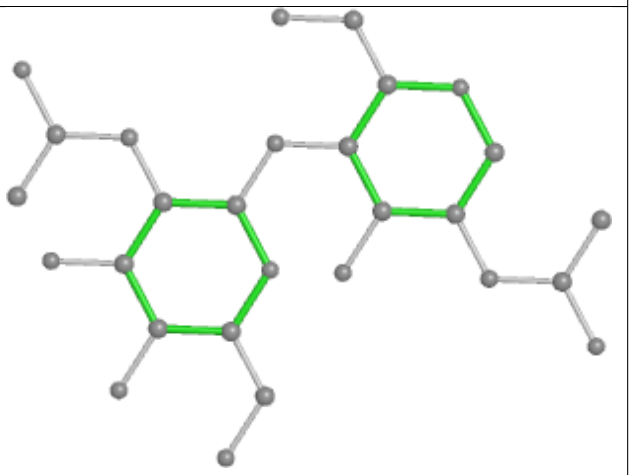
Bond lengths



Bond angles

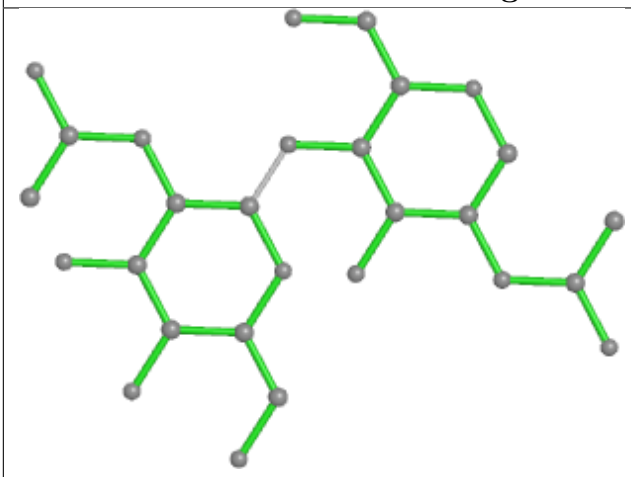


Torsions

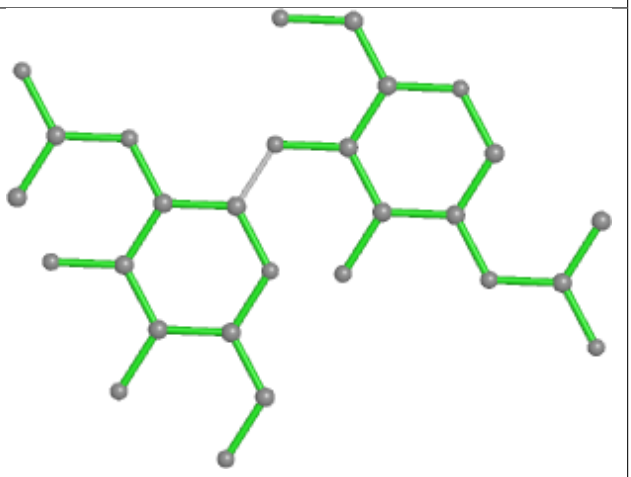


Rings

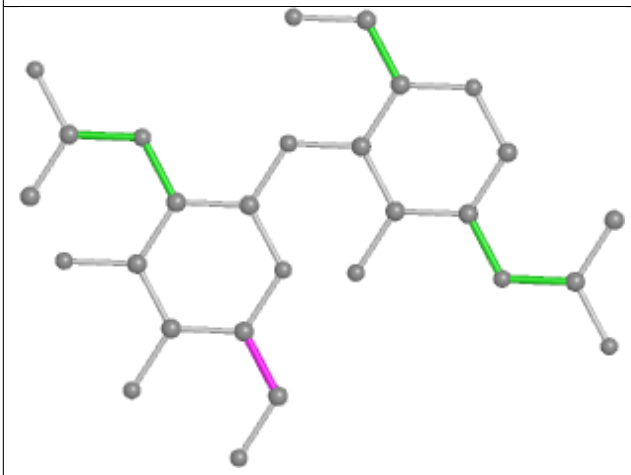
Oligosaccharide Chain I



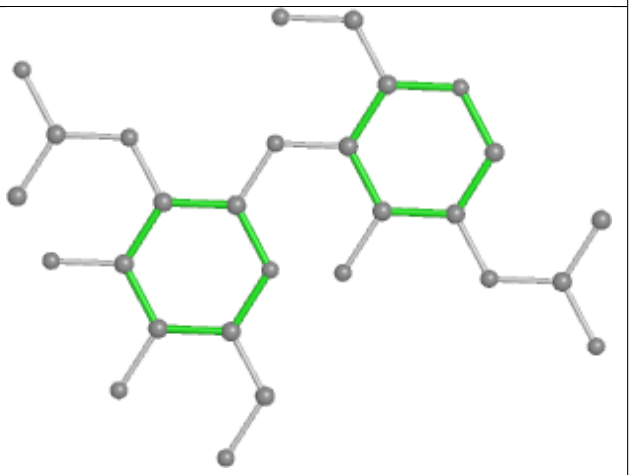
Bond lengths



Bond angles

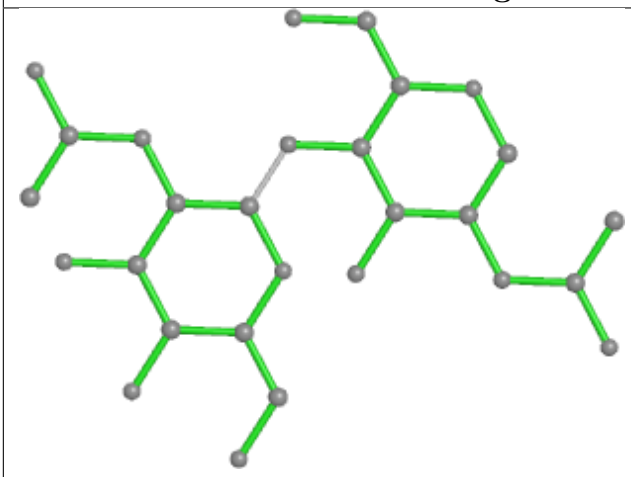


Torsions

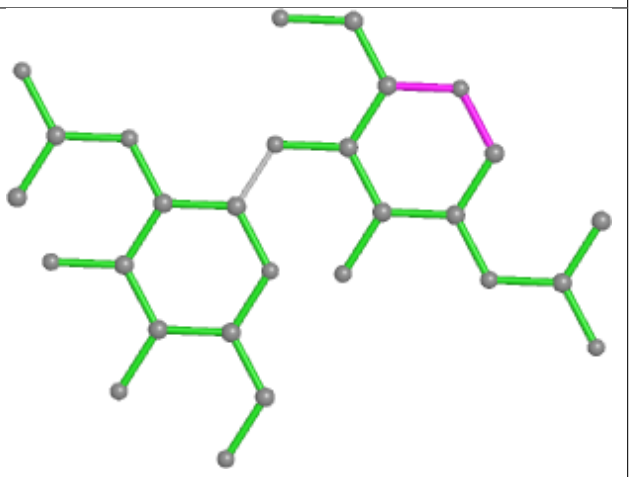


Rings

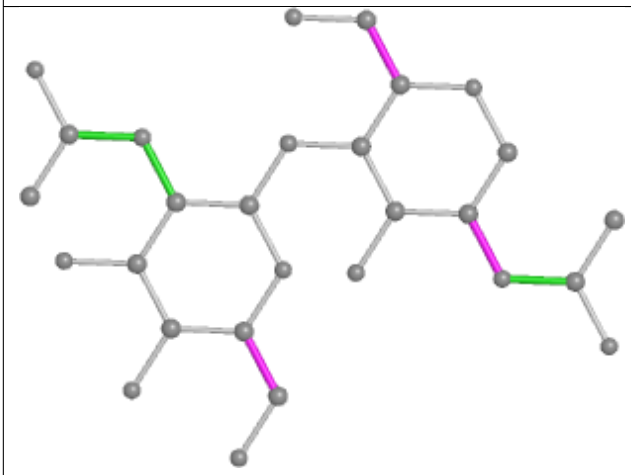
Oligosaccharide Chain K



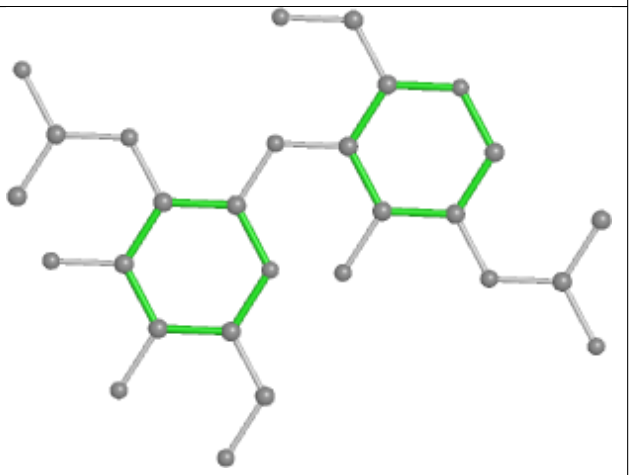
Bond lengths



Bond angles

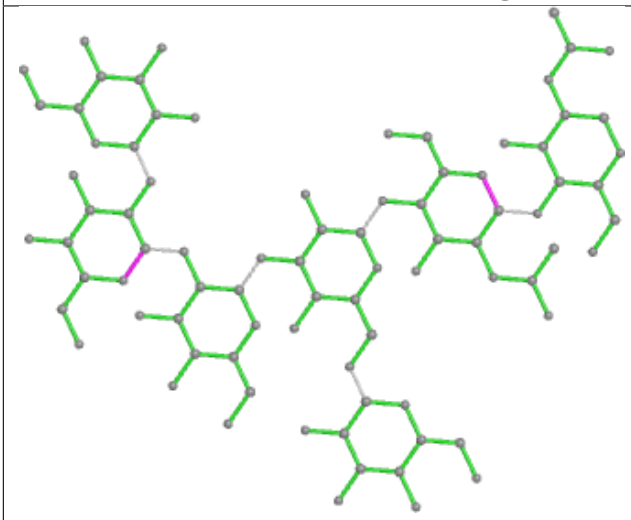


Torsions

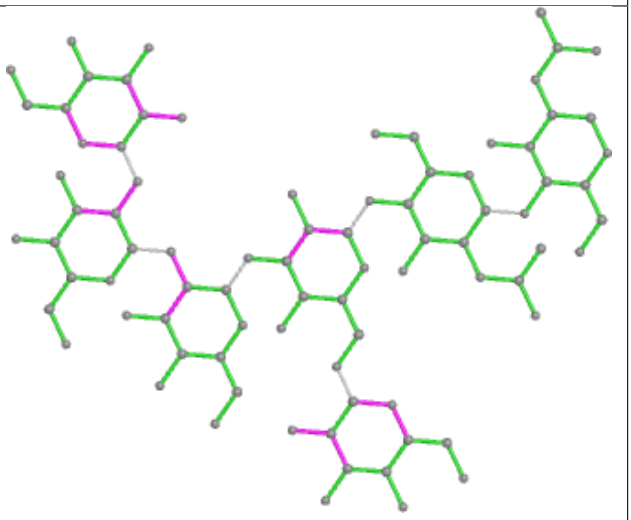


Rings

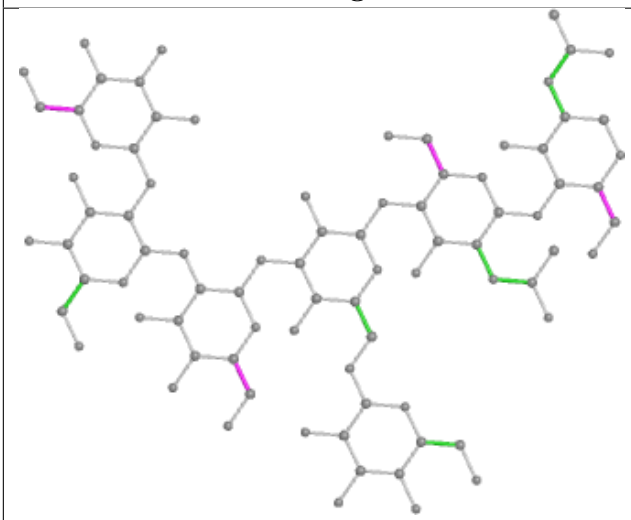
Oligosaccharide Chain F



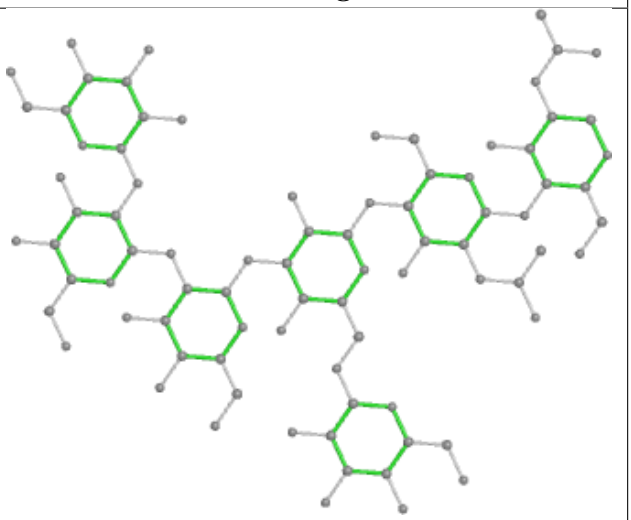
Bond lengths



Bond angles

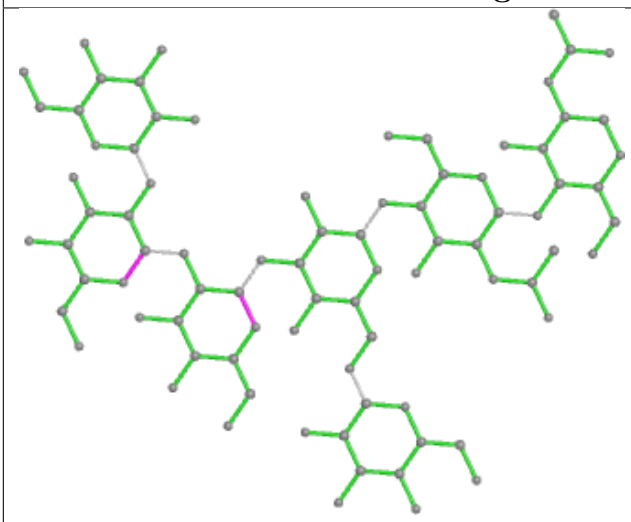


Torsions

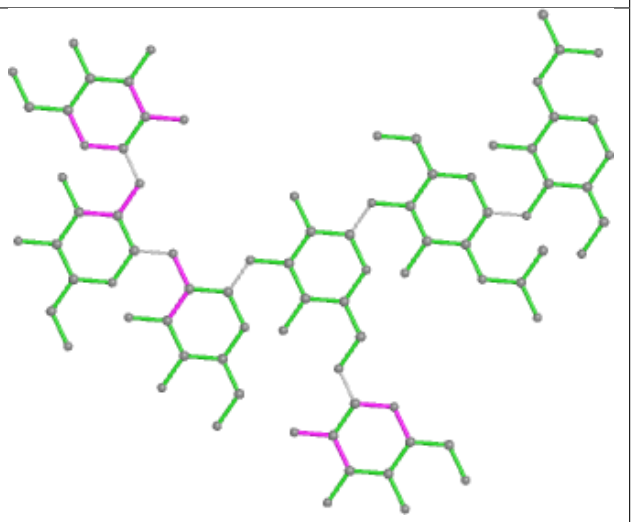


Rings

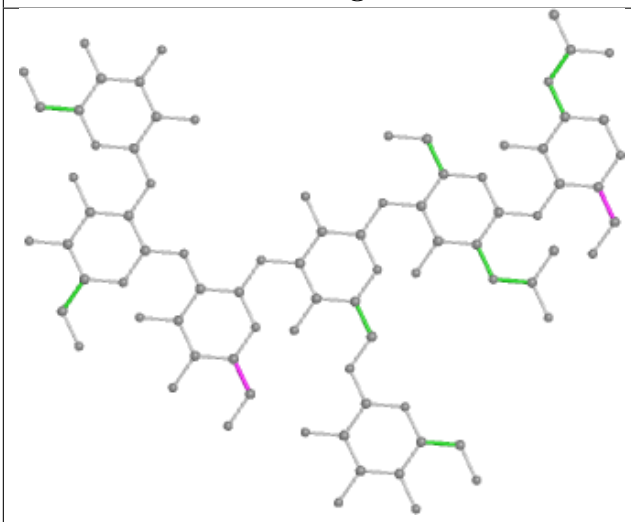
Oligosaccharide Chain H



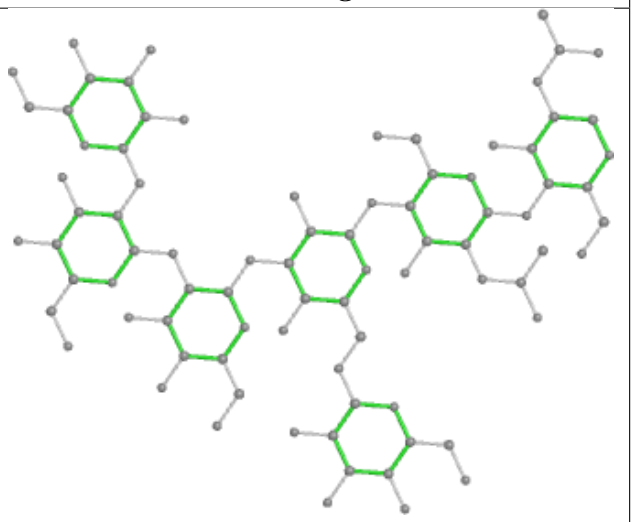
Bond lengths



Bond angles

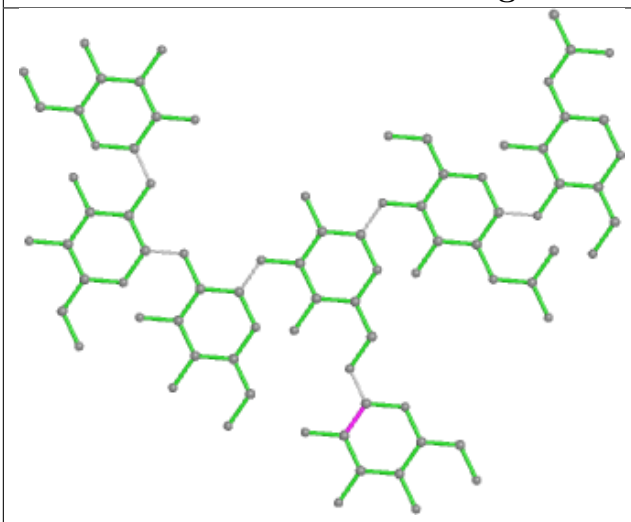


Torsions

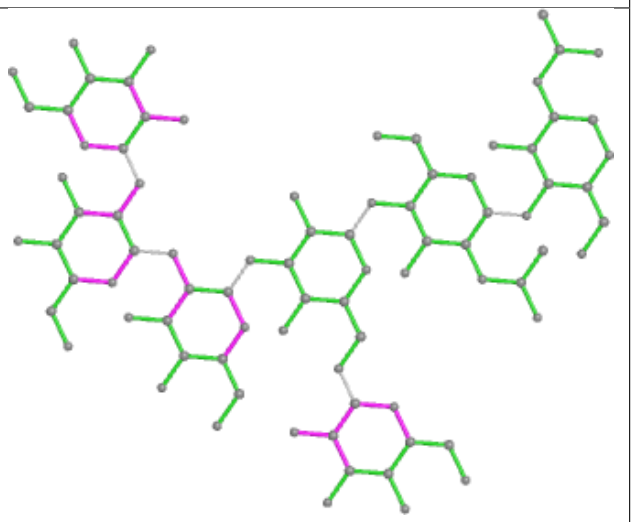


Rings

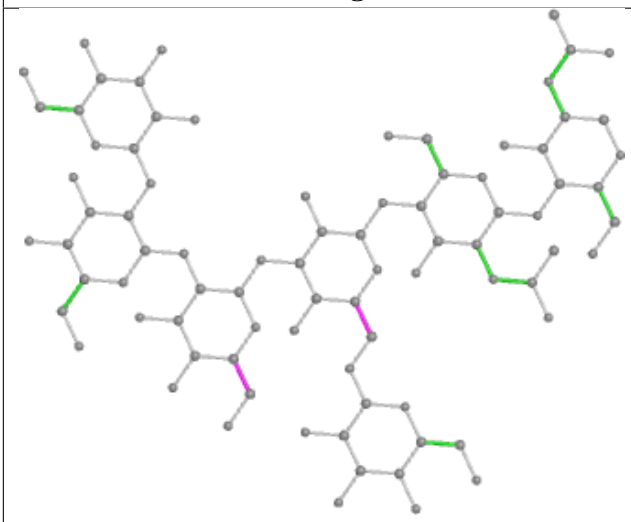
Oligosaccharide Chain J



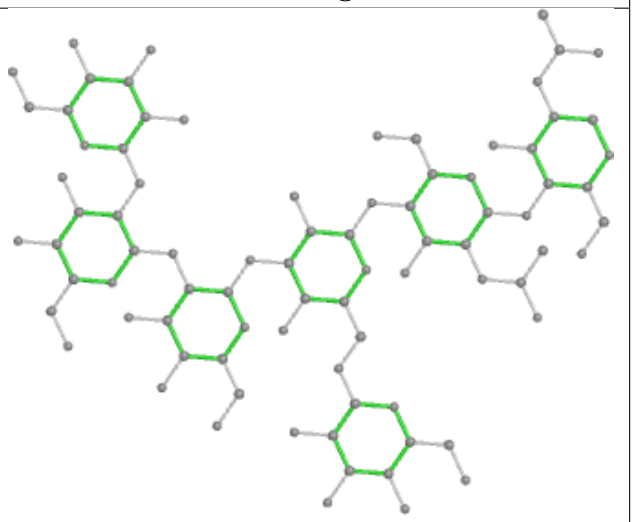
Bond lengths



Bond angles

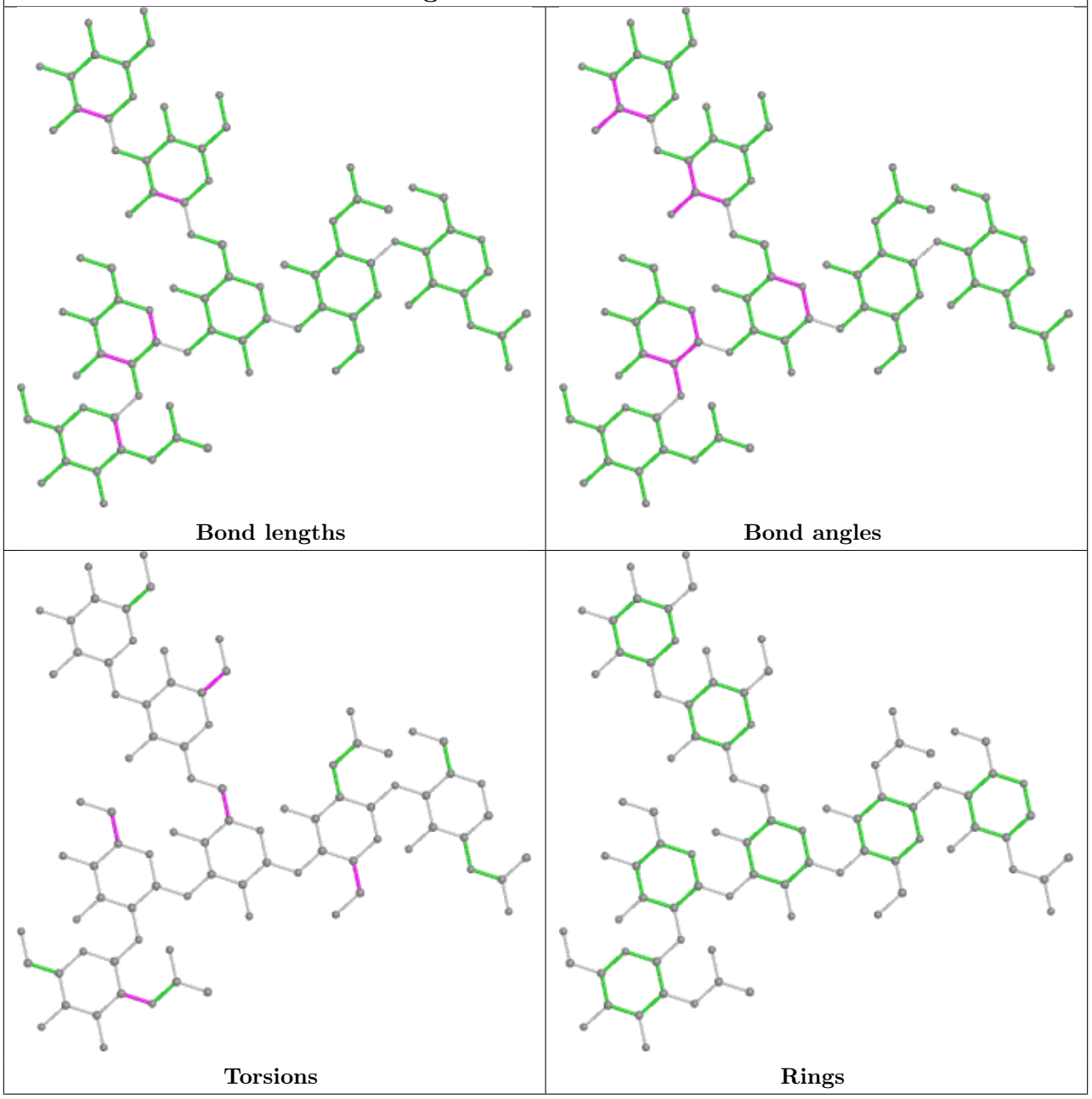


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

18 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	$\#\|Z\|>2$
5	NAG	D	504	1	14,14,15	0.63	0	17,19,21	1.36	2 (11%)
5	NAG	A	501	1	14,14,15	0.36	0	17,19,21	0.67	0
5	NAG	A	503	1	14,14,15	0.36	0	17,19,21	0.42	0
5	NAG	C	501	1	14,14,15	0.84	1 (7%)	17,19,21	0.84	1 (5%)
5	NAG	C	505	-	14,14,15	0.39	0	17,19,21	0.82	1 (5%)
5	NAG	C	503	1	14,14,15	0.23	0	17,19,21	0.96	1 (5%)
5	NAG	C	504	1	14,14,15	0.56	0	17,19,21	0.89	1 (5%)
5	NAG	B	505	-	14,14,15	1.52	1 (7%)	17,19,21	1.03	1 (5%)
5	NAG	B	504	-	14,14,15	0.42	0	17,19,21	0.65	0
5	NAG	B	503	1	14,14,15	0.33	0	17,19,21	0.39	0
5	NAG	D	503	-	14,14,15	0.49	0	17,19,21	0.79	1 (5%)
5	NAG	A	502	1	14,14,15	0.35	0	17,19,21	0.87	1 (5%)
5	NAG	B	501	-	14,14,15	0.88	1 (7%)	17,19,21	0.93	1 (5%)
5	NAG	B	502	1	14,14,15	0.37	0	17,19,21	0.77	1 (5%)
5	NAG	D	501	1	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	A	504	1	14,14,15	0.64	0	17,19,21	0.83	1 (5%)
5	NAG	D	502	1	14,14,15	0.25	0	17,19,21	0.55	0
5	NAG	C	502	1	14,14,15	0.47	0	17,19,21	0.81	1 (5%)

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
5	NAG	D	504	1	-	2/6/23/26	0/1/1/1
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	A	503	1	-	0/6/23/26	0/1/1/1
5	NAG	C	501	1	-	3/6/23/26	0/1/1/1
5	NAG	C	505	-	-	2/6/23/26	0/1/1/1
5	NAG	C	503	1	-	5/6/23/26	0/1/1/1
5	NAG	C	504	1	-	4/6/23/26	0/1/1/1
5	NAG	B	505	-	-	0/6/23/26	0/1/1/1
5	NAG	B	504	-	-	2/6/23/26	0/1/1/1
5	NAG	B	503	1	-	2/6/23/26	0/1/1/1
5	NAG	D	503	-	-	4/6/23/26	0/1/1/1
5	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	NAG	B	501	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	502	1	-	2/6/23/26	0/1/1/1
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	504	1	-	1/6/23/26	0/1/1/1
5	NAG	D	502	1	-	0/6/23/26	0/1/1/1
5	NAG	C	502	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	NAG	O5-C1	-5.37	1.35	1.43
5	B	501	NAG	O5-C1	-2.91	1.39	1.43
5	C	501	NAG	C1-C2	2.55	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	504	NAG	C1-O5-C5	4.22	117.91	112.19
5	B	505	NAG	C3-C4-C5	3.56	116.60	110.24
5	C	504	NAG	C1-O5-C5	3.16	116.47	112.19
5	C	501	NAG	C1-O5-C5	2.89	116.11	112.19
5	A	502	NAG	C1-O5-C5	2.88	116.09	112.19
5	C	503	NAG	C2-N2-C7	2.84	126.94	122.90
5	C	502	NAG	C1-O5-C5	2.82	116.02	112.19
5	D	503	NAG	C1-O5-C5	2.73	115.89	112.19
5	B	502	NAG	C1-O5-C5	2.52	115.61	112.19
5	C	505	NAG	C1-O5-C5	2.43	115.48	112.19
5	A	504	NAG	C1-O5-C5	2.34	115.37	112.19
5	B	501	NAG	C1-O5-C5	2.32	115.33	112.19
5	D	504	NAG	C3-C4-C5	2.06	113.92	110.24

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	502	NAG	O5-C5-C6-O6
5	A	502	NAG	O5-C5-C6-O6
5	D	503	NAG	C4-C5-C6-O6
5	A	502	NAG	C4-C5-C6-O6
5	C	503	NAG	O5-C5-C6-O6
5	D	503	NAG	O5-C5-C6-O6
5	B	502	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	501	NAG	O5-C5-C6-O6
5	C	505	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	B	504	NAG	C8-C7-N2-C2
5	B	504	NAG	O7-C7-N2-C2
5	C	503	NAG	C8-C7-N2-C2
5	C	503	NAG	O7-C7-N2-C2
5	C	504	NAG	C8-C7-N2-C2
5	C	504	NAG	O7-C7-N2-C2
5	D	503	NAG	C8-C7-N2-C2
5	D	503	NAG	O7-C7-N2-C2
5	D	504	NAG	C4-C5-C6-O6
5	C	501	NAG	O5-C5-C6-O6
5	C	503	NAG	C4-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	C	501	NAG	C4-C5-C6-O6
5	C	505	NAG	C4-C5-C6-O6
5	B	501	NAG	C1-C2-N2-C7
5	D	504	NAG	O5-C5-C6-O6
5	B	503	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	B	503	NAG	O5-C5-C6-O6
5	C	504	NAG	C4-C5-C6-O6
5	C	501	NAG	C1-C2-N2-C7
5	A	504	NAG	C3-C2-N2-C7
5	C	503	NAG	C3-C2-N2-C7
5	C	502	NAG	O5-C5-C6-O6
5	B	501	NAG	C3-C2-N2-C7
5	C	504	NAG	O5-C5-C6-O6

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	NAG	3	0
5	C	501	NAG	4	0
5	C	503	NAG	2	0
5	C	504	NAG	1	0
5	B	505	NAG	2	0
5	B	504	NAG	1	0
5	B	503	NAG	2	0
5	A	502	NAG	1	0

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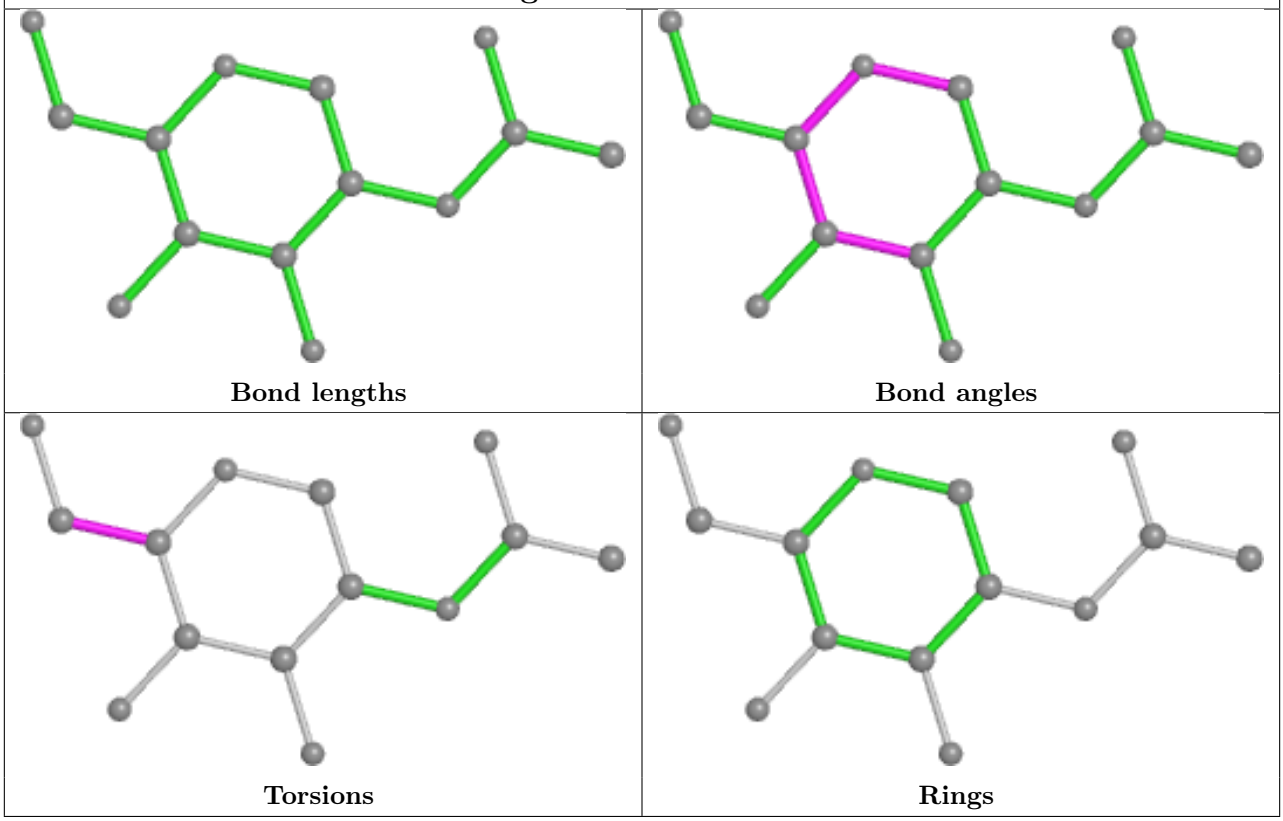
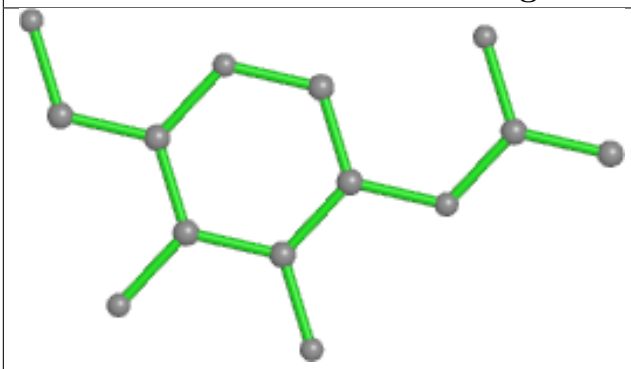
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	NAG	5	0
5	B	502	NAG	2	0
5	A	504	NAG	1	0
5	C	502	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

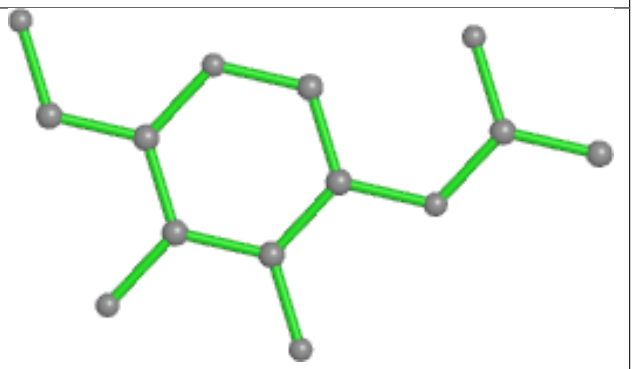
Ligand NAG D 504



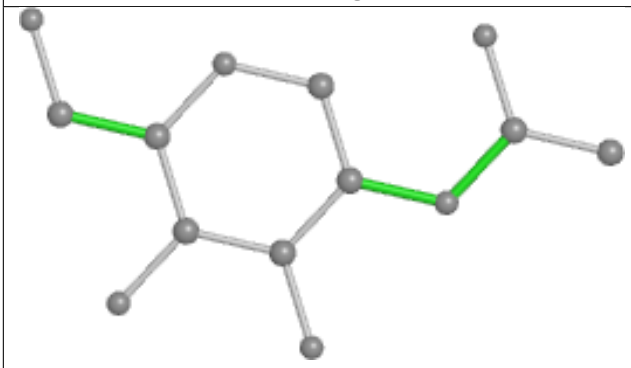
Ligand NAG A 501



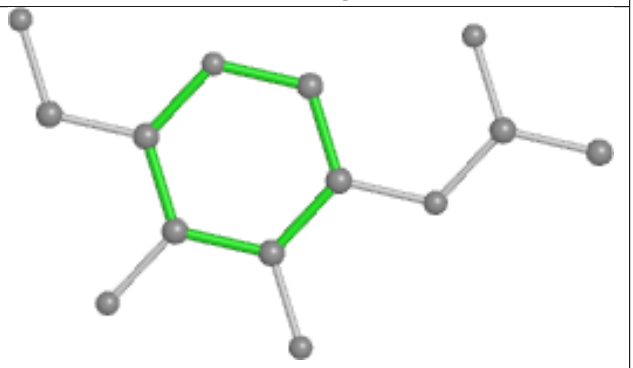
Bond lengths



Bond angles

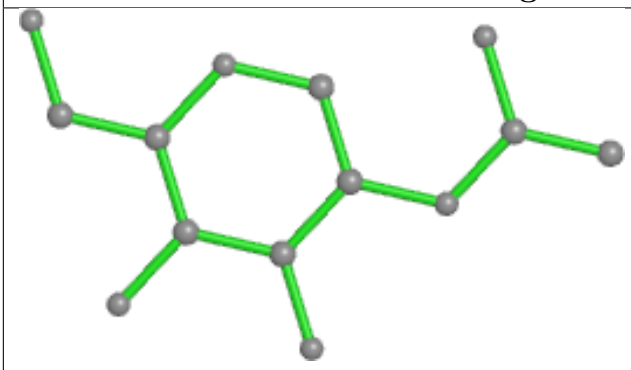


Torsions



Rings

Ligand NAG A 503



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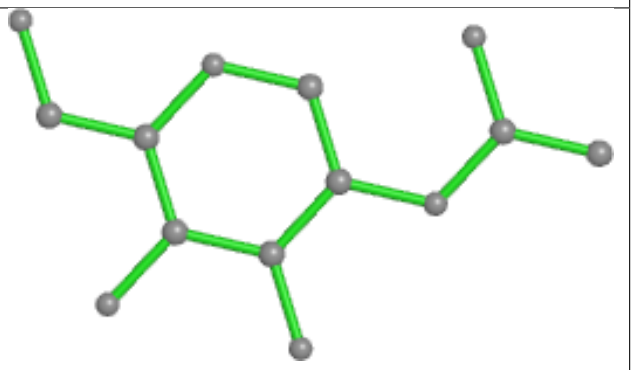
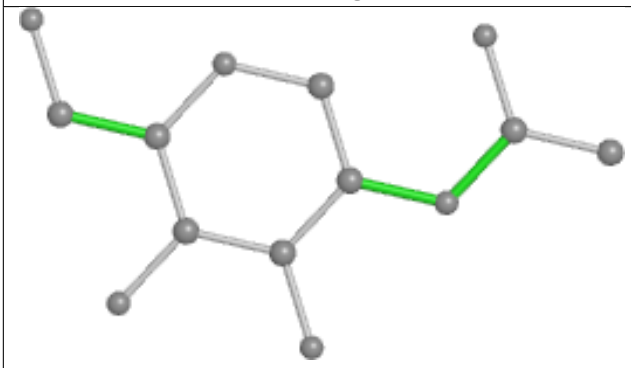


Bond angles



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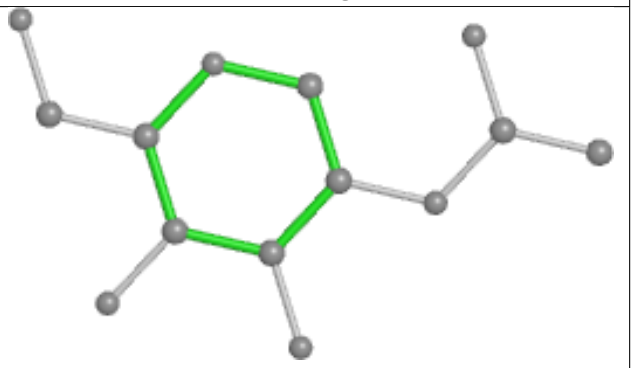
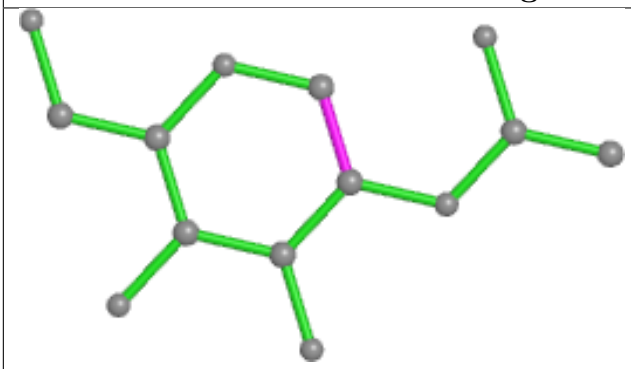
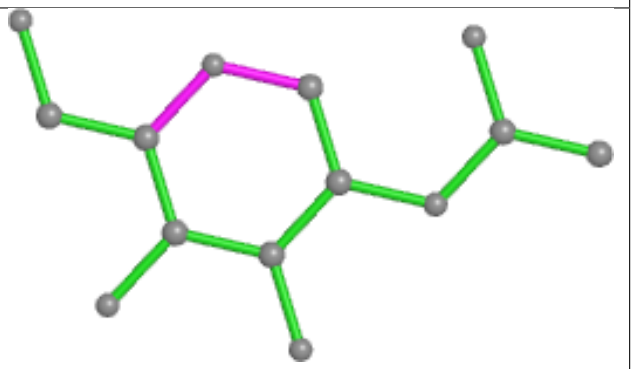


Rings

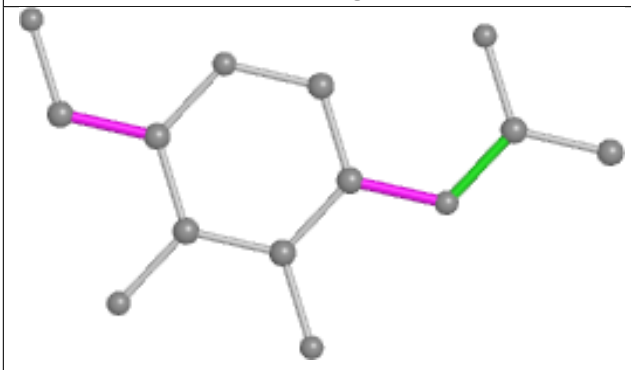
Ligand NAG C 501



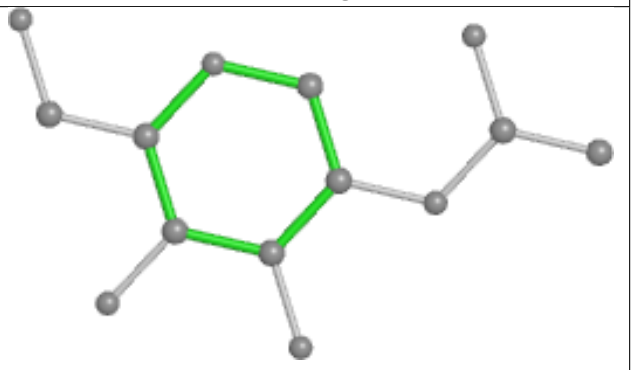
Bond lengths



Bond angles



Torsions



Rings

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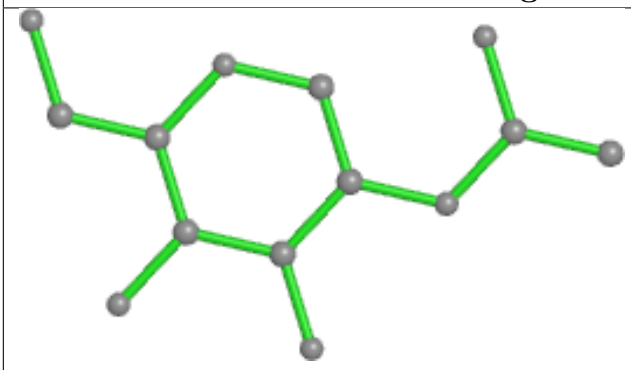

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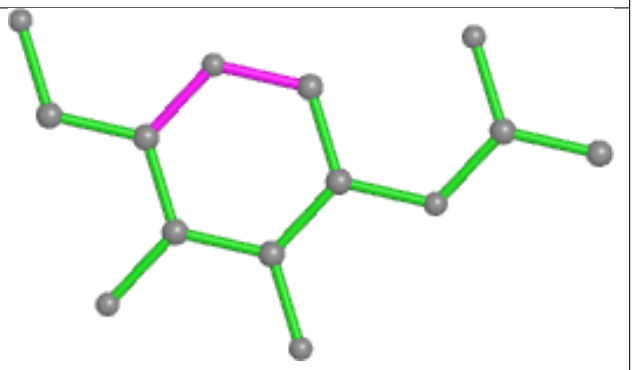

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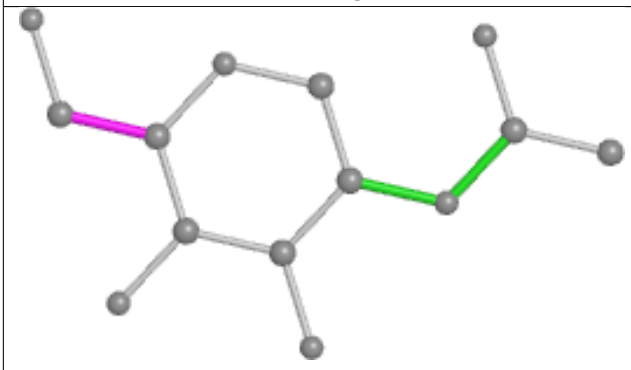

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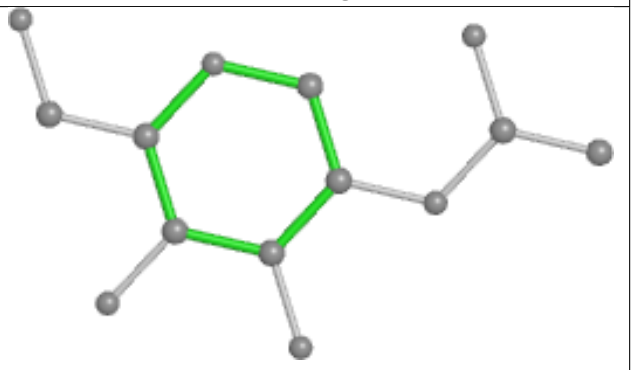
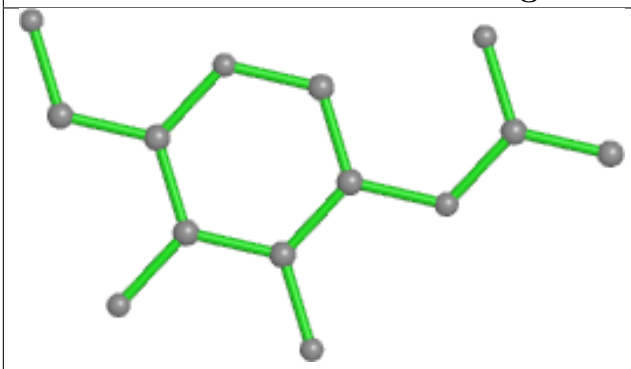


Rings

Ligand NAG C 503



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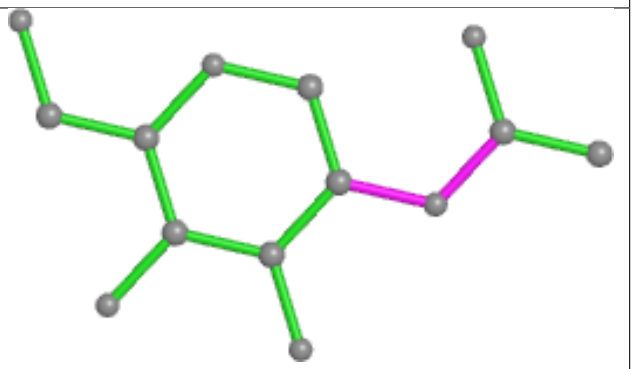

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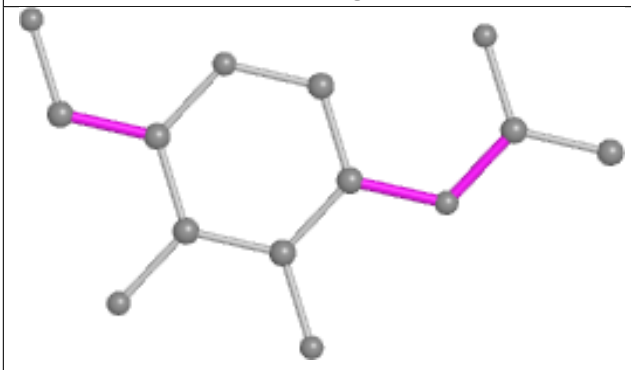

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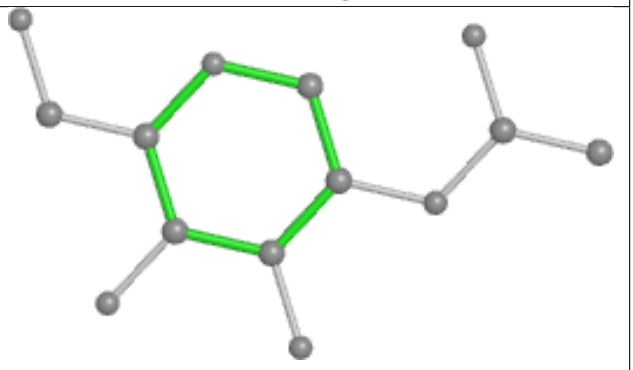

Rings

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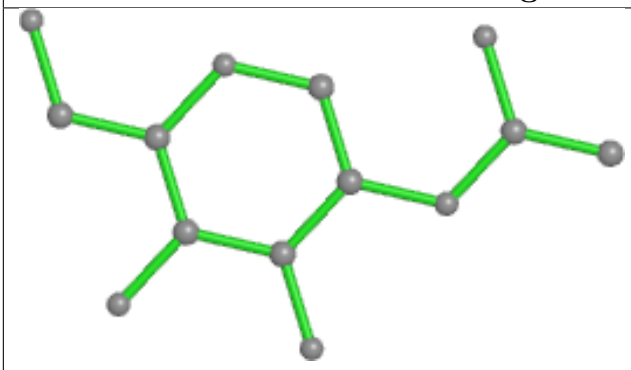

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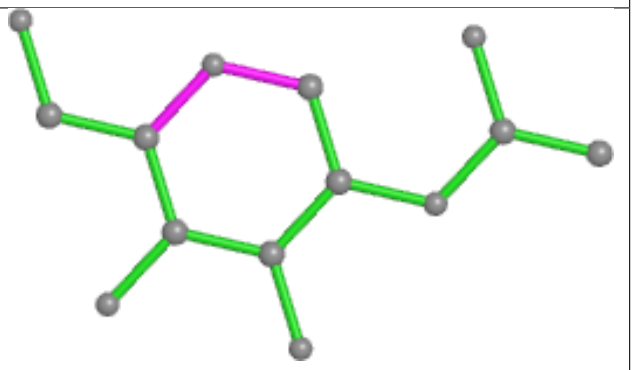
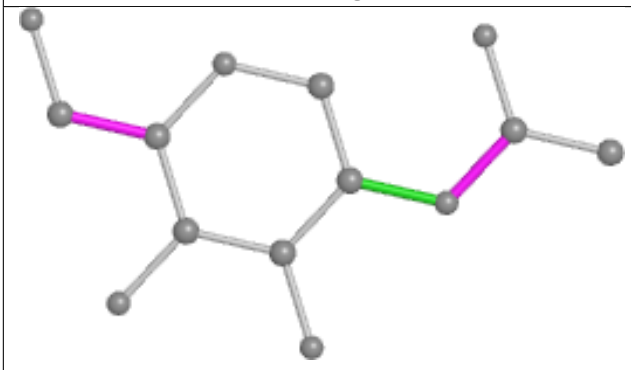


Bond angles



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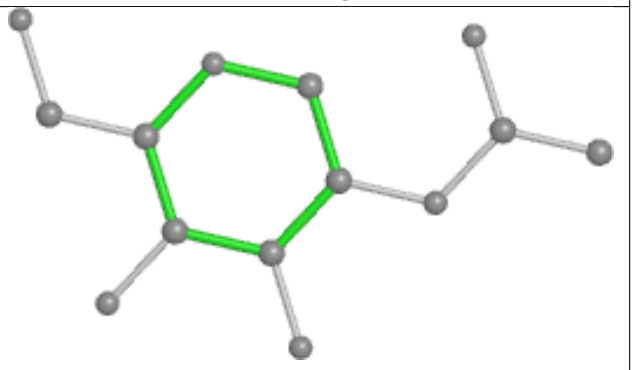

Rings

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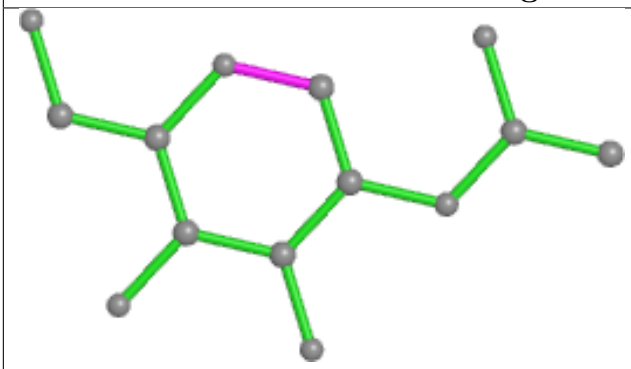

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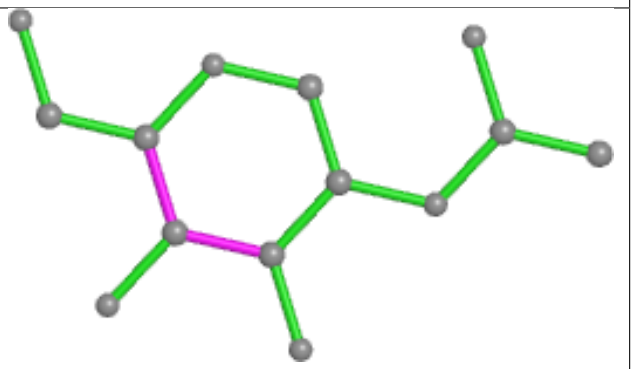

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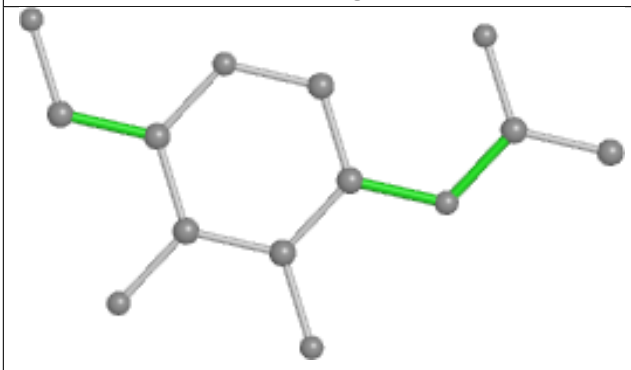

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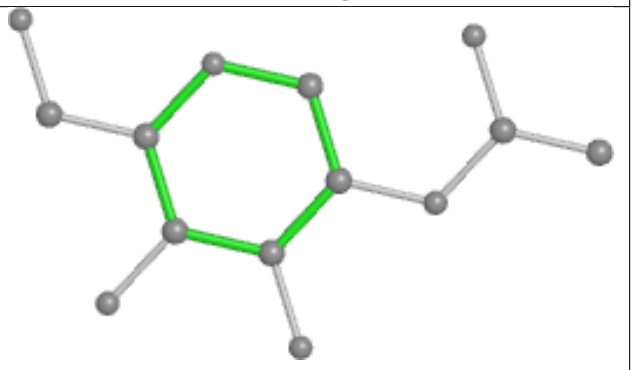

Rings

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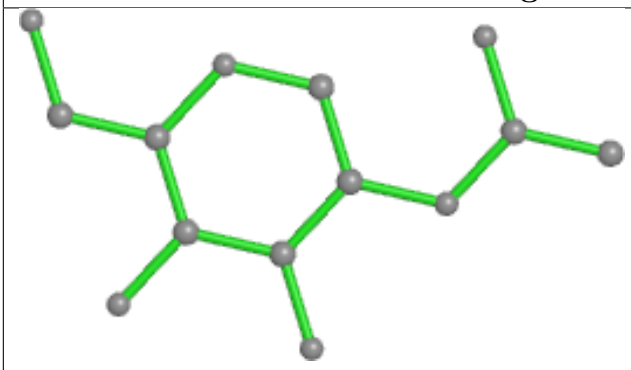

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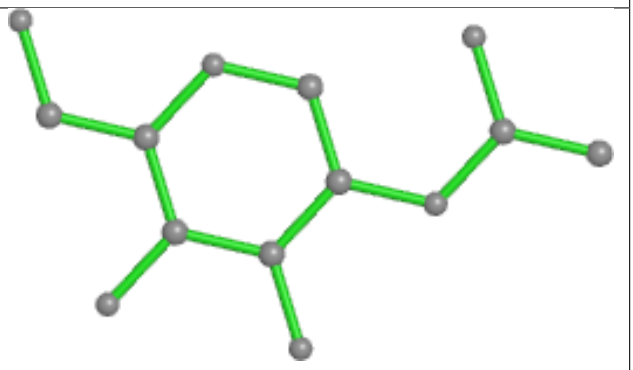
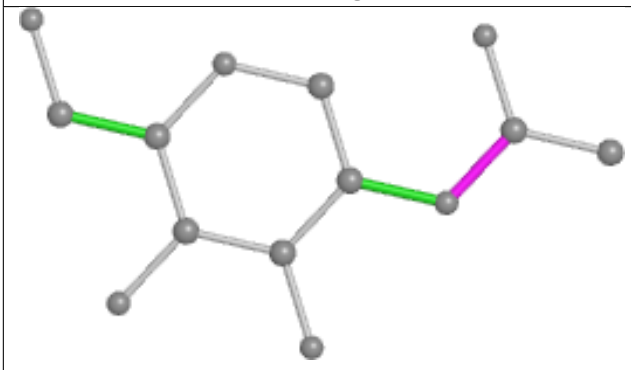


Bond angles



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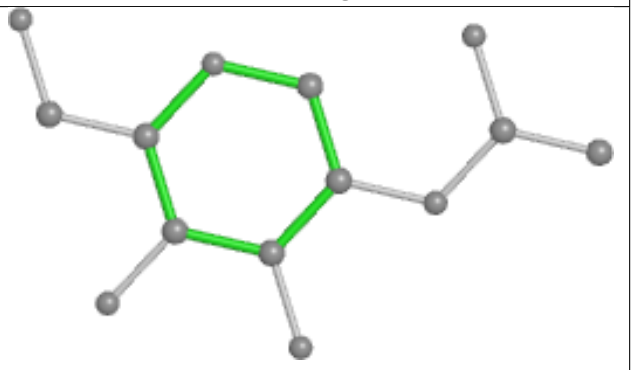
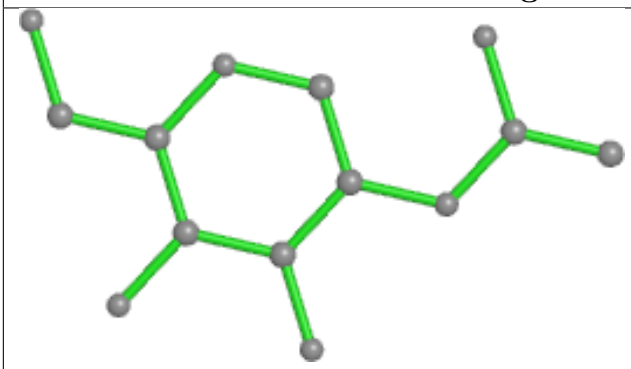


Rings

Ligand NAG B 503



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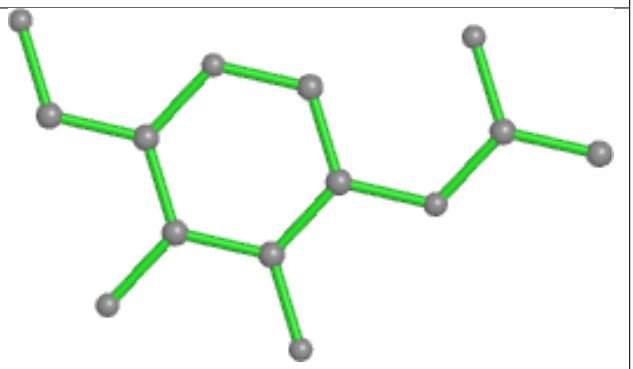
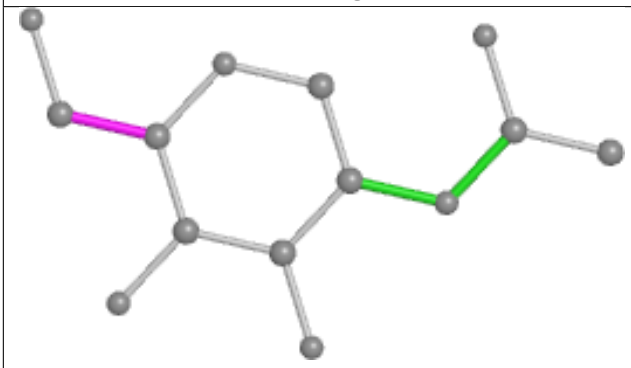
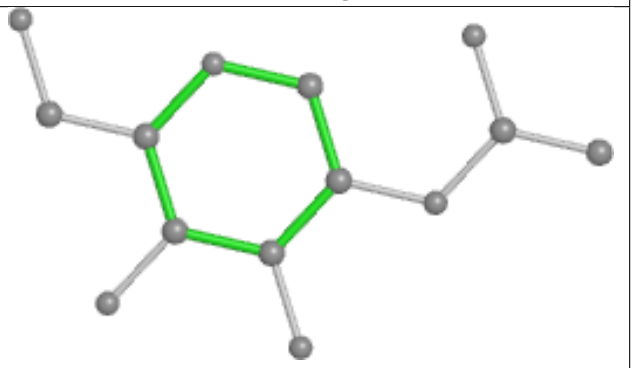


Bond angles

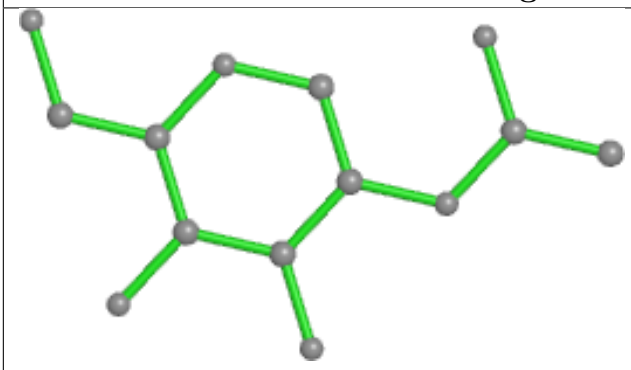


Torsions



Rings

Ligand NAG D 503



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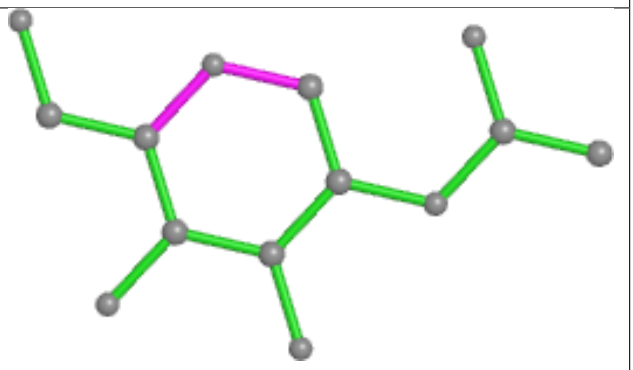

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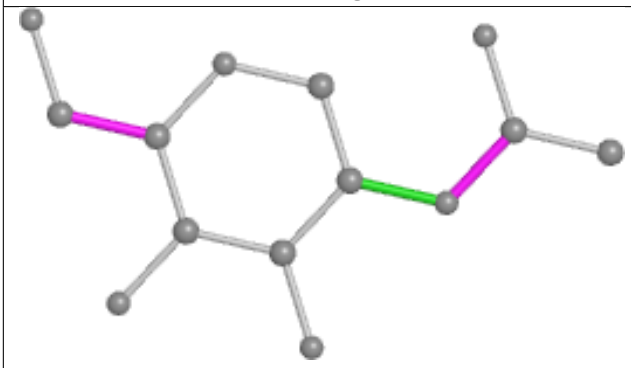

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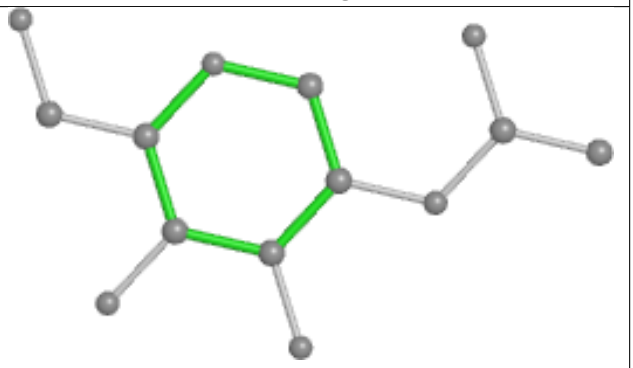
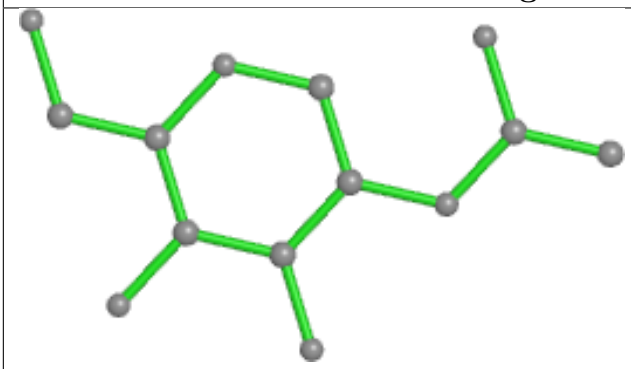
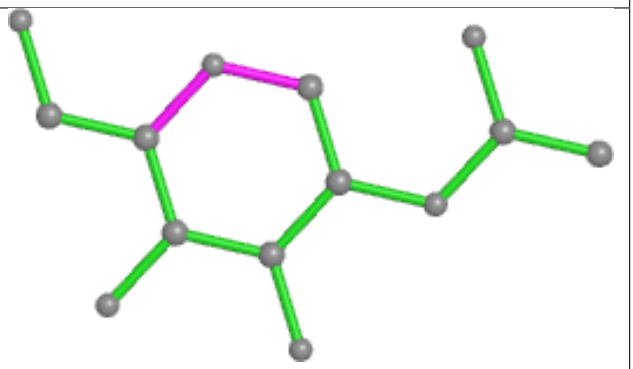


Rings

Ligand NAG A 502



Bond lengths



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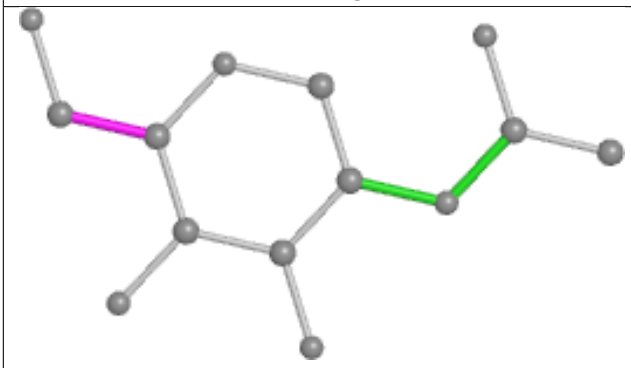

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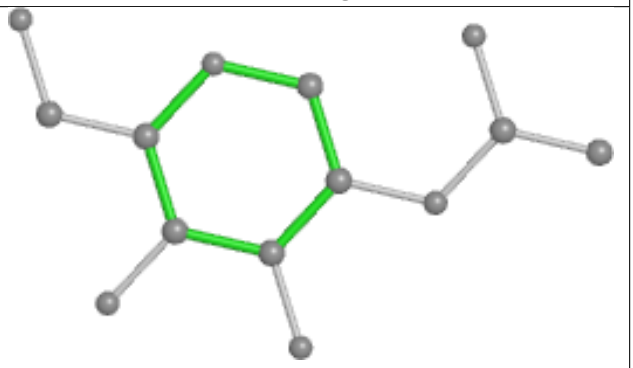
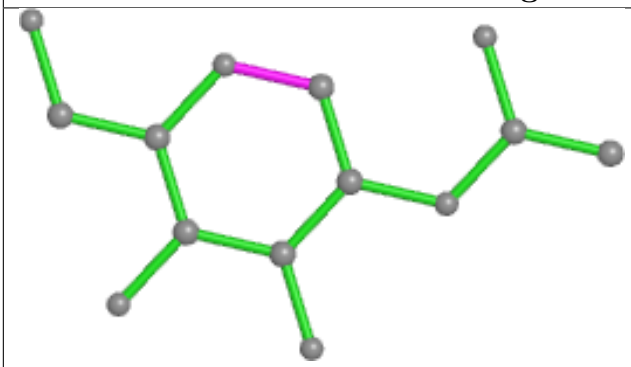
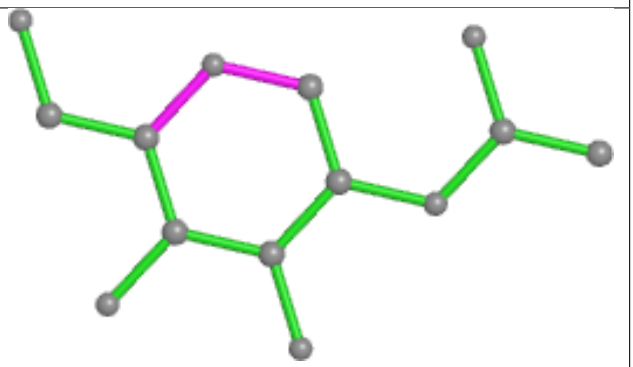


Rings

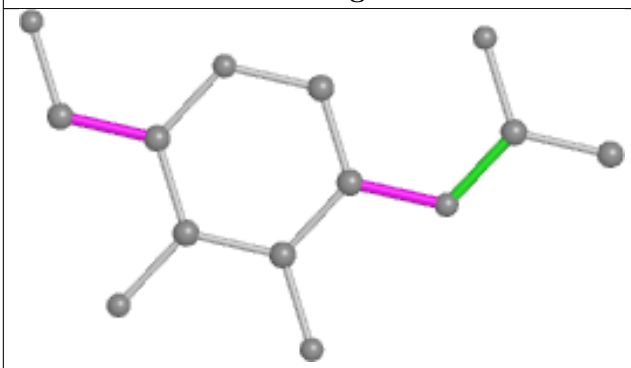
Ligand NAG B 501



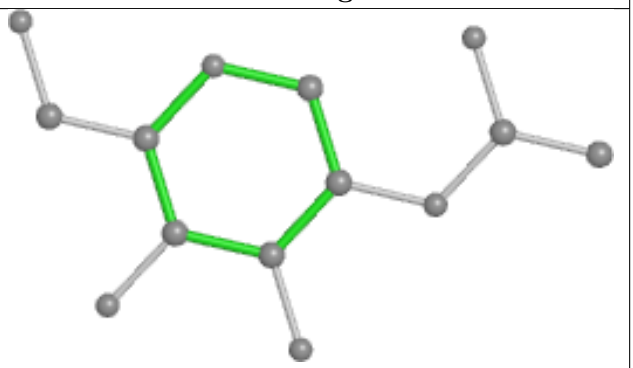
Bond lengths



Bond angles

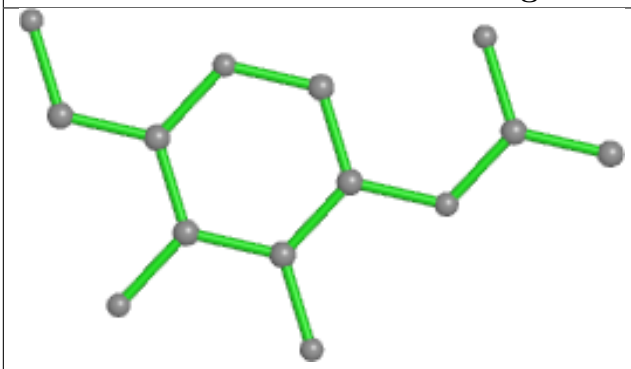


Torsions

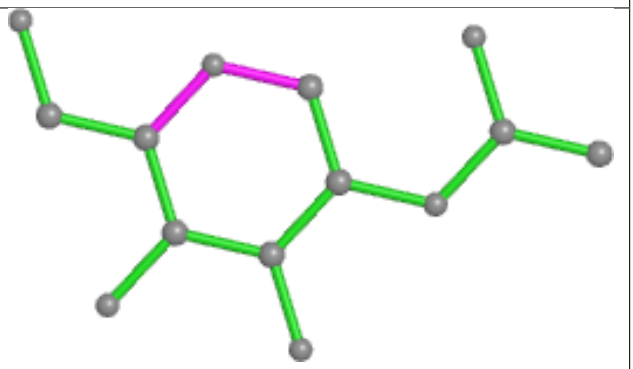


Rings

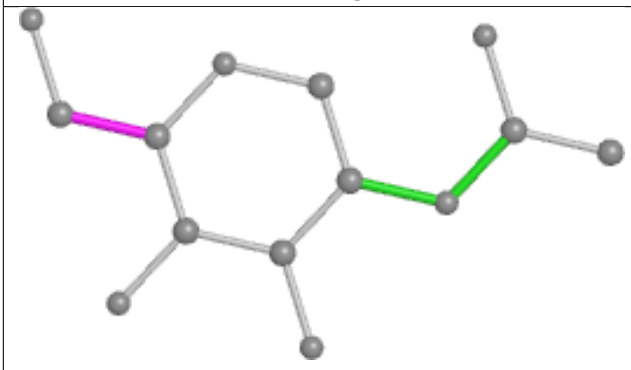
Ligand NAG B 502



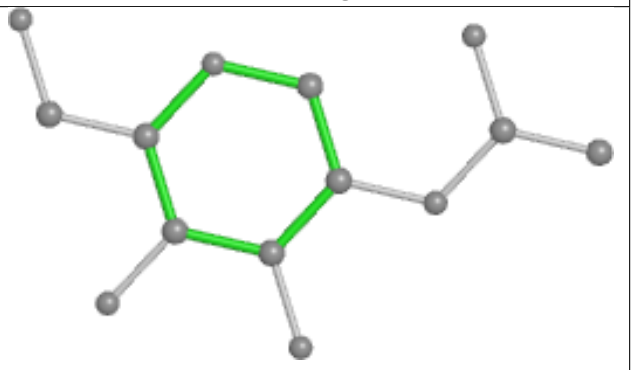
Bond lengths



Bond angles

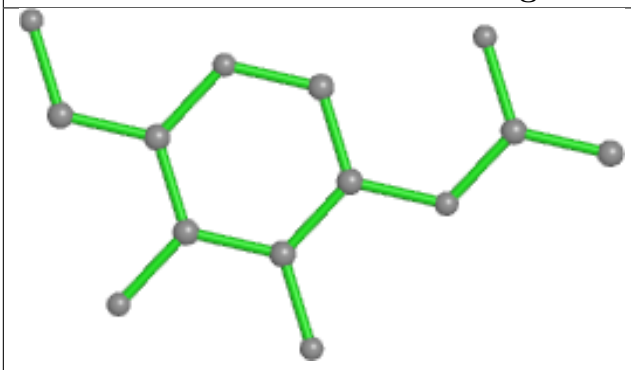


Torsions

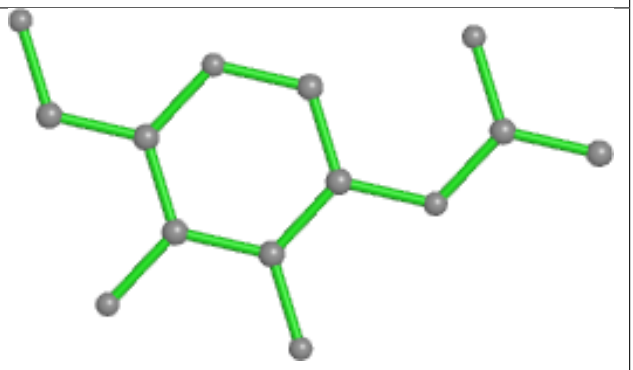


Rings

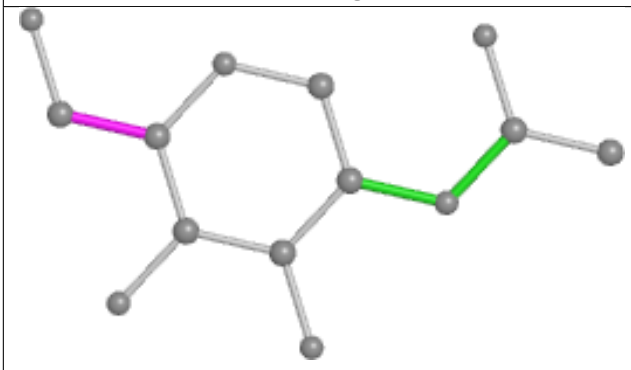
Ligand NAG D 501



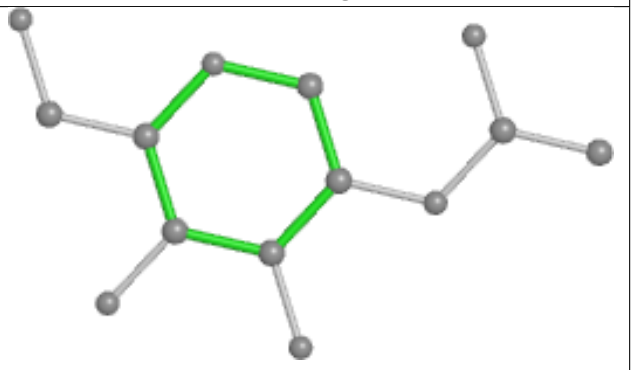
Bond lengths



Bond angles

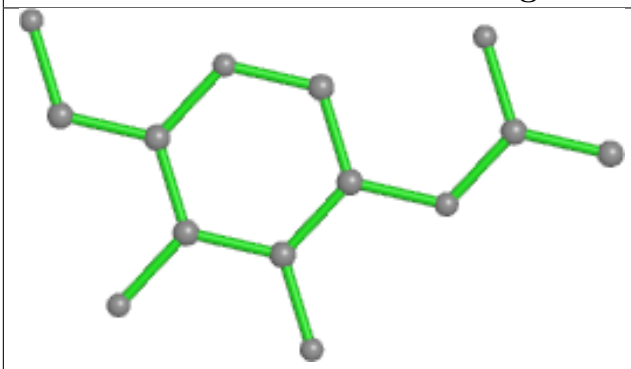


Torsions

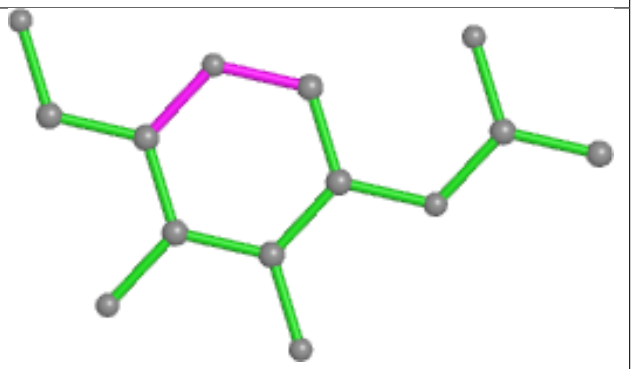


Rings

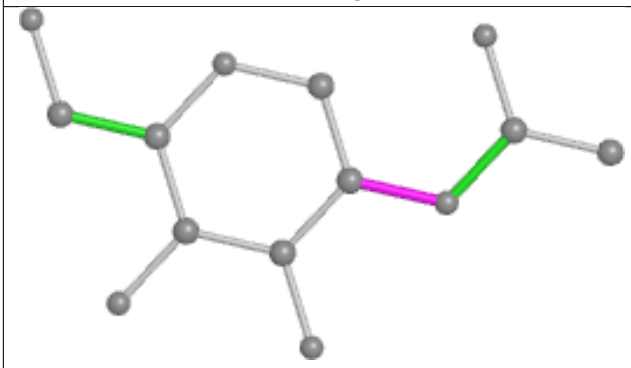
Ligand NAG A 504



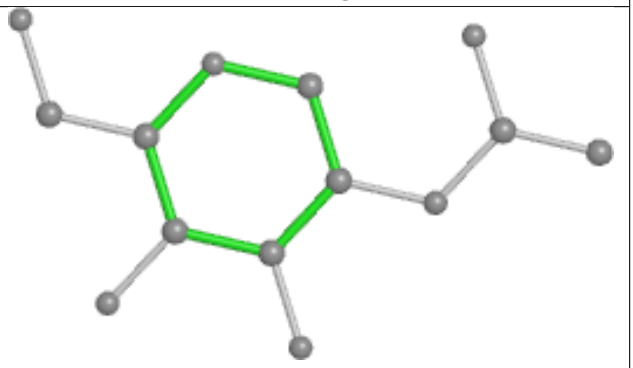
Bond lengths



Bond angles

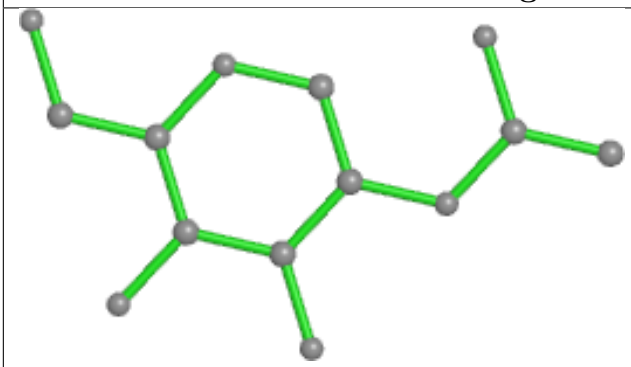


Torsions

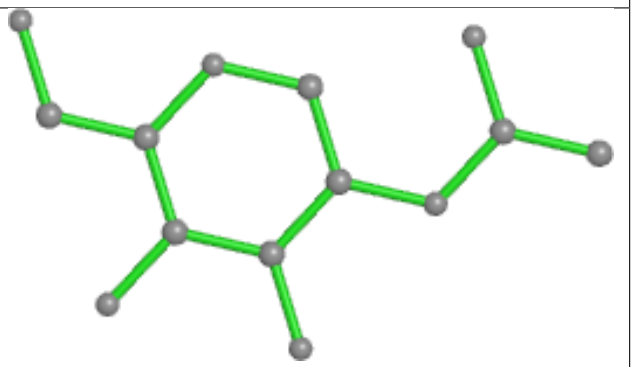


Rings

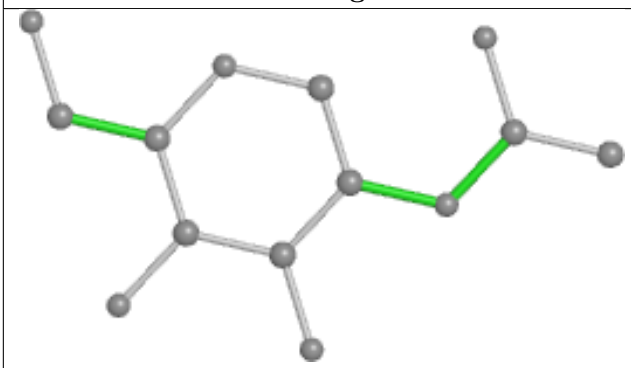
Ligand NAG D 502



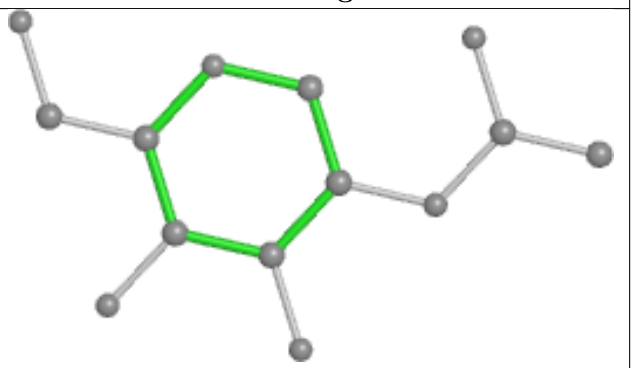
Bond lengths



Bond angles

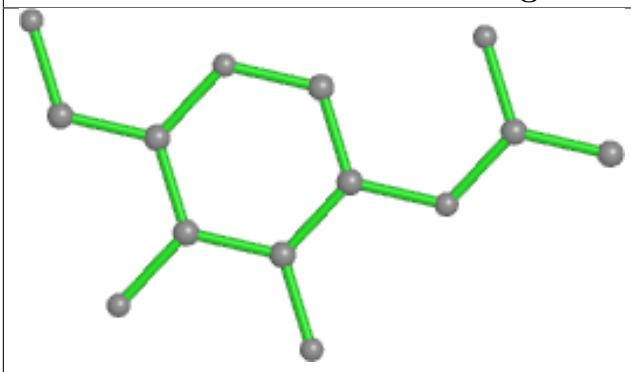


Torsions

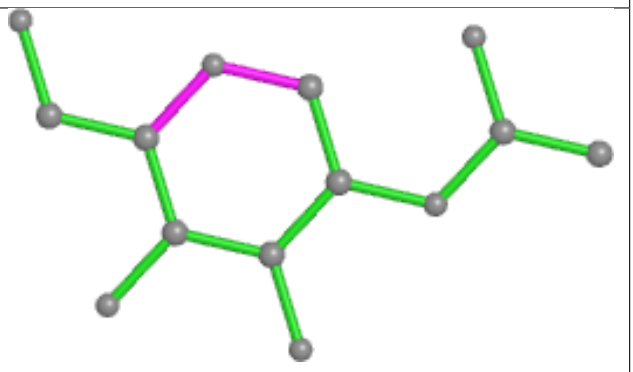


Rings

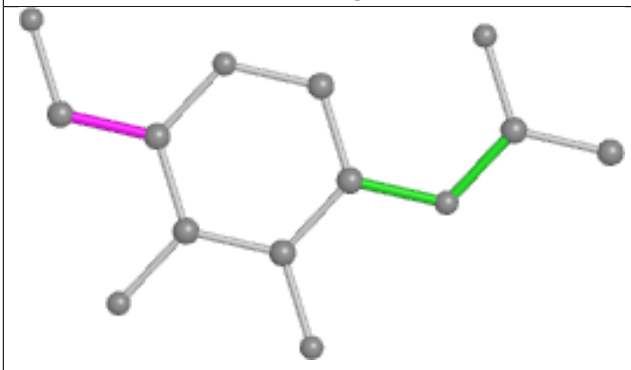
Ligand NAG C 502



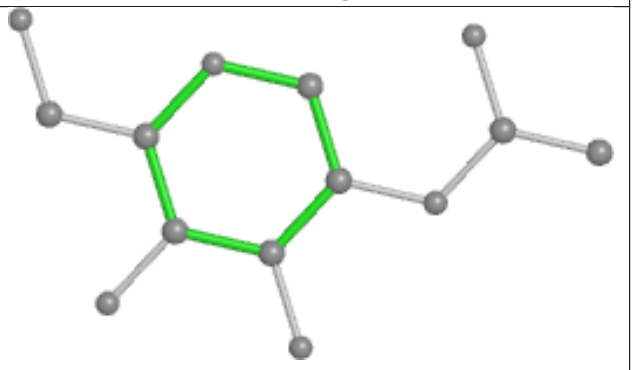
Bond lengths



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	393/424 (92%)	0.30	11 (2%) 53 55	23, 41, 74, 94	0
1	B	394/424 (92%)	0.26	4 (1%) 82 83	27, 39, 63, 87	0
1	C	394/424 (92%)	0.19	3 (0%) 86 86	24, 38, 64, 82	0
1	D	392/424 (92%)	0.27	7 (1%) 68 70	23, 42, 69, 82	0
All	All	1573/1696 (92%)	0.25	25 (1%) 72 73	23, 40, 68, 94	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	GLY	3.8
1	B	134	ARG	3.1
1	A	67	PHE	3.1
1	C	134	ARG	2.9
1	A	80	ASN	2.9
1	D	351	LYS	2.8
1	D	134	ARG	2.8
1	C	84	ILE	2.6
1	D	302	SER	2.5
1	A	355	GLN	2.5
1	A	134	ARG	2.5
1	A	155	ARG	2.4
1	C	85	ARG	2.4
1	A	112	VAL	2.4
1	D	27	ASN	2.4
1	A	119	ALA	2.3
1	D	272	THR	2.2
1	D	269	GLU	2.2
1	A	116	GLN	2.2
1	B	270	GLY	2.1
1	B	155	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	125	LEU	2.0
1	A	31	PHE	2.0
1	A	277	LEU	2.0
1	B	84	ILE	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
3	MAN	F	7	11/12	0.58	0.28	77,92,107,113	0
2	NAG	G	2	14/15	0.67	0.37	73,89,105,112	0
4	MAN	L	6	11/12	0.77	0.21	75,91,109,112	0
2	NAG	K	2	14/15	0.78	0.20	63,77,93,96	0
3	MAN	J	7	11/12	0.79	0.23	125,139,165,167	0
4	NAG	L	5	14/15	0.80	0.22	62,78,95,95	0
2	NAG	E	2	14/15	0.80	0.24	66,81,96,103	0
4	MAN	L	7	11/12	0.82	0.28	78,93,110,116	0
3	BMA	J	3	11/12	0.83	0.15	51,72,124,124	0
2	NAG	E	1	14/15	0.84	0.26	45,68,82,94	0
3	MAN	H	7	11/12	0.85	0.17	63,79,97,105	0
2	NAG	I	2	14/15	0.85	0.22	59,81,98,109	0
4	MAN	L	4	11/12	0.86	0.22	59,71,84,85	0
2	NAG	I	1	14/15	0.87	0.18	49,60,72,81	0
3	MAN	F	6	11/12	0.88	0.17	60,74,85,94	0
2	NAG	K	1	14/15	0.89	0.16	48,62,75,85	0
3	MAN	J	5	11/12	0.89	0.18	52,63,76,91	0
3	NAG	J	2	14/15	0.89	0.18	42,54,68,76	0
4	BMA	L	3	11/12	0.89	0.19	50,61,92,92	0
2	NAG	G	1	14/15	0.90	0.17	44,58,81,89	0
3	MAN	J	6	11/12	0.90	0.23	52,63,73,85	0
3	NAG	F	2	14/15	0.90	0.15	46,57,69,86	0
3	MAN	H	6	11/12	0.90	0.22	60,72,86,88	0
3	MAN	F	5	11/12	0.91	0.10	55,66,81,84	0

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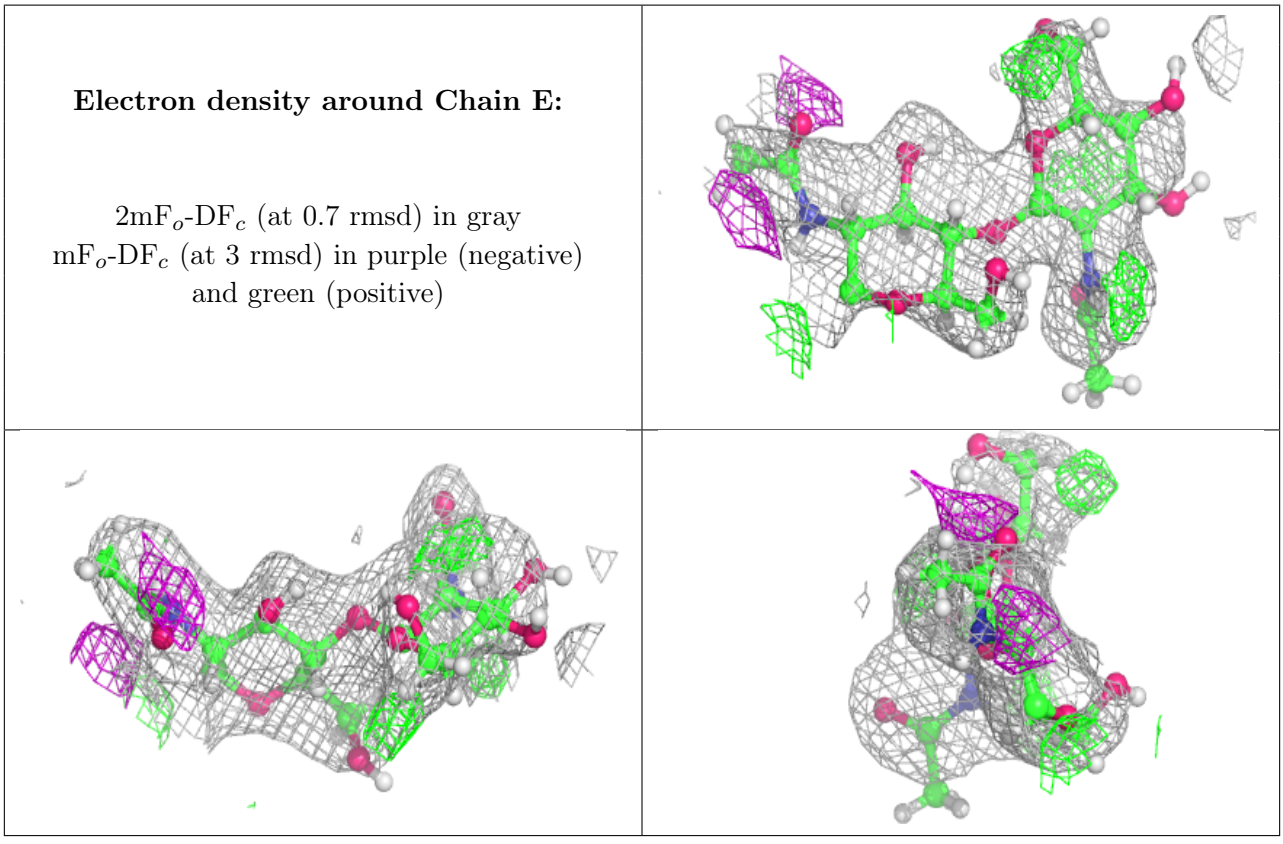
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	J	4	11/12	0.91	0.15	45,57,70,73	0
4	NAG	L	2	14/15	0.91	0.13	40,51,64,66	0
3	BMA	F	3	11/12	0.91	0.14	50,64,88,88	0
3	MAN	F	4	11/12	0.93	0.13	47,56,68,73	0
3	MAN	H	5	11/12	0.93	0.20	50,63,76,80	0
3	MAN	H	4	11/12	0.94	0.12	47,56,71,82	0
3	BMA	H	3	11/12	0.94	0.15	45,52,65,68	0
3	NAG	H	2	14/15	0.95	0.12	38,44,51,57	0
3	NAG	F	1	14/15	0.95	0.14	38,46,56,64	0
4	NAG	L	1	14/15	0.95	0.15	31,38,47,50	0
3	NAG	H	1	14/15	0.96	0.15	23,36,42,50	0
3	NAG	J	1	14/15	0.97	0.14	36,47,57,72	0

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

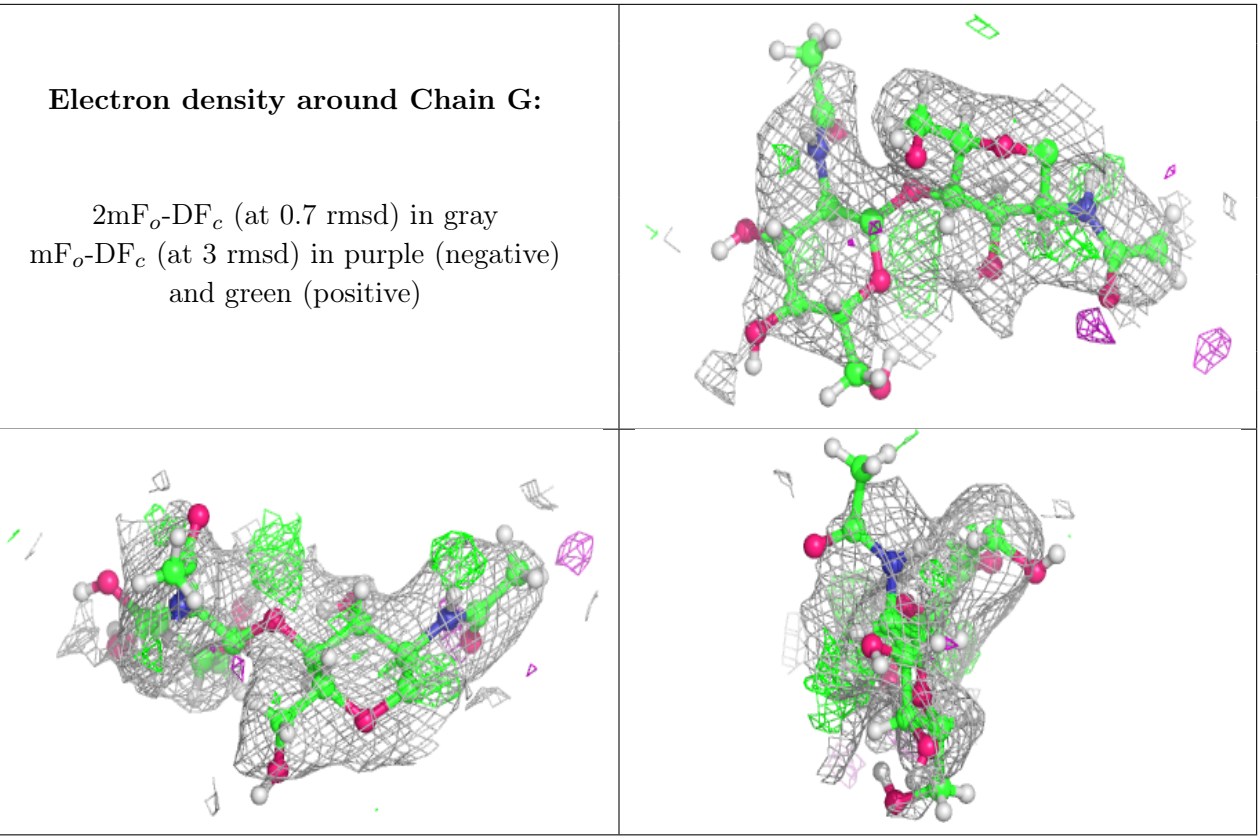
Electron density around Chain E:

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



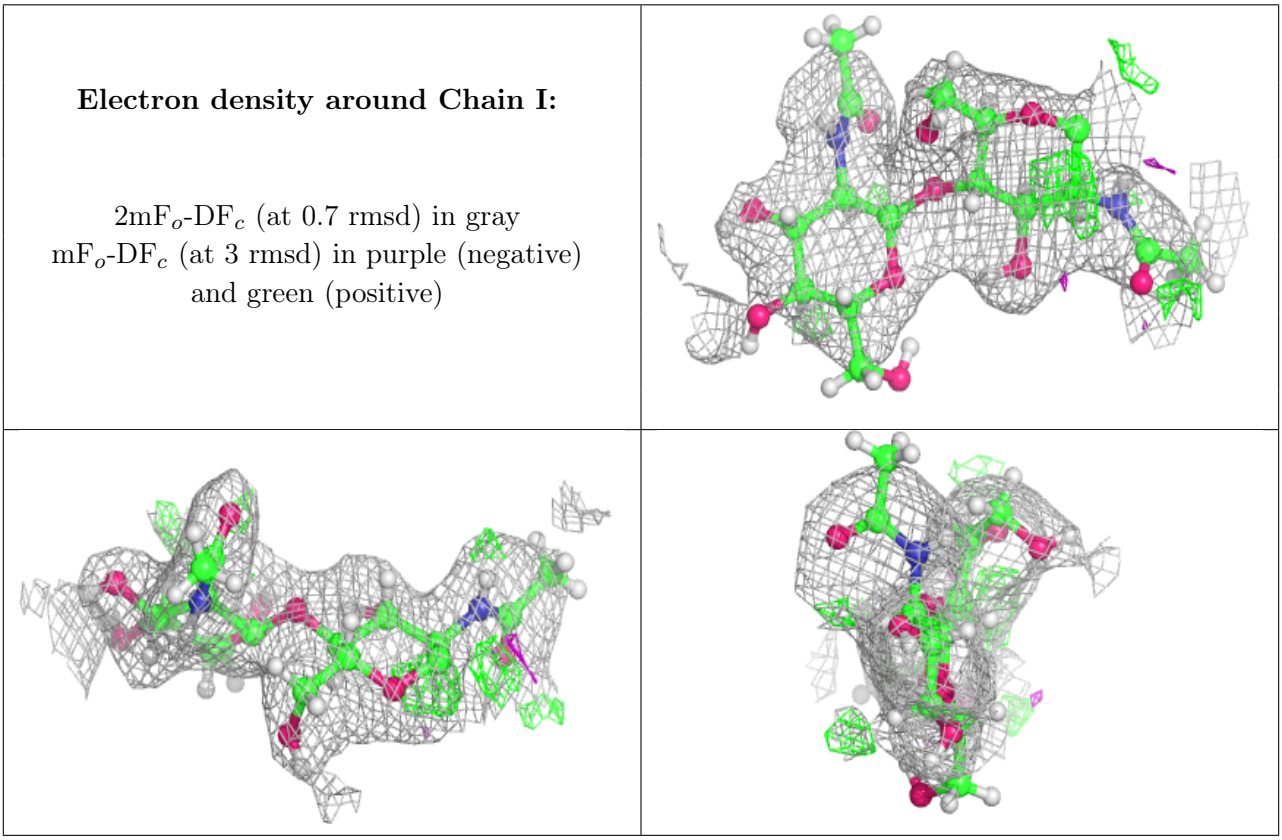
Electron density around Chain G:

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



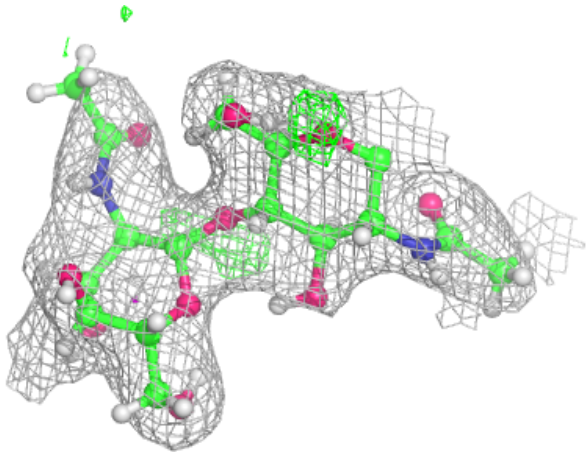
Electron density around Chain I:

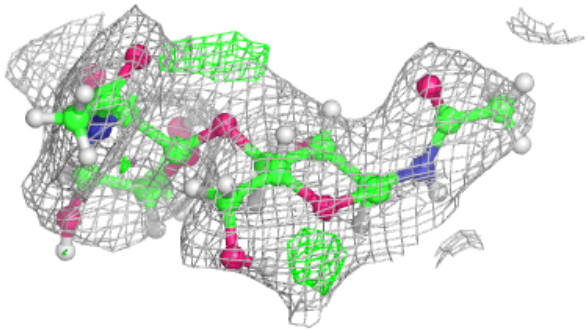
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

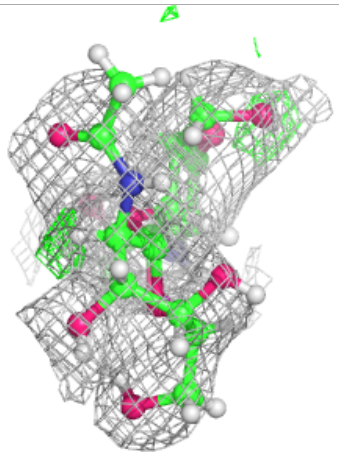


Electron density around Chain K:

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

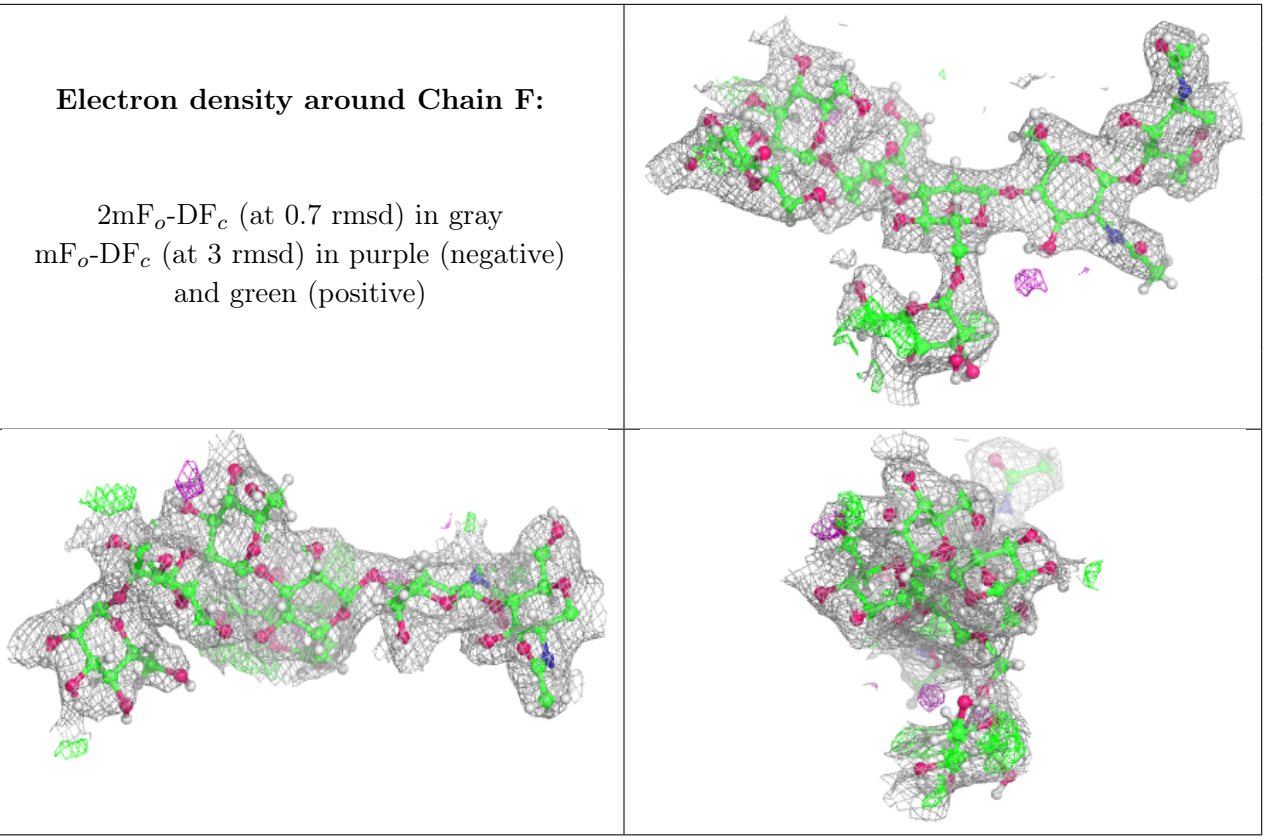






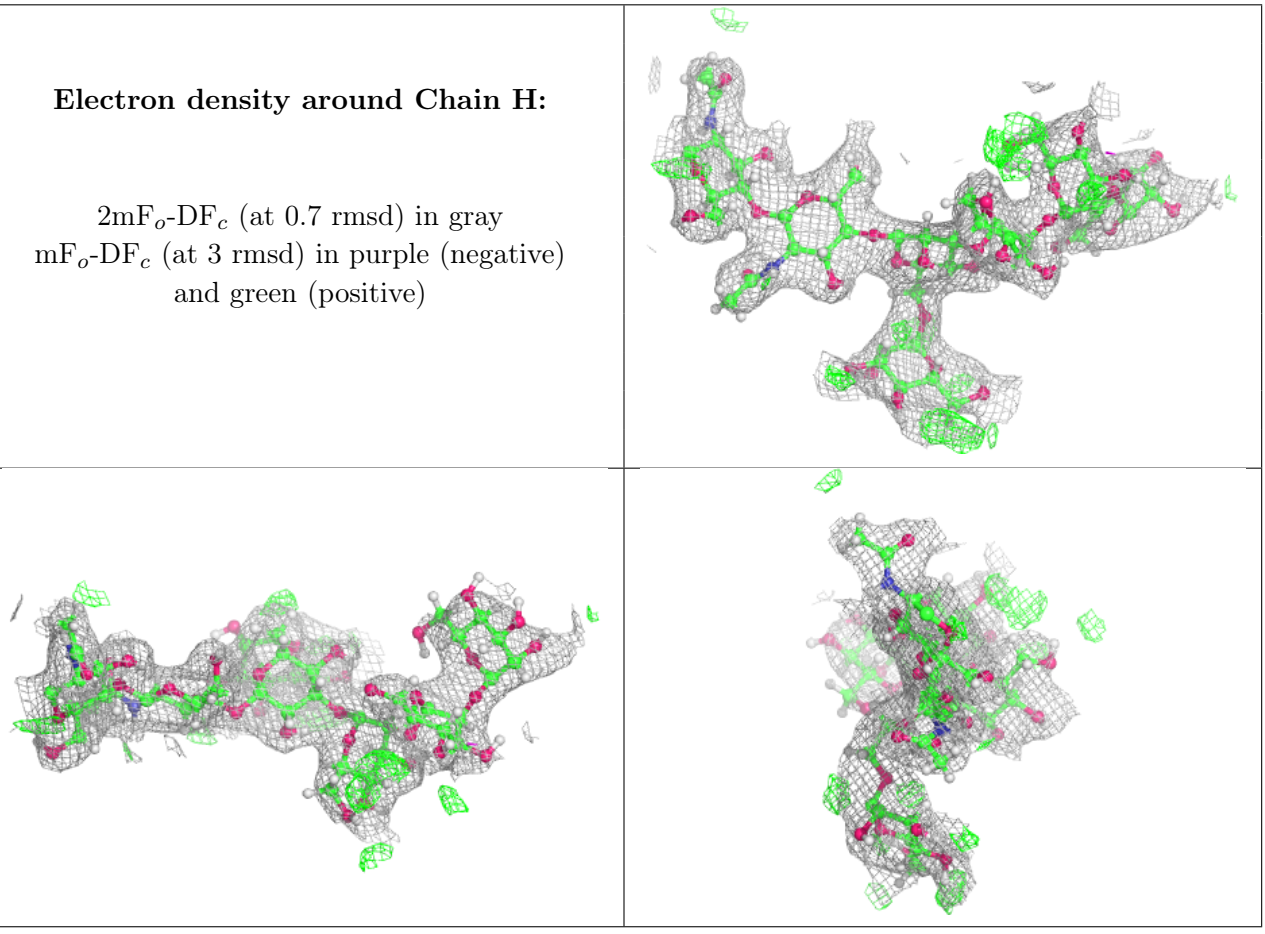
Electron density around Chain F:

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



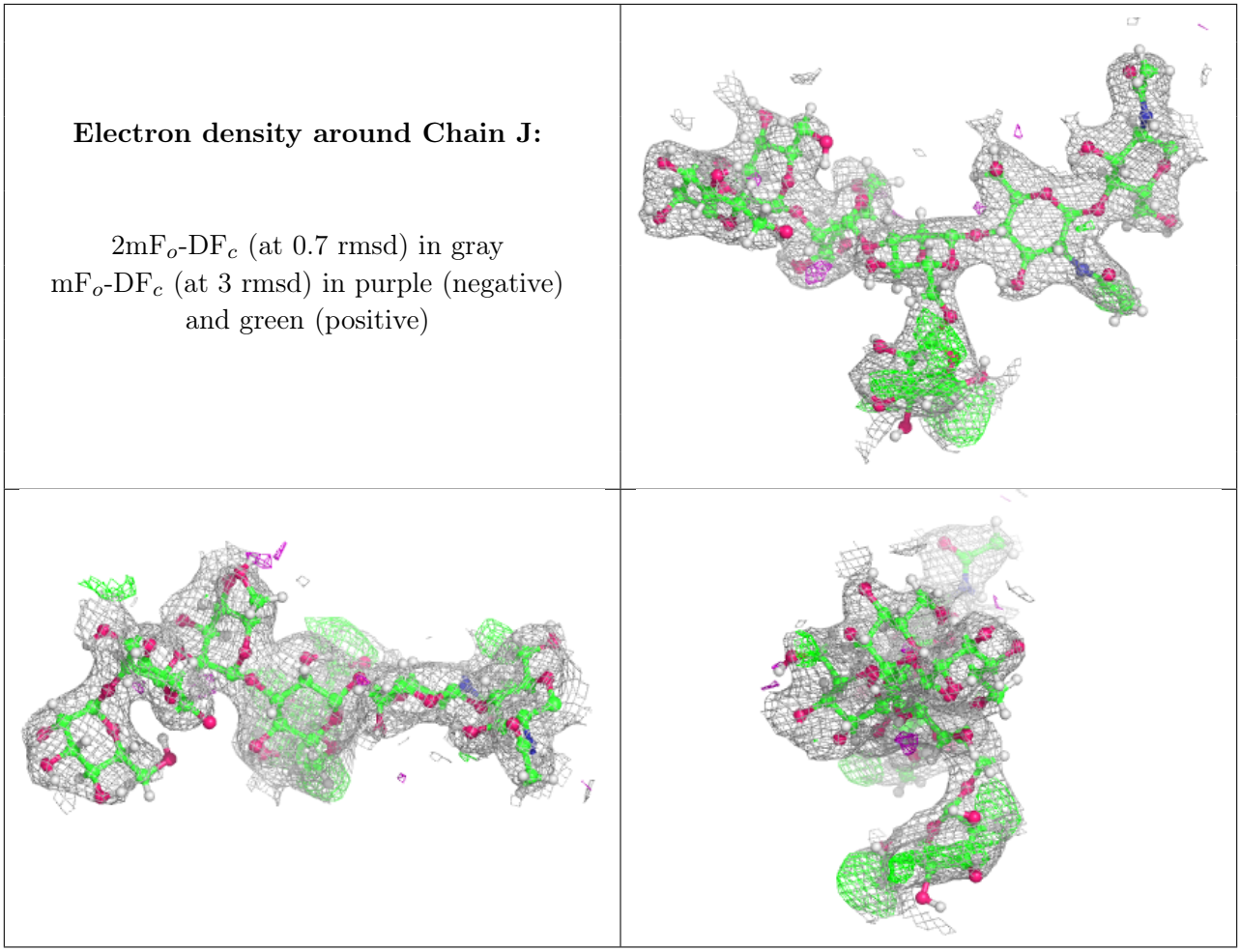
Electron density around Chain H:

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



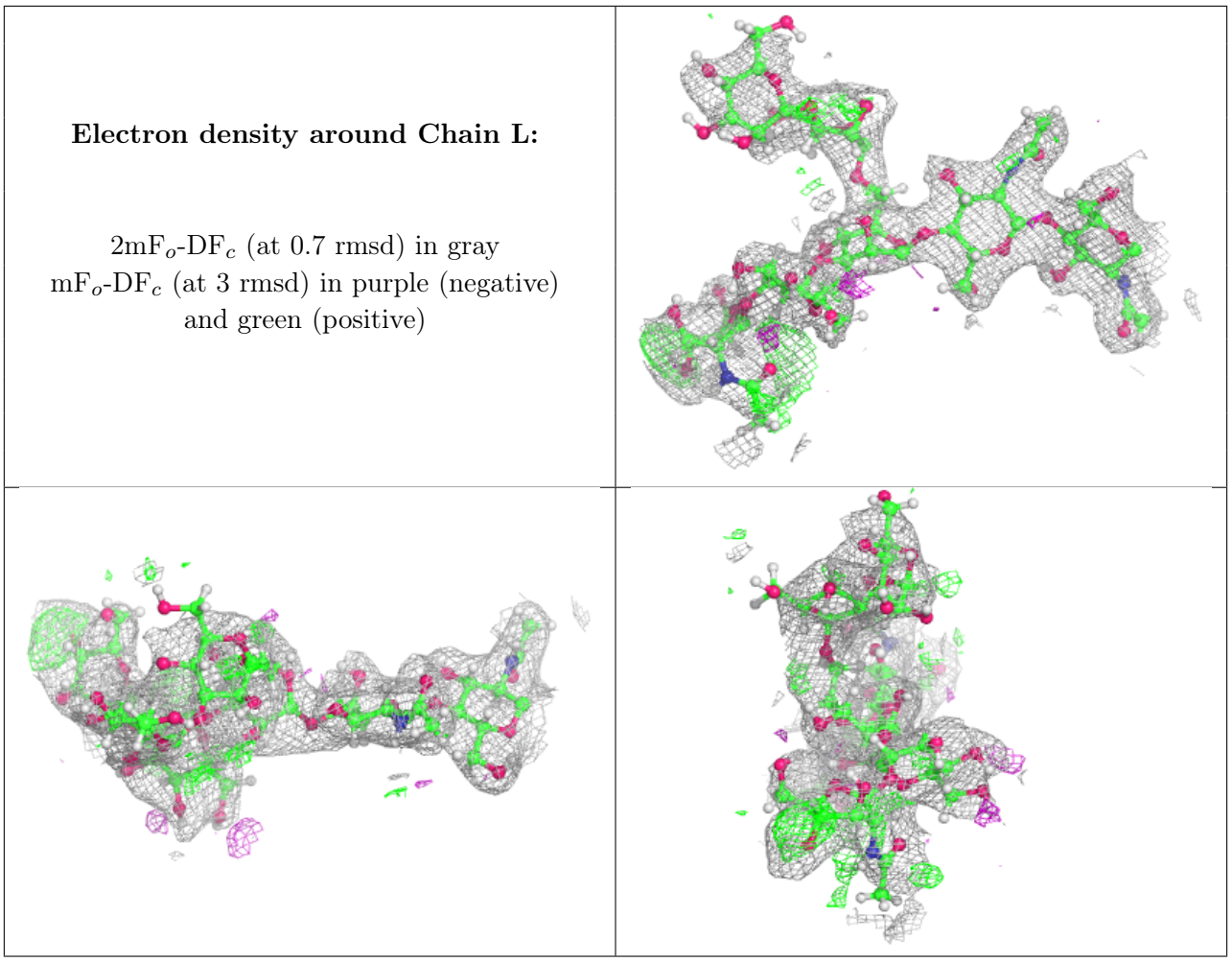
Electron density around Chain J:

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



Electron density around Chain L:

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



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
5	NAG	C	501	14/15	0.65	0.51	75,93,114,118	0
5	NAG	D	503	14/15	0.69	0.32	81,93,110,117	0
5	NAG	B	504	14/15	0.70	0.39	56,77,94,104	0
5	NAG	D	501	14/15	0.71	0.28	59,78,98,101	0
5	NAG	B	501	14/15	0.71	0.25	68,87,100,104	0
5	NAG	A	502	14/15	0.73	0.22	48,69,82,88	0
5	NAG	B	502	14/15	0.74	0.30	54,75,90,90	0
5	NAG	C	505	14/15	0.76	0.30	70,80,96,111	0
5	NAG	A	501	14/15	0.77	0.41	75,94,113,121	0
5	NAG	B	503	14/15	0.77	0.20	70,83,100,100	0

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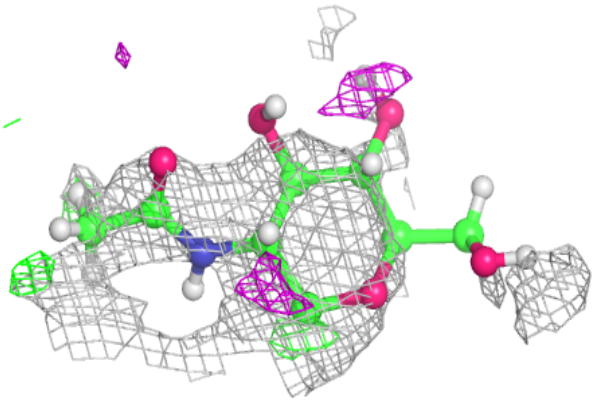
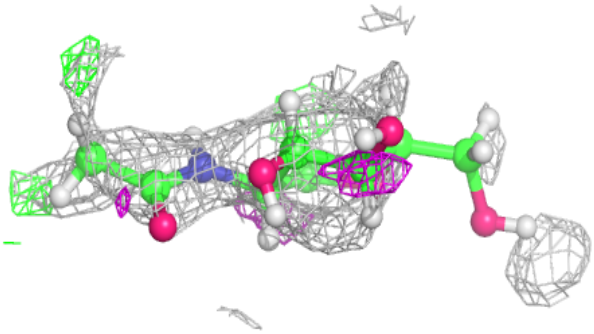
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	C	502	14/15	0.77	0.32	56,73,86,92	0
5	NAG	B	505	14/15	0.79	0.28	72,87,103,111	0
5	NAG	A	504	14/15	0.79	0.24	65,83,107,109	0
5	NAG	C	503	14/15	0.80	0.26	63,78,94,94	0
5	NAG	C	504	14/15	0.81	0.39	67,82,100,110	0
5	NAG	D	504	14/15	0.85	0.21	87,100,124,124	0
5	NAG	A	503	14/15	0.86	0.20	50,69,88,93	0
5	NAG	D	502	14/15	0.87	0.17	47,61,75,76	0

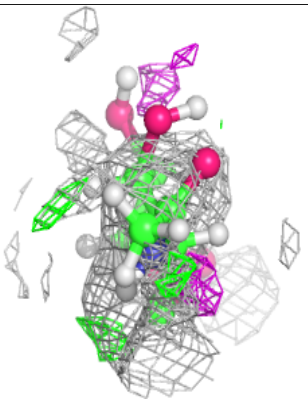
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAG 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)

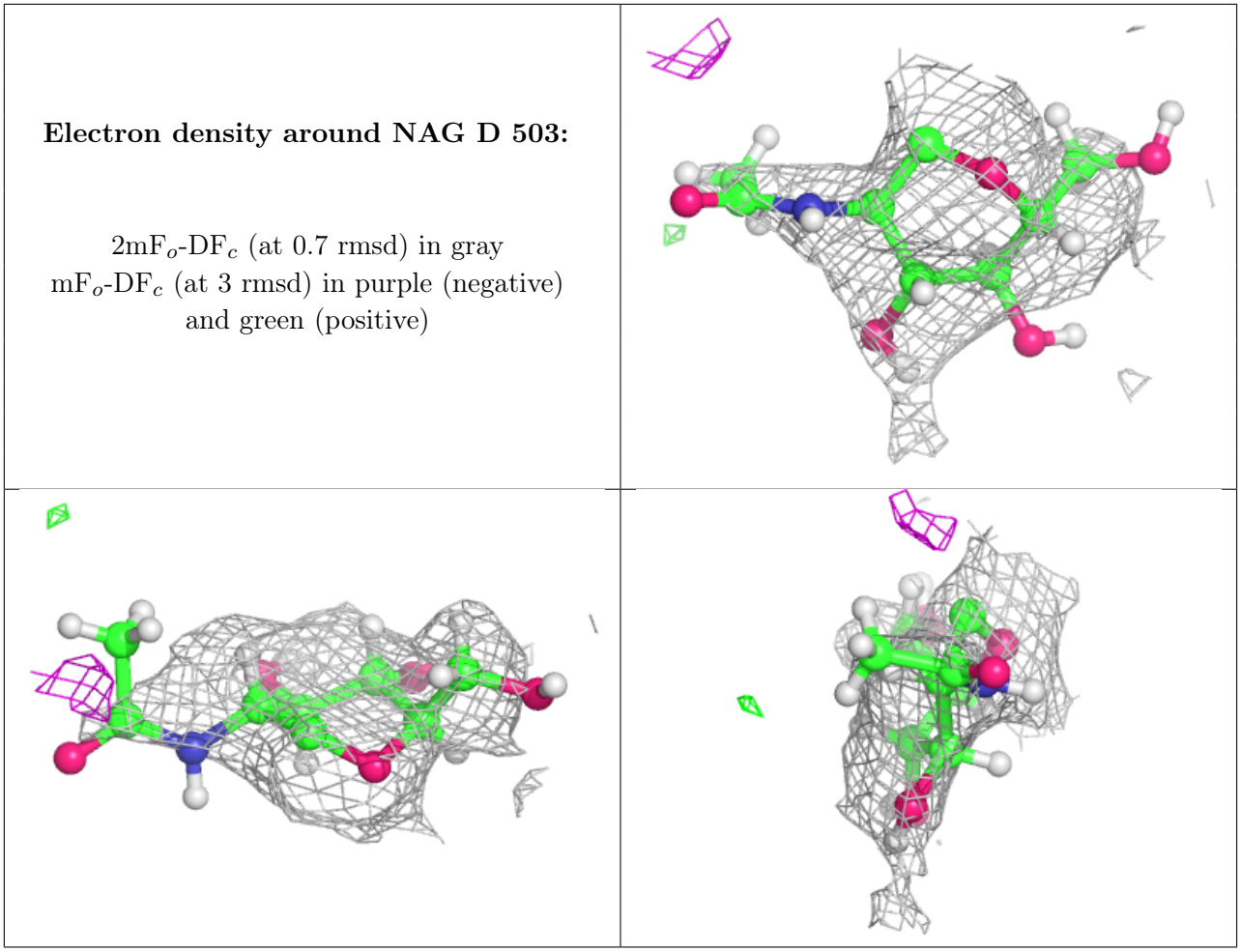






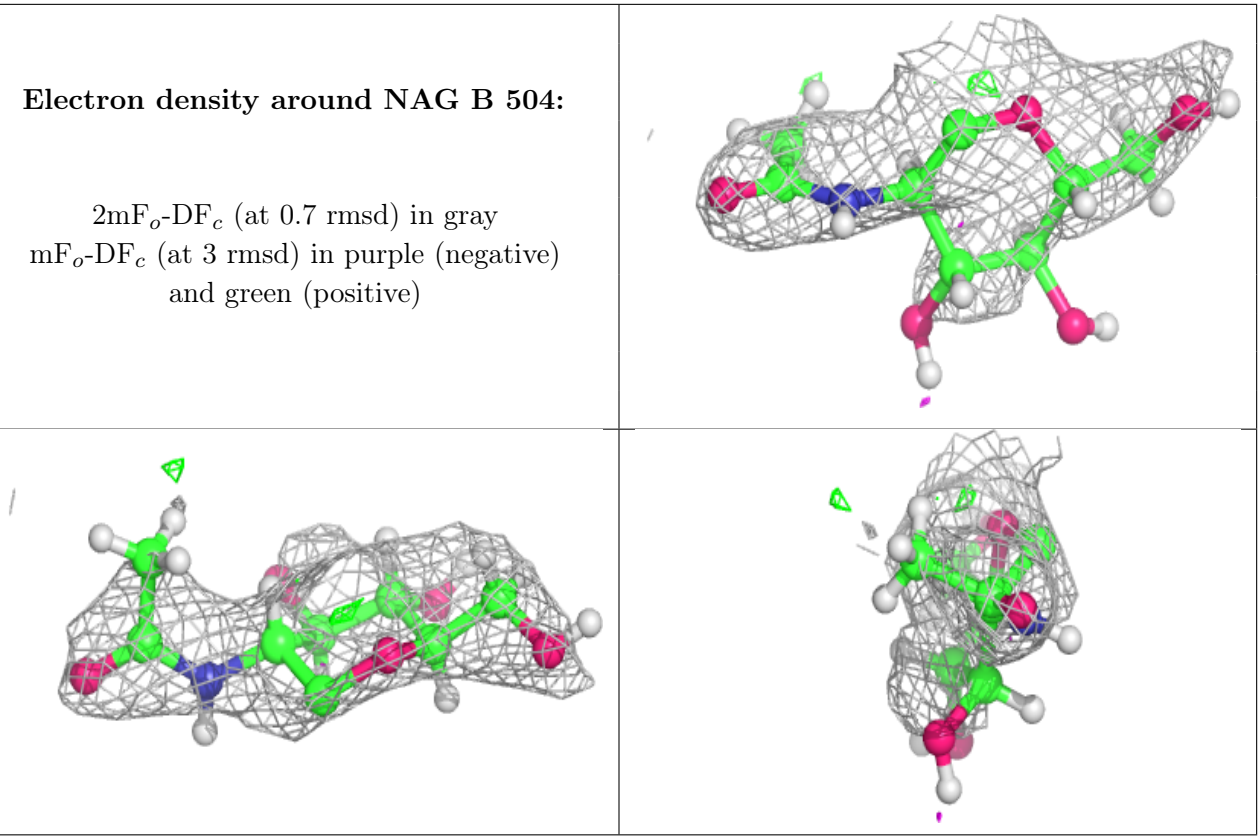
Electron density around NAG D 503:

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



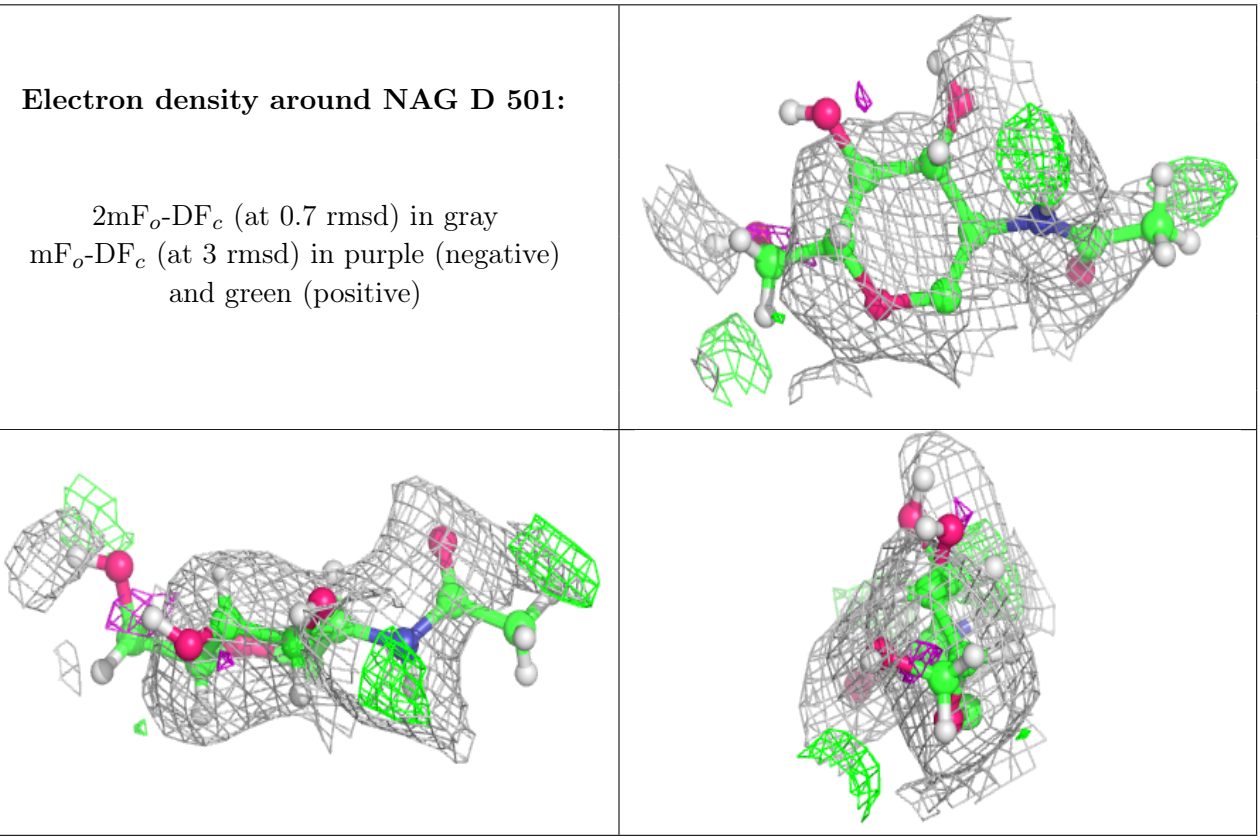
Electron density around NAG B 504:

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



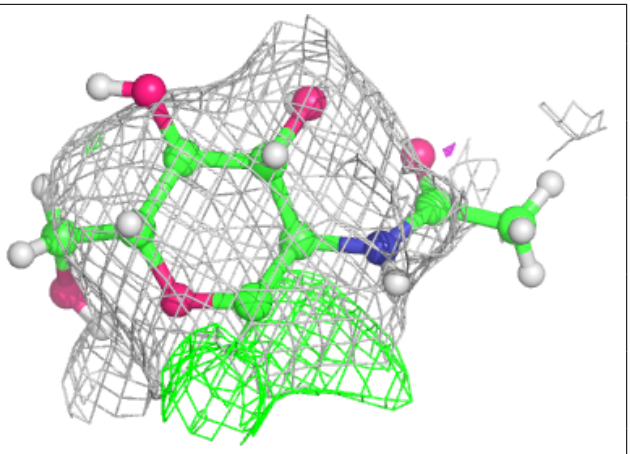
Electron density around NAG D 501:

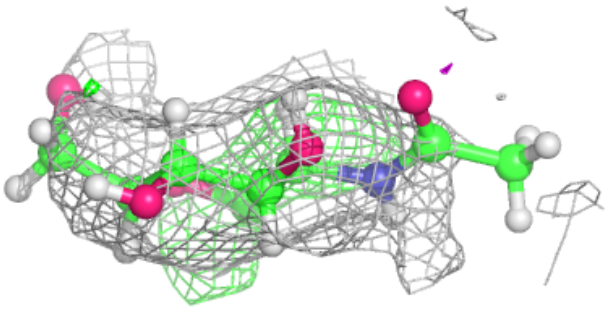
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

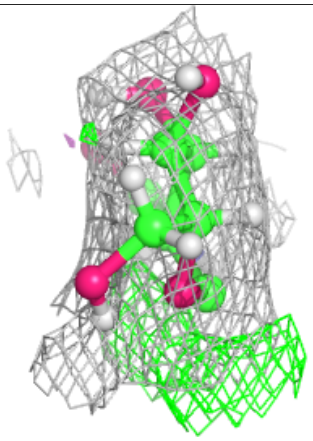


Electron density around NAG B 501:

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

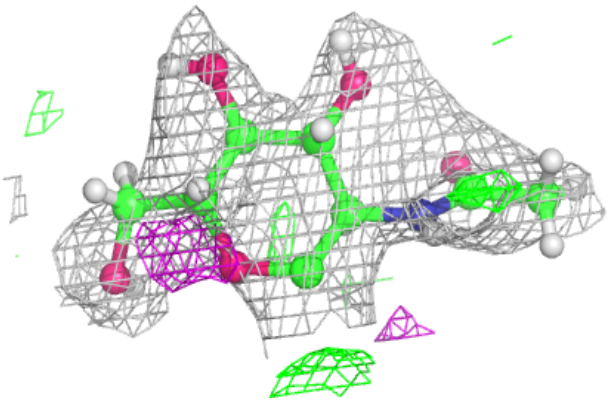


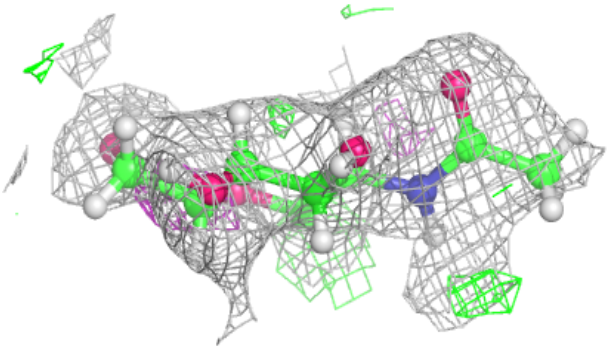


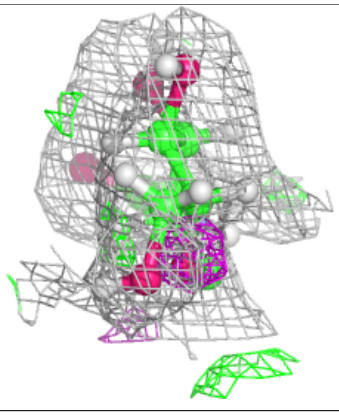


Electron density around NAG A 502:

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

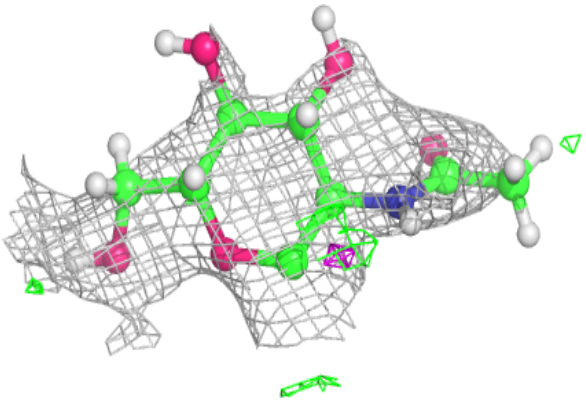


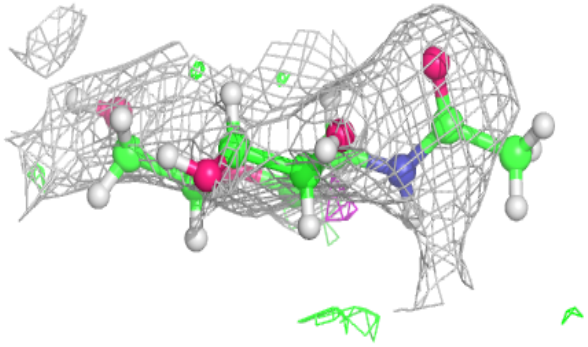


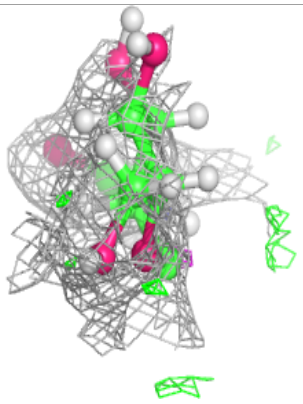


Electron density around NAG B 502:

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

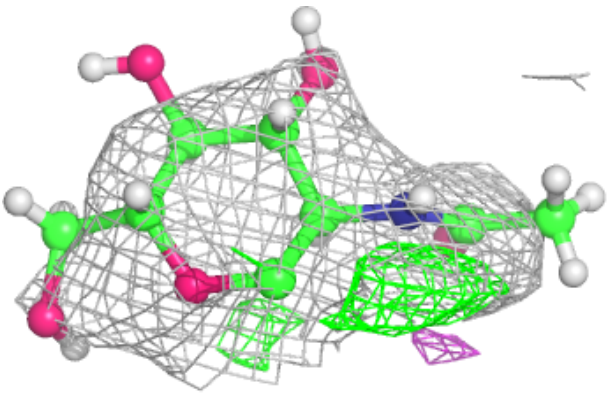


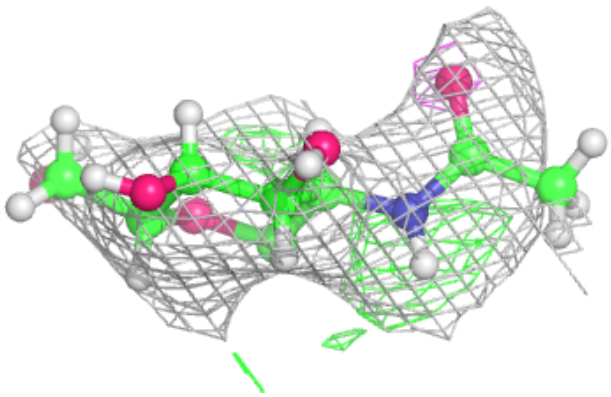


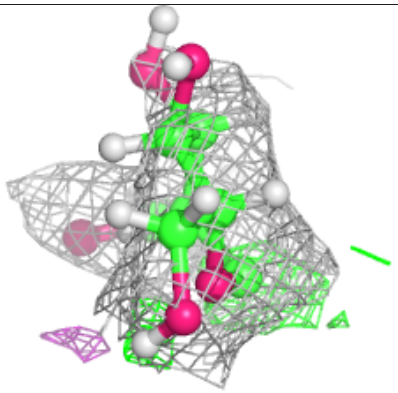


Electron density around NAG C 505:

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

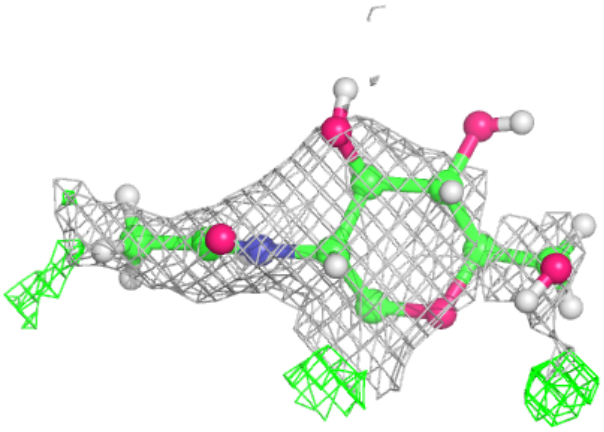


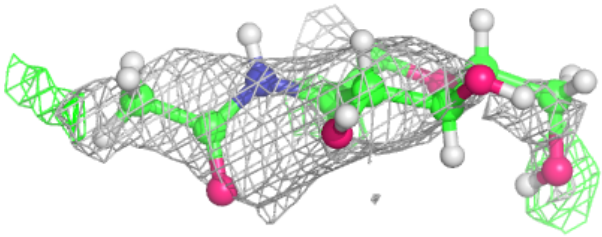


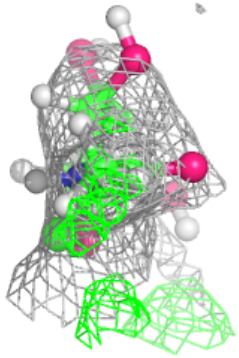


Electron density around NAG A 501:

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

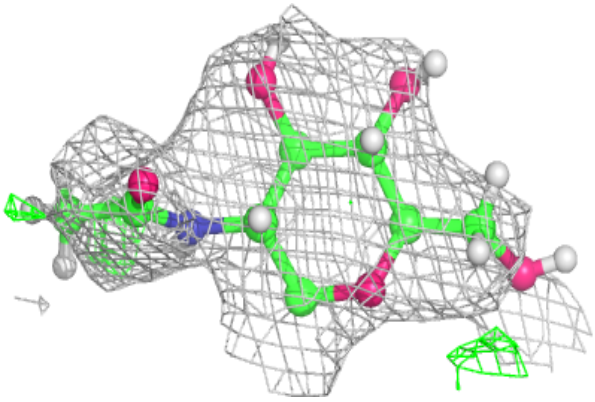


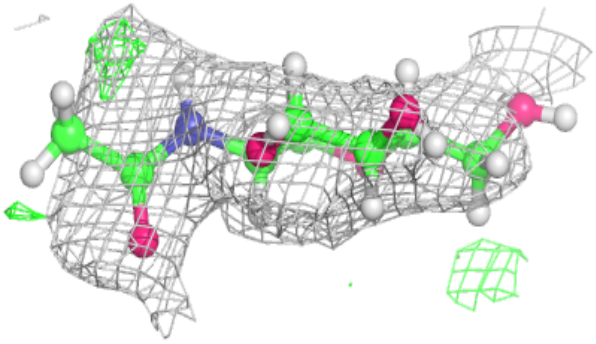


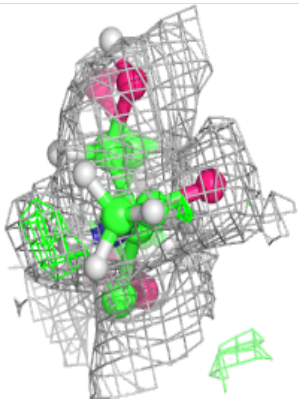


Electron density around NAG B 503:

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

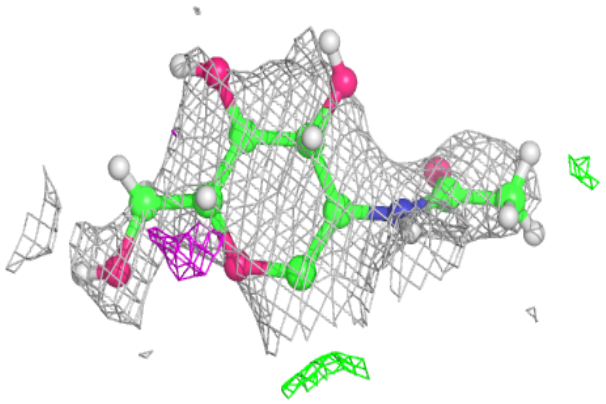


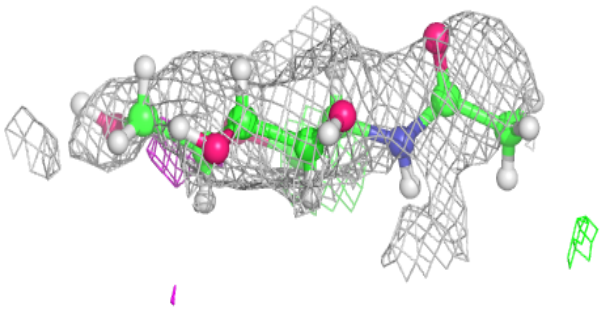


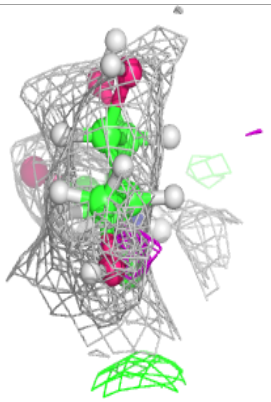


Electron density around NAG C 502:

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

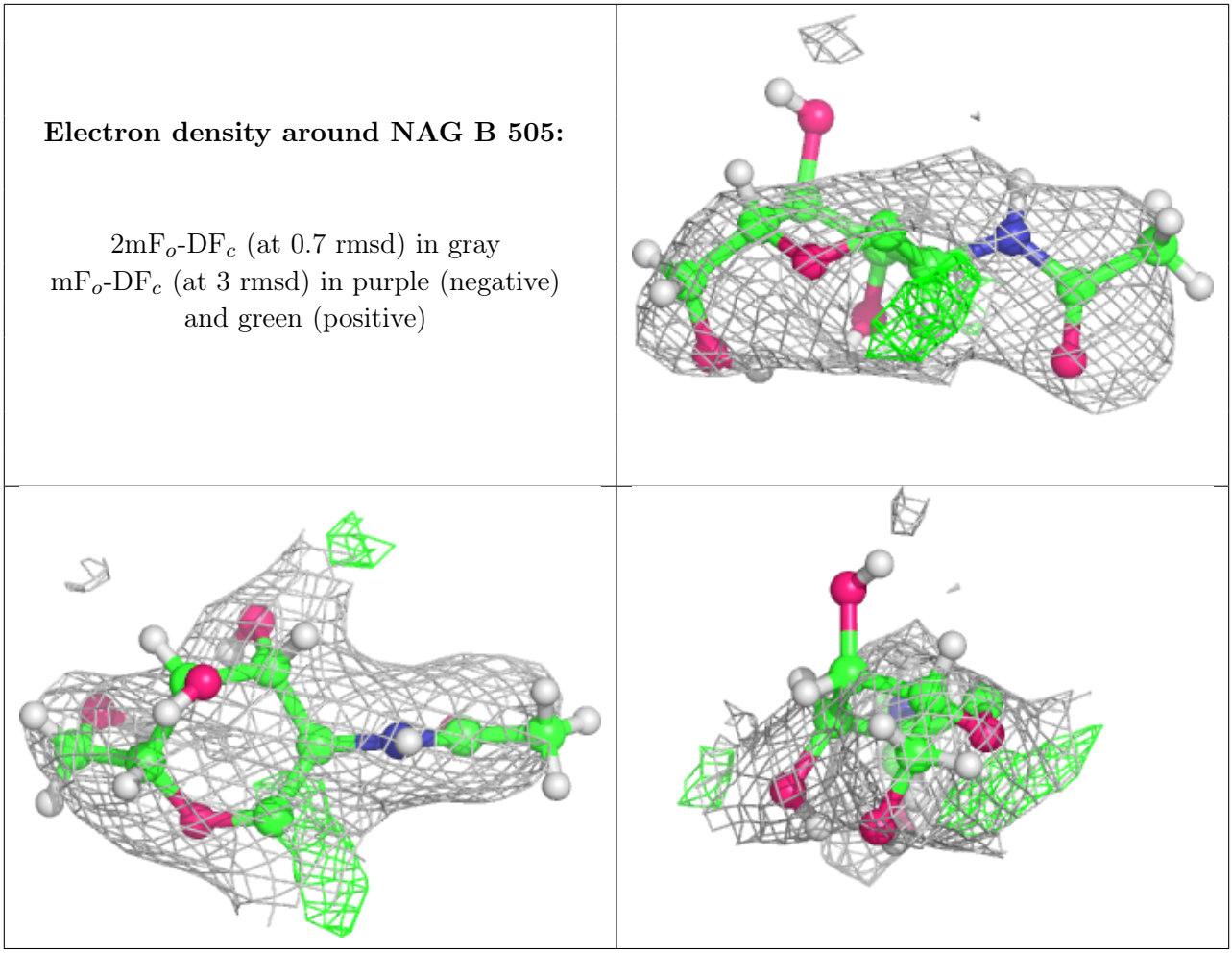






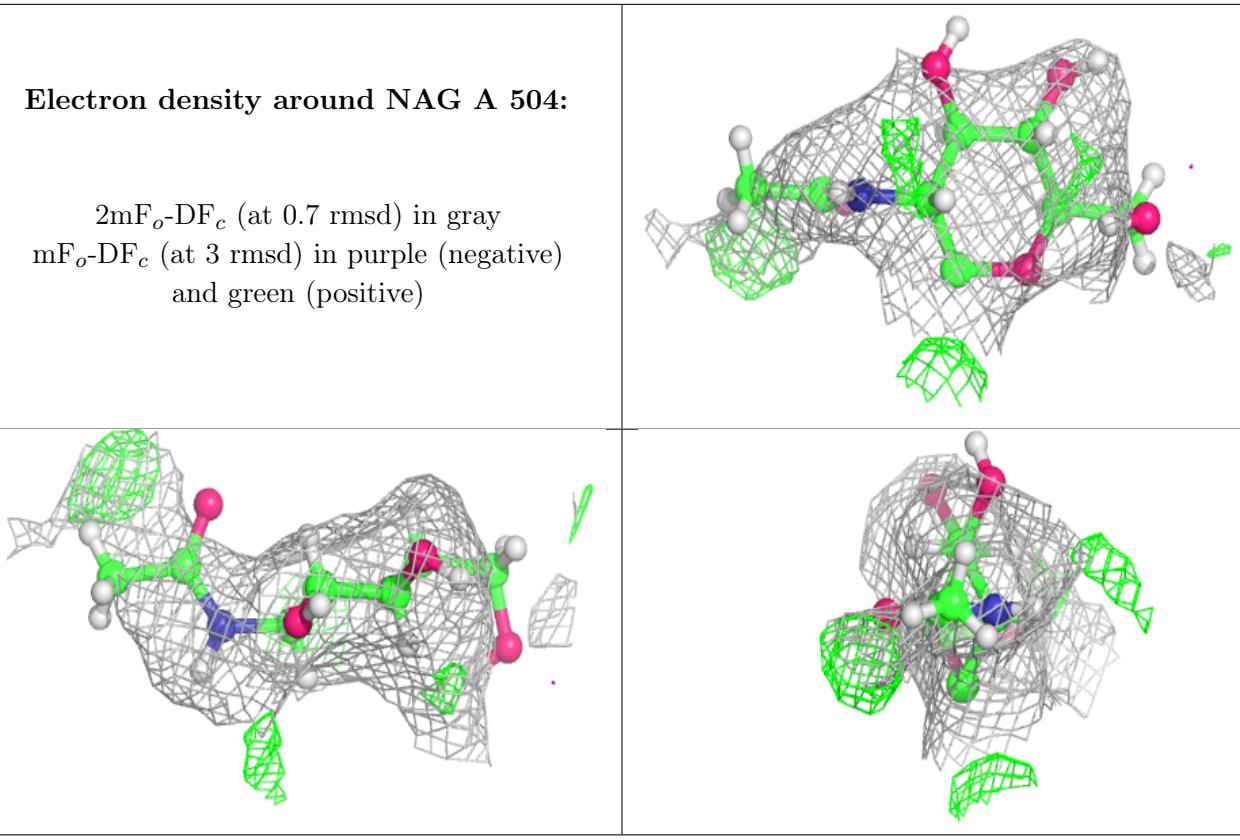
Electron density around NAG B 505:

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



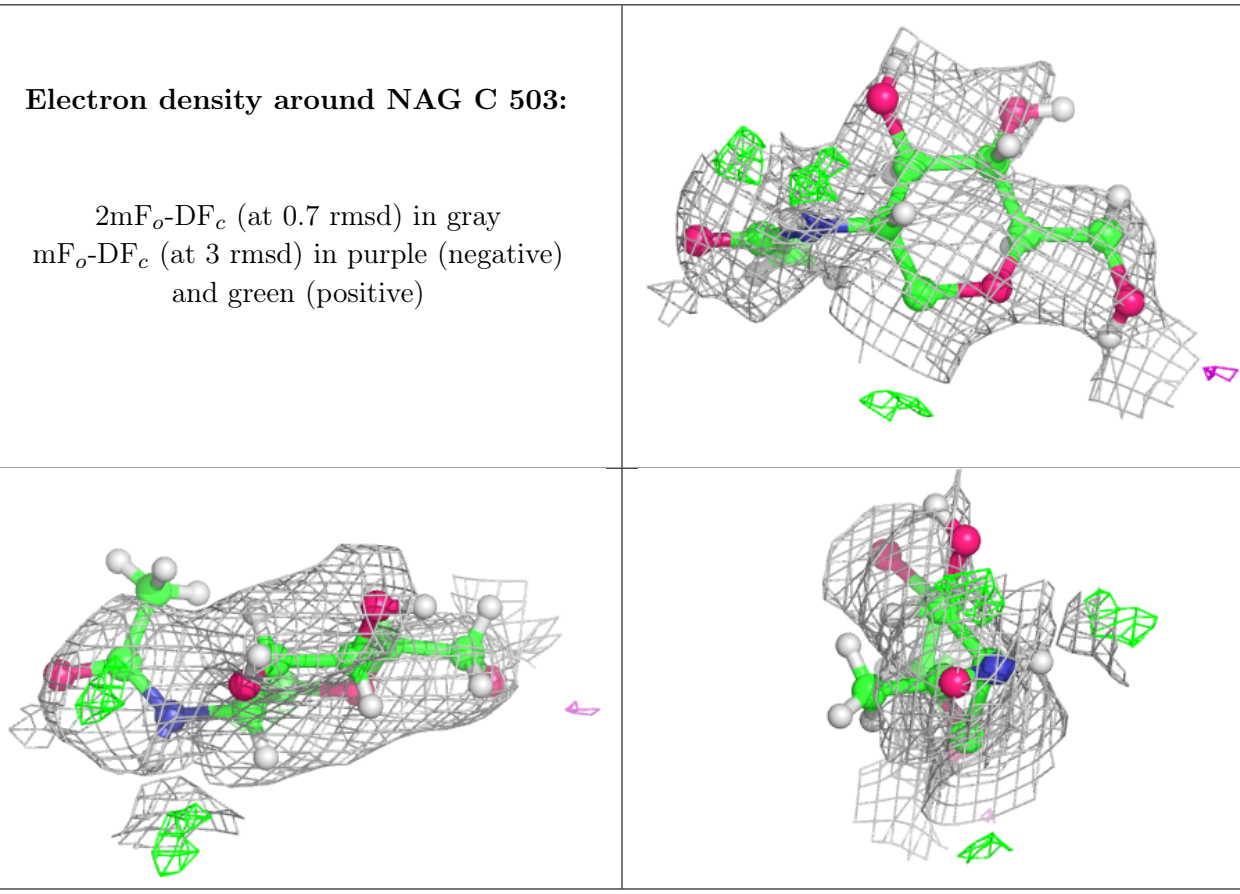
Electron density around NAG A 504:

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



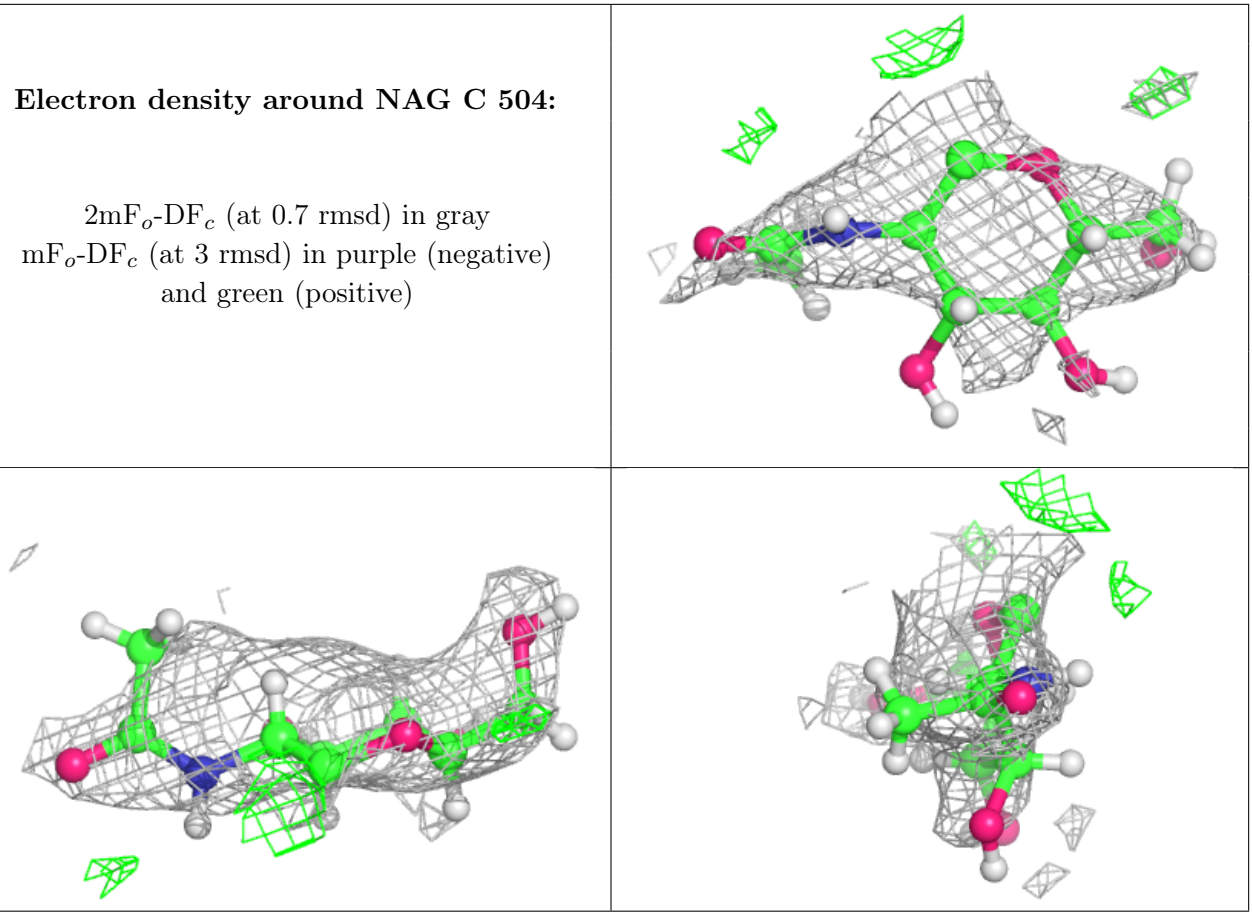
Electron density around NAG C 503:

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



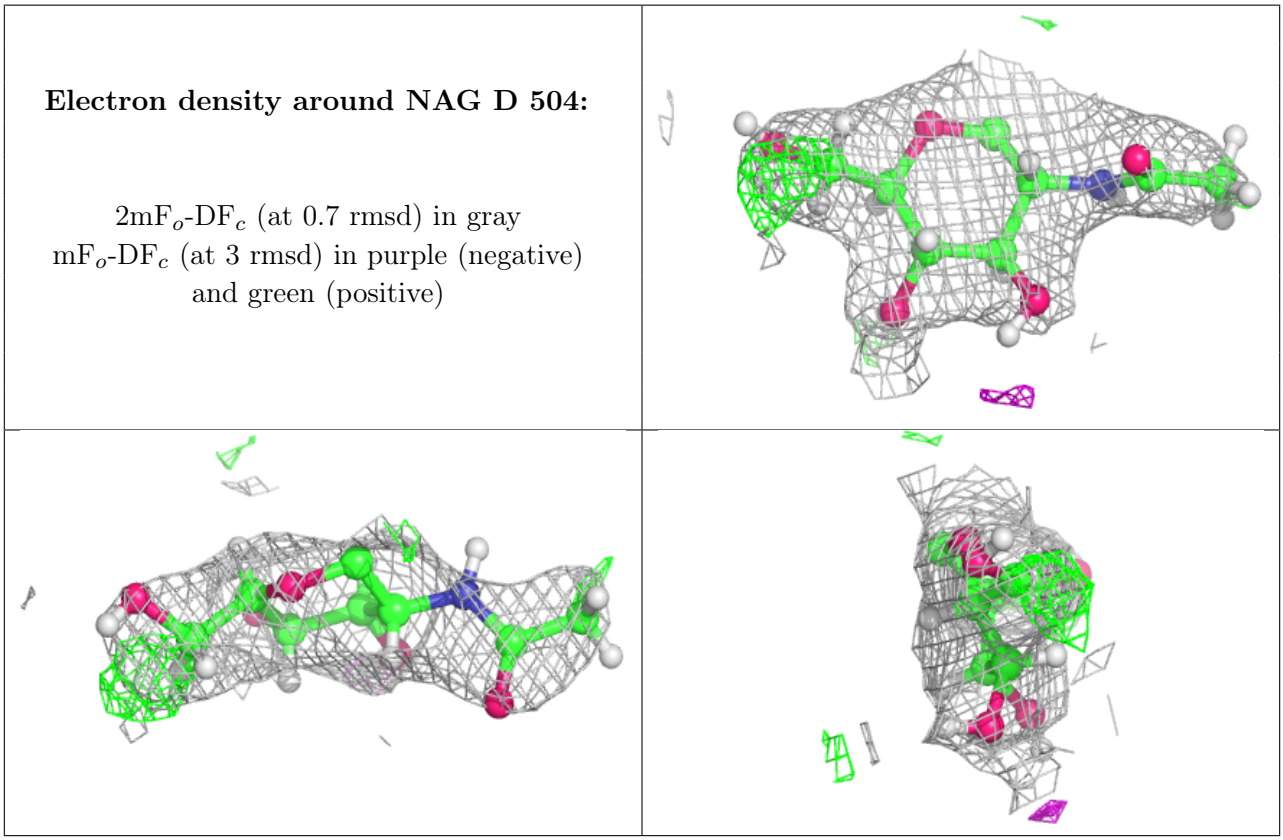
Electron density around NAG C 504:

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



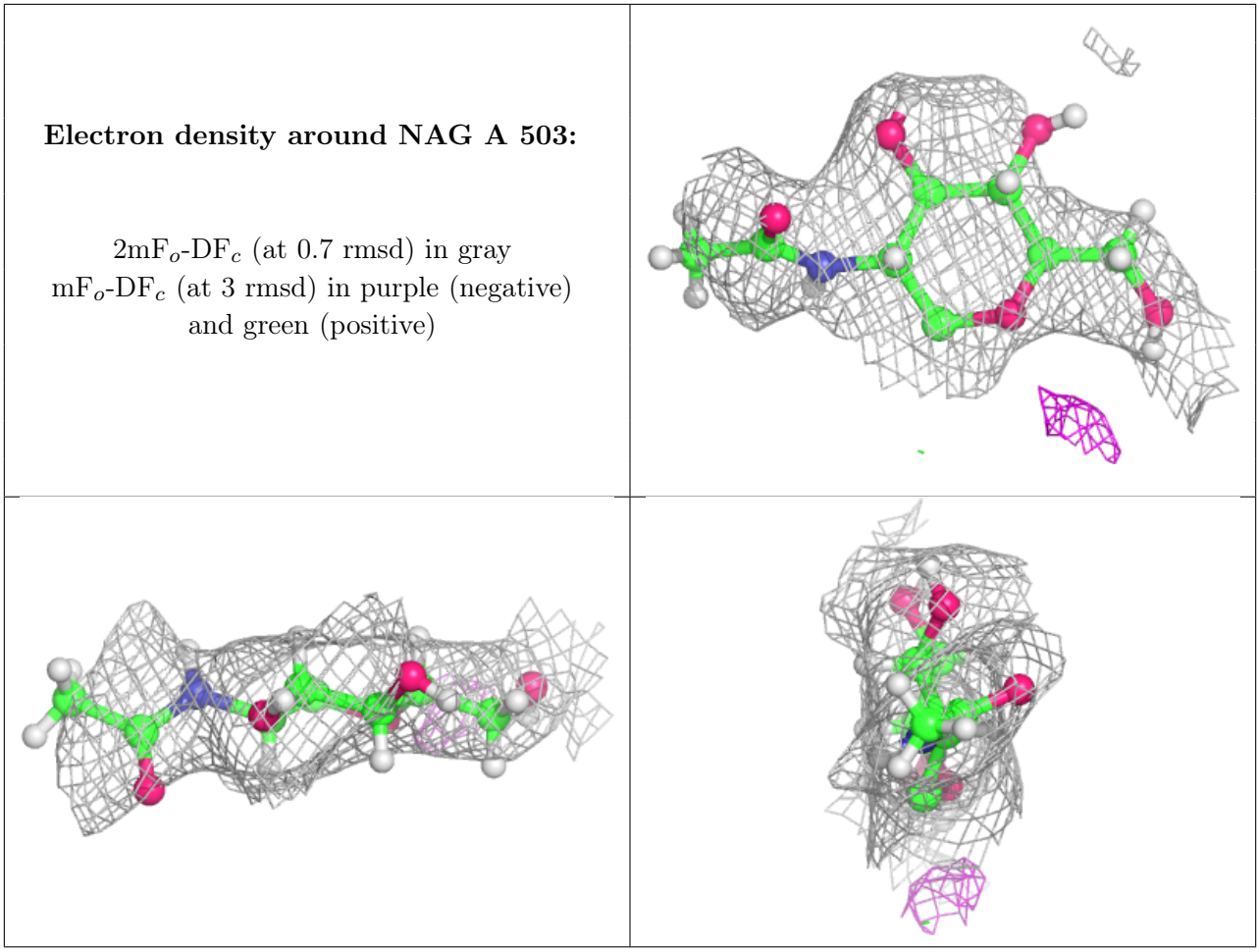
Electron density around NAG D 504:

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



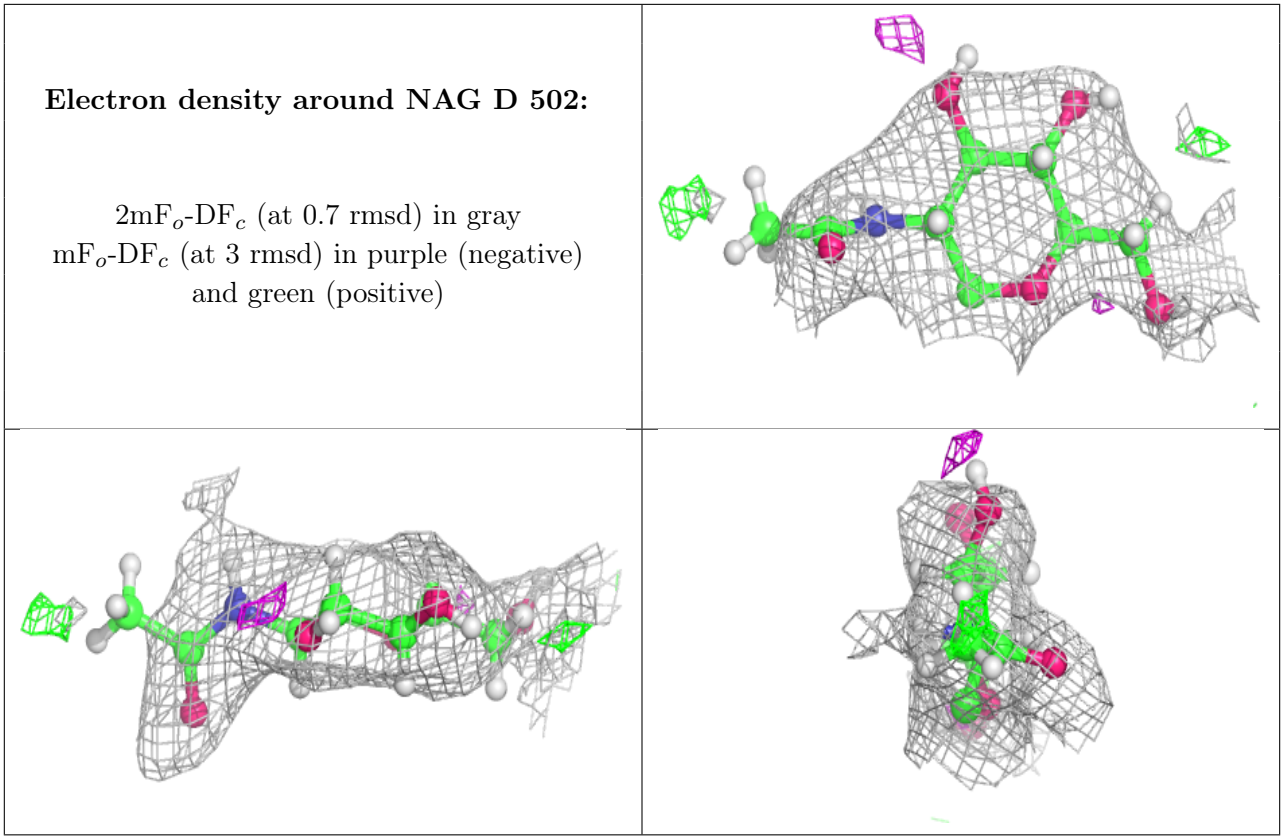
Electron density around NAG A 503:

$2mF_o$-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 D 502:

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



6.5 Other polymers (i)

There are no such residues in this entry.