Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 12:16 AM JST

PDB ID	:	8HFZ
EMDB ID	:	EMD-34729
Title	:	Cryo-EM structure of SARS-CoV-2 prototype spike protein in complex with white-tailed deer ACE2
Authors	:	Han, P.; Meng, Y.M.; Qi, J.X.
Deposited on	:	2022-11-13
Resolution	:	2.71 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

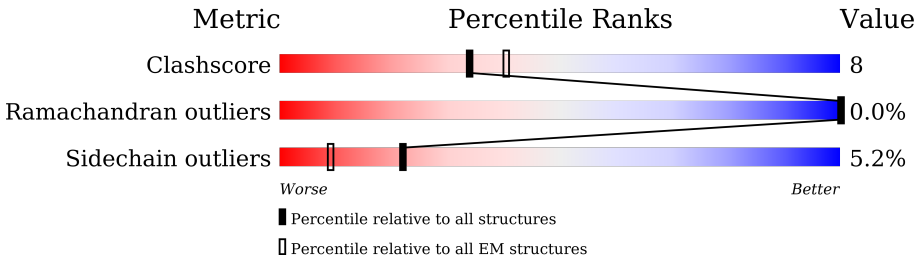
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.71 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	1217	71% 14% • 13%
1	B	1217	71% 15% • 13%
1	C	1217	70% 16% • 12%
2	E	661	59% 28% • 10%
3	D	2	100%
3	F	2	50% 50%
3	G	2	100%
3	H	2	100%
3	I	2	100%

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Mol	Chain	Length	Quality of chain
3	J	2	50% 50%
3	K	2	50% 50%
3	L	2	100%
3	M	2	100%
3	N	2	50% 50%
3	O	2	100%
3	P	2	100%
3	Q	2	100%
3	R	2	50% 50%
3	S	2	100%
3	T	2	50% 50%
3	U	2	50% 50%
3	V	2	50% 50%
3	W	2	50% 50%
3	X	2	50% 50%
3	Y	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30704 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0
			8290	5290	1383	1580	37		
1	B	1061	Total	C	N	O	S	0	0
			8292	5292	1383	1579	38		
1	C	1065	Total	C	N	O	S	0	0
			8322	5312	1388	1584	38		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	595	Total	C	N	O	S	0	0
			4889	3124	804	931	30		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		

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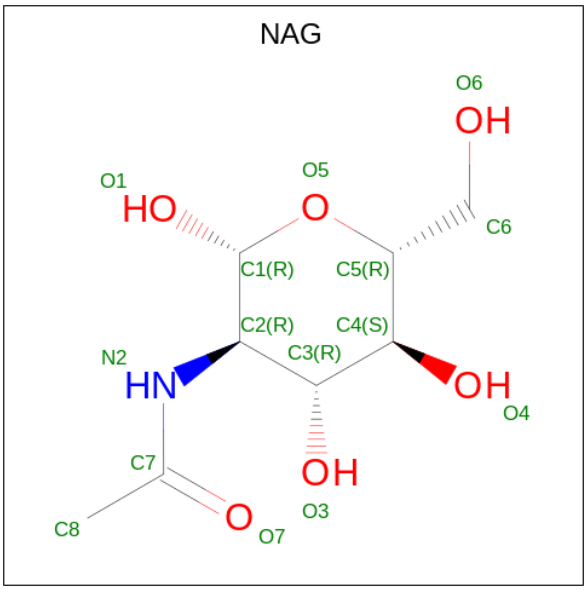
Mol	Chain	Residues	Atoms	AltConf	Trace
3	Q	2	Total C N O 28 16 2 10	0	0
3	R	2	Total C N O 28 16 2 10	0	0
3	S	2	Total C N O 28 16 2 10	0	0
3	T	2	Total C N O 28 16 2 10	0	0
3	U	2	Total C N O 28 16 2 10	0	0
3	V	2	Total C N O 28 16 2 10	0	0
3	W	2	Total C N O 28 16 2 10	0	0
3	X	2	Total C N O 28 16 2 10	0	0
3	Y	2	Total C N O 28 16 2 10	0	0

- Molecule 4 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	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

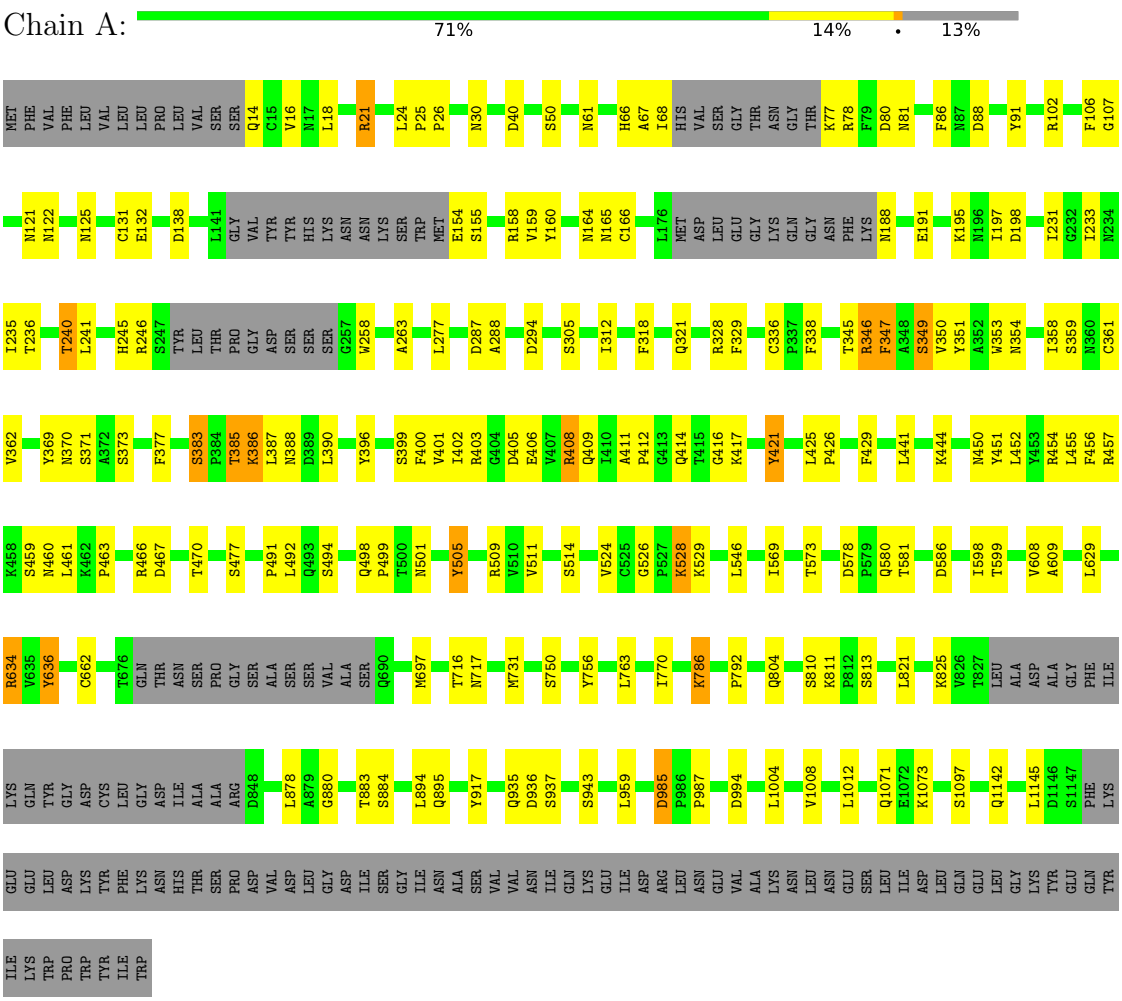
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	E	1	1	1	0

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. 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. 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.

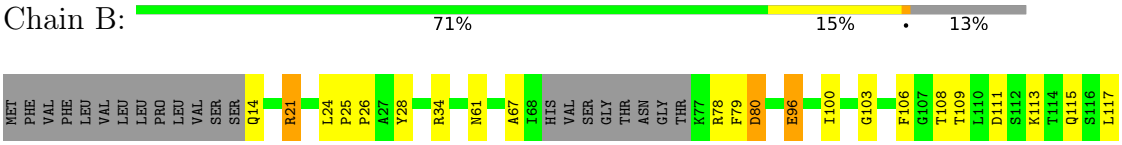
- Molecule 1: Spike glycoprotein

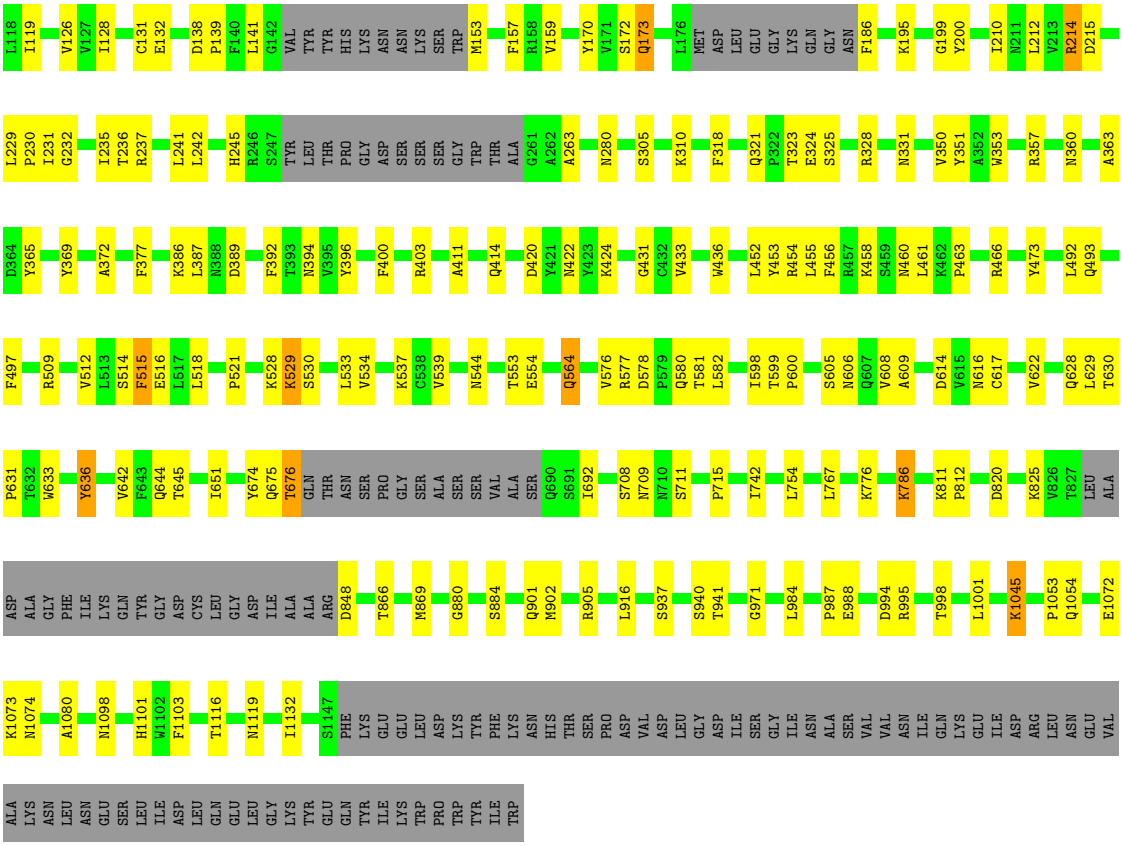
Chain A:



- Molecule 1: Spike glycoprotein

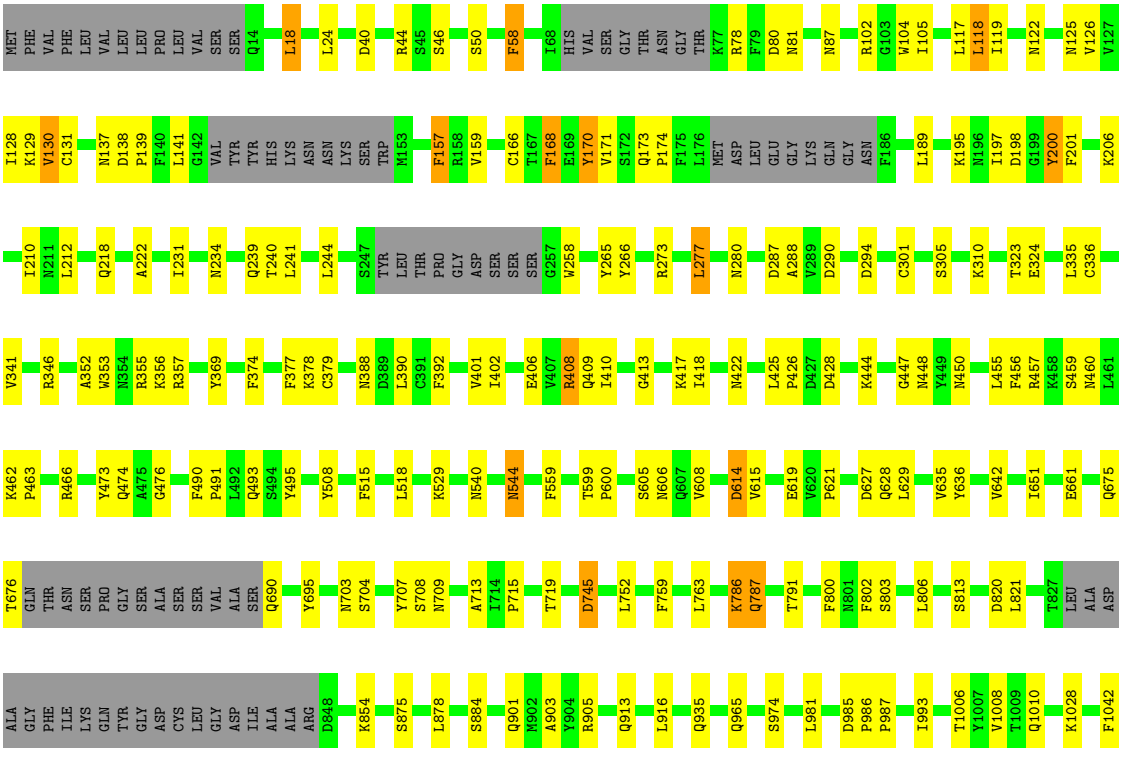
Chain B:

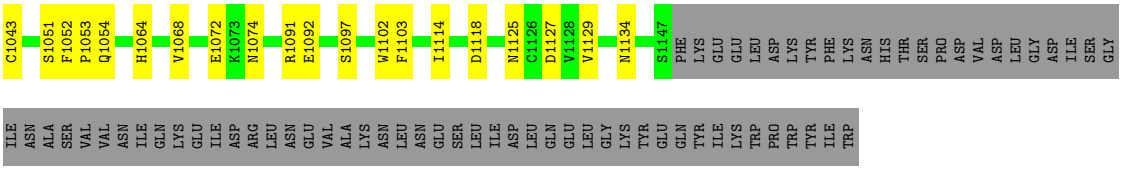




• Molecule 1: Spike glycoprotein

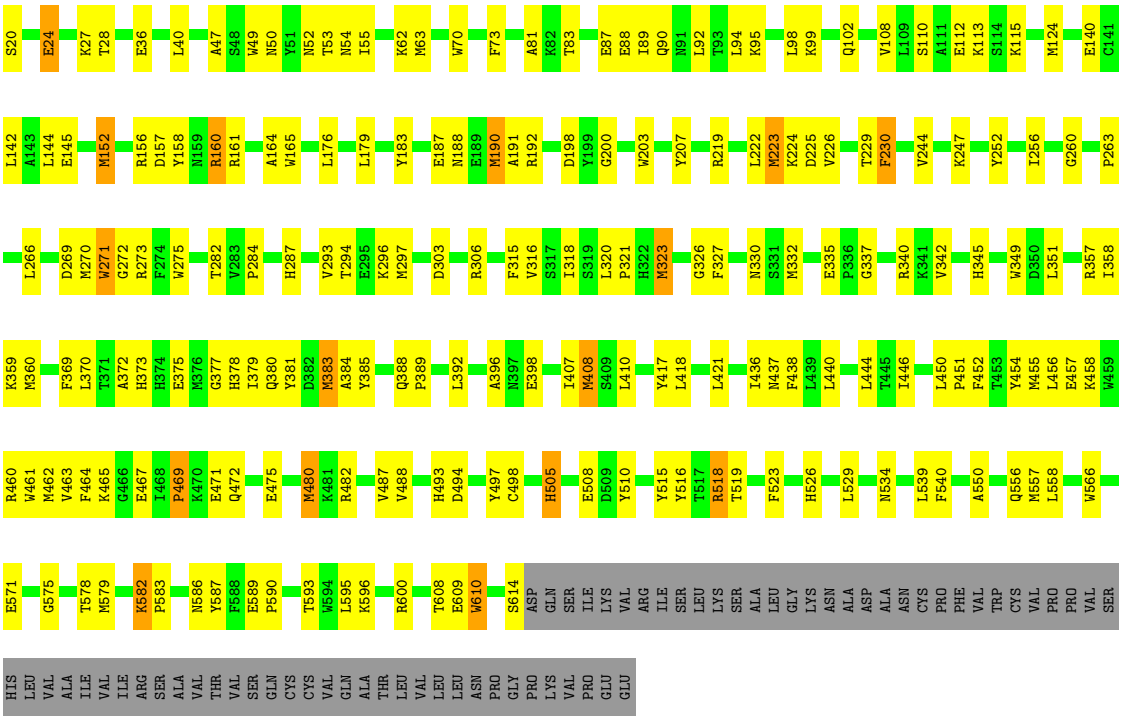
Chain C:





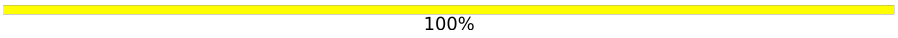
• Molecule 2: Angiotensin-converting enzyme

Chain E:



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

Chain D:



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

Chain F:

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

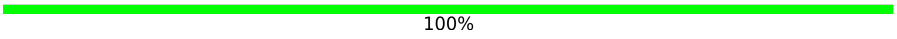
Chain G:

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

Chain H:

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

Chain I:



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

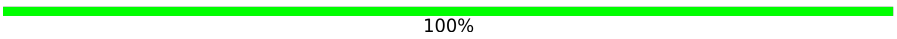
Chain J:

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

Chain K:

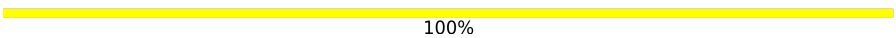
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain M:

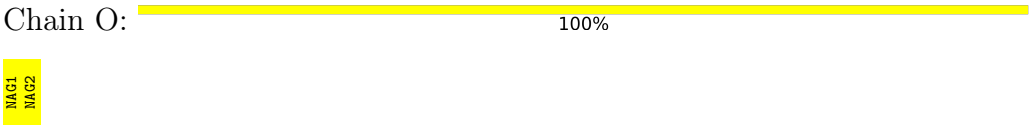


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

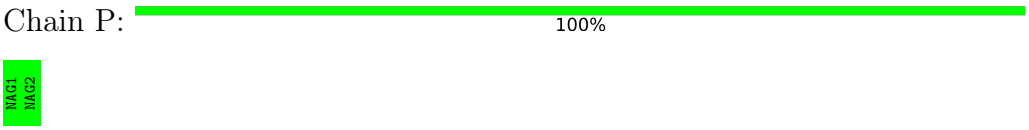
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



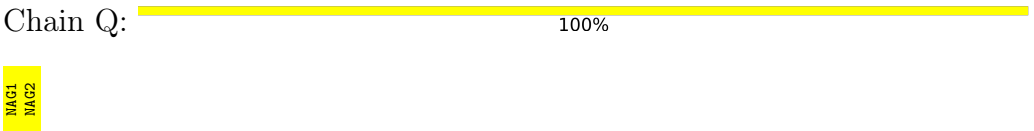
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



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

Chain Q:

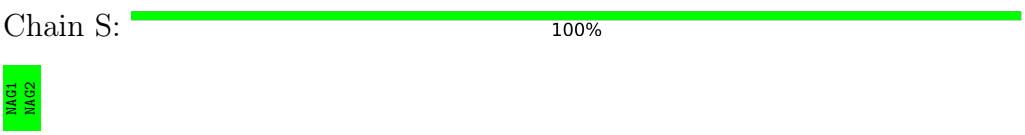


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

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

Chain S:



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

Chain T:

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

Chain U:

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

Chain V:

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

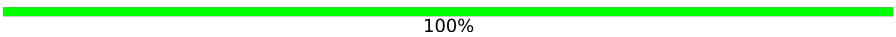
Chain W:

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

Chain X:

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

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123232	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.36	0/8483	0.53	0/11556
1	B	0.37	0/8484	0.54	1/11553 (0.0%)
1	C	0.35	0/8516	0.54	2/11598 (0.0%)
2	E	0.31	1/5024 (0.0%)	0.58	2/6812 (0.0%)
All	All	0.35	1/30507 (0.0%)	0.54	5/41519 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	469	PRO	CG-CD	-5.30	1.33	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	469	PRO	CA-N-CD	-13.12	93.14	111.50
2	E	469	PRO	N-CD-CG	-8.32	90.72	103.20
1	B	614	ASP	CB-CG-OD1	6.79	124.42	118.30
1	C	614	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	629	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8290	0	8083	114	0
1	B	8292	0	8089	118	0
1	C	8322	0	8118	125	0
2	E	4889	0	4657	122	0
3	D	28	0	25	1	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	2	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	1	0
3	O	28	0	25	1	0
3	P	28	0	25	0	0
3	Q	28	0	25	3	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	25	2	0
3	U	28	0	25	2	0
3	V	28	0	25	1	0
3	W	28	0	25	3	0
3	X	28	0	25	1	0
3	Y	28	0	25	0	0
4	A	56	0	52	0	0
4	B	126	0	117	2	0
4	C	98	0	91	6	0
4	E	42	0	39	5	0
5	E	1	0	0	0	0
All	All	30704	0	29771	482	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 8.

All (482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:THR:HG1	1:C:690:GLN:N	1.70	0.89
2:E:207:TYR:HB3	2:E:219:ARG:HD3	1.56	0.85
2:E:436:ILE:HG22	2:E:438:PHE:H	1.46	0.78
1:C:457:ARG:NH1	1:C:459:SER:OG	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ASN:HD21	1:B:454:ARG:H	1.35	0.74
2:E:342:VAL:HG21	2:E:359:LYS:HG2	1.71	0.72
2:E:27:LYS:HE3	2:E:98:LEU:HD11	1.71	0.72
1:C:676:THR:HG23	1:C:690:GLN:HG2	1.71	0.72
2:E:269:ASP:HB3	2:E:272:GLY:H	1.55	0.72
1:B:24:LEU:HD12	1:B:78:ARG:HE	1.54	0.71
1:A:426:PRO:HA	1:A:463:PRO:HB3	1.72	0.71
2:E:110:SER:HB3	2:E:113:LYS:HG3	1.70	0.70
1:C:1103:PHE:HZ	3:W:1:NAG:H61	1.56	0.70
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.09	0.70
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.72	0.70
1:A:634:ARG:NH1	1:A:636:TYR:O	2.25	0.69
1:C:125:ASN:HA	1:C:174:PRO:HD3	1.73	0.69
3:T:1:NAG:H61	3:T:2:NAG:HN2	1.57	0.69
1:C:40:ASP:OD2	1:C:44:ARG:NH2	2.23	0.68
1:C:417:LYS:HE2	1:C:455:LEU:HD23	1.75	0.68
1:C:105:ILE:HG23	1:C:241:LEU:HD11	1.74	0.68
1:C:189:LEU:HB2	1:C:210:ILE:HD11	1.74	0.68
1:B:321:GLN:H	1:B:628:GLN:HE22	1.41	0.68
2:E:372:ALA:HA	2:E:375:GLU:HB2	1.75	0.68
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.27	0.68
2:E:90:GLN:OE1	2:E:90:GLN:N	2.21	0.68
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.27	0.67
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.41	0.67
1:B:987:PRO:HD3	1:C:413:GLY:HA3	1.77	0.66
1:A:501:ASN:HB3	1:A:505:TYR:HB3	1.76	0.66
1:A:578:ASP:OD2	1:A:581:THR:N	2.28	0.66
1:C:117:LEU:HA	1:C:130:VAL:HA	1.78	0.65
1:A:452:LEU:HD21	1:A:492:LEU:HD12	1.78	0.65
1:B:1098:ASN:OD1	3:Q:1:NAG:N2	2.29	0.65
2:E:482:ARG:HD3	2:E:488:VAL:HG13	1.78	0.65
1:B:21:ARG:HE	1:B:21:ARG:H	1.44	0.65
1:C:356:LYS:NZ	1:C:357:ARG:O	2.30	0.65
1:A:155:SER:HB3	1:A:158:ARG:HB2	1.78	0.65
1:A:318:PHE:HA	1:A:629:LEU:HD22	1.78	0.64
2:E:505:HIS:HB3	2:E:510:TYR:HB3	1.79	0.64
1:C:1051:SER:HG	1:C:1064:HIS:HD1	1.46	0.64
2:E:335:GLU:HG3	2:E:337:GLY:H	1.62	0.64
1:B:323:THR:HB	1:B:539:VAL:HG12	1.79	0.64
1:B:436:TRP:HB3	1:B:509:ARG:HB2	1.79	0.63
1:C:605:SER:OG	1:C:606:ASN:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:703:NAG:H3	4:E:703:NAG:H83	1.79	0.63
1:A:454:ARG:NH1	1:A:467:ASP:OD2	2.33	0.62
1:C:206:LYS:NZ	1:C:222:ALA:O	2.31	0.62
2:E:494:ASP:H	2:E:497:TYR:HD2	1.47	0.62
1:A:336:CYS:N	1:A:361:CYS:SG	2.72	0.62
1:C:615:VAL:HG13	1:C:619:GLU:HG2	1.81	0.62
1:B:521:PRO:HG3	1:B:564:GLN:HG3	1.80	0.62
1:B:394:ASN:ND2	1:C:200:TYR:OH	2.32	0.62
1:C:745:ASP:OD1	1:C:745:ASP:N	2.22	0.62
1:A:236:THR:HG22	3:D:1:NAG:HN2	1.63	0.62
1:A:386:LYS:HD2	1:A:390:LEU:HD22	1.80	0.62
2:E:24:GLU:O	2:E:28:THR:OG1	2.16	0.61
1:A:498:GLN:OE1	1:A:501:ASN:ND2	2.26	0.61
1:B:577:ARG:HD3	1:B:582:LEU:HD12	1.82	0.61
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.81	0.61
2:E:407:ILE:HG23	2:E:526:HIS:HA	1.83	0.61
2:E:244:VAL:HG22	2:E:440:LEU:HD21	1.82	0.61
2:E:282:THR:O	2:E:437:ASN:ND2	2.34	0.61
1:C:409:GLN:HE22	1:C:417:LYS:H	1.48	0.60
2:E:95:LYS:HA	2:E:98:LEU:HD12	1.82	0.60
1:C:635:VAL:HG23	1:C:636:TYR:HD2	1.65	0.60
2:E:571:GLU:HA	2:E:575:GLY:HA2	1.83	0.60
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.84	0.60
1:C:418:ILE:HG22	1:C:422:ASN:HD22	1.65	0.60
1:B:96:GLU:OE1	1:B:100:ILE:N	2.33	0.59
1:A:122:ASN:OD1	1:A:125:ASN:N	2.36	0.59
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.85	0.59
1:C:1134:ASN:OD1	3:X:1:NAG:N2	2.35	0.59
1:A:1142:GLN:HE22	1:A:1145:LEU:HD13	1.68	0.59
3:H:2:NAG:H3	3:H:2:NAG:H83	1.85	0.59
1:C:703:ASN:OD1	1:C:704:SER:N	2.36	0.58
1:B:674:TYR:HD1	1:B:692:ILE:HG12	1.68	0.58
1:C:1125:ASN:ND2	1:C:1127:ASP:OD1	2.36	0.58
1:B:389:ASP:OD1	1:B:389:ASP:N	2.36	0.58
3:W:1:NAG:H83	3:W:1:NAG:H3	1.85	0.58
1:C:1092:GLU:N	1:C:1092:GLU:OE1	2.36	0.58
2:E:27:LYS:HD2	2:E:94:LEU:HD23	1.86	0.58
1:C:139:PRO:HB3	1:C:159:VAL:HG12	1.84	0.57
2:E:188:ASN:HD21	2:E:464:PHE:HB3	1.69	0.57
2:E:358:ILE:HD11	2:E:379:ILE:HG21	1.86	0.57
1:A:86:PHE:N	1:A:236:THR:O	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:471:GLU:OE1	2:E:471:GLU:N	2.35	0.57
2:E:81:ALA:O	2:E:102:GLN:NE2	2.31	0.57
1:A:546:LEU:HD21	1:A:573:THR:HG21	1.87	0.57
1:B:424:LYS:HG2	1:B:463:PRO:HG3	1.86	0.57
1:A:353:TRP:O	1:A:466:ARG:NH2	2.36	0.57
2:E:383:MET:CE	2:E:383:MET:H	2.18	0.57
3:H:1:NAG:H83	3:H:1:NAG:H3	1.87	0.57
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.87	0.57
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.87	0.57
1:B:642:VAL:HG22	1:B:651:ILE:HG12	1.87	0.57
1:C:323:THR:OG1	1:C:324:GLU:OE1	2.22	0.57
1:C:1127:ASP:OD1	1:C:1127:ASP:N	2.36	0.57
1:A:529:LYS:HE3	1:A:529:LYS:HA	1.87	0.56
1:A:461:LEU:HD21	1:A:467:ASP:HB2	1.87	0.56
1:A:154:GLU:HA	1:A:245:HIS:HA	1.86	0.56
1:C:118:LEU:N	1:C:129:LYS:O	2.25	0.56
1:B:866:THR:H	1:B:869:MET:HE2	1.70	0.56
1:C:141:LEU:HD23	1:C:157:PHE:HA	1.86	0.56
1:A:477:SER:HG	2:E:20:SER:N	2.02	0.56
1:B:403:ARG:HD3	1:B:497:PHE:HE1	1.71	0.56
1:A:294:ASP:OD1	1:A:294:ASP:N	2.38	0.56
2:E:87:GLU:O	2:E:88:GLU:HG3	2.06	0.56
1:B:372:ALA:HB3	1:B:436:TRP:HH2	1.71	0.55
2:E:515:TYR:HA	2:E:518:ARG:HG2	1.87	0.55
1:C:81:ASN:O	1:C:239:GLN:NE2	2.40	0.55
2:E:388:GLN:HB3	2:E:392:LEU:HB2	1.86	0.55
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.70	0.55
1:A:132:GLU:HB2	1:A:164:ASN:HB2	1.89	0.55
1:B:80:ASP:N	1:B:80:ASP:OD1	2.39	0.55
1:C:125:ASN:HD21	4:C:1303:NAG:H62	1.70	0.55
1:B:138:ASP:OD1	1:B:138:ASP:N	2.39	0.55
1:A:361:CYS:SG	1:A:362:VAL:N	2.80	0.55
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.88	0.55
1:A:354:ASN:OD1	1:A:354:ASN:N	2.40	0.54
1:C:168:PHE:CE2	1:C:170:TYR:HB2	2.42	0.54
2:E:87:GLU:O	2:E:89:ILE:HG12	2.08	0.54
2:E:582:LYS:H	2:E:582:LYS:HD3	1.72	0.54
1:A:16:VAL:O	1:A:18:LEU:HD12	2.07	0.54
1:C:277:LEU:HD12	1:C:277:LEU:H	1.71	0.54
1:A:491:PRO:HG2	1:A:492:LEU:HD22	1.90	0.54
1:B:323:THR:HG22	1:B:324:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:VAL:HA	1:B:636:TYR:HE2	1.73	0.54
1:C:195:LYS:HG2	1:C:197:ILE:HG13	1.90	0.54
1:C:448:ASN:HD22	1:C:450:ASN:HD22	1.55	0.54
1:C:1103:PHE:CZ	3:W:1:NAG:H61	2.41	0.54
1:B:67:ALA:HB3	1:B:263:ALA:HB3	1.91	0.54
1:C:802:PHE:N	3:U:1:NAG:O7	2.41	0.54
2:E:260:GLY:HA2	2:E:610:TRP:CH2	2.43	0.54
1:A:716:THR:HG21	1:A:1073:LYS:HE2	1.90	0.53
2:E:145:GLU:N	2:E:145:GLU:OE1	2.40	0.53
1:C:138:ASP:N	1:C:138:ASP:OD1	2.40	0.53
2:E:200:GLY:HA2	2:E:203:TRP:CE3	2.44	0.53
1:B:516:GLU:HG2	1:B:518:LEU:HG	1.90	0.53
1:B:984:LEU:HD11	1:B:988:GLU:OE1	2.08	0.53
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.89	0.53
2:E:384:ALA:HB1	2:E:558:LEU:HB3	1.91	0.53
1:B:529:LYS:HG2	1:B:530:SER:N	2.24	0.53
1:A:67:ALA:HB3	1:A:263:ALA:HB3	1.90	0.53
1:A:406:GLU:N	1:A:406:GLU:OE1	2.41	0.53
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.90	0.53
2:E:142:LEU:HD21	2:E:164:ALA:HA	1.89	0.53
1:B:199:GLY:HA2	1:B:232:GLY:HA2	1.91	0.52
1:B:742:ILE:HD11	1:B:1001:LEU:HD13	1.89	0.52
1:B:1073:LYS:HG2	1:B:1074:ASN:H	1.74	0.52
1:B:811:LYS:NZ	1:B:812:PRO:O	2.28	0.52
1:B:599:THR:HB	1:B:608:VAL:HG12	1.90	0.52
1:C:903:ALA:HB1	1:C:913:GLN:HG2	1.92	0.52
1:B:848:ASP:OD1	1:B:848:ASP:N	2.42	0.52
1:C:402:ILE:HG23	1:C:406:GLU:HG2	1.91	0.52
2:E:389:PRO:HD2	2:E:392:LEU:HD12	1.92	0.52
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.28	0.51
1:C:378:LYS:HZ3	1:C:379:CYS:C	2.13	0.51
2:E:593:THR:HA	2:E:596:LYS:HE2	1.92	0.51
1:B:386:LYS:NZ	1:C:981:LEU:O	2.43	0.51
2:E:87:GLU:OE1	2:E:87:GLU:N	2.40	0.51
1:A:526:GLY:O	1:A:528:LYS:NZ	2.37	0.51
1:B:328:ARG:HH11	1:B:533:LEU:HB2	1.75	0.51
1:C:802:PHE:H	3:U:1:NAG:H81	1.75	0.51
2:E:396:ALA:HB1	2:E:566:TRP:HB3	1.93	0.51
1:B:880:GLY:O	1:B:884:SER:OG	2.24	0.51
1:C:80:ASP:O	1:C:265:TYR:OH	2.17	0.51
2:E:92:LEU:HD12	2:E:95:LYS:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:1:NAG:H61	3:T:2:NAG:N2	2.26	0.51
1:A:383:SER:OG	1:A:385:THR:O	2.28	0.51
2:E:326:GLY:O	2:E:330:ASN:ND2	2.44	0.51
1:B:786:LYS:H	1:B:786:LYS:HD3	1.76	0.50
2:E:303:ASP:OD1	2:E:303:ASP:N	2.44	0.50
1:C:128:ILE:O	1:C:129:LYS:HD2	2.11	0.50
1:C:456:PHE:HD2	1:C:491:PRO:HA	1.74	0.50
1:A:21:ARG:NH2	1:A:81:ASN:OD1	2.44	0.50
1:A:345:THR:O	1:A:509:ARG:NH2	2.40	0.50
2:E:608:THR:HG22	2:E:609:GLU:HG2	1.94	0.50
2:E:271:TRP:HD1	2:E:273:ARG:HH11	1.59	0.50
1:A:408:ARG:HH21	1:A:414:GLN:HE22	1.59	0.50
1:B:245:HIS:H	1:B:245:HIS:CD2	2.30	0.50
1:C:173:GLN:OE1	1:C:174:PRO:HD2	2.12	0.50
1:C:786:LYS:HG2	1:C:787:GLN:HG2	1.93	0.50
2:E:226:VAL:HG13	2:E:454:TYR:CE1	2.47	0.50
1:B:1103:PHE:HZ	3:Q:1:NAG:H61	1.77	0.50
1:B:108:THR:HG22	1:B:236:THR:HG23	1.94	0.50
4:C:1307:NAG:H5	4:C:1307:NAG:HN2	1.75	0.50
1:B:436:TRP:N	1:B:509:ARG:O	2.37	0.50
1:B:994:ASP:O	1:B:998:THR:OG1	2.24	0.50
1:C:104:TRP:N	1:C:119:ILE:O	2.39	0.50
1:C:474:GLN:NE2	1:C:476:GLY:O	2.44	0.50
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.35	0.50
2:E:190:MET:SD	2:E:191:ALA:N	2.85	0.50
1:A:102:ARG:HE	1:A:121:ASN:HD22	1.58	0.49
1:A:336:CYS:HB2	1:A:338:PHE:CE2	2.47	0.49
1:A:287:ASP:OD1	1:A:288:ALA:N	2.45	0.49
2:E:315:PHE:HZ	2:E:373:HIS:HA	1.78	0.49
2:E:378:HIS:HD2	2:E:378:HIS:O	1.95	0.49
1:A:470:THR:HG21	1:A:492:LEU:HD11	1.94	0.49
1:B:186:PHE:HB3	1:B:212:LEU:HD11	1.94	0.49
1:C:752:LEU:HD11	1:C:993:ILE:HD11	1.95	0.49
1:A:350:VAL:HG13	1:A:402:ILE:HD11	1.95	0.49
1:B:629:LEU:H	1:B:629:LEU:HD23	1.77	0.49
1:B:21:ARG:H	1:B:21:ARG:NE	2.08	0.49
1:B:605:SER:OG	1:B:606:ASN:N	2.46	0.49
1:C:24:LEU:HD22	1:C:78:ARG:HD2	1.93	0.49
2:E:156:ARG:HB3	2:E:252:TYR:HE2	1.78	0.49
2:E:369:PHE:HZ	2:E:417:TYR:HH	1.61	0.49
2:E:540:PHE:HE1	2:E:590:PRO:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:SER:OG	1:A:811:LYS:NZ	2.41	0.49
2:E:480:MET:SD	2:E:480:MET:N	2.67	0.49
1:A:66:HIS:O	1:A:80:ASP:HB2	2.13	0.49
1:B:111:ASP:OD1	1:B:113:LYS:HG2	2.13	0.49
1:B:331:ASN:HB3	1:B:580:GLN:HG2	1.95	0.48
1:C:128:ILE:O	1:C:128:ILE:HD12	2.12	0.48
2:E:263:PRO:HA	2:E:487:VAL:HG13	1.95	0.48
2:E:315:PHE:CZ	2:E:377:GLY:HA3	2.48	0.48
1:C:18:LEU:HA	1:C:137:ASN:HD21	1.79	0.48
2:E:475:GLU:CD	2:E:475:GLU:H	2.17	0.48
1:A:188:ASN:OD1	1:A:188:ASN:N	2.46	0.48
1:B:578:ASP:HB3	1:B:581:THR:O	2.13	0.48
1:B:622:VAL:HA	1:B:636:TYR:CE2	2.47	0.48
1:B:141:LEU:HD22	1:B:157:PHE:HA	1.95	0.48
1:B:357:ARG:CZ	1:B:357:ARG:HA	2.43	0.48
1:B:357:ARG:HA	1:B:357:ARG:NH1	2.29	0.48
1:C:406:GLU:HG3	1:C:418:ILE:HG12	1.96	0.48
1:B:411:ALA:HB3	1:B:414:GLN:HB3	1.95	0.48
1:C:821:LEU:HD22	1:C:935:GLN:HG3	1.96	0.48
2:E:157:ASP:OD1	2:E:157:ASP:N	2.47	0.48
1:B:754:LEU:HD23	1:B:754:LEU:H	1.78	0.48
1:A:195:LYS:HG2	1:A:197:ILE:HD13	1.95	0.48
1:A:786:LYS:CD	1:A:786:LYS:H	2.26	0.48
2:E:460:ARG:HA	2:E:463:VAL:HG12	1.96	0.48
1:A:936:ASP:N	1:A:936:ASP:OD1	2.47	0.48
1:C:719:THR:N	1:C:1068:VAL:O	2.42	0.48
1:A:346:ARG:HA	1:A:346:ARG:NH1	2.29	0.47
1:C:1074:ASN:OD1	3:V:1:NAG:N2	2.47	0.47
2:E:161:ARG:HA	2:E:266:LEU:HD21	1.96	0.47
2:E:192:ARG:NH2	2:E:465:LYS:O	2.47	0.47
1:B:103:GLY:H	1:B:241:LEU:HB2	1.80	0.47
1:C:125:ASN:HD22	1:C:171:VAL:HG22	1.78	0.47
1:C:210:ILE:HG22	1:C:212:LEU:H	1.80	0.47
2:E:383:MET:H	2:E:383:MET:HE3	1.79	0.47
1:A:359:SER:HA	1:A:524:VAL:HG12	1.95	0.47
1:C:122:ASN:OD1	4:C:1303:NAG:N2	2.47	0.47
1:C:294:ASP:OD1	1:C:294:ASP:N	2.48	0.47
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.61	0.47
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.97	0.47
1:B:28:TYR:HB3	1:B:61:ASN:OD1	2.14	0.47
1:B:436:TRP:HA	1:B:436:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:ARG:NH1	1:C:409:GLN:HG2	2.29	0.47
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.96	0.47
1:B:452:LEU:HD13	1:B:492:LEU:HB3	1.96	0.47
1:B:629:LEU:HG	1:B:631:PRO:HG3	1.95	0.47
1:A:763:LEU:HD22	1:A:1008:VAL:HG21	1.96	0.47
1:C:675:GLN:O	1:C:690:GLN:N	2.47	0.47
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.97	0.47
2:E:36:GLU:HB3	2:E:73:PHE:HE2	1.79	0.47
1:B:200:TYR:CZ	1:B:230:PRO:HB3	2.49	0.47
1:B:458:LYS:HA	1:B:473:TYR:CD1	2.49	0.47
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.96	0.46
1:C:417:LYS:O	1:C:417:LYS:NZ	2.46	0.46
2:E:144:LEU:HD22	2:E:144:LEU:H	1.79	0.46
1:A:444:LYS:C	1:A:499:PRO:HD3	2.36	0.46
1:C:986:PRO:N	1:C:987:PRO:HD2	2.30	0.46
2:E:293:VAL:O	2:E:418:LEU:HD22	2.15	0.46
1:A:985:ASP:OD2	1:A:987:PRO:HD2	2.14	0.46
1:B:172:SER:OG	1:B:173:GLN:N	2.48	0.46
1:C:661:GLU:O	1:C:695:TYR:OH	2.21	0.46
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.97	0.46
2:E:40:LEU:HD13	2:E:70:TRP:HA	1.96	0.46
1:A:599:THR:HB	1:A:608:VAL:HG12	1.98	0.46
1:B:420:ASP:O	1:B:461:LEU:N	2.44	0.46
1:A:138:ASP:N	1:A:138:ASP:OD1	2.47	0.46
2:E:27:LYS:HE2	4:E:703:NAG:O3	2.16	0.46
1:B:353:TRP:HB2	1:B:466:ARG:HH21	1.80	0.46
1:C:131:CYS:HB3	1:C:166:CYS:HA	1.96	0.46
2:E:94:LEU:HB2	4:E:703:NAG:H4	1.97	0.46
1:B:363:ALA:HB1	1:B:365:TYR:CE2	2.51	0.46
1:B:1101:HIS:ND1	3:Q:1:NAG:H5	2.31	0.46
1:C:218:GLN:OE1	1:C:218:GLN:HA	2.16	0.46
2:E:176:LEU:HB3	2:E:498:CYS:SG	2.56	0.46
1:A:401:VAL:O	1:A:402:ILE:HD13	2.15	0.46
1:A:457:ARG:NE	1:A:459:SER:O	2.48	0.46
1:A:569:ILE:HD12	1:A:569:ILE:H	1.81	0.46
1:B:453:TYR:HE1	1:B:493:GLN:HB2	1.80	0.46
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.97	0.45
1:B:529:LYS:HG2	1:B:530:SER:H	1.81	0.45
1:C:125:ASN:ND2	1:C:171:VAL:HG22	2.31	0.45
2:E:321:PRO:O	2:E:380:GLN:HG2	2.16	0.45
2:E:452:PHE:CE2	2:E:456:LEU:HD22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.99	0.45
1:A:30:ASN:HA	1:A:61:ASN:HA	1.98	0.45
1:A:102:ARG:NE	1:A:121:ASN:HD22	2.14	0.45
1:C:614:ASP:O	1:C:614:ASP:OD2	2.34	0.45
1:C:456:PHE:HB3	1:C:473:TYR:CD2	2.52	0.45
1:C:854:LYS:HB2	1:C:854:LYS:HE3	1.81	0.45
1:B:420:ASP:HB3	1:B:460:ASN:HB3	1.99	0.45
1:A:450:ASN:N	1:A:450:ASN:OD1	2.50	0.45
1:B:108:THR:O	1:B:237:ARG:NH1	2.50	0.45
1:C:444:LYS:HG3	1:C:447:GLY:H	1.82	0.45
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.52	0.45
2:E:36:GLU:HB3	2:E:73:PHE:CE2	2.51	0.45
1:A:336:CYS:HB2	1:A:338:PHE:CZ	2.51	0.45
1:B:21:ARG:HB3	1:B:79:PHE:CE1	2.51	0.45
1:C:280:ASN:ND2	4:C:1305:NAG:H82	2.32	0.45
2:E:47:ALA:HB1	2:E:50:ASN:HB2	1.98	0.45
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.99	0.44
1:A:329:PHE:O	1:A:580:GLN:NE2	2.50	0.44
1:B:1080:ALA:O	1:B:1132:ILE:HG13	2.17	0.44
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.99	0.44
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.16	0.44
2:E:222:LEU:HB3	2:E:223:MET:HE1	1.99	0.44
2:E:49:TRP:HE1	4:E:701:NAG:C8	2.30	0.44
2:E:225:ASP:OD1	2:E:225:ASP:N	2.51	0.44
2:E:586:ASN:HA	2:E:589:GLU:HG2	1.98	0.44
1:A:457:ARG:HH21	1:A:460:ASN:HA	1.81	0.44
1:B:528:LYS:HB2	1:B:528:LYS:HE3	1.53	0.44
1:B:786:LYS:H	1:B:786:LYS:CD	2.30	0.44
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.99	0.44
1:A:821:LEU:HD13	1:A:935:GLN:HE21	1.82	0.44
2:E:140:GLU:OE1	2:E:160:ARG:HB2	2.17	0.44
2:E:508:GLU:N	2:E:508:GLU:OE1	2.50	0.44
2:E:589:GLU:HB2	2:E:590:PRO:HD3	2.00	0.44
1:B:1119:ASN:OD1	1:B:1119:ASN:N	2.47	0.44
1:A:403:ARG:HE	1:A:505:TYR:HA	1.82	0.44
1:A:429:PHE:HE1	1:A:514:SER:HA	1.83	0.44
1:B:351:TYR:HA	1:B:454:ARG:NH2	2.33	0.44
1:C:708:SER:OG	1:C:709:ASN:N	2.50	0.44
2:E:53:THR:OG1	4:E:701:NAG:H2	2.18	0.44
2:E:316:VAL:HA	2:E:320:LEU:H	1.83	0.44
2:E:458:LYS:HG2	2:E:461:TRP:CZ3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LYS:O	1:A:421:TYR:HB2	2.18	0.44
1:B:96:GLU:OE2	1:B:100:ILE:HB	2.18	0.44
1:C:457:ARG:NH1	1:C:460:ASN:O	2.50	0.44
2:E:349:TRP:HE3	2:E:351:LEU:HD21	1.83	0.44
1:A:14:GLN:HE21	1:A:18:LEU:HD11	1.82	0.43
1:A:370:ASN:OD1	1:A:371:SER:N	2.51	0.43
1:B:215:ASP:OD1	1:B:215:ASP:N	2.44	0.43
2:E:458:LYS:HA	2:E:461:TRP:CE3	2.53	0.43
1:A:240:THR:OG1	1:A:241:LEU:N	2.50	0.43
1:B:61:ASN:HD21	4:B:1308:NAG:H83	1.82	0.43
1:B:675:GLN:HB3	1:B:676:THR:H	1.51	0.43
1:B:708:SER:HB3	1:B:711:SER:HB3	2.00	0.43
1:A:349:SER:OG	1:A:350:VAL:N	2.51	0.43
2:E:165:TRP:CZ2	2:E:493:HIS:HE1	2.37	0.43
2:E:318:ILE:HG22	2:E:550:ALA:HB3	2.01	0.43
1:A:346:ARG:CZ	1:A:347:PHE:H	2.31	0.43
1:B:229:LEU:HD12	1:B:231:ILE:HD11	2.00	0.43
1:B:455:LEU:HG	1:B:456:PHE:HD1	1.84	0.43
1:C:117:LEU:H	1:C:117:LEU:HD23	1.84	0.43
2:E:294:THR:HG22	2:E:296:LYS:HB2	1.99	0.43
2:E:377:GLY:HA2	2:E:380:GLN:OE1	2.18	0.43
1:C:455:LEU:HB3	1:C:493:GLN:HE22	1.84	0.43
1:C:273:ARG:NH1	1:C:290:ASP:OD2	2.51	0.43
1:A:231:ILE:HG22	1:A:233:ILE:HG13	2.00	0.43
1:A:351:TYR:OH	1:A:454:ARG:HG2	2.18	0.43
1:A:717:ASN:HB2	1:A:1071:GLN:HB2	2.01	0.43
1:C:627:ASP:OD1	1:C:627:ASP:N	2.51	0.43
1:C:1114:ILE:H	1:C:1114:ILE:HG12	1.66	0.43
4:C:1307:NAG:H5	4:C:1307:NAG:N2	2.33	0.43
1:A:245:HIS:O	1:A:258:TRP:HB2	2.18	0.43
1:A:498:GLN:CD	1:A:498:GLN:H	2.22	0.43
1:B:119:ILE:HG12	1:B:128:ILE:HG12	2.01	0.43
1:B:360:ASN:OD1	1:B:360:ASN:O	2.37	0.43
1:C:346:ARG:NH1	1:C:346:ARG:HA	2.34	0.43
1:C:409:GLN:NE2	1:C:417:LYS:H	2.14	0.43
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.84	0.43
1:C:599:THR:HB	1:C:608:VAL:HG12	2.01	0.43
2:E:179:LEU:HD23	2:E:179:LEU:HA	1.82	0.42
2:E:457:GLU:OE1	2:E:461:TRP:NE1	2.52	0.42
1:A:388:ASN:OD1	1:A:528:LYS:NZ	2.47	0.42
1:B:115:GLN:HA	1:B:132:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:HD13	1:C:198:ASP:OD2	2.19	0.42
1:C:353:TRP:HZ3	1:C:355:ARG:HB2	1.85	0.42
2:E:446:ILE:HD13	2:E:523:PHE:HZ	1.84	0.42
2:E:518:ARG:HG3	2:E:519:THR:N	2.33	0.42
1:A:399:SER:HB3	1:A:511:VAL:HG22	2.00	0.42
2:E:418:LEU:HA	2:E:421:LEU:HD12	2.01	0.42
2:E:529:LEU:HD23	2:E:529:LEU:HA	1.88	0.42
1:B:940:SER:OG	1:B:941:THR:N	2.53	0.42
2:E:582:LYS:HD3	2:E:583:PRO:HD3	2.01	0.42
1:A:107:GLY:H	1:A:235:ILE:HG23	1.85	0.42
1:A:321:GLN:HE21	1:A:629:LEU:HB2	1.84	0.42
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.84	0.42
1:B:387:LEU:H	1:B:387:LEU:HD12	1.84	0.42
1:B:1045:LYS:HE2	1:B:1045:LYS:HB2	1.81	0.42
1:C:401:VAL:O	1:C:402:ILE:HD13	2.20	0.42
2:E:230:PHE:HZ	2:E:451:PRO:HG3	1.85	0.42
2:E:408:MET:CE	2:E:408:MET:H	2.33	0.42
1:C:117:LEU:HD13	1:C:231:ILE:HG21	2.01	0.42
1:C:806:LEU:HD23	1:C:806:LEU:HA	1.86	0.42
1:C:884:SER:O	1:C:884:SER:OG	2.33	0.42
1:A:825:LYS:HA	1:A:825:LYS:HD2	1.89	0.42
1:C:280:ASN:HD22	4:C:1305:NAG:H82	1.85	0.42
1:C:426:PRO:HD3	1:C:463:PRO:HB3	2.01	0.42
1:C:428:ASP:OD1	1:C:428:ASP:N	2.45	0.42
2:E:370:LEU:O	2:E:373:HIS:ND1	2.43	0.42
2:E:407:ILE:HG21	2:E:529:LEU:HD12	2.01	0.42
1:A:40:ASP:OD1	1:A:40:ASP:N	2.52	0.42
1:A:411:ALA:H	1:A:425:LEU:HD22	1.85	0.42
1:A:880:GLY:O	1:A:884:SER:OG	2.28	0.42
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.87	0.42
1:B:776:LYS:HB3	1:B:776:LYS:HE3	1.82	0.42
1:C:81:ASN:HB3	1:C:239:GLN:HE21	1.85	0.42
2:E:108:VAL:HG11	2:E:190:MET:HG2	2.02	0.42
1:A:883:THR:O	1:A:895:GLN:HA	2.20	0.42
1:A:917:TYR:HB3	1:C:1129:VAL:HG13	2.02	0.42
1:B:139:PRO:HB3	1:B:159:VAL:HB	2.00	0.42
1:B:616:ASN:OD1	1:B:617:CYS:N	2.53	0.42
1:C:58:PHE:HD1	1:C:58:PHE:HA	1.77	0.42
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.53	0.42
2:E:225:ASP:O	2:E:229:THR:HG23	2.19	0.42
2:E:539:LEU:HD12	2:E:587:TYR:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:HG23	1:A:77:LYS:HA	2.02	0.41
1:B:453:TYR:CE1	1:B:493:GLN:HB2	2.54	0.41
1:C:119:ILE:HG13	1:C:128:ILE:HG22	2.01	0.41
1:C:287:ASP:OD1	1:C:288:ALA:N	2.50	0.41
2:E:578:THR:OG1	2:E:579:MET:N	2.53	0.41
1:A:336:CYS:HB3	1:A:358:ILE:HG12	2.02	0.41
1:A:1142:GLN:NE2	1:A:1145:LEU:HD13	2.35	0.41
1:B:109:THR:OG1	1:B:111:ASP:OD1	2.38	0.41
2:E:589:GLU:O	2:E:593:THR:HG23	2.20	0.41
1:B:433:VAL:HG22	1:B:512:VAL:HG13	2.02	0.41
1:C:529:LYS:HE2	1:C:529:LYS:HB2	1.89	0.41
2:E:152:MET:HB3	2:E:156:ARG:HH12	1.86	0.41
2:E:188:ASN:ND2	2:E:464:PHE:HB3	2.33	0.41
2:E:450:LEU:HD23	2:E:450:LEU:HA	1.90	0.41
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.90	0.41
1:A:159:VAL:HG23	1:A:160:TYR:CD1	2.53	0.41
1:C:544:ASN:OD1	1:C:544:ASN:N	2.53	0.41
1:C:417:LYS:CE	1:C:455:LEU:HD23	2.47	0.41
2:E:275:TRP:HB2	2:E:444:LEU:HB3	2.02	0.41
2:E:323:MET:SD	2:E:327:PHE:HB3	2.60	0.41
2:E:467:GLU:H	2:E:467:GLU:CD	2.21	0.41
1:A:195:LYS:HE3	1:A:195:LYS:HB3	1.84	0.41
1:A:1004:LEU:HD23	1:A:1004:LEU:HA	1.90	0.41
1:C:401:VAL:C	1:C:402:ILE:HD13	2.41	0.41
2:E:198:ASP:OD1	2:E:198:ASP:N	2.54	0.41
1:B:644:GLN:NE2	1:B:645:THR:O	2.53	0.41
1:C:985:ASP:HB3	1:C:987:PRO:HD2	2.02	0.41
1:B:25:PRO:HA	1:B:26:PRO:HD3	1.99	0.41
1:B:280:ASN:HD22	4:B:1303:NAG:H82	1.86	0.41
2:E:160:ARG:HH22	2:E:270:MET:HA	1.86	0.41
1:A:312:ILE:HD12	1:A:598:ILE:HG13	2.01	0.41
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.79	0.41
1:B:14:GLN:N	1:B:14:GLN:OE1	2.54	0.41
1:B:186:PHE:N	1:B:210:ILE:O	2.53	0.41
1:B:431:GLY:HA2	1:B:515:PHE:HD2	1.86	0.41
1:B:537:LYS:HB3	1:B:537:LYS:HE2	1.79	0.41
1:C:341:VAL:H	1:C:341:VAL:HG22	1.60	0.41
1:C:352:ALA:HA	1:C:466:ARG:HE	1.86	0.41
1:C:878:LEU:HD21	1:C:1052:PHE:HB3	2.02	0.41
2:E:99:LYS:HE2	2:E:99:LYS:HB3	1.90	0.41
2:E:247:LYS:HE2	2:E:284:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:HIS:HE1	2:E:349:TRP:CZ2	2.39	0.41
1:A:409:GLN:HB3	1:A:416:GLY:HA3	2.01	0.41
1:A:455:LEU:HD23	1:A:455:LEU:HA	1.95	0.41
2:E:340:ARG:HH12	2:E:342:VAL:HG23	1.86	0.41
1:B:106:PHE:HB3	1:B:235:ILE:HD13	2.03	0.40
1:B:214:ARG:HA	1:B:214:ARG:HD3	1.85	0.40
1:B:328:ARG:NH1	1:B:533:LEU:HB2	2.35	0.40
1:B:630:THR:N	1:B:631:PRO:HD3	2.36	0.40
2:E:161:ARG:HH21	2:E:266:LEU:HD13	1.86	0.40
1:A:387:LEU:HD12	1:A:390:LEU:HD21	2.03	0.40
1:C:310:LYS:HG3	1:C:600:PRO:HA	2.03	0.40
2:E:161:ARG:HH22	2:E:256:ILE:HD11	1.85	0.40
2:E:183:TYR:O	2:E:187:GLU:HB2	2.20	0.40
1:A:943:SER:O	1:A:943:SER:OG	2.39	0.40
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.40	0.40
1:C:335:LEU:HD23	1:C:336:CYS:N	2.36	0.40
1:C:621:PRO:HB3	1:C:628:GLN:NE2	2.36	0.40
2:E:398:GLU:H	2:E:398:GLU:HG2	1.63	0.40
3:O:1:NAG:O3	3:O:2:NAG:O5	2.34	0.40
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.03	0.40
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.96	0.40
1:C:410:ILE:H	1:C:410:ILE:HD12	1.85	0.40
2:E:55:ILE:O	2:E:55:ILE:HD12	2.22	0.40
2:E:62:LYS:HE2	2:E:62:LYS:HB3	1.91	0.40
2:E:378:HIS:O	2:E:378:HIS:CD2	2.74	0.40
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.87	0.40
3:N:1:NAG:H61	3:N:2:NAG:HN2	1.87	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 PDB entries followed by that with respect to all EM entries.

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	1047/1217 (86%)	999 (95%)	48 (5%)	0	100	100
1	B	1047/1217 (86%)	994 (95%)	53 (5%)	0	100	100
1	C	1051/1217 (86%)	993 (94%)	58 (6%)	0	100	100
2	E	593/661 (90%)	556 (94%)	36 (6%)	1 (0%)	44	67
All	All	3738/4312 (87%)	3542 (95%)	195 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	469	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 PDB entries followed by that with respect to all EM entries.

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	930/1065 (87%)	889 (96%)	41 (4%)	24	49
1	B	931/1065 (87%)	893 (96%)	38 (4%)	26	52
1	C	933/1065 (88%)	882 (94%)	51 (6%)	18	40
2	E	527/585 (90%)	484 (92%)	43 (8%)	9	22
All	All	3321/3780 (88%)	3148 (95%)	173 (5%)	22	42

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	24	LEU
1	A	50	SER
1	A	78	ARG
1	A	88	ASP
1	A	165	ASN
1	A	198	ASP
1	A	240	THR
1	A	246	ARG
1	A	277	LEU

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Mol	Chain	Res	Type
1	A	305	SER
1	A	346	ARG
1	A	347	PHE
1	A	349	SER
1	A	369	TYR
1	A	373	SER
1	A	377	PHE
1	A	383	SER
1	A	385	THR
1	A	386	LYS
1	A	400	PHE
1	A	405	ASP
1	A	408	ARG
1	A	421	TYR
1	A	441	LEU
1	A	451	TYR
1	A	456	PHE
1	A	494	SER
1	A	505	TYR
1	A	528	LYS
1	A	586	ASP
1	A	634	ARG
1	A	636	TYR
1	A	731	MET
1	A	750	SER
1	A	786	LYS
1	A	813	SER
1	A	878	LEU
1	A	937	SER
1	A	985	ASP
1	A	1097	SER
1	B	21	ARG
1	B	34	ARG
1	B	80	ASP
1	B	96	GLU
1	B	126	VAL
1	B	131	CYS
1	B	153	MET
1	B	173	GLN
1	B	195	LYS
1	B	214	ARG
1	B	242	LEU

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Mol	Chain	Res	Type
1	B	305	SER
1	B	318	PHE
1	B	325	SER
1	B	350	VAL
1	B	369	TYR
1	B	377	PHE
1	B	392	PHE
1	B	400	PHE
1	B	515	PHE
1	B	529	LYS
1	B	544	ASN
1	B	553	THR
1	B	554	GLU
1	B	564	GLN
1	B	576	VAL
1	B	633	TRP
1	B	636	TYR
1	B	676	THR
1	B	709	ASN
1	B	786	LYS
1	B	820	ASP
1	B	825	LYS
1	B	902	MET
1	B	916	LEU
1	B	937	SER
1	B	1045	LYS
1	B	1116	THR
1	C	18	LEU
1	C	46	SER
1	C	50	SER
1	C	58	PHE
1	C	87	ASN
1	C	102	ARG
1	C	118	LEU
1	C	130	VAL
1	C	157	PHE
1	C	168	PHE
1	C	170	TYR
1	C	200	TYR
1	C	201	PHE
1	C	234	ASN
1	C	240	THR

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Mol	Chain	Res	Type
1	C	244	LEU
1	C	258	TRP
1	C	266	TYR
1	C	277	LEU
1	C	301	CYS
1	C	305	SER
1	C	369	TYR
1	C	374	PHE
1	C	377	PHE
1	C	388	ASN
1	C	390	LEU
1	C	392	PHE
1	C	408	ARG
1	C	462	LYS
1	C	490	PHE
1	C	495	TYR
1	C	508	TYR
1	C	515	PHE
1	C	518	LEU
1	C	540	ASN
1	C	544	ASN
1	C	559	PHE
1	C	745	ASP
1	C	759	PHE
1	C	786	LYS
1	C	787	GLN
1	C	791	THR
1	C	800	PHE
1	C	803	SER
1	C	813	SER
1	C	820	ASP
1	C	875	SER
1	C	916	LEU
1	C	965	GLN
1	C	974	SER
1	C	1043	CYS
2	E	24	GLU
2	E	52	ASN
2	E	54	ASN
2	E	63	MET
2	E	83	THR
2	E	112	GLU

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Mol	Chain	Res	Type
2	E	115	LYS
2	E	124	MET
2	E	152	MET
2	E	158	TYR
2	E	160	ARG
2	E	190	MET
2	E	223	MET
2	E	224	LYS
2	E	230	PHE
2	E	271	TRP
2	E	287	HIS
2	E	297	MET
2	E	306	ARG
2	E	323	MET
2	E	332	MET
2	E	357	ARG
2	E	360	MET
2	E	381	TYR
2	E	383	MET
2	E	385	TYR
2	E	408	MET
2	E	410	LEU
2	E	455	MET
2	E	462	MET
2	E	472	GLN
2	E	480	MET
2	E	505	HIS
2	E	516	TYR
2	E	518	ARG
2	E	534	ASN
2	E	556	GLN
2	E	557	MET
2	E	582	LYS
2	E	595	LEU
2	E	600	ARG
2	E	610	TRP
2	E	614	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN

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Mol	Chain	Res	Type
1	A	121	ASN
1	A	188	ASN
1	A	314	GLN
1	A	343	ASN
1	A	414	GLN
1	A	437	ASN
1	A	613	GLN
1	A	675	GLN
1	A	762	GLN
1	A	804	GLN
1	A	935	GLN
1	A	953	ASN
1	A	957	GLN
1	A	1142	GLN
1	B	14	GLN
1	B	173	GLN
1	B	218	GLN
1	B	245	HIS
1	B	317	ASN
1	B	354	ASN
1	B	360	ASN
1	B	394	ASN
1	B	422	ASN
1	B	448	ASN
1	B	493	GLN
1	B	519	HIS
1	B	544	ASN
1	B	628	GLN
1	B	658	ASN
1	B	901	GLN
1	B	955	ASN
1	B	1002	GLN
1	C	87	ASN
1	C	137	ASN
1	C	239	GLN
1	C	422	ASN
1	C	450	ASN
1	C	519	HIS
1	C	580	GLN
1	C	658	ASN
1	C	675	GLN
1	C	901	GLN

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Mol	Chain	Res	Type
1	C	965	GLN
1	C	1002	GLN
2	E	43	GLN
2	E	59	ASN
2	E	61	GLN
2	E	64	ASN
2	E	330	ASN
2	E	345	HIS
2	E	493	HIS
2	E	524	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

42 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	$\#\|Z\|>2$
3	NAG	D	1	3,1	14,14,15	0.17	0	17,19,21	0.44	0
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.20	0	17,19,21	0.65	0
3	NAG	F	2	3	14,14,15	0.38	0	17,19,21	0.73	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.32	0	17,19,21	0.53	0
3	NAG	G	2	3	14,14,15	0.36	0	17,19,21	0.40	0
3	NAG	H	1	3,1	14,14,15	0.41	0	17,19,21	1.36	2 (11%)
3	NAG	H	2	3	14,14,15	0.41	0	17,19,21	1.22	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	I	1	3,1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	I	2	3	14,14,15	0.32	0	17,19,21	0.58	0
3	NAG	J	1	3,1	14,14,15	0.25	0	17,19,21	0.59	0
3	NAG	J	2	3	14,14,15	0.61	1 (7%)	17,19,21	0.77	1 (5%)
3	NAG	K	1	3,1	14,14,15	0.63	1 (7%)	17,19,21	0.49	0
3	NAG	K	2	3	14,14,15	0.68	0	17,19,21	0.51	0
3	NAG	L	1	3,1	14,14,15	0.27	0	17,19,21	0.45	0
3	NAG	L	2	3	14,14,15	0.27	0	17,19,21	0.55	0
3	NAG	M	1	3,1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
3	NAG	M	2	3	14,14,15	0.92	1 (7%)	17,19,21	0.67	0
3	NAG	N	1	3,1	14,14,15	0.43	0	17,19,21	0.88	1 (5%)
3	NAG	N	2	3	14,14,15	0.41	0	17,19,21	0.55	0
3	NAG	O	1	3,1	14,14,15	0.23	0	17,19,21	0.37	0
3	NAG	O	2	3	14,14,15	0.52	0	17,19,21	0.42	0
3	NAG	P	1	3,1	14,14,15	0.37	0	17,19,21	0.78	0
3	NAG	P	2	3	14,14,15	0.40	0	17,19,21	0.53	0
3	NAG	Q	1	3,1	14,14,15	0.50	0	17,19,21	0.51	0
3	NAG	Q	2	3	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
3	NAG	R	1	3,1	14,14,15	0.20	0	17,19,21	0.67	1 (5%)
3	NAG	R	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	S	1	3,1	14,14,15	0.22	0	17,19,21	0.57	0
3	NAG	S	2	3	14,14,15	0.19	0	17,19,21	0.39	0
3	NAG	T	1	3,1	14,14,15	0.25	0	17,19,21	0.67	1 (5%)
3	NAG	T	2	3	14,14,15	0.54	0	17,19,21	0.48	0
3	NAG	U	1	3,1	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	U	2	3	14,14,15	0.32	0	17,19,21	0.36	0
3	NAG	V	1	3,1	14,14,15	0.33	0	17,19,21	0.46	0
3	NAG	V	2	3	14,14,15	0.27	0	17,19,21	0.59	0
3	NAG	W	1	3,1	14,14,15	0.52	0	17,19,21	1.24	1 (5%)
3	NAG	W	2	3	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	X	1	3,1	14,14,15	0.26	0	17,19,21	0.64	1 (5%)
3	NAG	X	2	3	14,14,15	0.34	0	17,19,21	0.59	0
3	NAG	Y	1	3,2	14,14,15	0.39	0	17,19,21	0.50	0
3	NAG	Y	2	3	14,14,15	0.55	0	17,19,21	0.54	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
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	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	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	1/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	M	2	3	-	4/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	4/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	4/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	4/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Y	1	3,2	-	4/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	NAG	O5-C1	2.82	1.48	1.43
3	K	1	NAG	O5-C1	-2.29	1.40	1.43
3	J	2	NAG	O5-C1	-2.06	1.40	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1	NAG	C2-N2-C7	4.43	129.21	122.90
3	W	1	NAG	C2-N2-C7	4.21	128.89	122.90
3	H	2	NAG	C2-N2-C7	3.89	128.44	122.90
3	J	2	NAG	C1-O5-C5	2.91	116.13	112.19
3	N	1	NAG	C1-O5-C5	2.86	116.07	112.19
3	Q	2	NAG	C1-O5-C5	2.59	115.70	112.19
3	F	2	NAG	C1-O5-C5	2.42	115.47	112.19
3	M	1	NAG	C1-O5-C5	2.27	115.27	112.19
3	H	2	NAG	C1-C2-N2	2.25	114.34	110.49
3	D	2	NAG	C1-O5-C5	2.24	115.22	112.19
3	R	1	NAG	C1-O5-C5	2.18	115.14	112.19
3	H	1	NAG	C1-O5-C5	2.18	115.14	112.19
3	T	1	NAG	C1-O5-C5	2.11	115.06	112.19
3	X	1	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	W	2	NAG	O5-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	M	1	NAG	C8-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	M	2	NAG	C8-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	P	2	NAG	C8-C7-N2-C2
3	P	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C3-C2-N2-C7
3	X	2	NAG	C3-C2-N2-C7
3	V	2	NAG	C1-C2-N2-C7
3	M	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	C1-C2-N2-C7
3	I	2	NAG	C4-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C3-C2-N2-C7
3	H	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	V	2	NAG	C3-C2-N2-C7
3	W	1	NAG	C3-C2-N2-C7

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	M	2	NAG	O5-C5-C6-O6
3	P	1	NAG	C1-C2-N2-C7

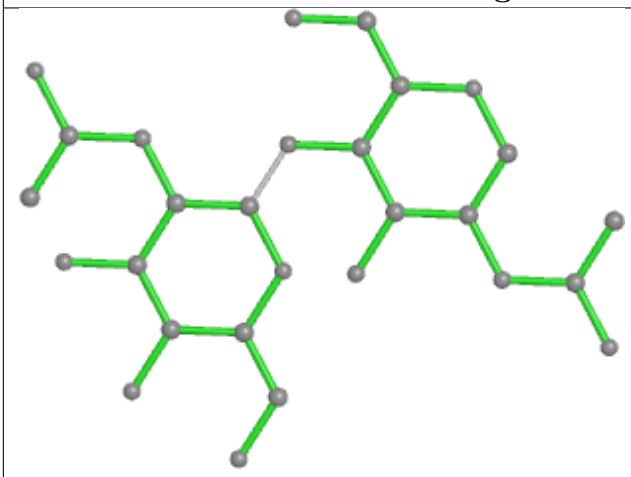
There are no ring outliers.

14 monomers are involved in 17 short contacts:

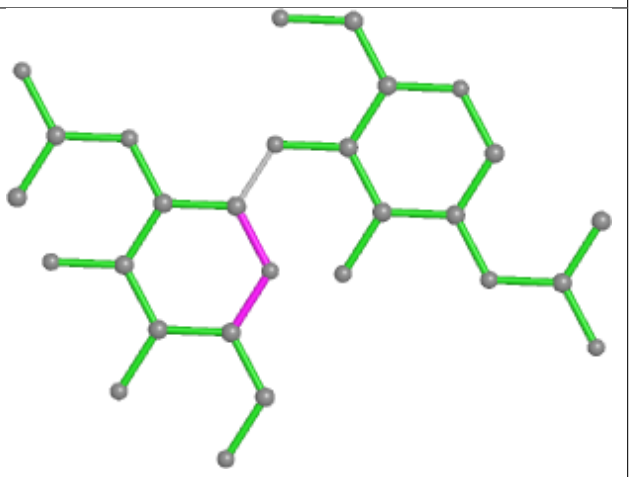
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	2	NAG	1	0
3	N	1	NAG	1	0
3	O	2	NAG	1	0
3	Q	1	NAG	3	0
3	T	2	NAG	2	0
3	H	2	NAG	1	0
3	H	1	NAG	1	0
3	W	1	NAG	3	0
3	X	1	NAG	1	0
3	D	1	NAG	1	0
3	U	1	NAG	2	0
3	V	1	NAG	1	0
3	T	1	NAG	2	0
3	O	1	NAG	1	0

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

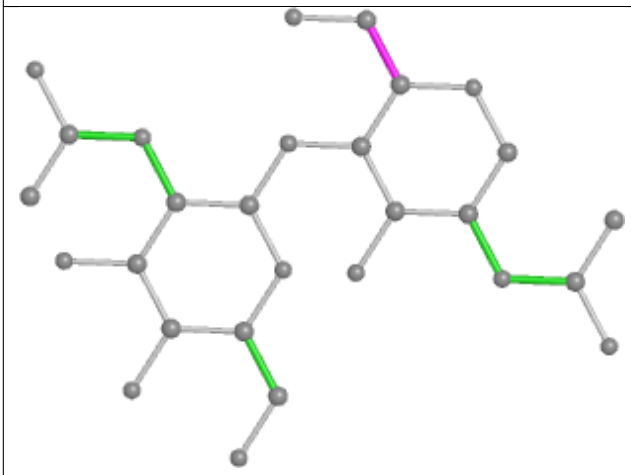
Oligosaccharide Chain D



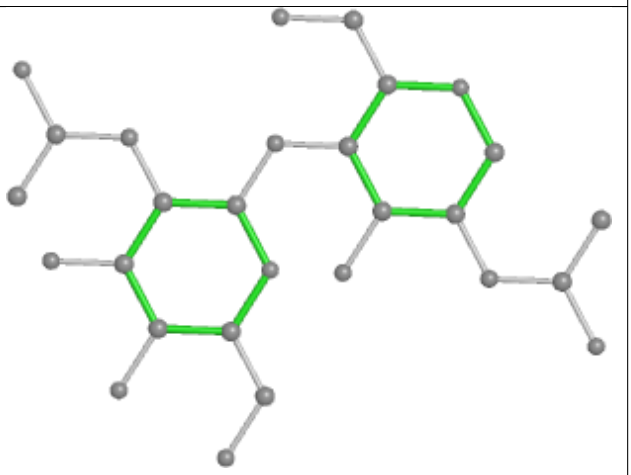
Bond lengths



Bond angles

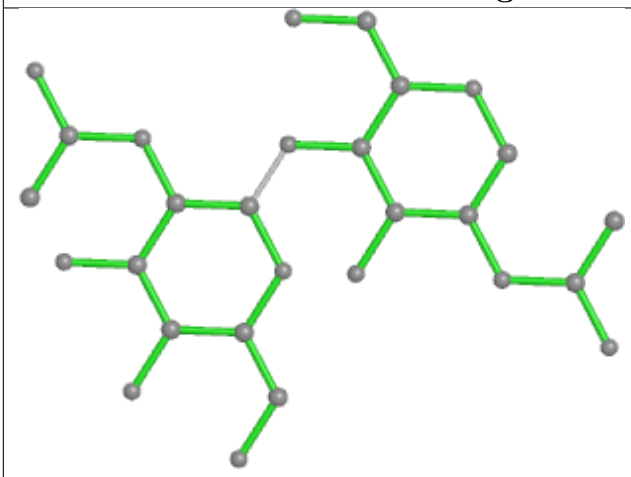


Torsions

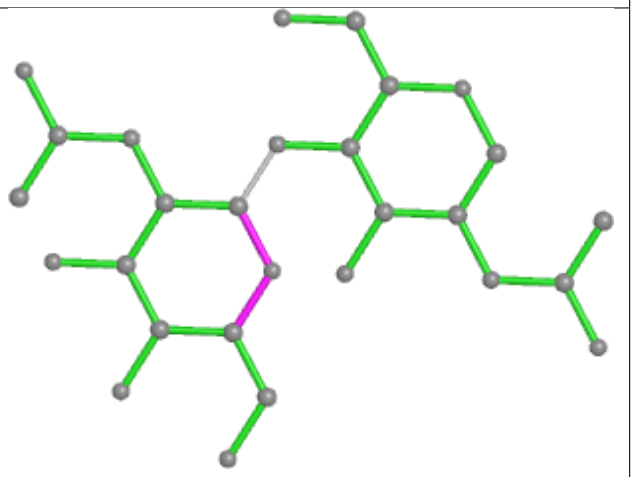


Rings

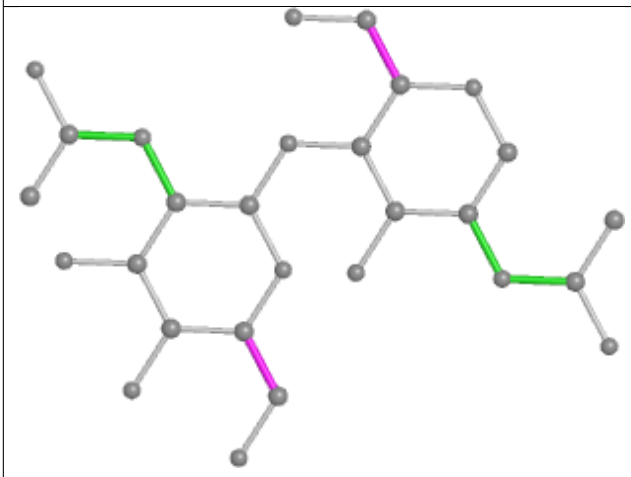
Oligosaccharide Chain F



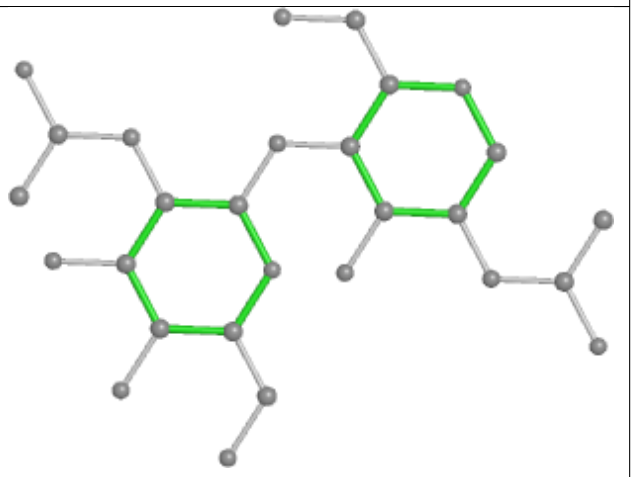
Bond lengths



Bond angles

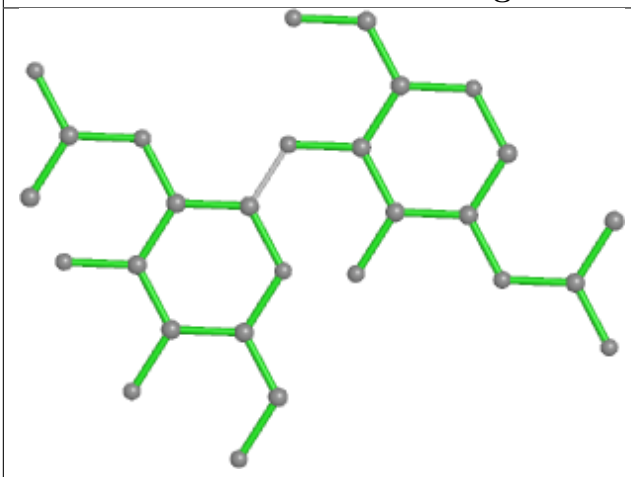


Torsions

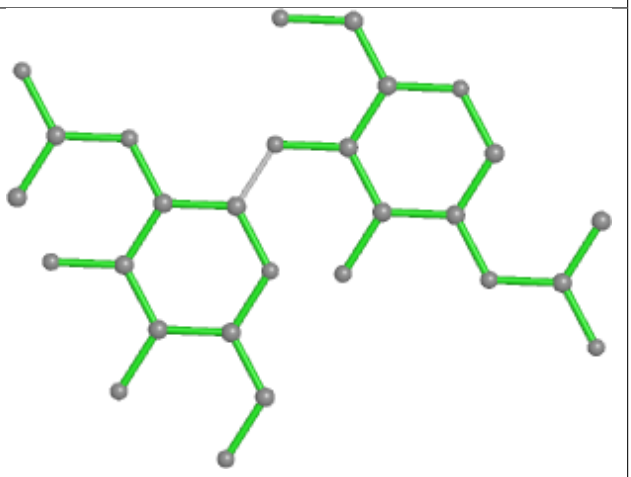


Rings

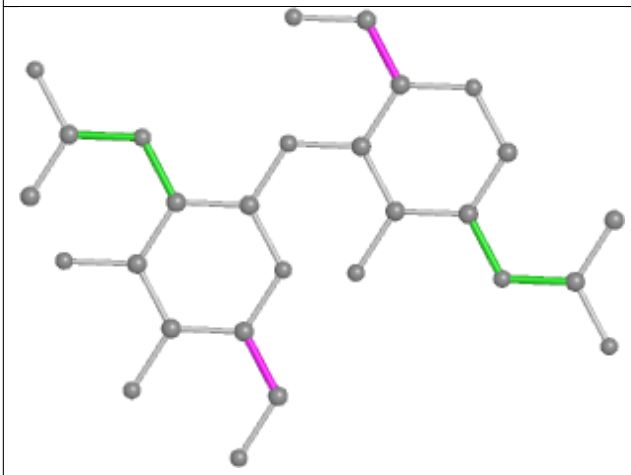
Oligosaccharide Chain G



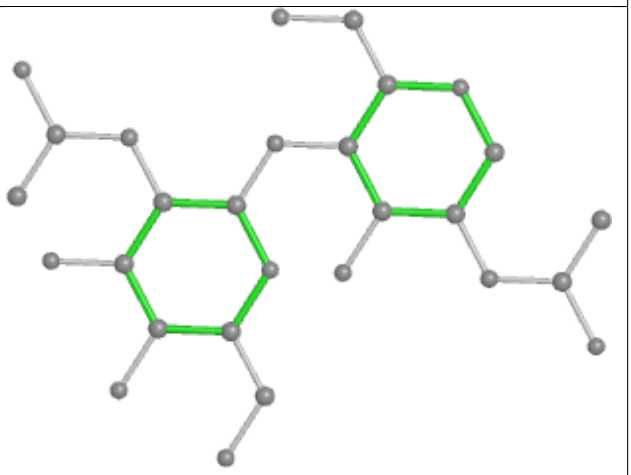
Bond lengths



Bond angles

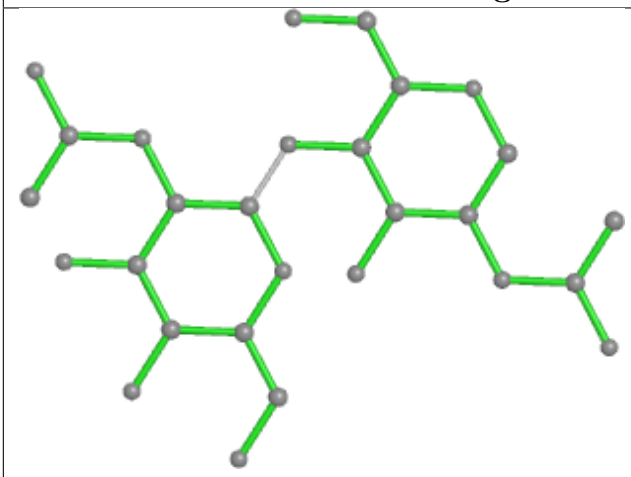


Torsions

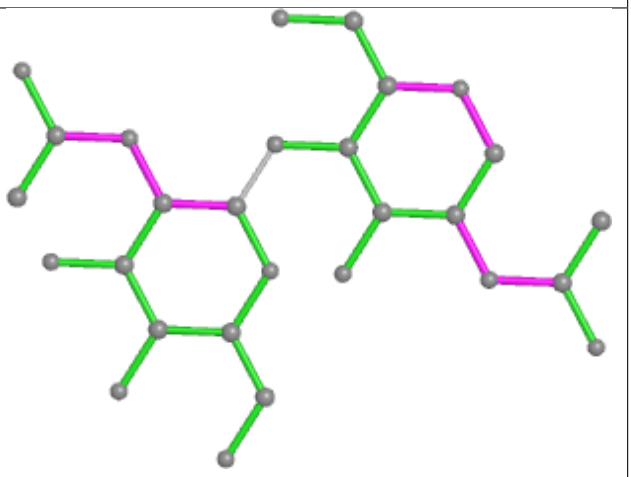


Rings

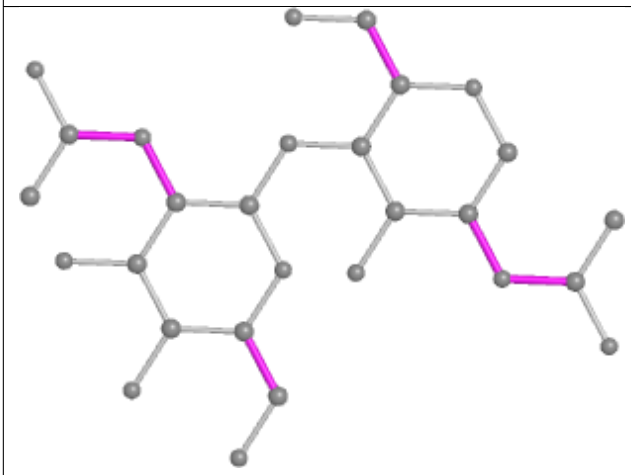
Oligosaccharide Chain H



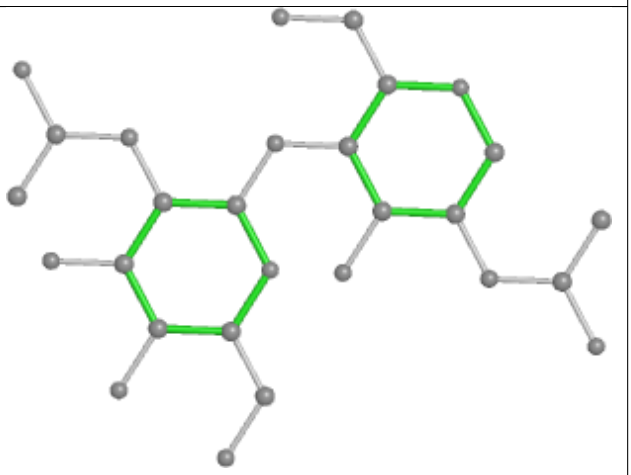
Bond lengths



Bond angles

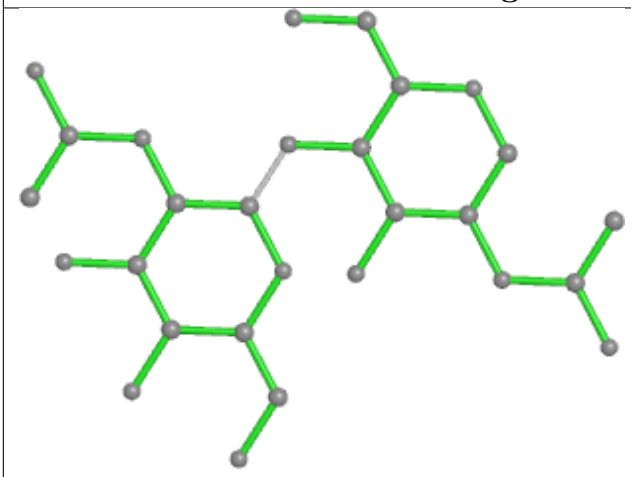


Torsions

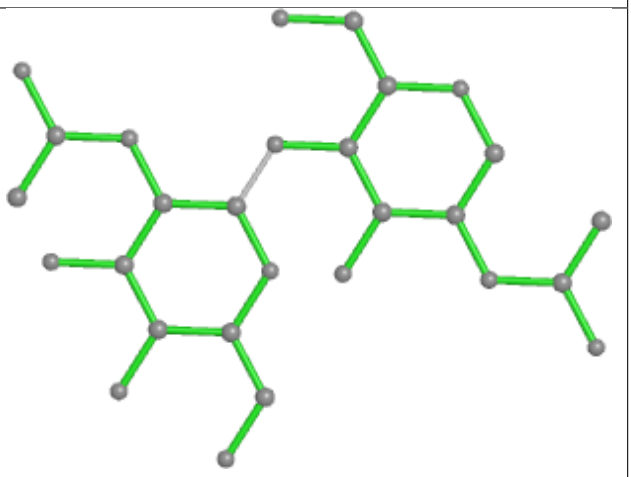


Rings

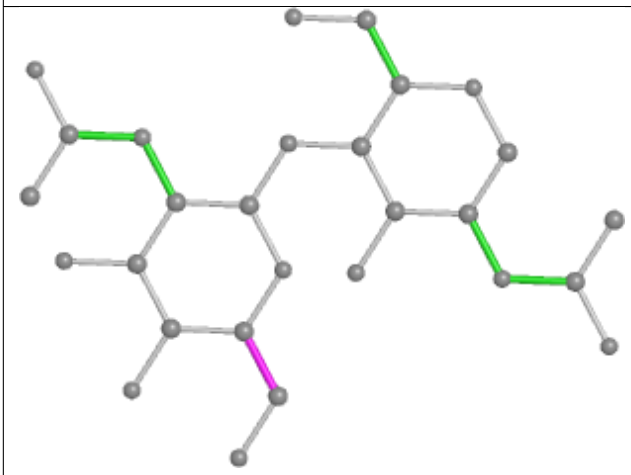
Oligosaccharide Chain I



Bond lengths



Bond angles



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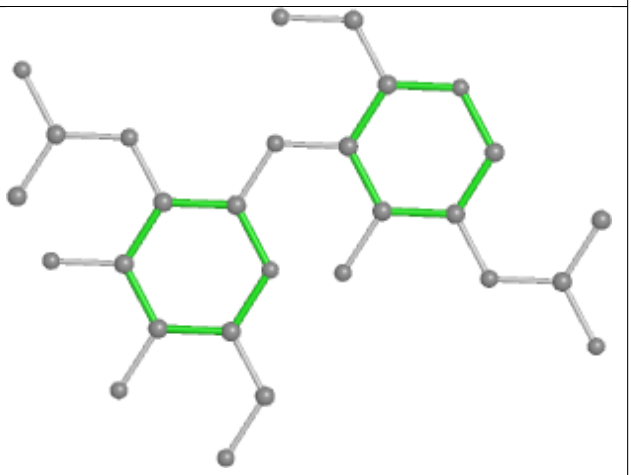
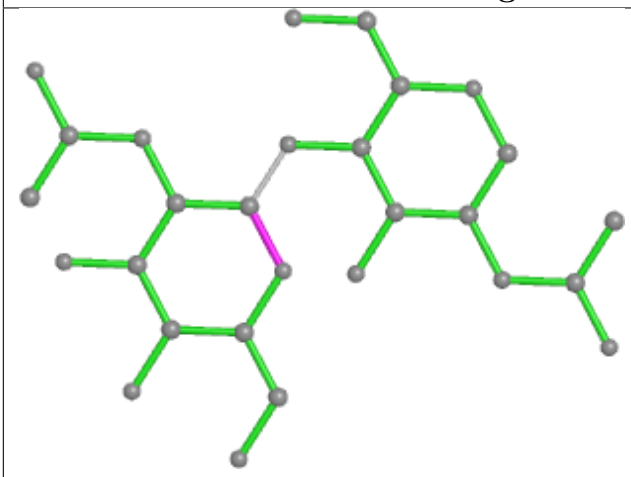
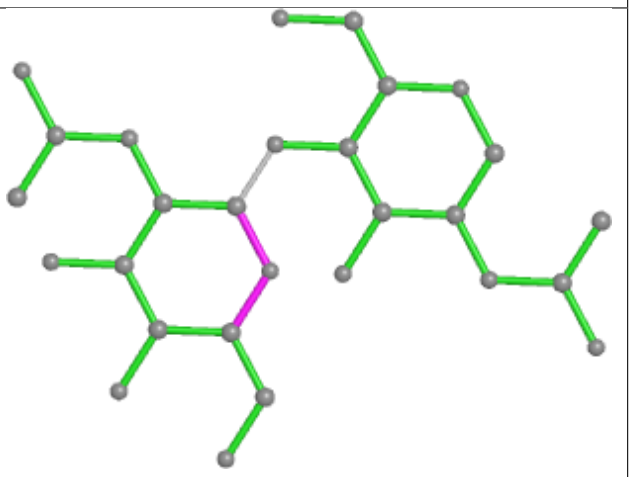


Rings

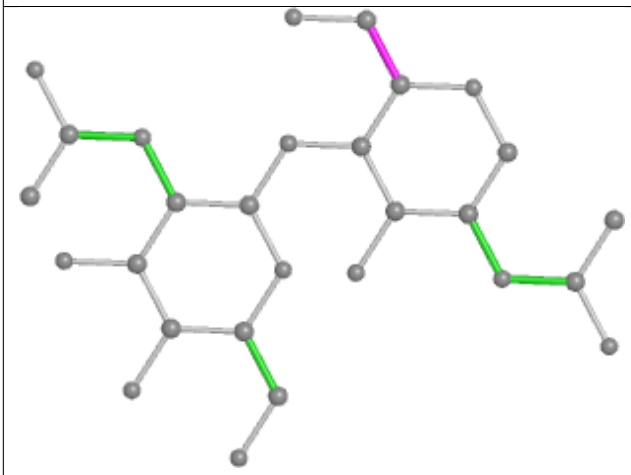
Oligosaccharide Chain J



Bond lengths



Bond angles



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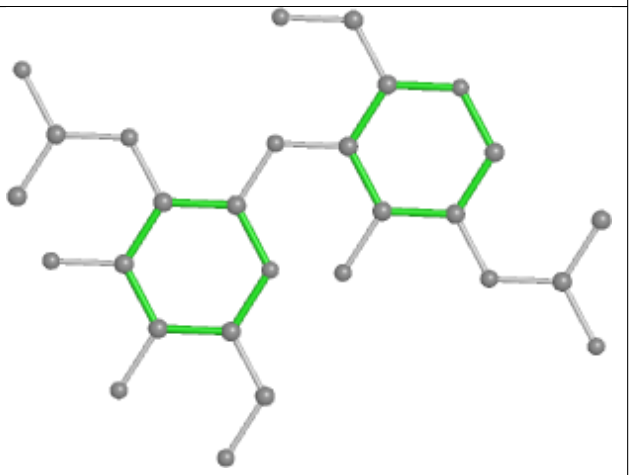
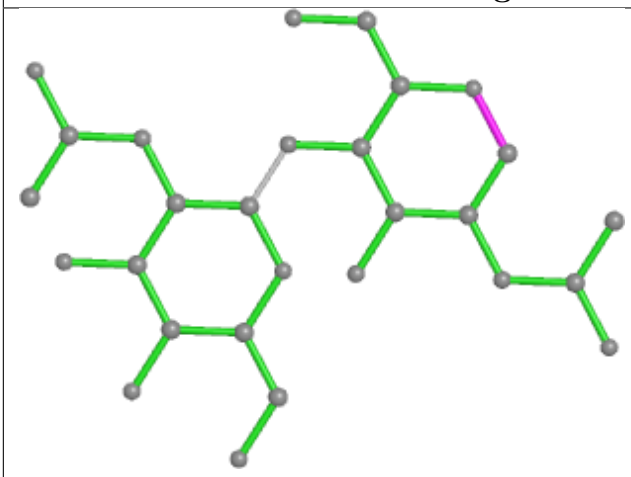
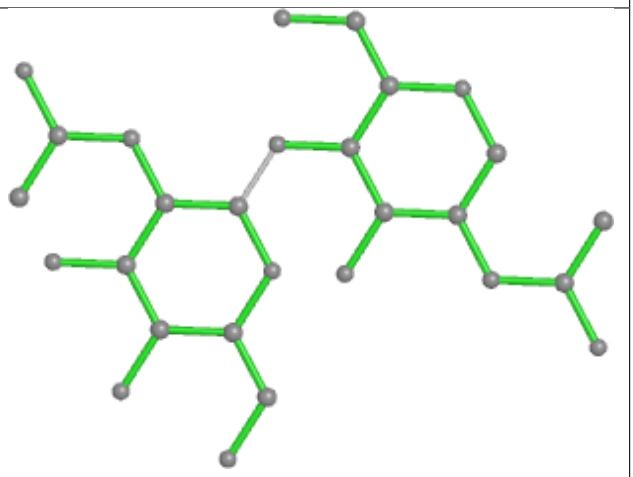


Rings

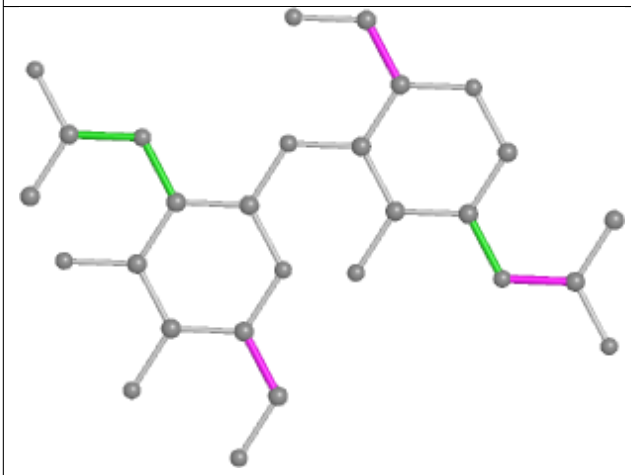
Oligosaccharide Chain K



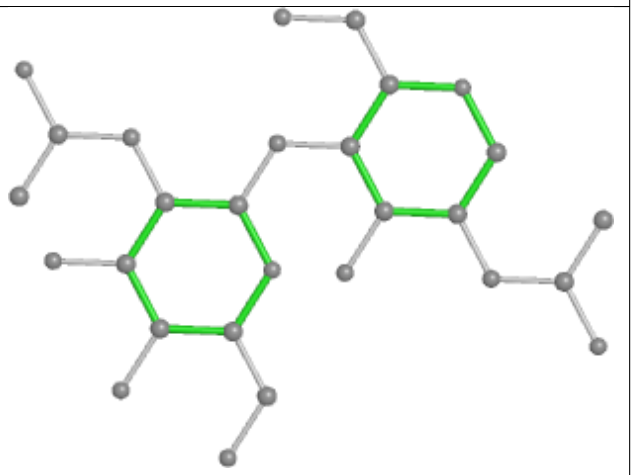
Bond lengths



Bond angles

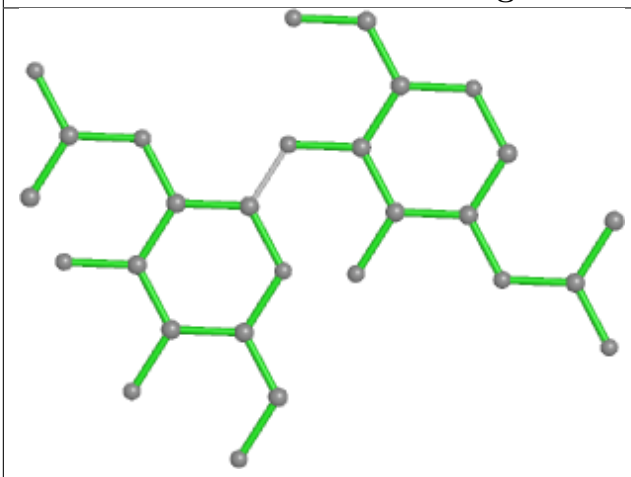


Torsions

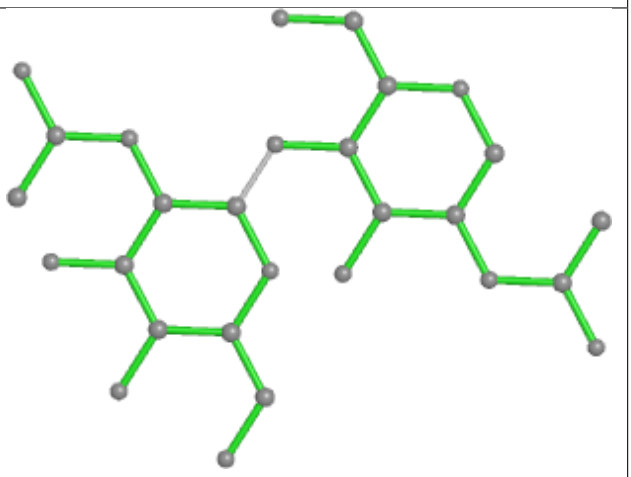


Rings

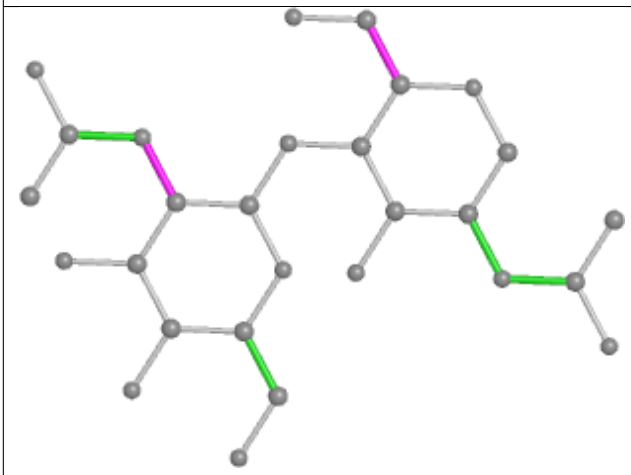
Oligosaccharide Chain L



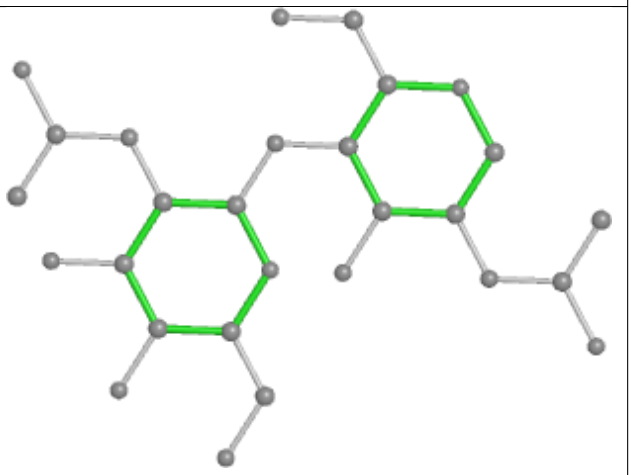
Bond lengths



Bond angles

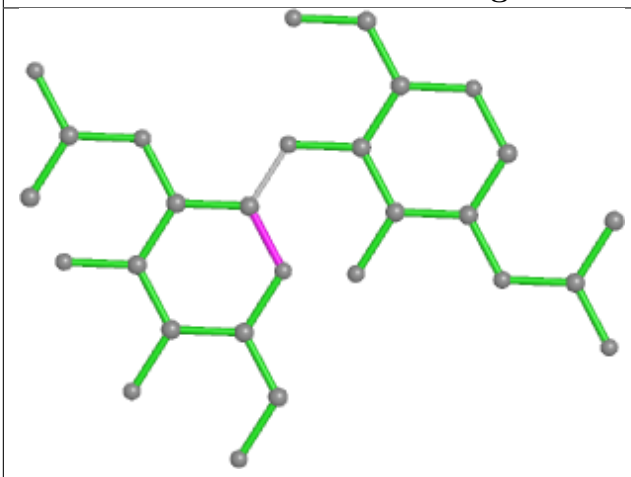


Torsions

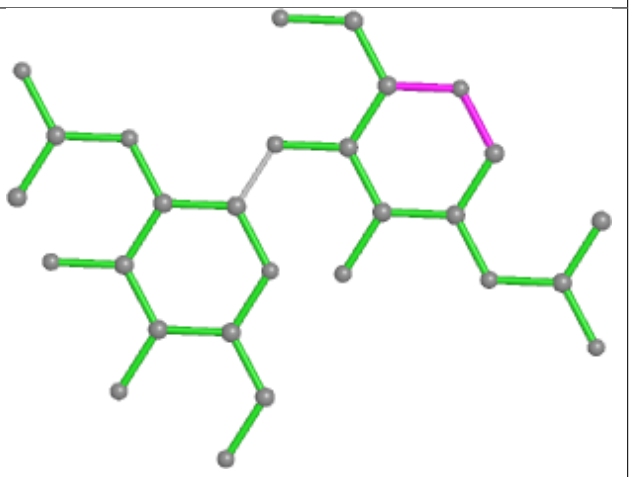


Rings

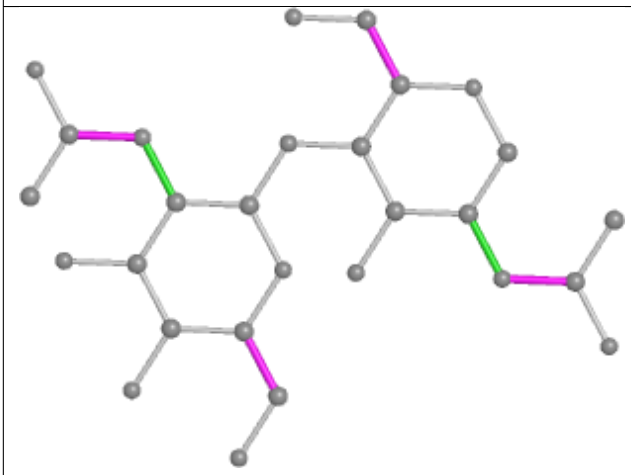
Oligosaccharide Chain M



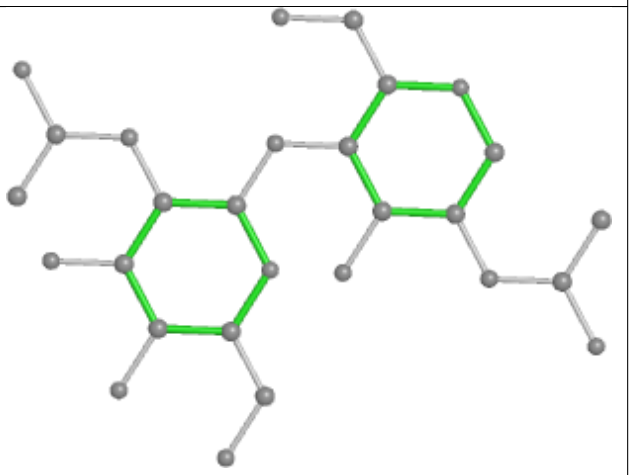
Bond lengths



Bond angles

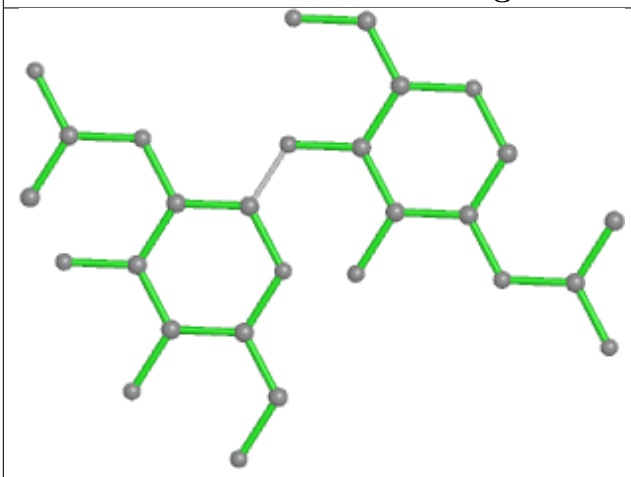


Torsions

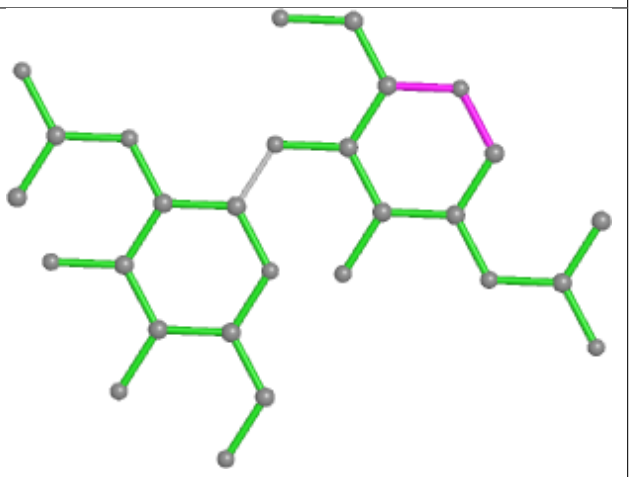


Rings

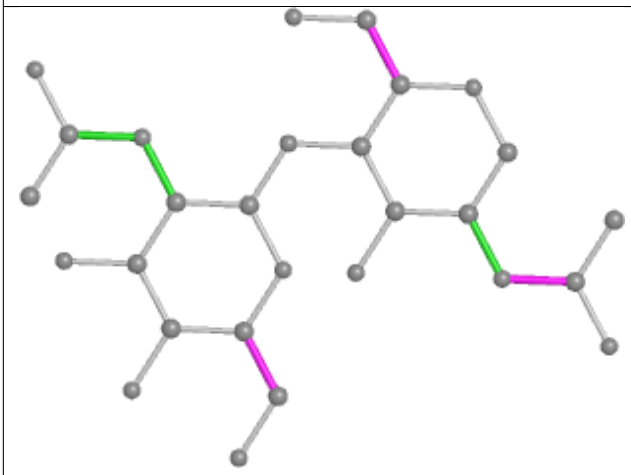
Oligosaccharide Chain N



Bond lengths



Bond angles



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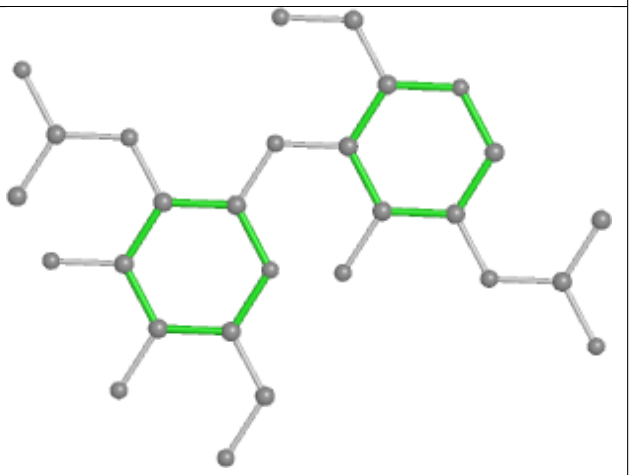
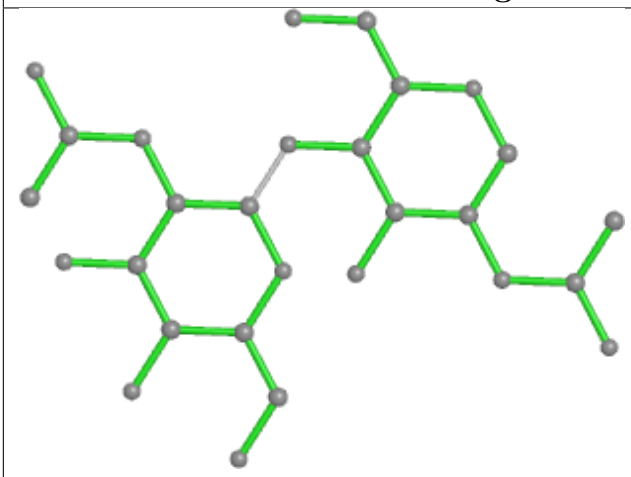
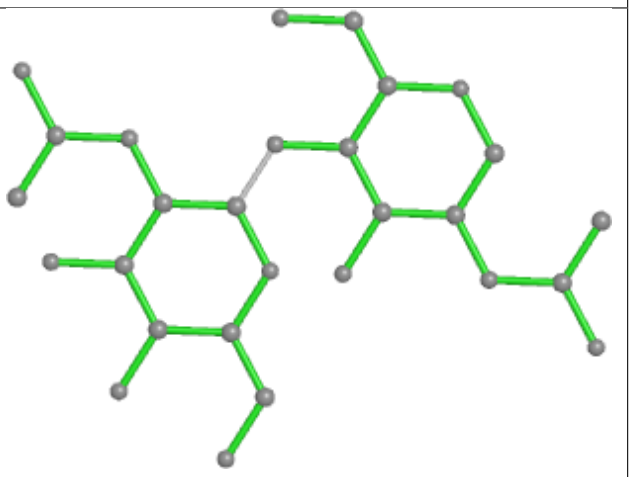


Rings

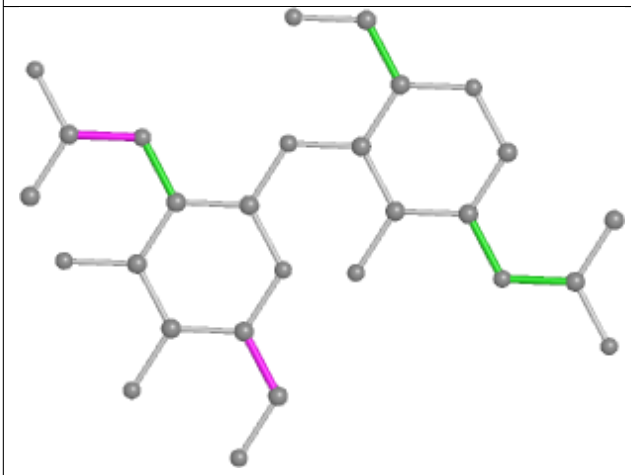
Oligosaccharide Chain O



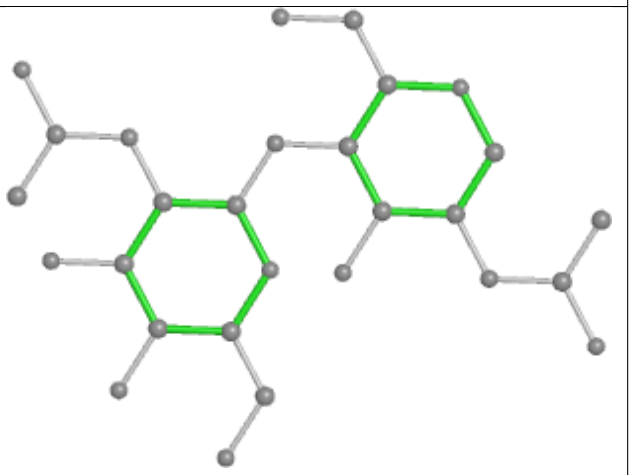
Bond lengths



Bond angles

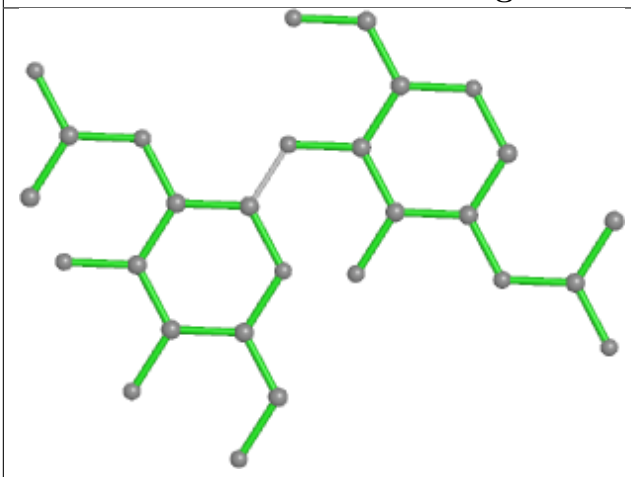


Torsions

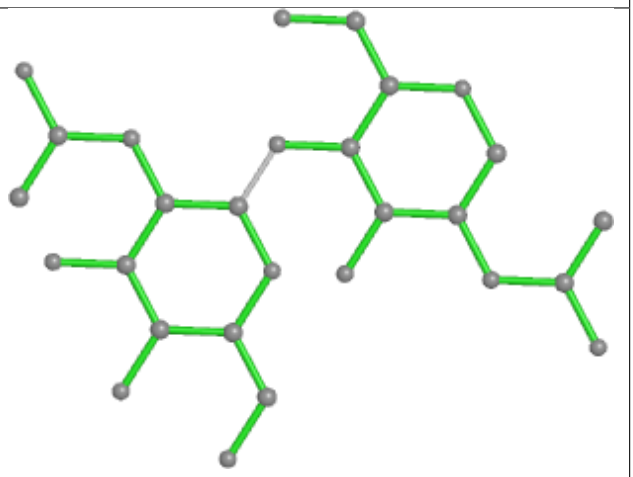


Rings

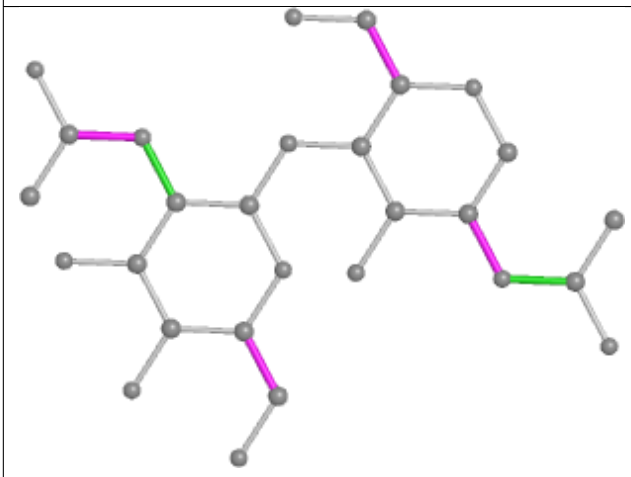
Oligosaccharide Chain P



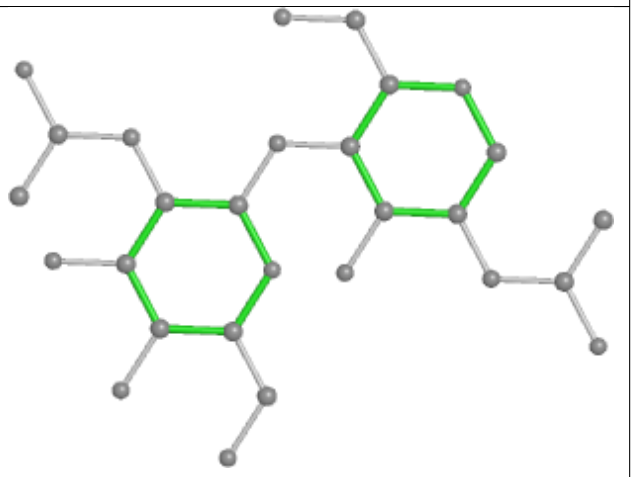
Bond lengths



Bond angles

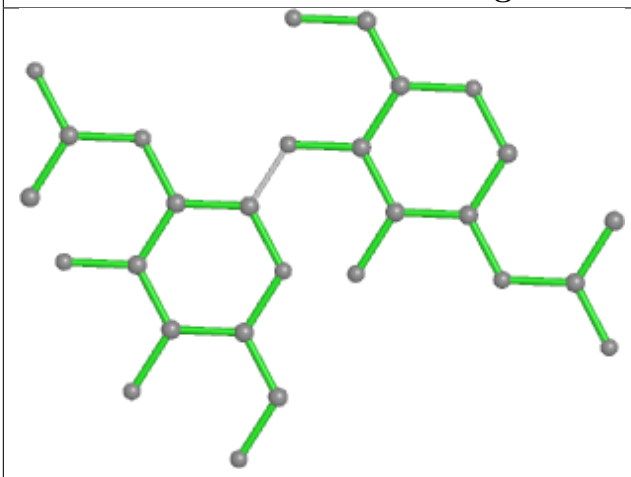


Torsions

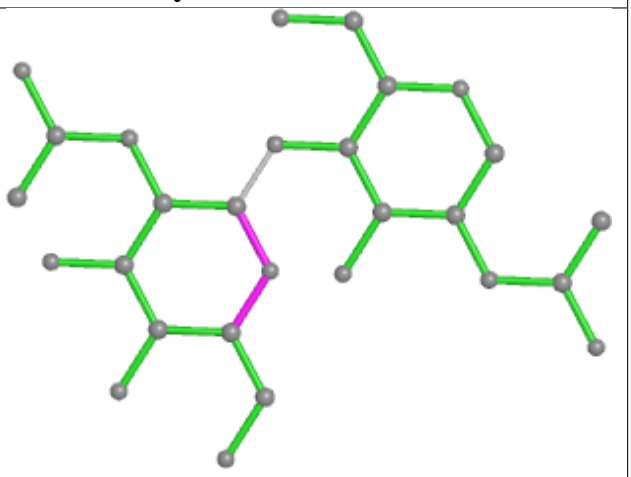


Rings

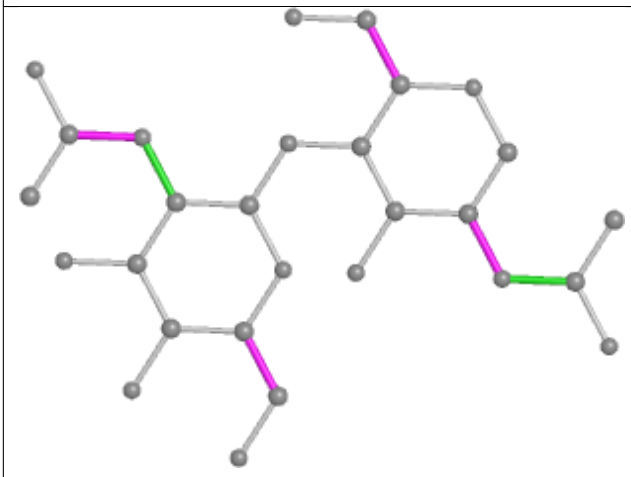
Oligosaccharide Chain Q



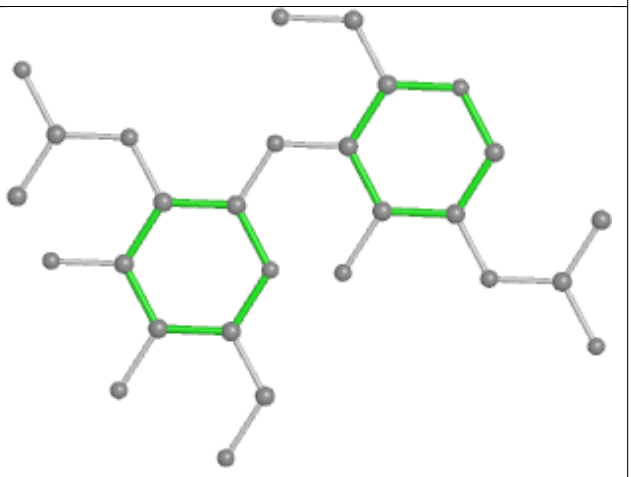
Bond lengths



Bond angles

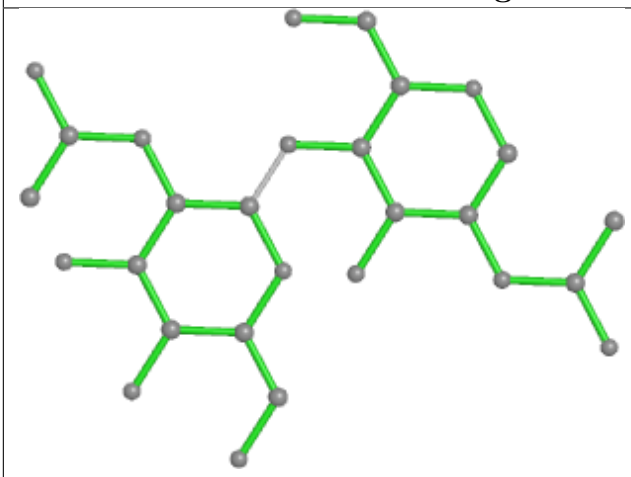


Torsions

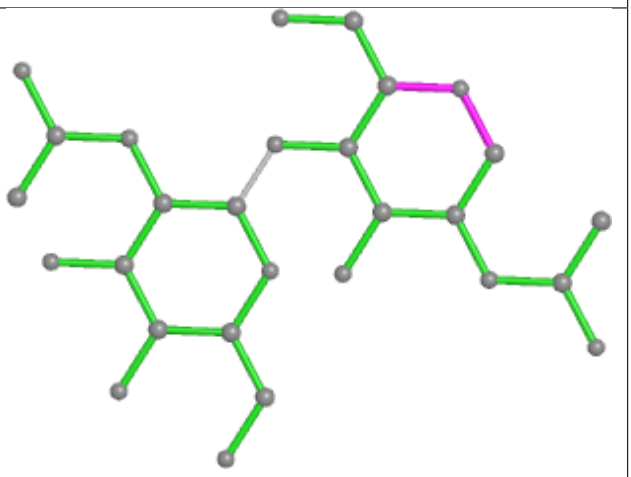


Rings

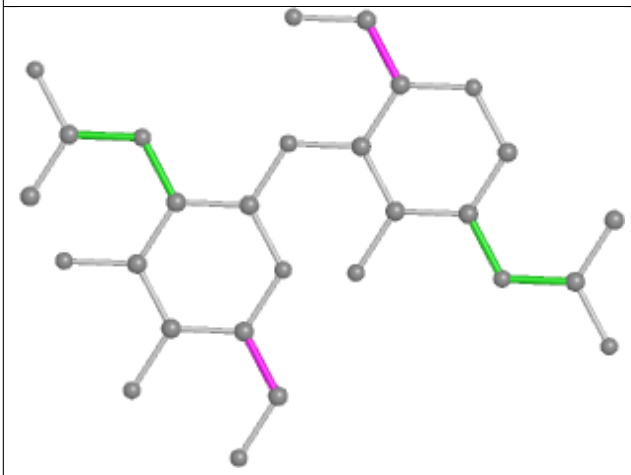
Oligosaccharide Chain R



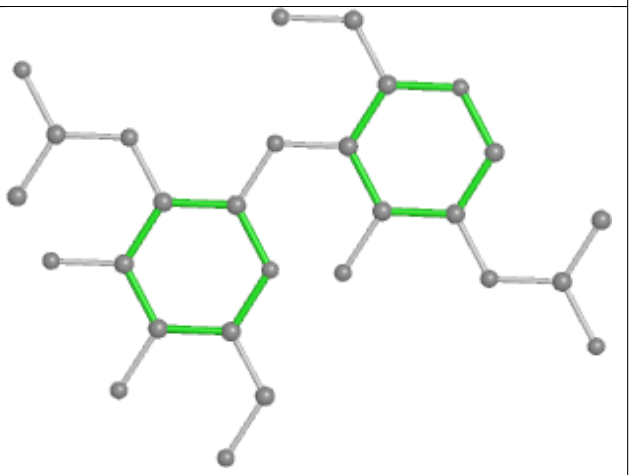
Bond lengths



Bond angles

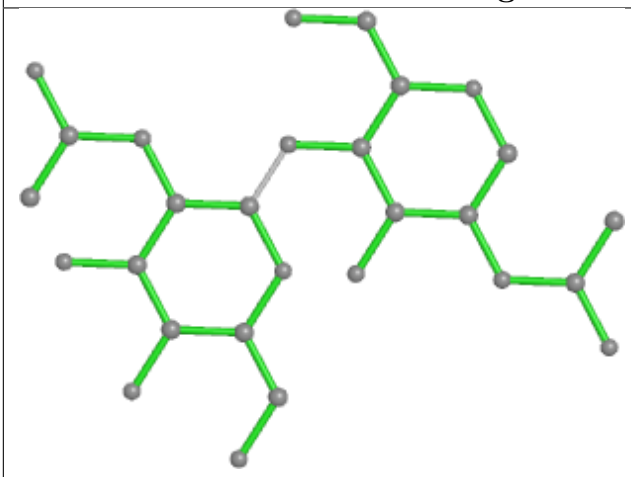


Torsions

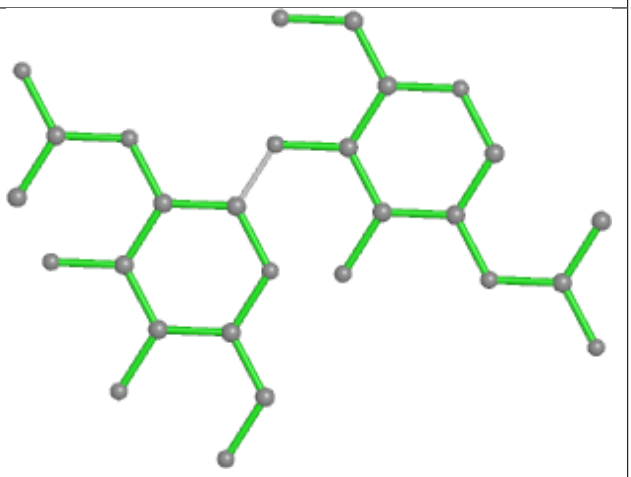


Rings

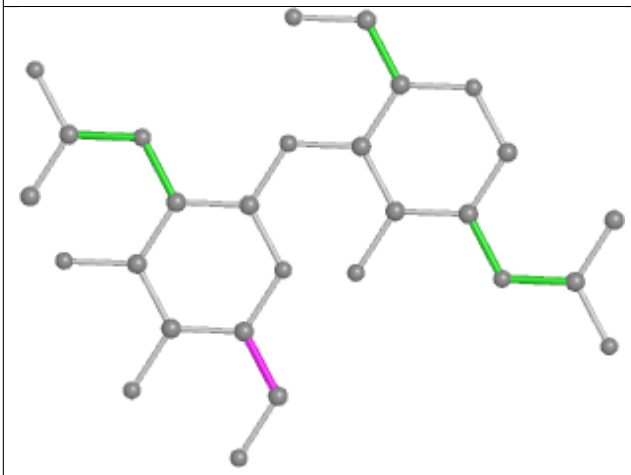
Oligosaccharide Chain S



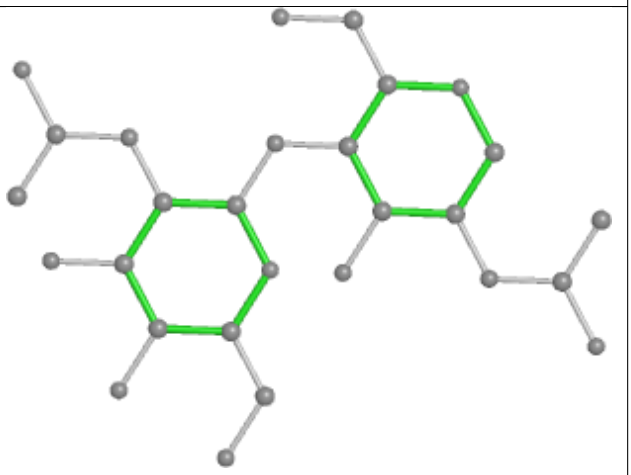
Bond lengths



Bond angles

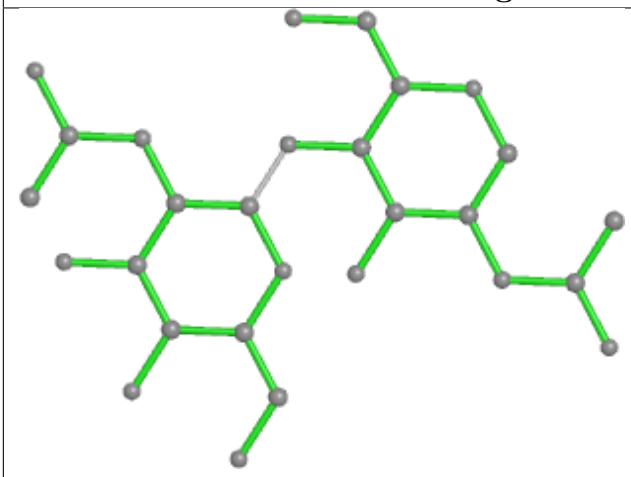


Torsions

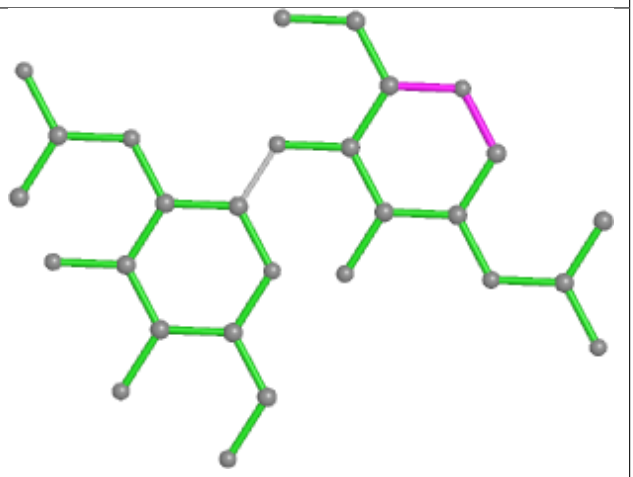


Rings

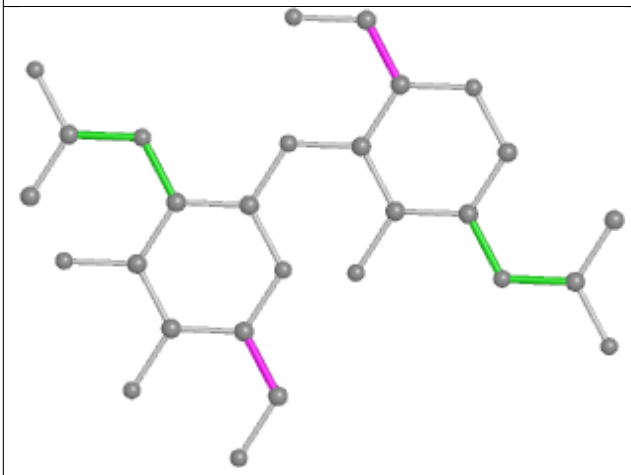
Oligosaccharide Chain T



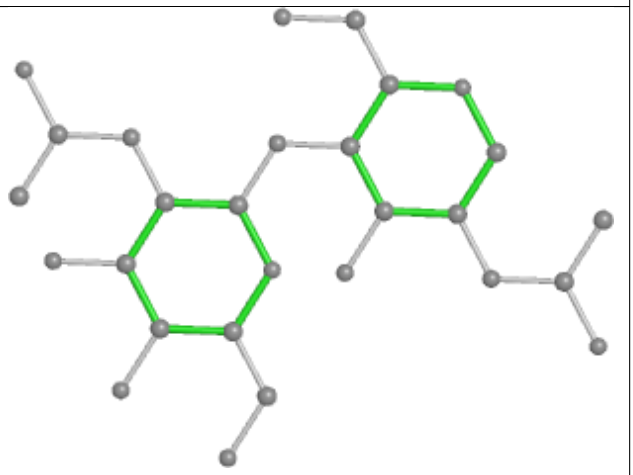
Bond lengths



Bond angles

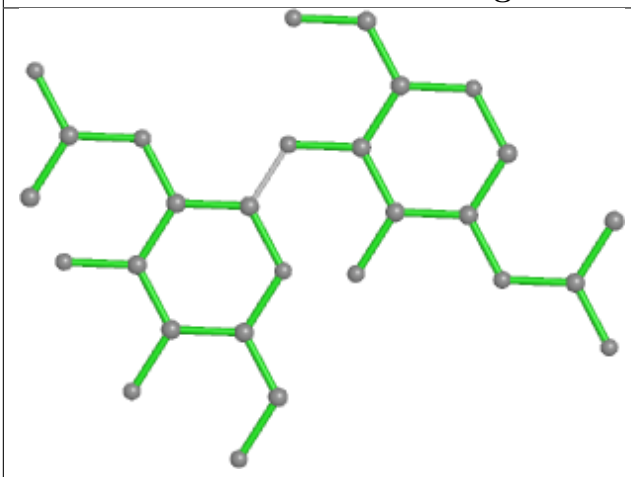


Torsions

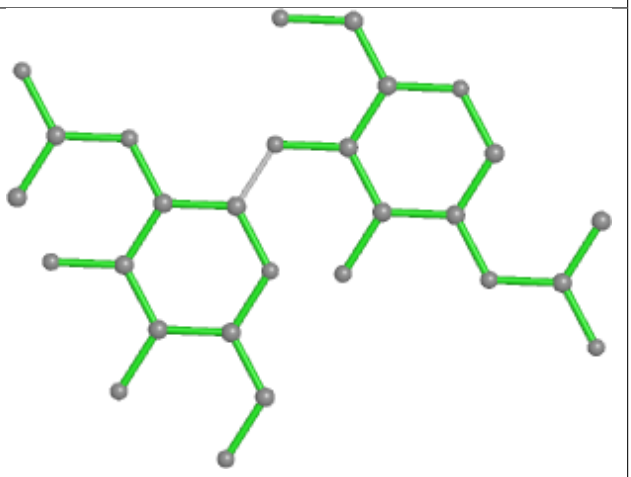


Rings

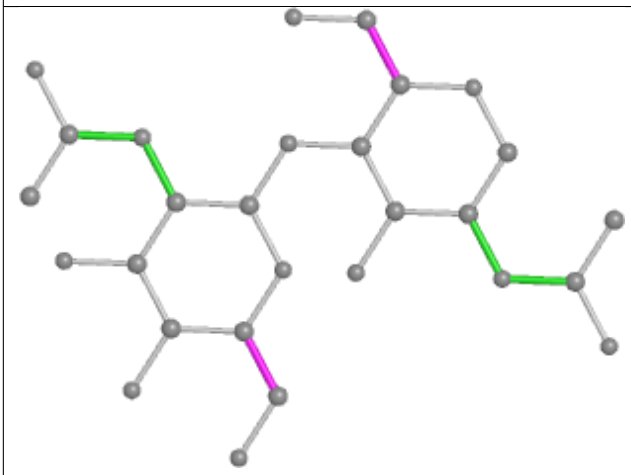
Oligosaccharide Chain U



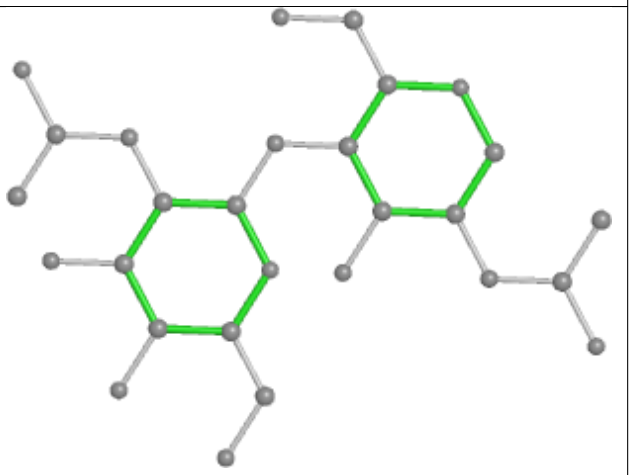
Bond lengths



Bond angles

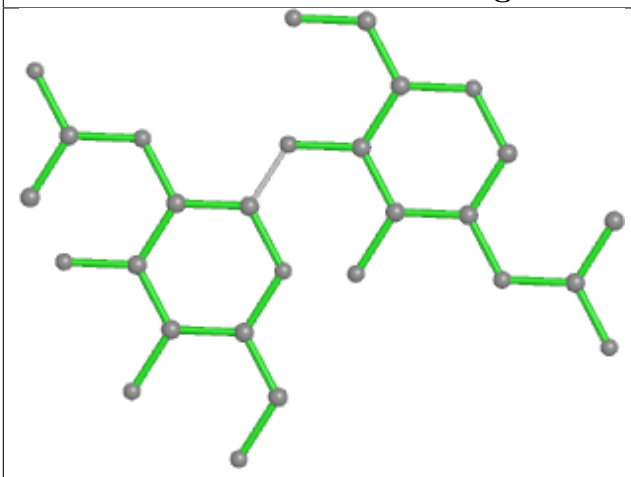


Torsions

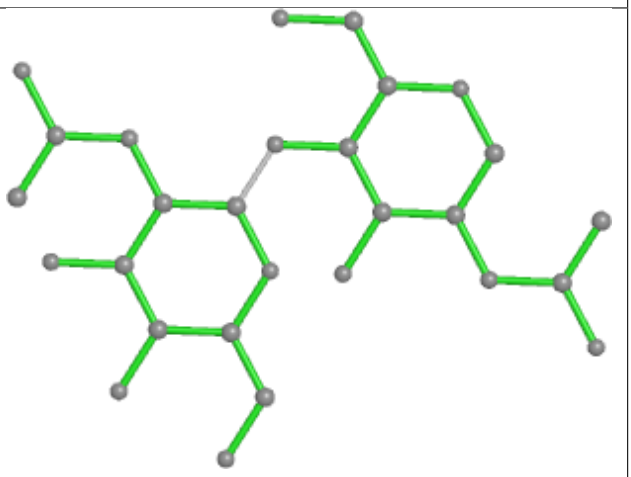


Rings

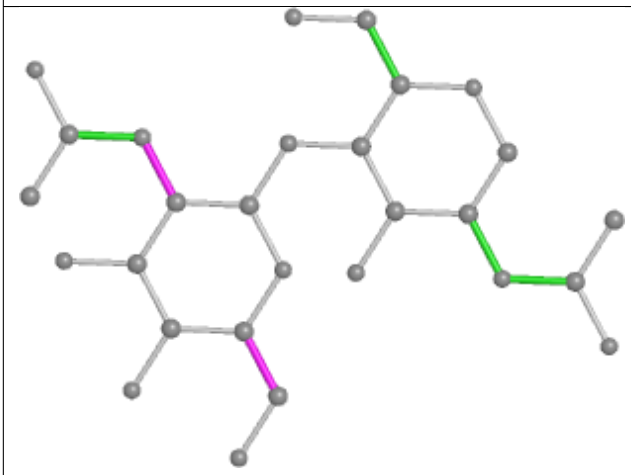
Oligosaccharide Chain V



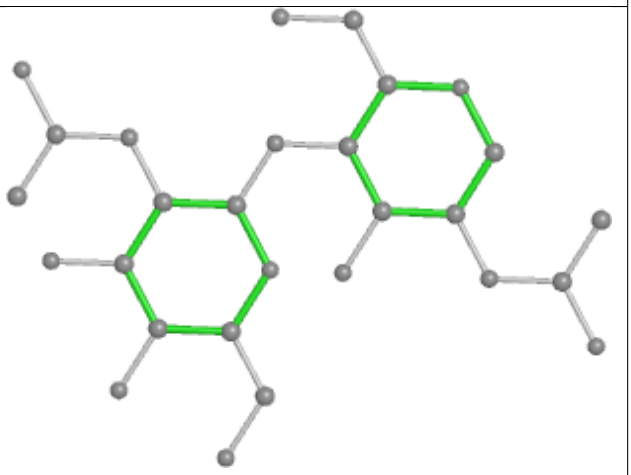
Bond lengths



Bond angles

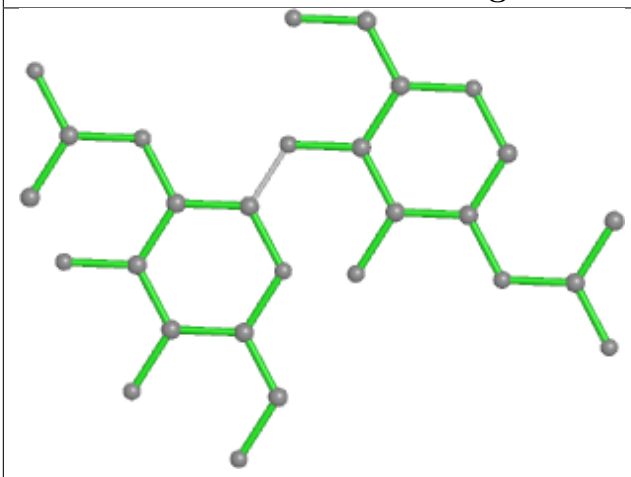


Torsions

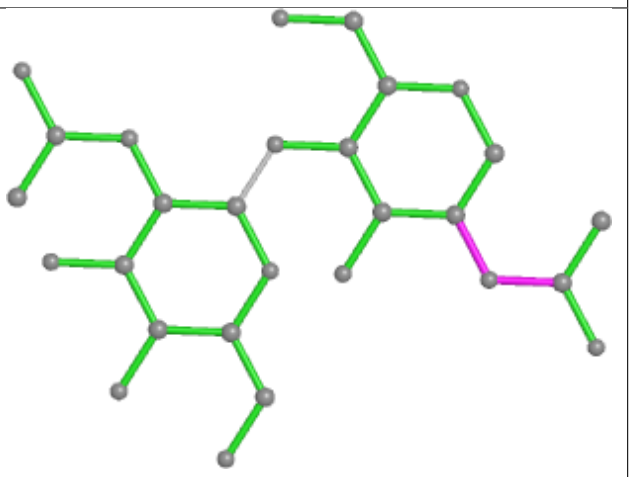


Rings

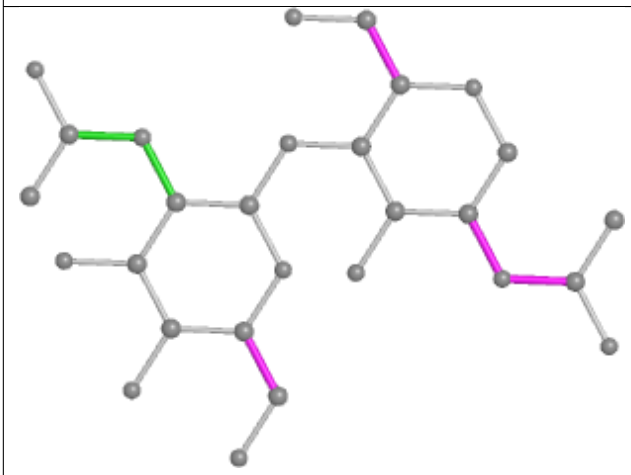
Oligosaccharide Chain W



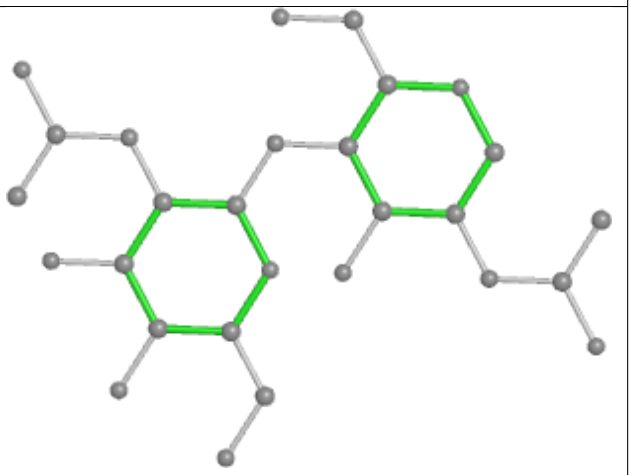
Bond lengths



Bond angles

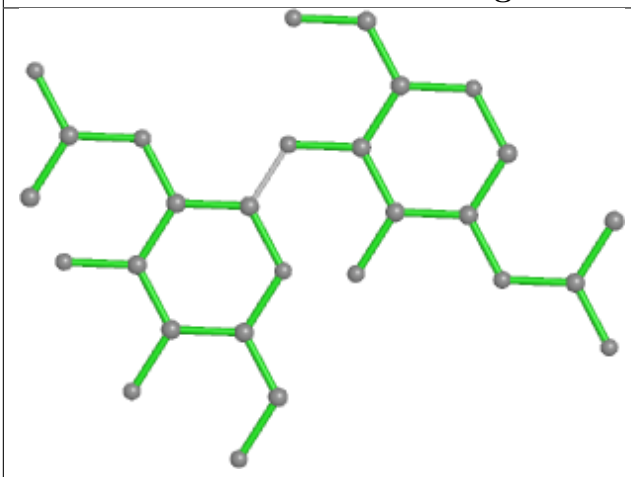


Torsions

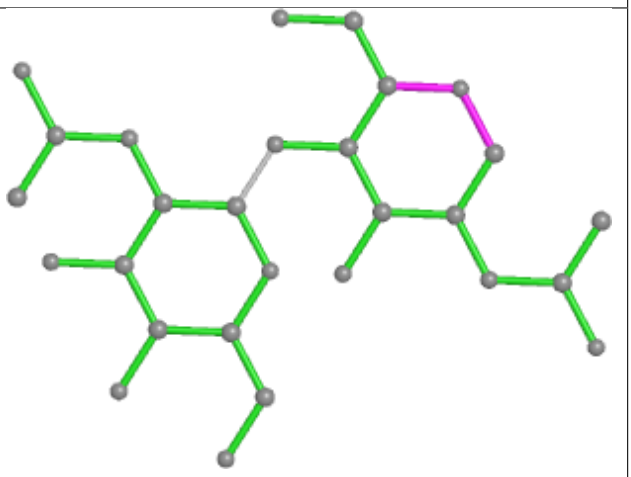


Rings

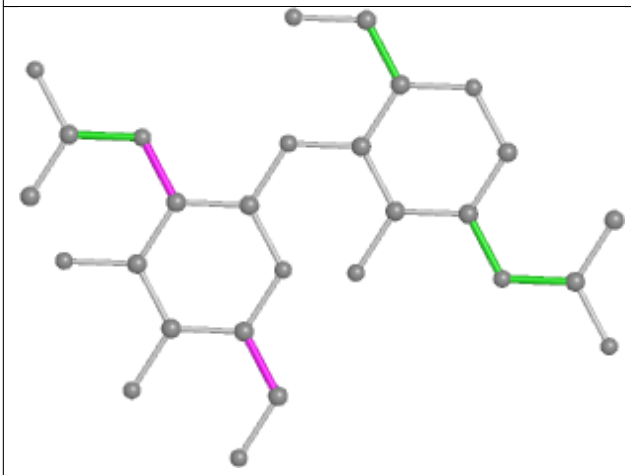
Oligosaccharide Chain X



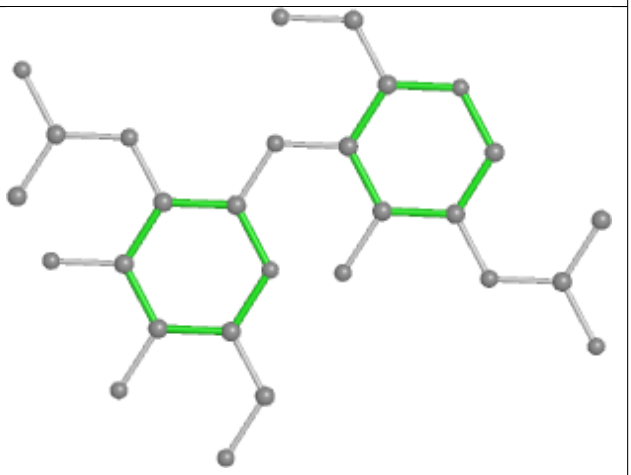
Bond lengths



Bond angles

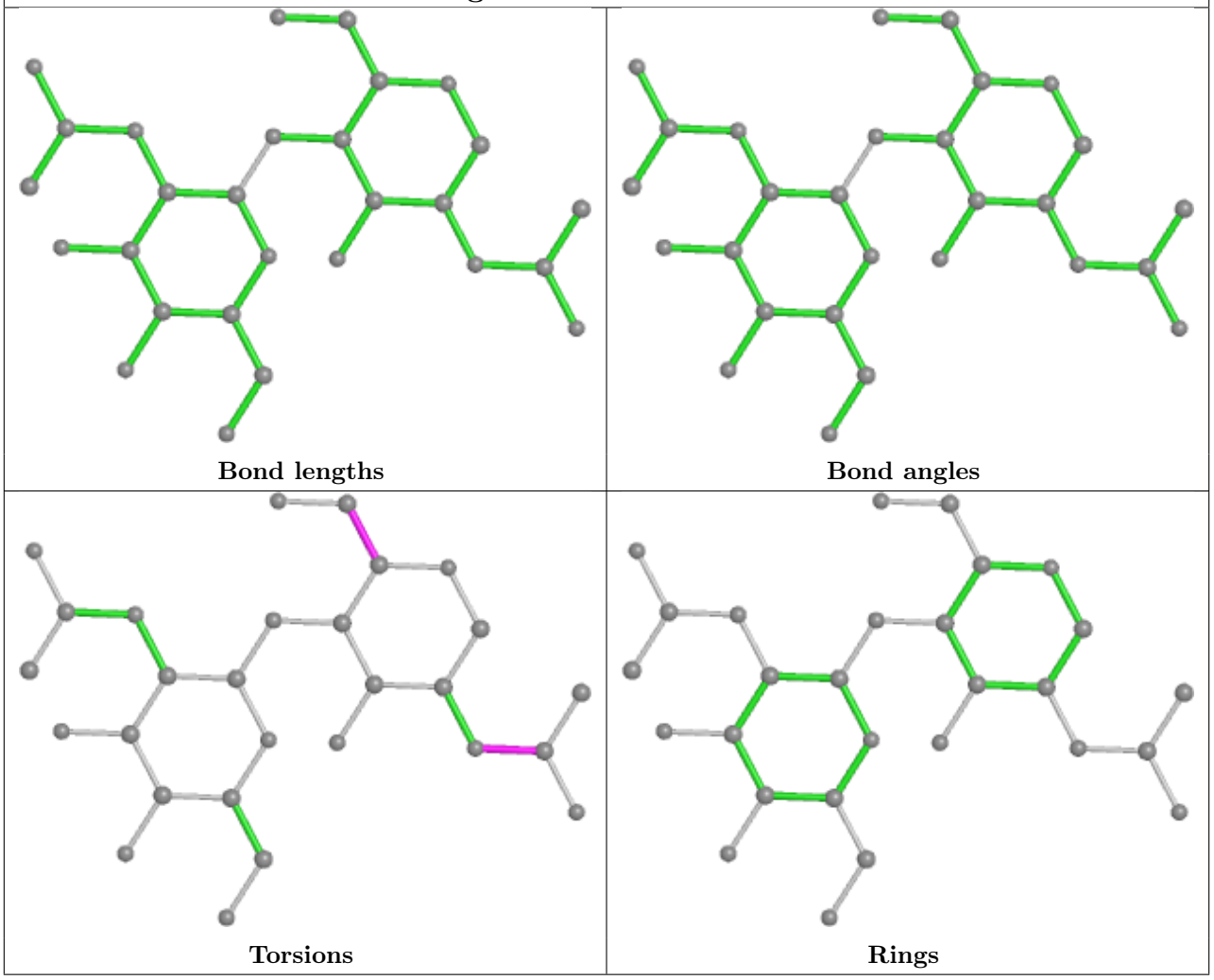


Torsions



Rings

Oligosaccharide Chain Y



5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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	$\#\|Z\| > 2$
4	NAG	A	1301	1	14,14,15	0.40	0	17,19,21	0.38	0
4	NAG	E	702	2	14,14,15	0.39	0	17,19,21	0.41	0
4	NAG	E	703	2	14,14,15	0.58	0	17,19,21	1.30	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1305	1	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	B	1302	1	14,14,15	0.75	1 (7%)	17,19,21	0.53	0
4	NAG	E	701	2	14,14,15	0.92	1 (7%)	17,19,21	0.76	1 (5%)
4	NAG	B	1301	1	14,14,15	0.17	0	17,19,21	0.56	0
4	NAG	B	1304	1	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	C	1304	1	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	A	1304	1	14,14,15	0.27	0	17,19,21	0.50	0
4	NAG	C	1307	1	14,14,15	0.97	2 (14%)	17,19,21	0.80	1 (5%)
4	NAG	C	1306	1	14,14,15	0.40	0	17,19,21	0.45	0
4	NAG	C	1302	1	14,14,15	0.44	0	17,19,21	0.64	0
4	NAG	B	1306	1	14,14,15	0.92	1 (7%)	17,19,21	1.41	1 (5%)
4	NAG	B	1305	1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	B	1307	1	14,14,15	0.29	0	17,19,21	0.52	0
4	NAG	B	1308	1	14,14,15	0.69	1 (7%)	17,19,21	0.57	0
4	NAG	A	1302	1	14,14,15	0.42	0	17,19,21	0.59	0
4	NAG	C	1301	1	14,14,15	0.61	0	17,19,21	1.03	1 (5%)
4	NAG	B	1309	1	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.54	0
4	NAG	C	1303	1	14,14,15	0.32	0	17,19,21	0.82	1 (5%)
4	NAG	A	1303	1	14,14,15	0.48	0	17,19,21	0.59	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
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	E	702	2	-	2/6/23/26	0/1/1/1
4	NAG	E	703	2	-	5/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	E	701	2	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1306	NAG	O5-C1	3.32	1.49	1.43
4	E	701	NAG	O5-C1	2.67	1.48	1.43
4	B	1302	NAG	O5-C1	2.66	1.48	1.43
4	C	1307	NAG	O5-C1	2.66	1.48	1.43
4	C	1307	NAG	C1-C2	2.34	1.55	1.52
4	B	1308	NAG	O5-C1	-2.27	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1306	NAG	C1-O5-C5	5.49	119.63	112.19
4	E	703	NAG	C2-N2-C7	4.40	129.16	122.90
4	C	1301	NAG	C1-O5-C5	3.74	117.26	112.19
4	C	1303	NAG	C1-O5-C5	2.90	116.12	112.19
4	C	1307	NAG	C1-O5-C5	2.64	115.76	112.19
4	E	701	NAG	C1-O5-C5	2.61	115.72	112.19

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	NAG	C4-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1302	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	E	703	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	B	1305	NAG	C8-C7-N2-C2
4	B	1305	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	E	702	NAG	C8-C7-N2-C2
4	E	702	NAG	O7-C7-N2-C2
4	E	703	NAG	C8-C7-N2-C2
4	E	703	NAG	O7-C7-N2-C2
4	B	1304	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	E	701	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	E	703	NAG	C4-C5-C6-O6
4	A	1301	NAG	C1-C2-N2-C7
4	C	1306	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6

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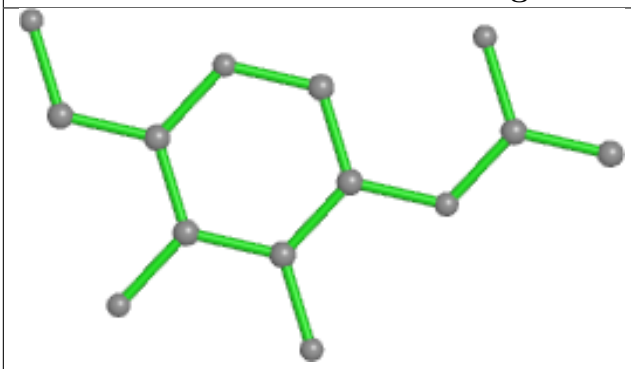
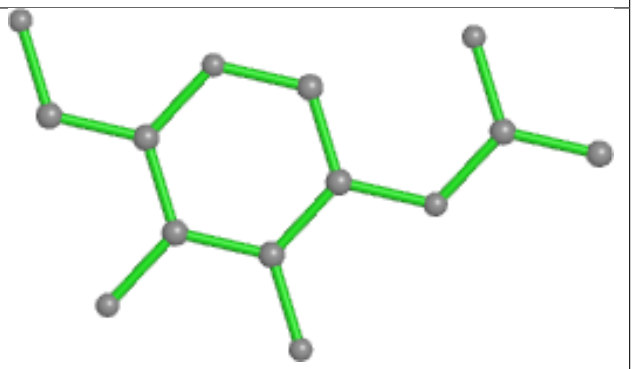
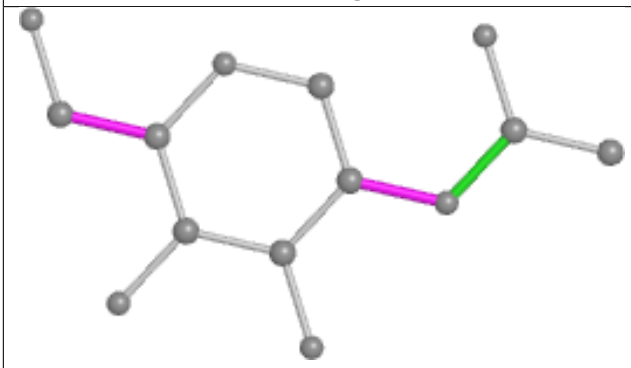
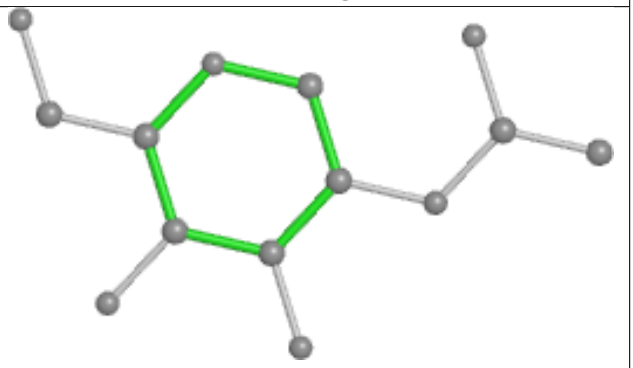
Mol	Chain	Res	Type	Atoms
4	A	1302	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	E	703	NAG	C3-C2-N2-C7
4	B	1309	NAG	C4-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	A	1301	NAG	C3-C2-N2-C7

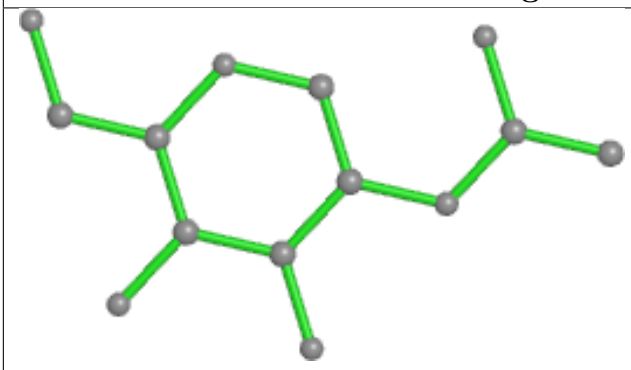
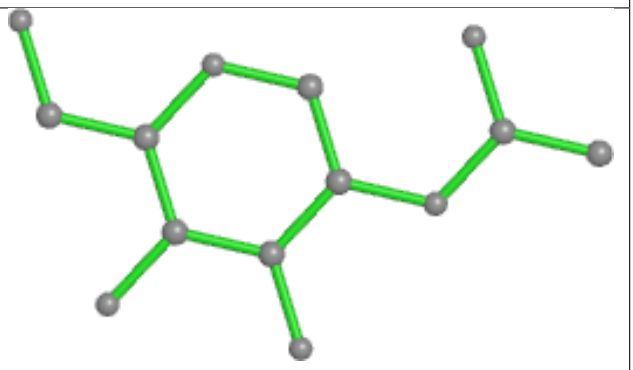
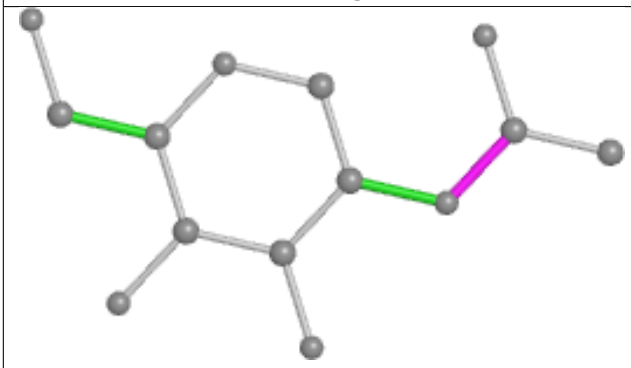
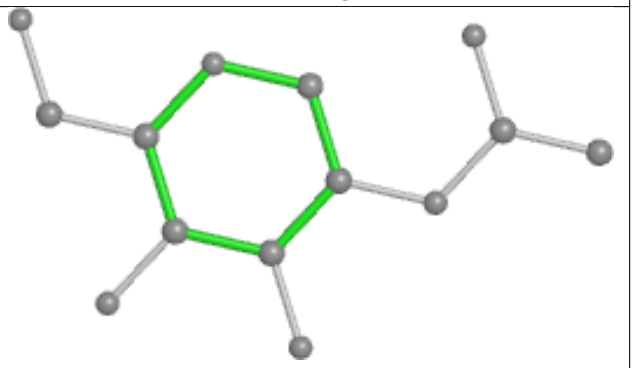
There are no ring outliers.

7 monomers are involved in 13 short contacts:

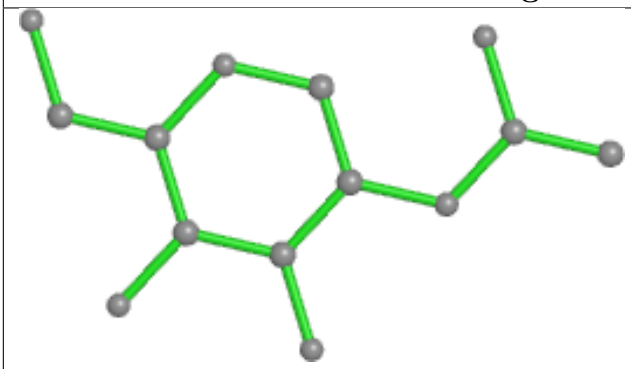
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	703	NAG	3	0
4	C	1305	NAG	2	0
4	E	701	NAG	2	0
4	C	1307	NAG	2	0
4	B	1308	NAG	1	0
4	B	1303	NAG	1	0
4	C	1303	NAG	2	0

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.

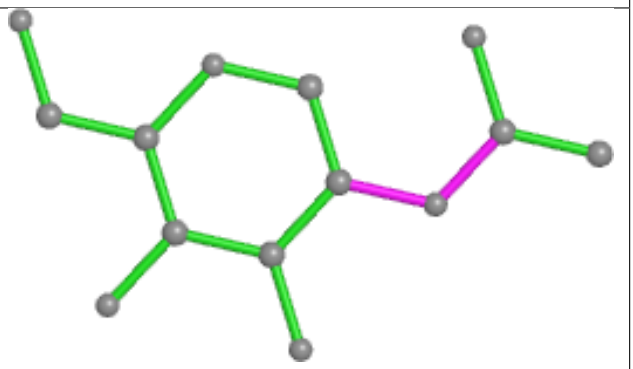
Ligand NAG A 1301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG E 702	
	
Bond lengths	Bond angles
	
Torsions	Rings

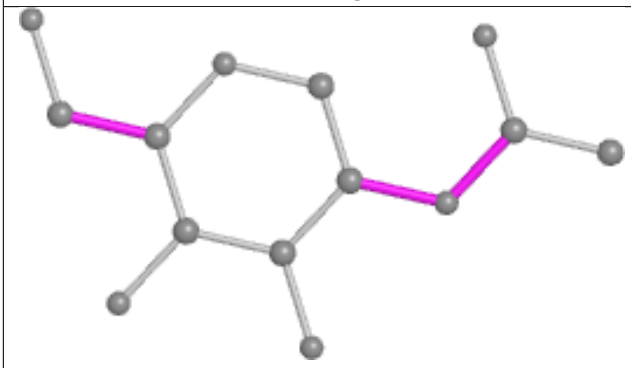
Ligand NAG E 703



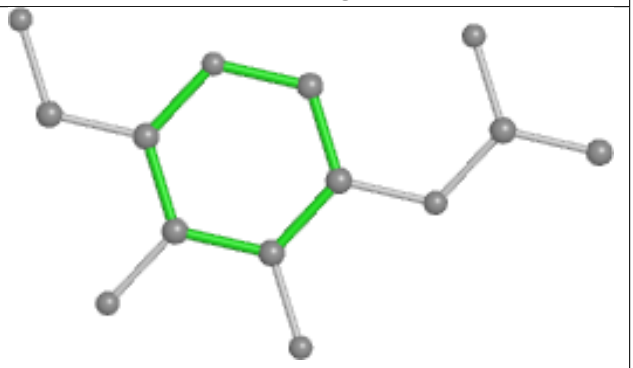
Bond lengths



Bond angles

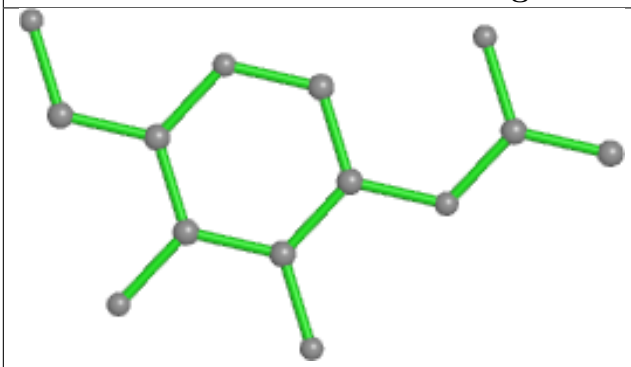


Torsions

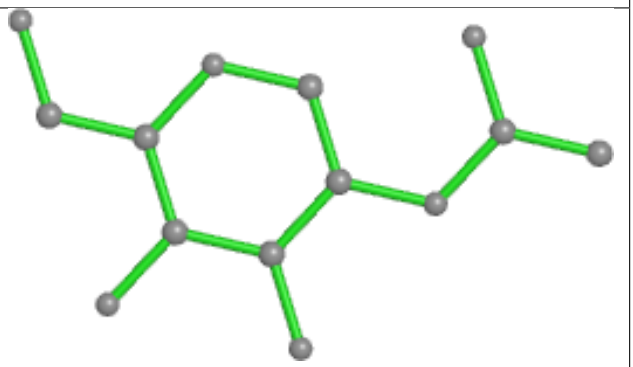


Rings

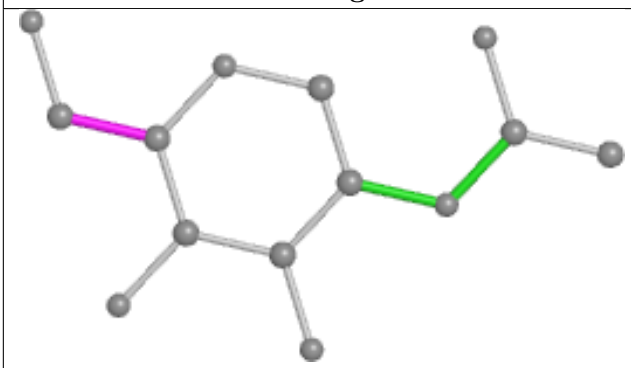
Ligand NAG C 1305



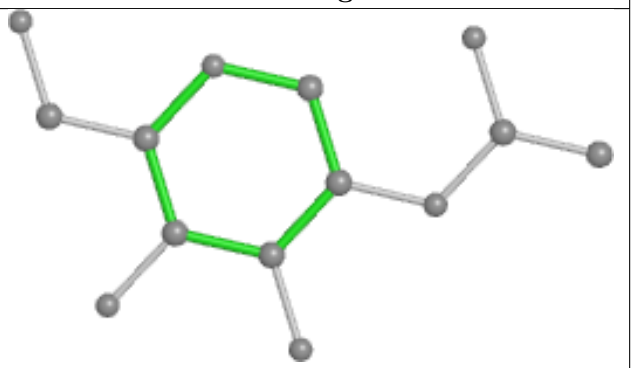
Bond lengths



Bond angles

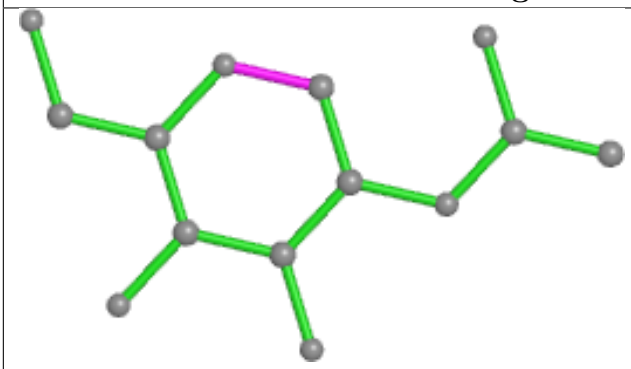


Torsions

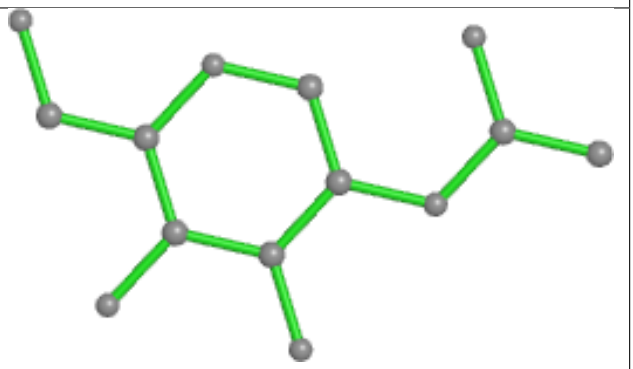


Rings

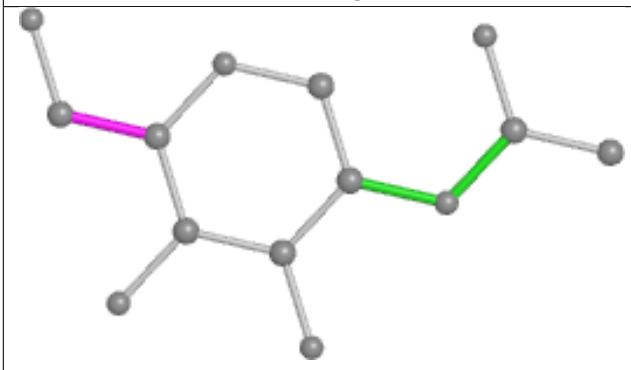
Ligand NAG B 1302



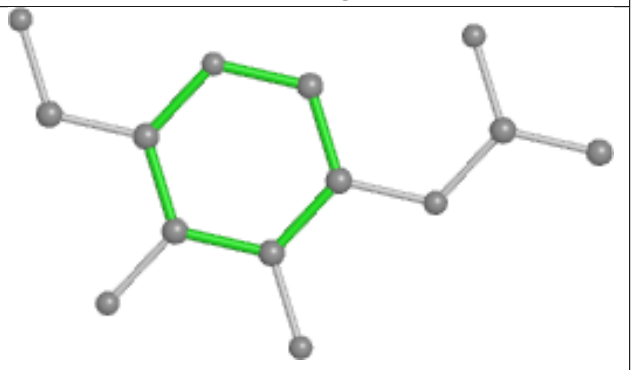
Bond lengths



Bond angles

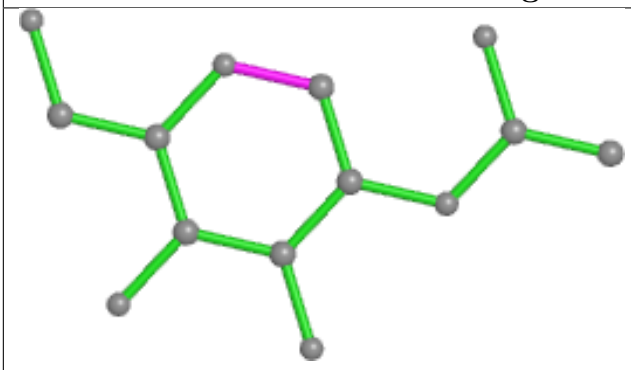


Torsions



Rings

Ligand NAG E 701



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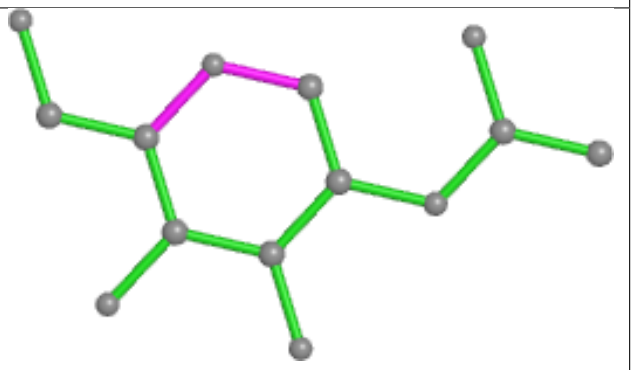
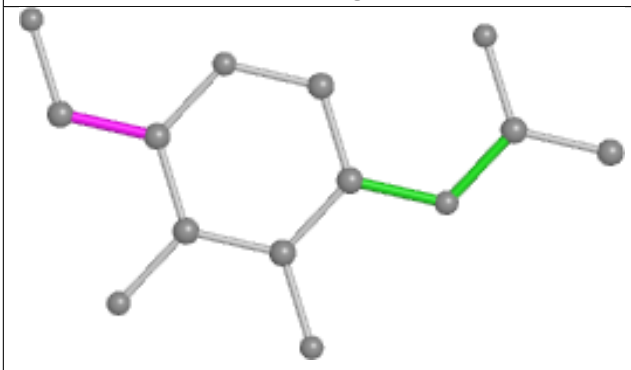


Bond angles



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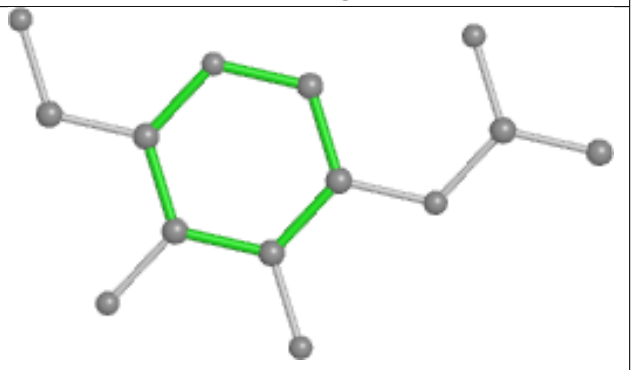
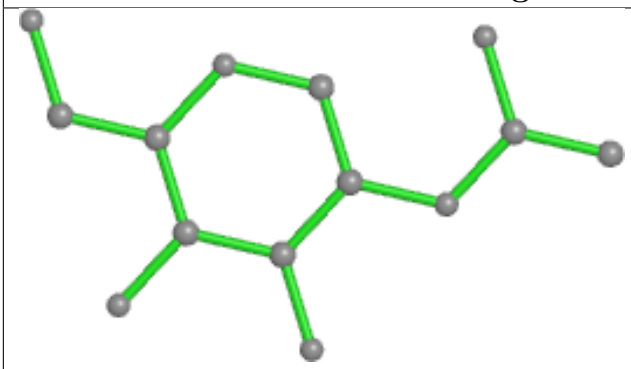


Rings

Ligand NAG B 1301



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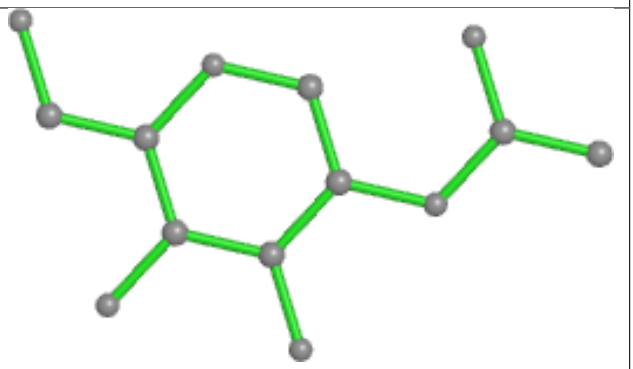
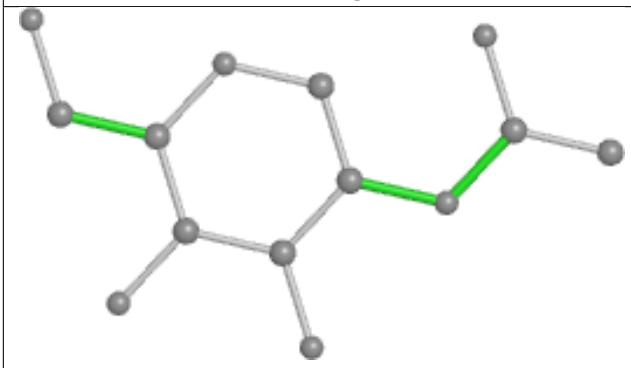


Bond angles



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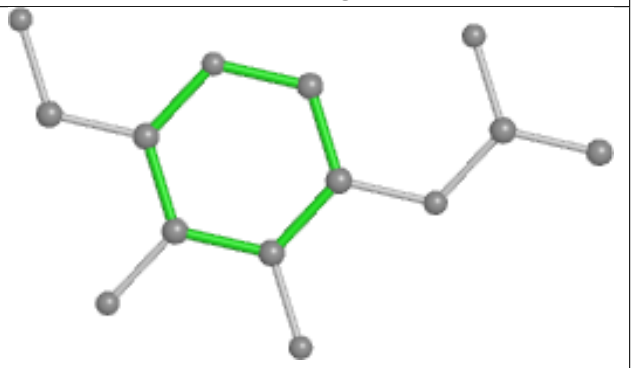
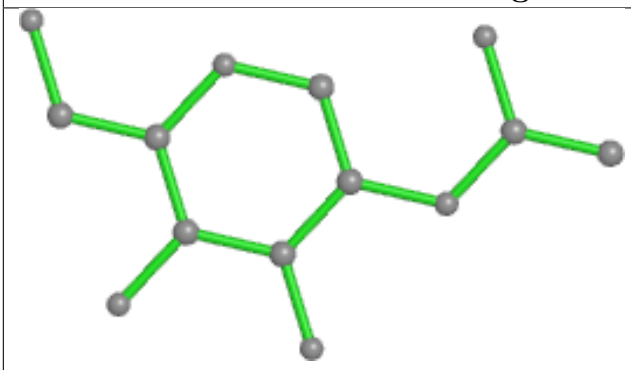


Rings

Ligand NAG B 1304



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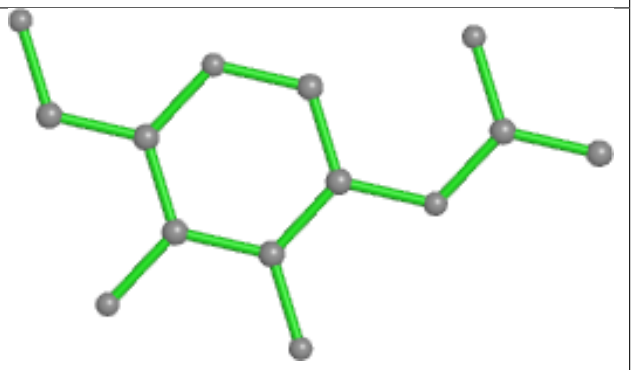
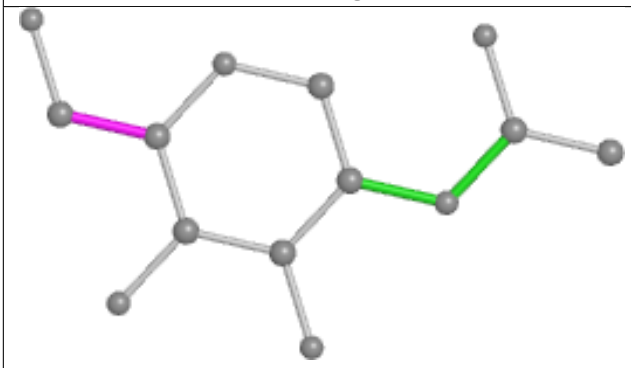
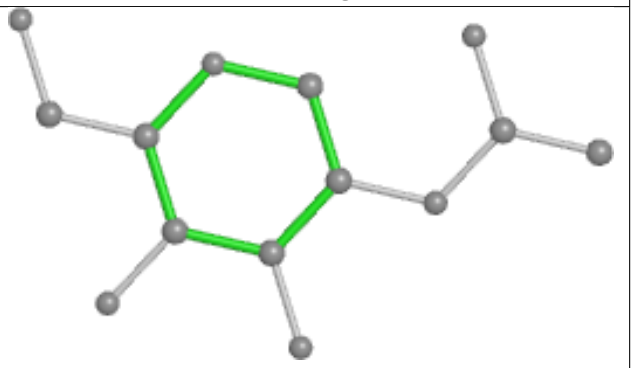


Bond angles

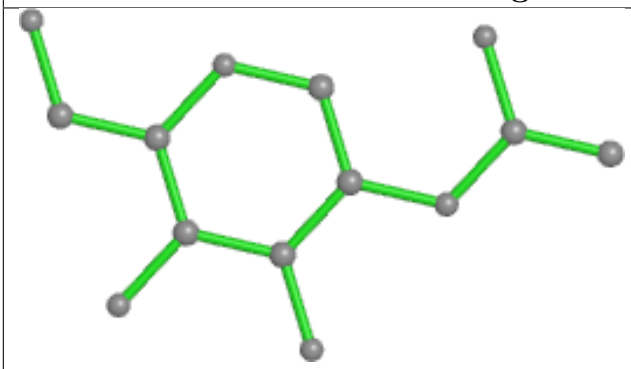


Torsions



Rings

Ligand NAG C 1304



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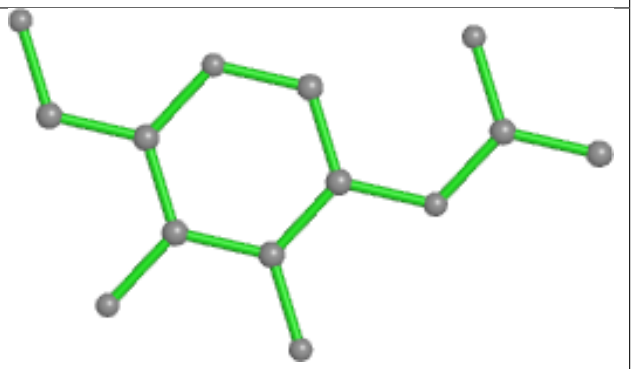
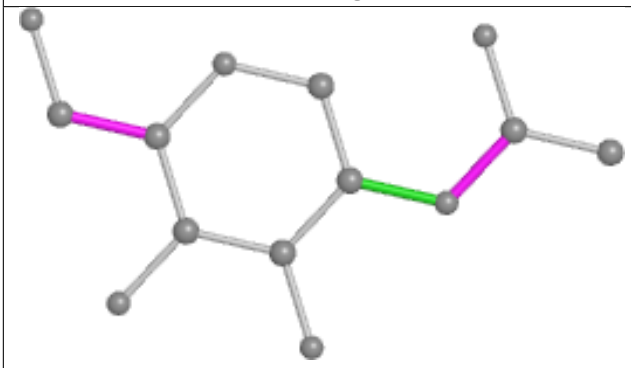
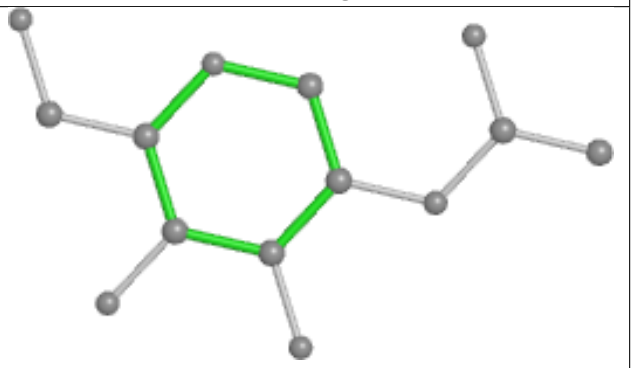


Bond angles

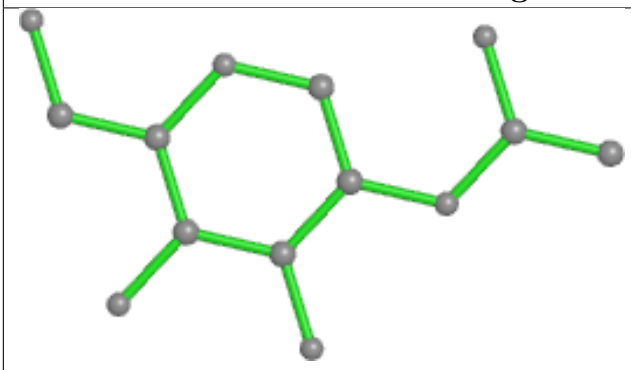


Torsions

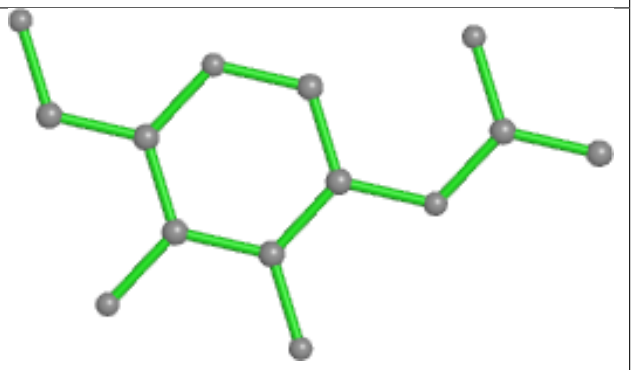


Rings

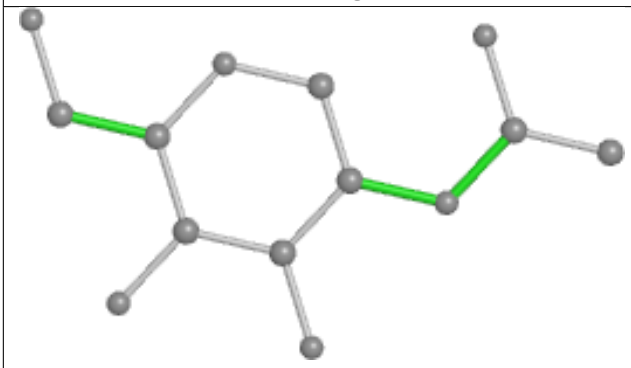
Ligand NAG A 1304



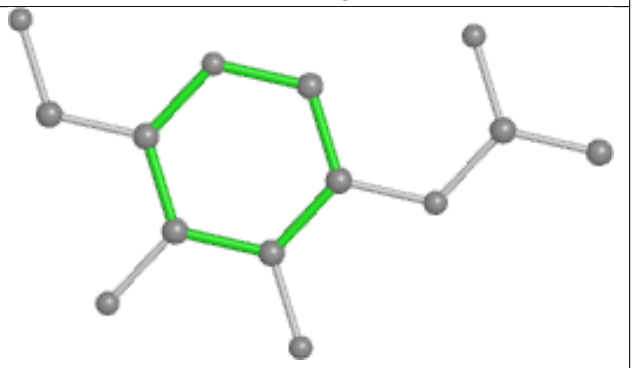
Bond lengths



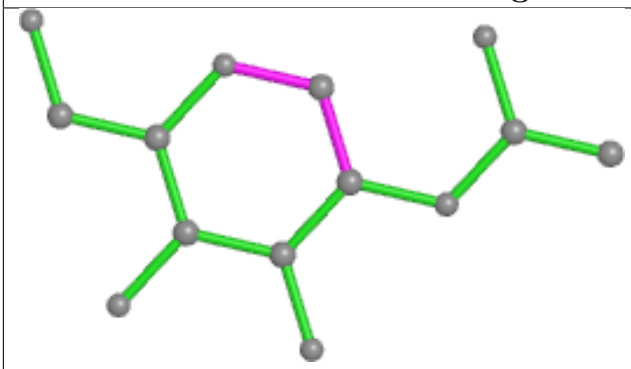
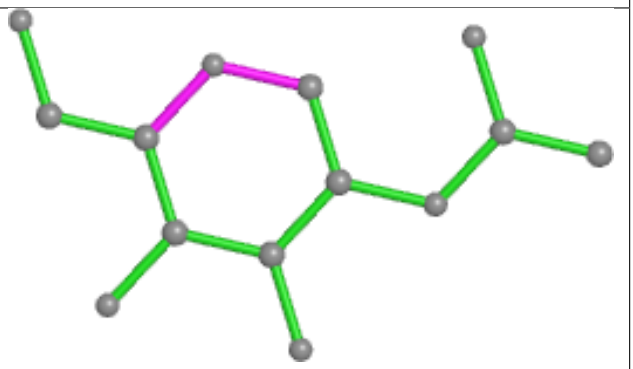
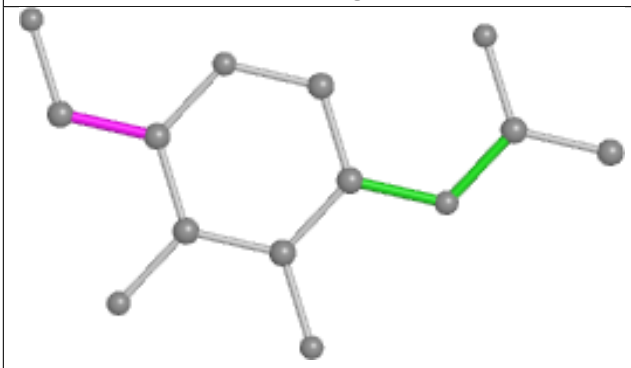
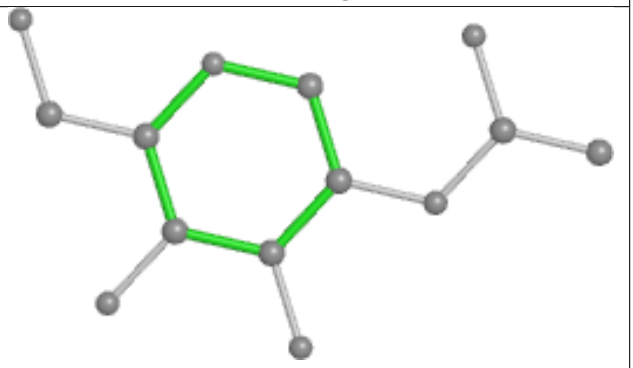
Bond angles

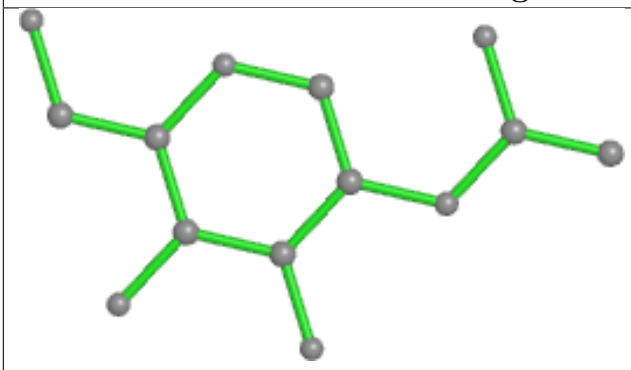
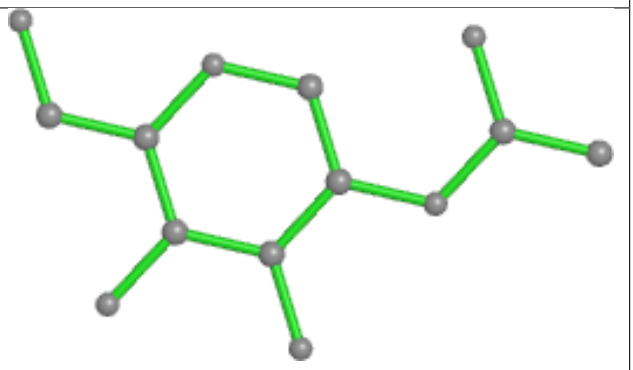
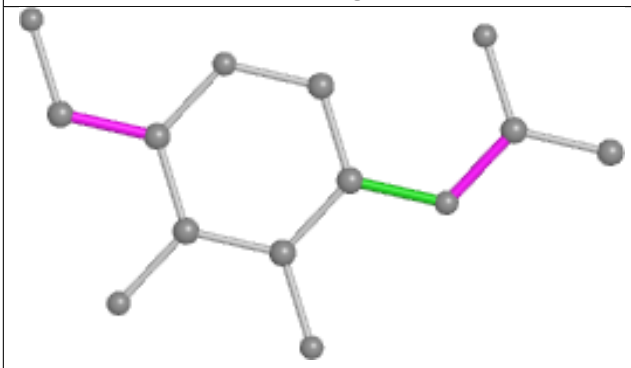
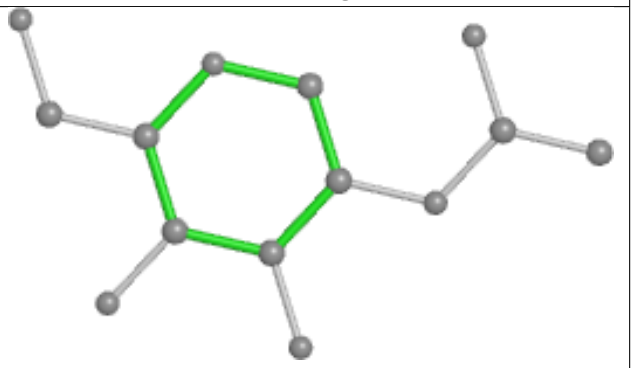


Torsions

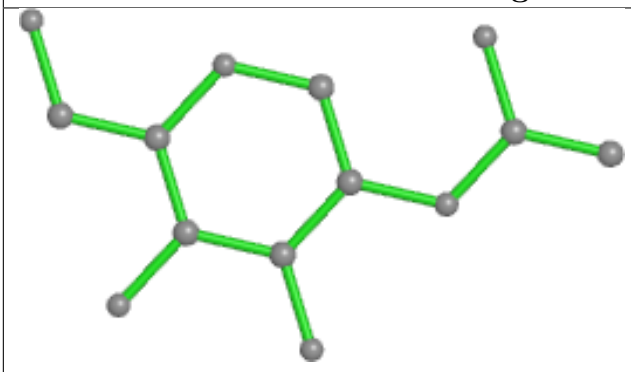


Rings

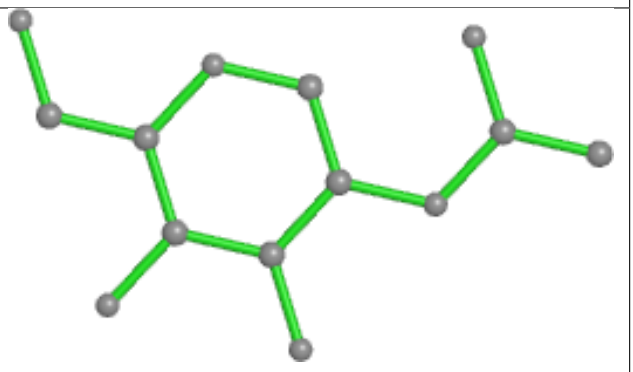
Ligand NAG C 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 1306	
 Bond lengths	 Bond angles
 Torsions	 Rings

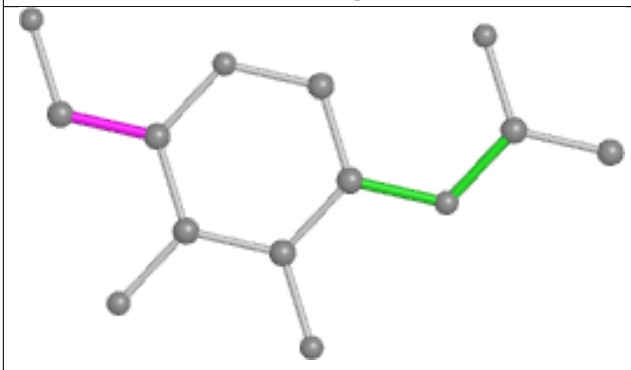
Ligand NAG C 1302



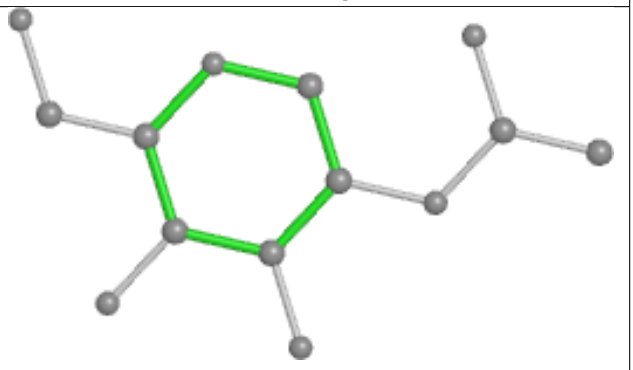
Bond lengths



Bond angles

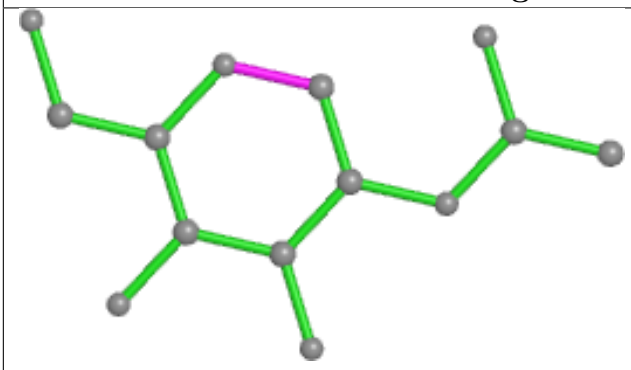


Torsions

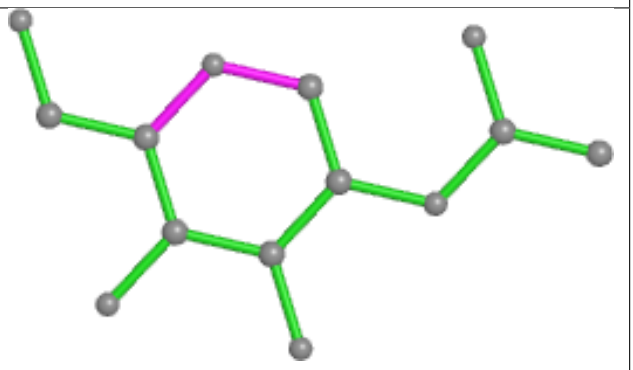


Rings

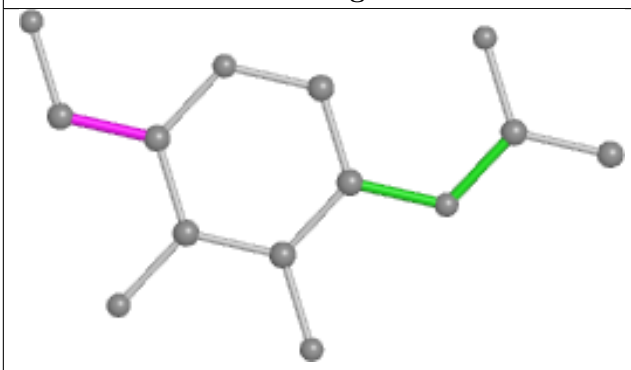
Ligand NAG B 1306



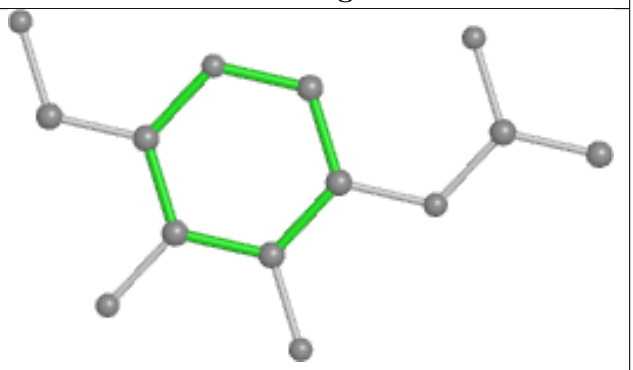
Bond lengths



Bond angles

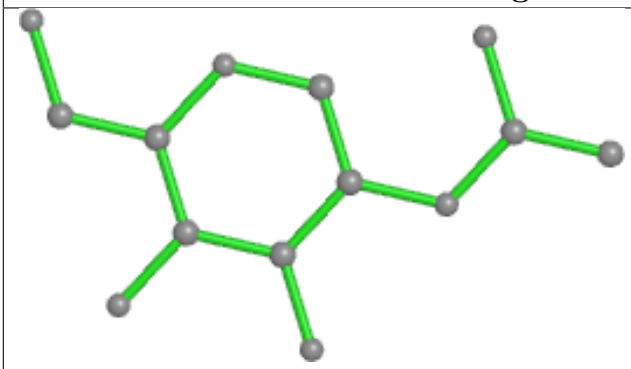


Torsions

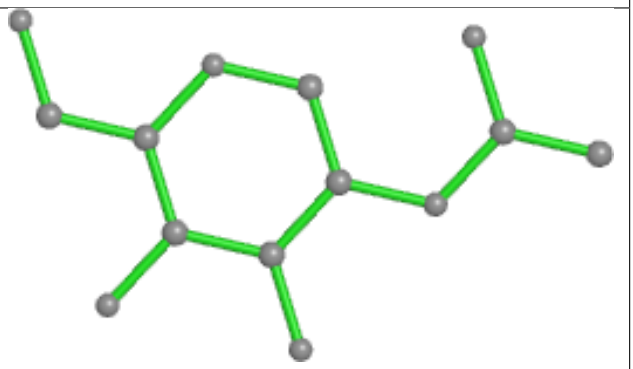


Rings

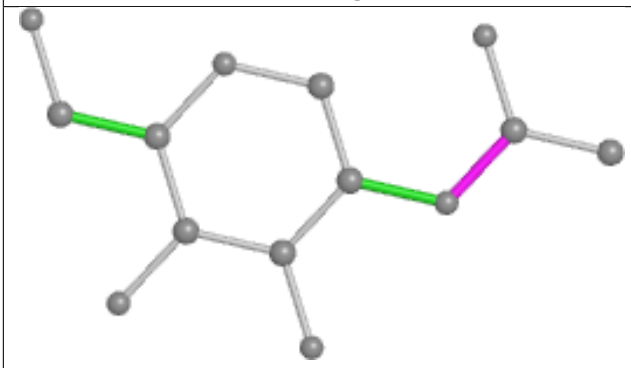
Ligand NAG B 1305



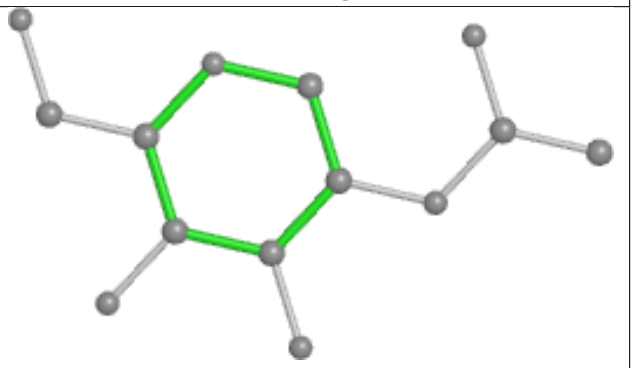
Bond lengths



Bond angles

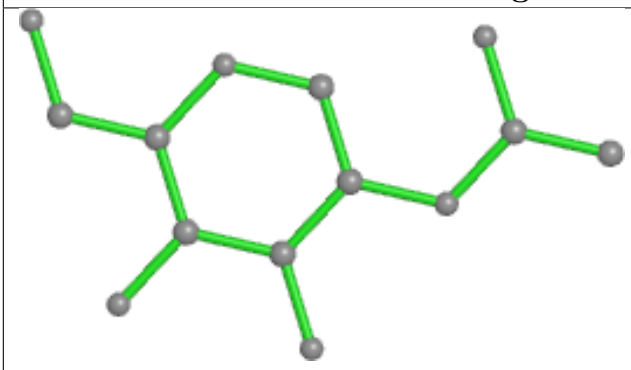


Torsions

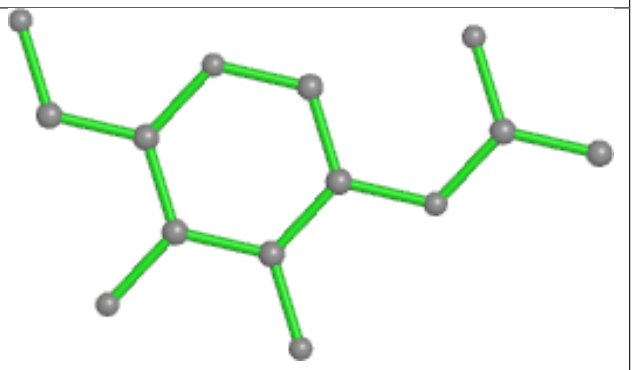


Rings

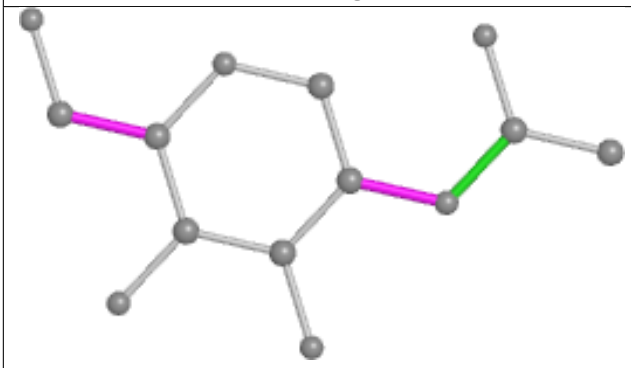
Ligand NAG B 1307



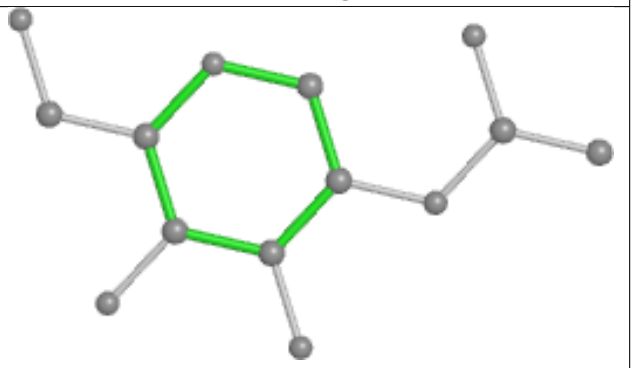
Bond lengths



Bond angles

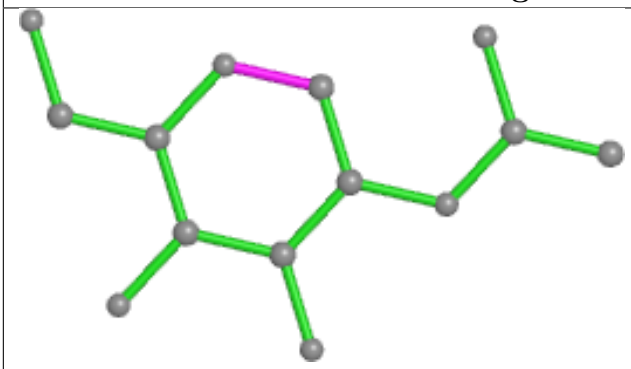


Torsions

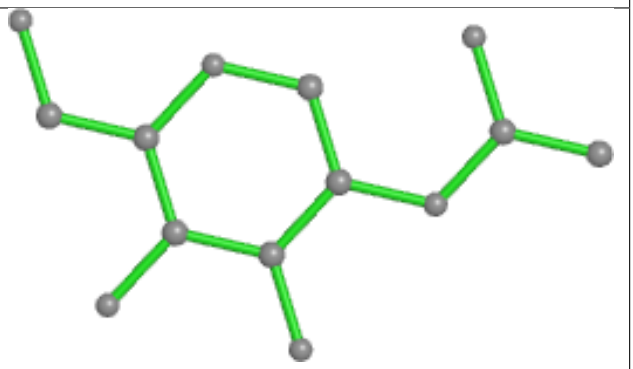


Rings

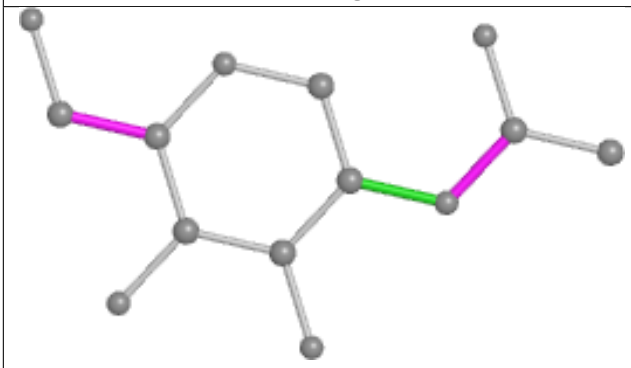
Ligand NAG B 1308



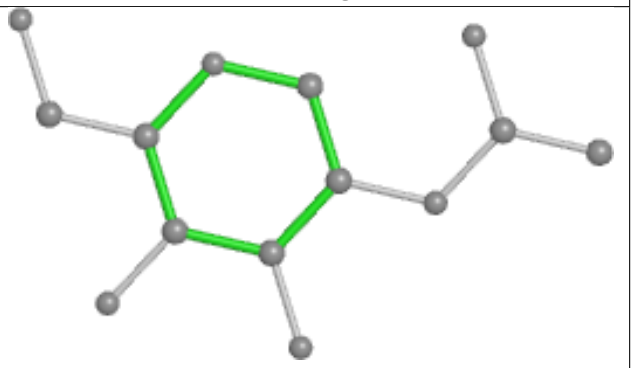
Bond lengths



Bond angles

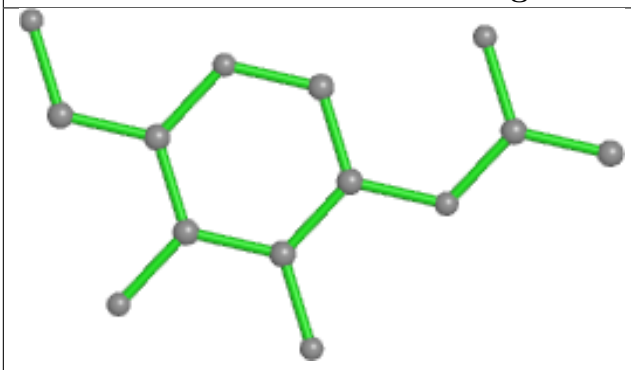


Torsions

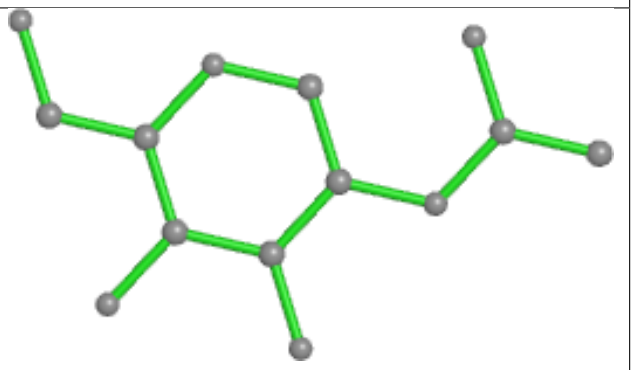


Rings

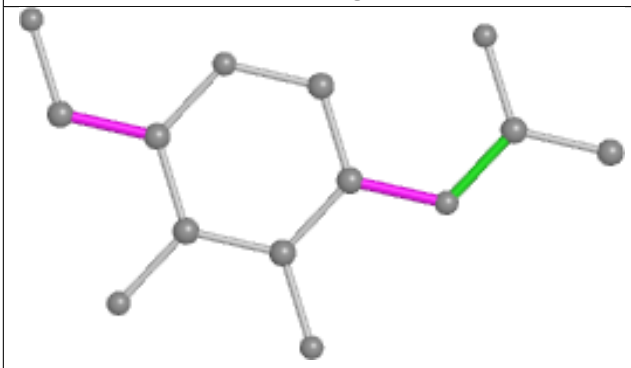
Ligand NAG A 1302



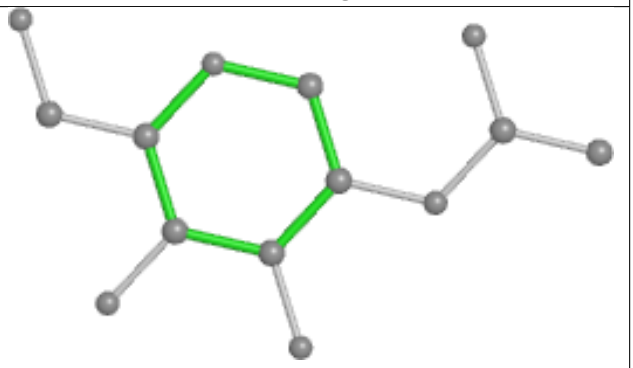
Bond lengths



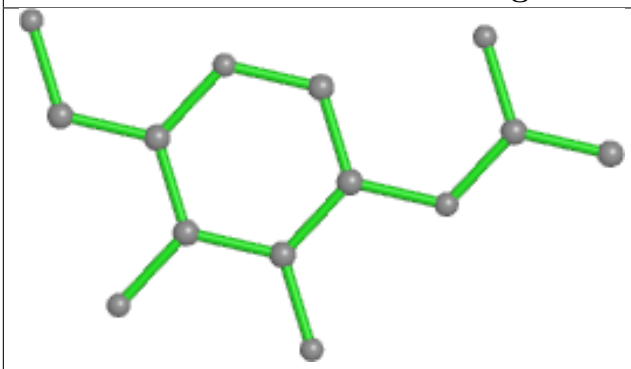
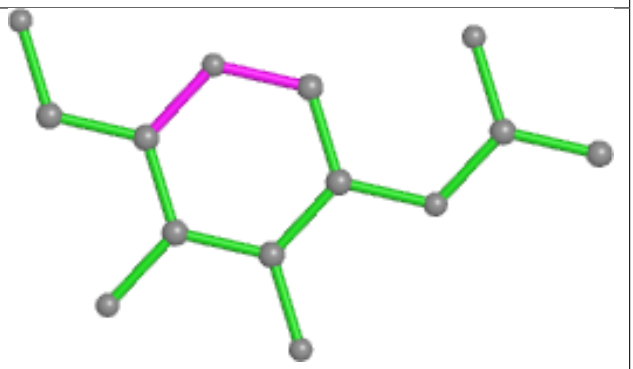
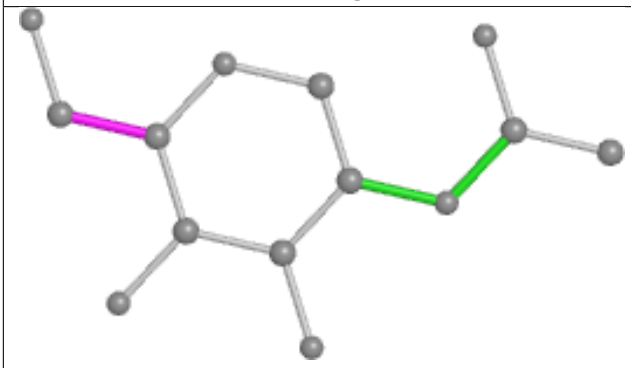
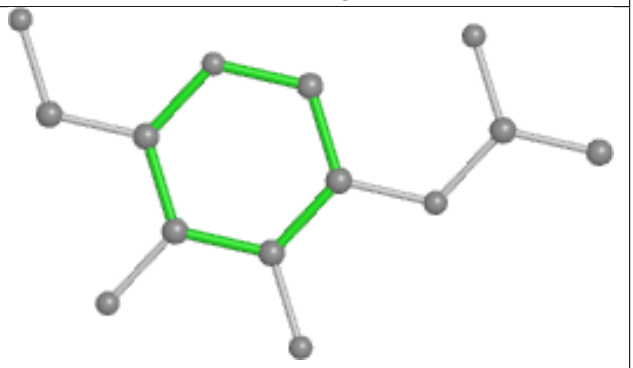
Bond angles

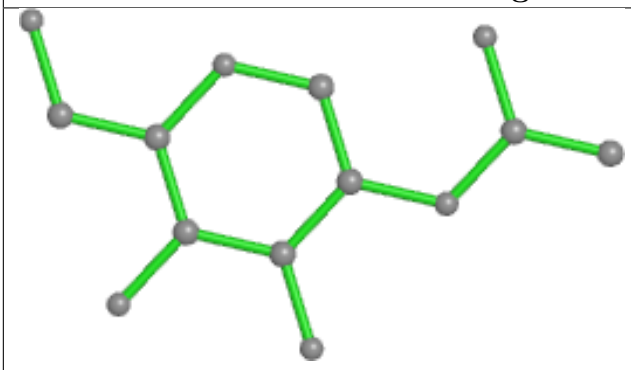
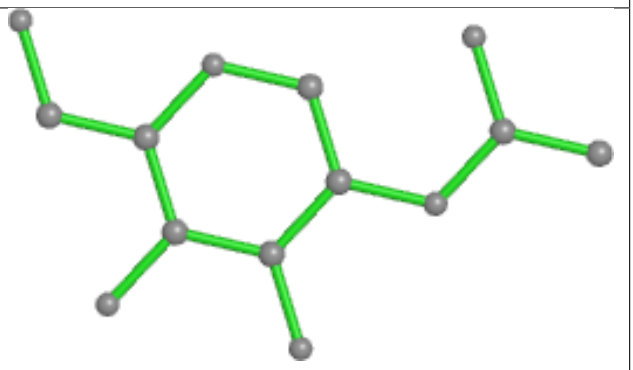
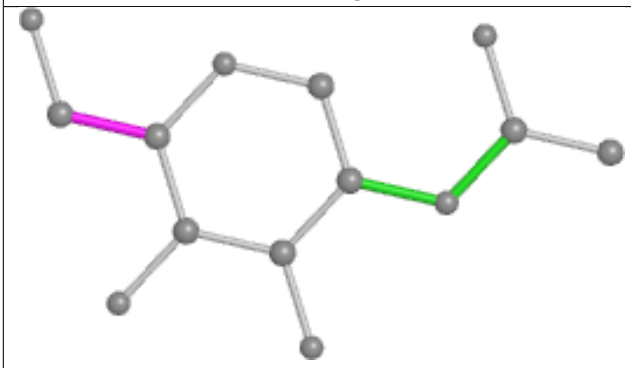
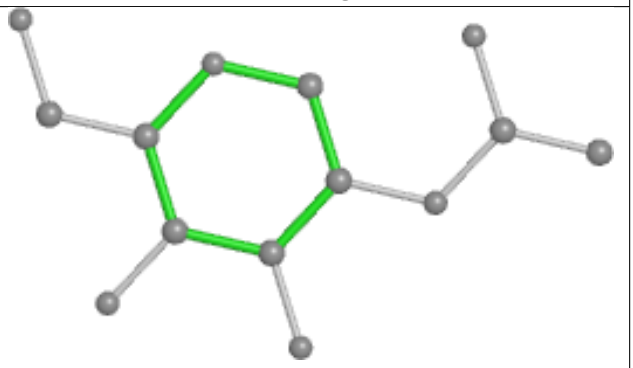


Torsions

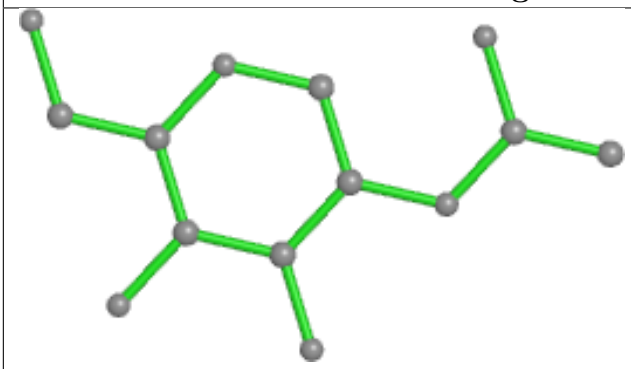


Rings

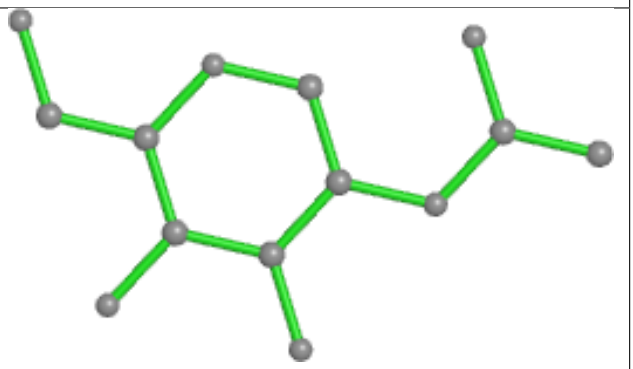
Ligand NAG C 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1309	
 Bond lengths	 Bond angles
 Torsions	 Rings

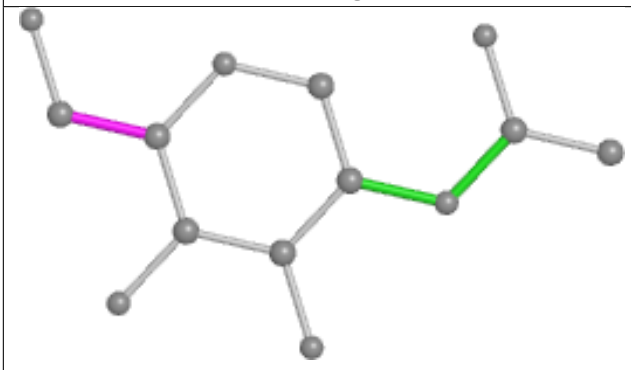
Ligand NAG B 1303



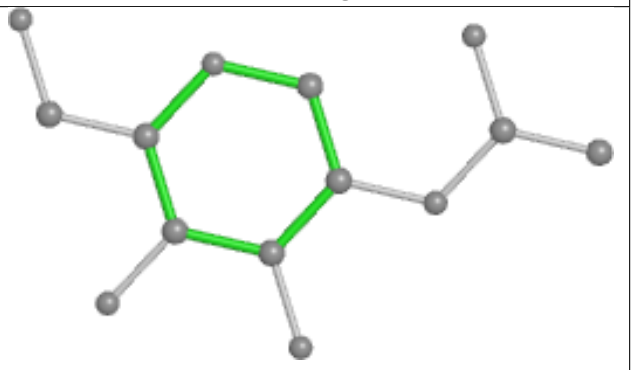
Bond lengths



Bond angles

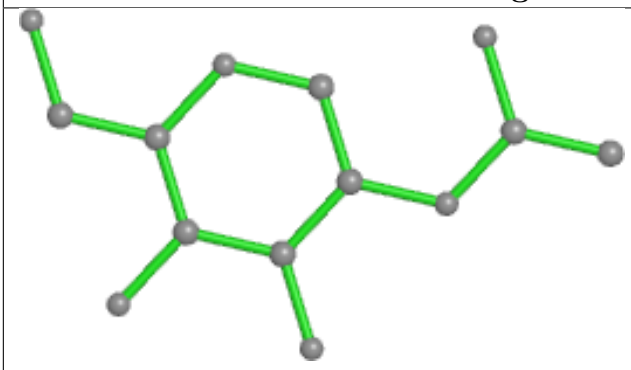


Torsions

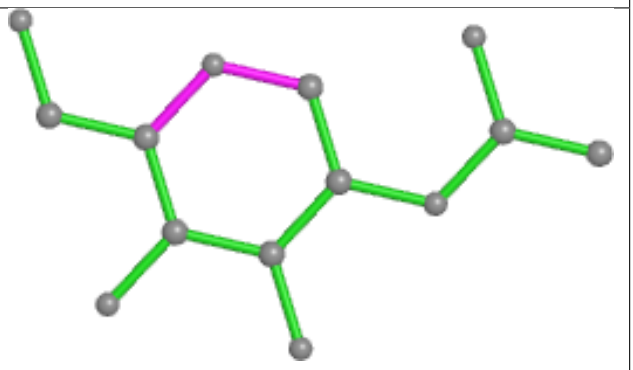


Rings

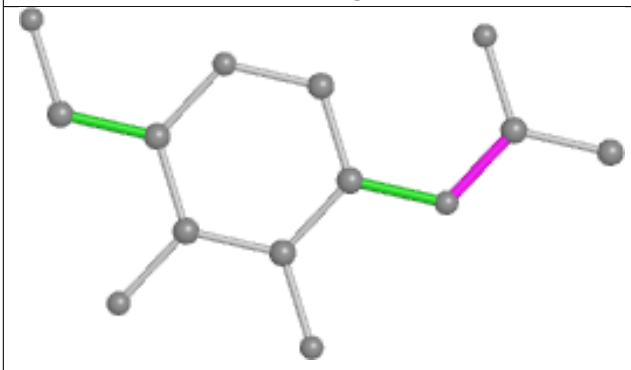
Ligand NAG C 1303



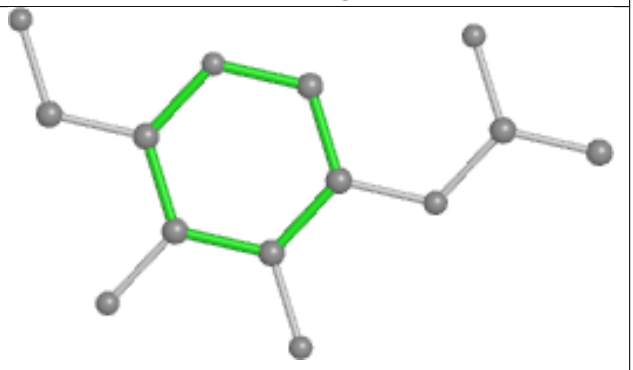
Bond lengths



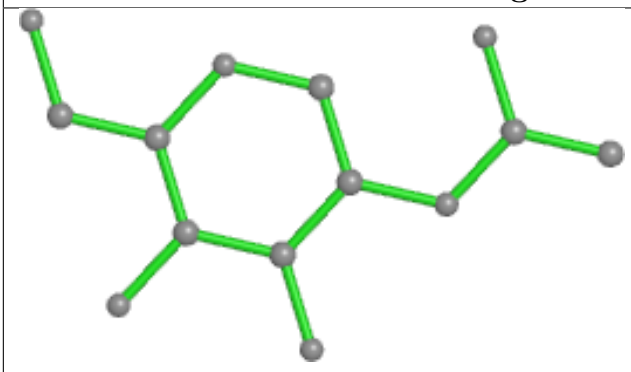
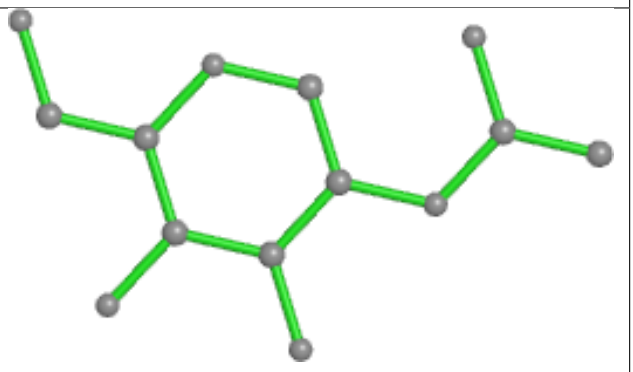
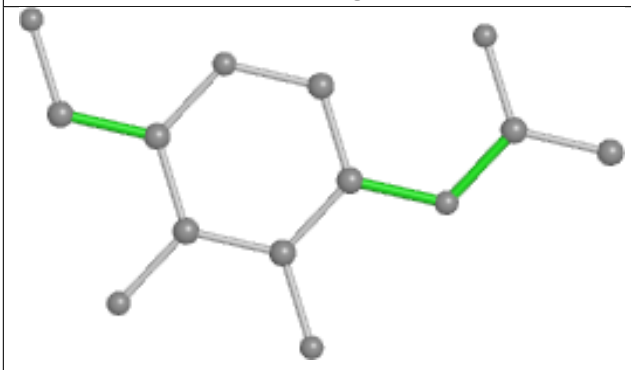
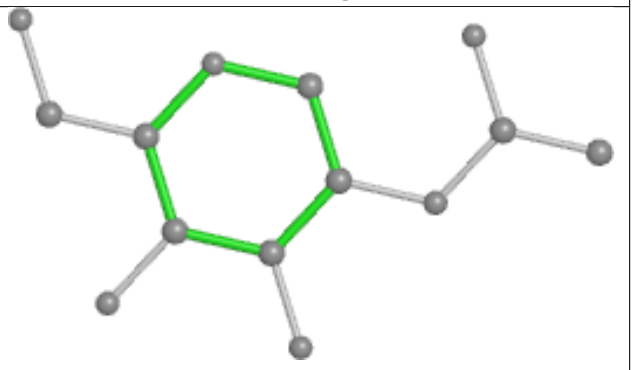
Bond angles



Torsions



Rings

Ligand NAG A 1303	
 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.