Full wwPDB EM Validation Report (i)

Feb 13, 2023 – 03:38 PM EST

PDB ID	:	7SC5
EMDB ID	:	EMD-25022
Title	:	Cytoplasmic tail deleted HIV Env trimer in nanodisc
Authors	:	Yang, S.; Walz, T.
Deposited on	:	2021-09-27
Resolution	:	3.88 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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

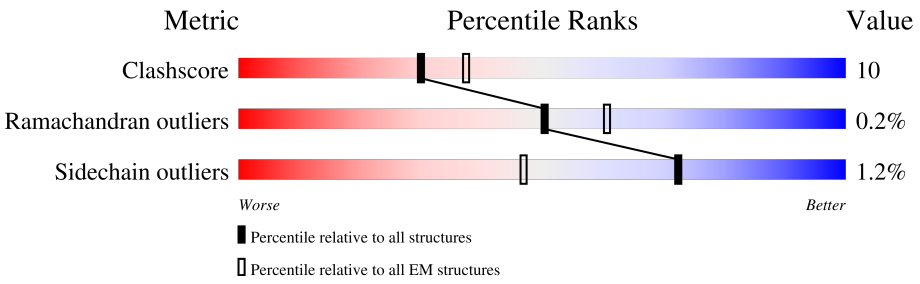
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.88 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	71% 22% 7%
1	C	474	69% 23% • 7%
1	E	474	70% 23% 7%
2	B	212	7% 53% 18% 29%
2	D	212	7% 52% 18% 29%
2	F	212	8% 52% 18% 29%
3	G	3	100%
3	I	3	67% 33% 33% 33%

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Mol	Chain	Length	Quality of chain
3	J	3	100%
3	L	3	67%, 33%, 33%, 33%
3	M	3	33%, 67%
3	O	3	67%, 33%, 33%, 33%
4	H	2	50%, 50%
4	K	2	50%, 50%
4	N	2	50%, 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14703 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	440	3464	2179	611	647	27	0	0
1	C	440	3464	2179	611	647	27	0	0
1	E	440	3464	2179	611	647	27	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ARG	LYS	conflict	UNP A0A6H1VID3
A	374	SER	TYR	conflict	UNP A0A6H1VID3
A	499	CYS	ALA	conflict	UNP A0A6H1VID3
C	59	ARG	LYS	conflict	UNP A0A6H1VID3
C	374	SER	TYR	conflict	UNP A0A6H1VID3
C	499	CYS	ALA	conflict	UNP A0A6H1VID3
E	59	ARG	LYS	conflict	UNP A0A6H1VID3
E	374	SER	TYR	conflict	UNP A0A6H1VID3
E	499	CYS	ALA	conflict	UNP A0A6H1VID3

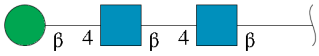
- Molecule 2 is a protein called Transmembrane protein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	150	1163	729	208	220	6	0	0
2	D	150	1163	729	208	220	6	0	0
2	F	150	1163	729	208	220	6	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP A0A173DX29
B	605	CYS	THR	conflict	UNP A0A173DX29
B	632	GLU	ASP	conflict	UNP A0A173DX29
B	641	LEU	ILE	conflict	UNP A0A173DX29
B	700	THR	ALA	conflict	UNP A0A173DX29
B	704	ILE	VAL	conflict	UNP A0A173DX29
B	705	VAL	ILE	conflict	UNP A0A173DX29
B	706	ASN	HIS	conflict	UNP A0A173DX29
B	720	HIS	LEU	conflict	UNP A0A173DX29
B	723	ALA	THR	conflict	UNP A0A173DX29
D	559	PRO	ILE	conflict	UNP A0A173DX29
D	605	CYS	THR	conflict	UNP A0A173DX29
D	632	GLU	ASP	conflict	UNP A0A173DX29
D	641	LEU	ILE	conflict	UNP A0A173DX29
D	700	THR	ALA	conflict	UNP A0A173DX29
D	704	ILE	VAL	conflict	UNP A0A173DX29
D	705	VAL	ILE	conflict	UNP A0A173DX29
D	706	ASN	HIS	conflict	UNP A0A173DX29
D	720	HIS	LEU	conflict	UNP A0A173DX29
D	723	ALA	THR	conflict	UNP A0A173DX29
F	559	PRO	ILE	conflict	UNP A0A173DX29
F	605	CYS	THR	conflict	UNP A0A173DX29
F	632	GLU	ASP	conflict	UNP A0A173DX29
F	641	LEU	ILE	conflict	UNP A0A173DX29
F	700	THR	ALA	conflict	UNP A0A173DX29
F	704	ILE	VAL	conflict	UNP A0A173DX29
F	705	VAL	ILE	conflict	UNP A0A173DX29
F	706	ASN	HIS	conflict	UNP A0A173DX29
F	720	HIS	LEU	conflict	UNP A0A173DX29
F	723	ALA	THR	conflict	UNP A0A173DX29

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	3	39	22	2	15	0	0
			Total	C	N	O		
3	I	3	39	22	2	15	0	0

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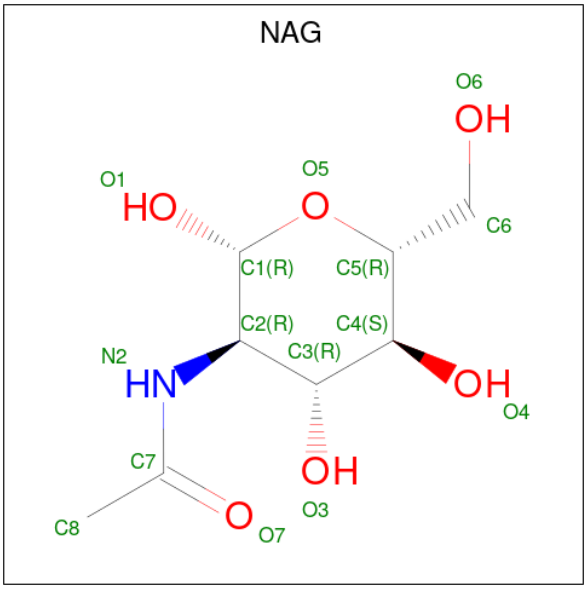
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	J	3	39	22	2	15	0	0
			Total	C	N	O		
3	L	3	39	22	2	15	0	0
			Total	C	N	O		
3	M	3	39	22	2	15	0	0
			Total	C	N	O		
3	O	3	39	22	2	15	0	0

- Molecule 4 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
			Total	C	N	O		
4	H	2	28	16	2	10	0	0
			Total	C	N	O		
4	K	2	28	16	2	10	0	0
			Total	C	N	O		
4	N	2	28	16	2	10	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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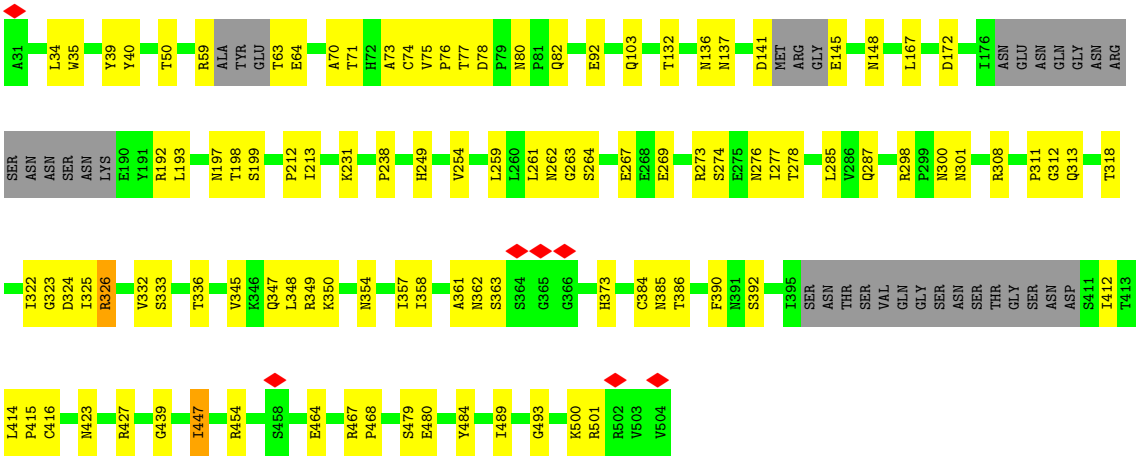
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	D	1	14	8	1	5	0
			Total	C	N	O	
5	D	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	E	1	14	8	1	5	0
			Total	C	N	O	
5	F	1	14	8	1	5	0
			Total	C	N	O	
5	F	1	14	8	1	5	0
			Total	C	N	O	
5	F	1	14	8	1	5	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

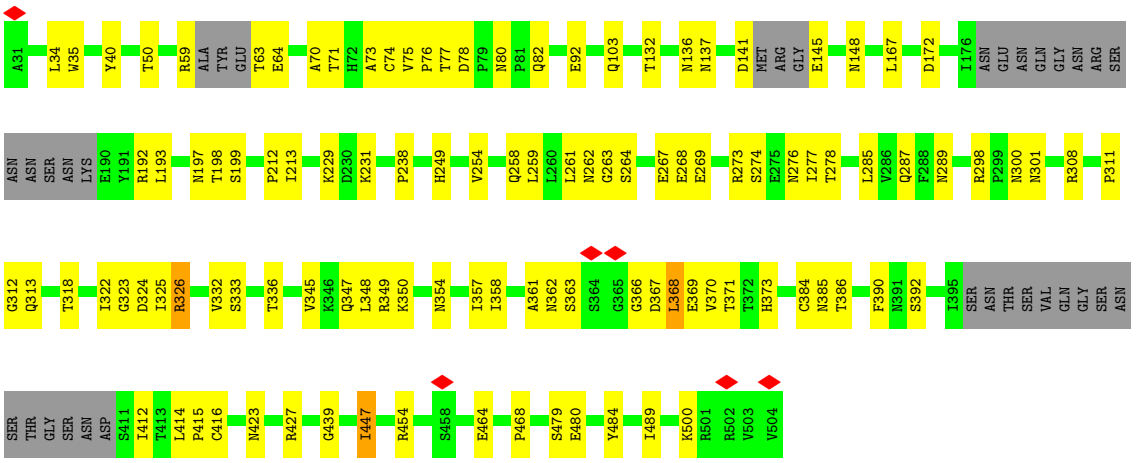
• Molecule 1: Envelope glycoprotein gp120

Chain A:



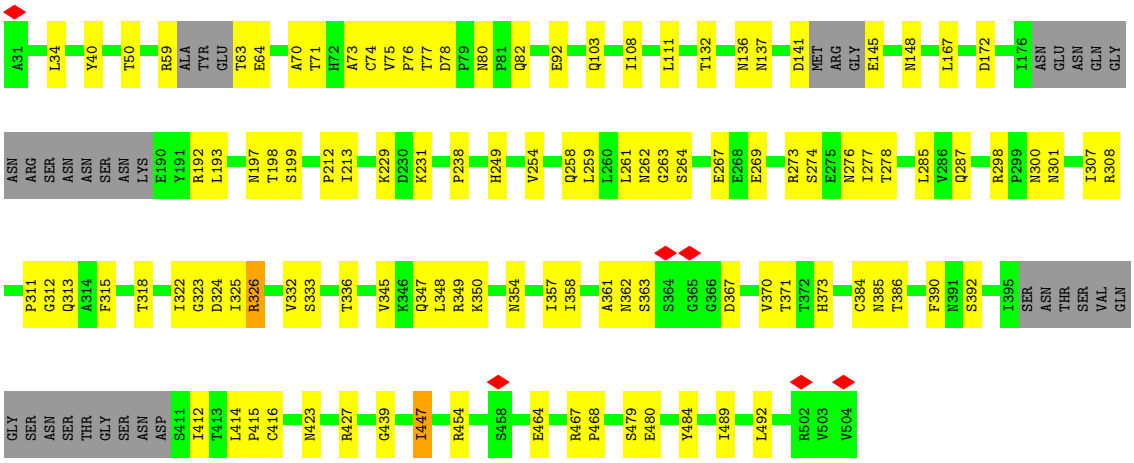
• Molecule 1: Envelope glycoprotein gp120

Chain C:



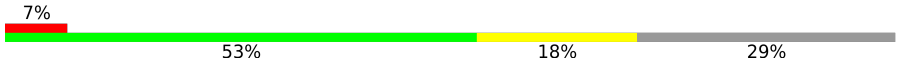
• Molecule 1: Envelope glycoprotein gp120

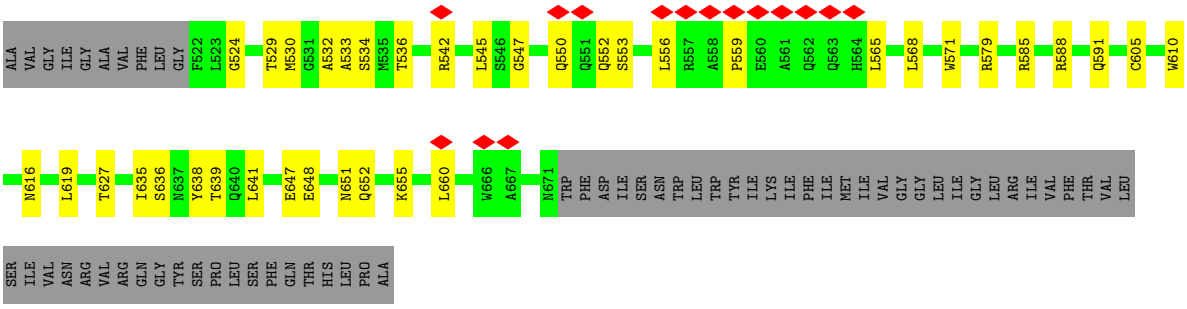
Chain E:



- Molecule 2: Transmembrane protein gp41

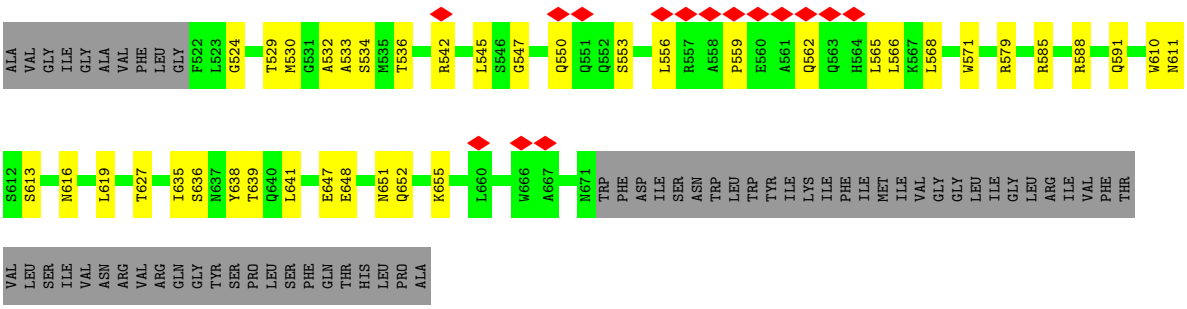
Chain B:





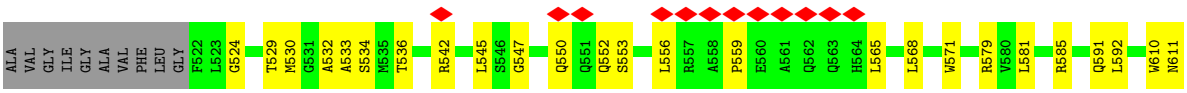
- Molecule 2: Transmembrane protein gp41

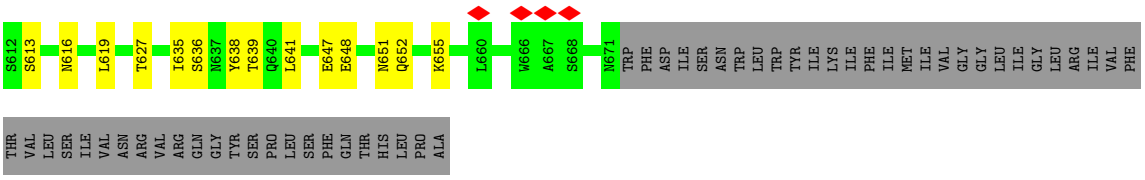
Chain D:



- Molecule 2: Transmembrane protein gp41

Chain F:





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

Chain G: 100%

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

Chain I: 67% 33% 33% 33%

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

Chain J: 100%

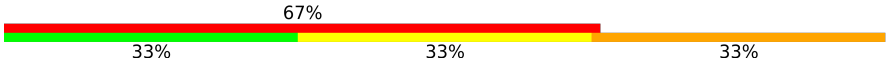
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 67% 33% 33% 33%

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

Chain M: 33% 67%

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

Chain O: 

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

Chain H:

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

Chain K:

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

Chain N:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47616	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0109	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.40	0/3535	0.57	0/4800
1	C	0.40	0/3535	0.57	0/4800
1	E	0.40	0/3535	0.58	0/4800
2	B	0.34	0/1182	0.57	0/1605
2	D	0.34	0/1182	0.57	0/1605
2	F	0.34	0/1182	0.57	0/1605
All	All	0.39	0/14151	0.57	0/19215

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3464	0	3411	69	0
1	C	3464	0	3411	74	0
1	E	3464	0	3411	77	0
2	B	1163	0	1127	29	0
2	D	1163	0	1127	29	0
2	F	1163	0	1127	29	0
3	G	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	39	0	34	1	0
3	J	39	0	34	1	0
3	L	39	0	34	1	0
3	M	39	0	34	2	0
3	O	39	0	34	1	0
4	H	28	0	25	0	0
4	K	28	0	25	0	0
4	N	28	0	25	0	0
5	A	126	0	117	3	0
5	B	42	0	39	0	0
5	C	126	0	117	3	0
5	D	42	0	39	0	0
5	E	126	0	117	3	0
5	F	42	0	39	0	0
All	All	14703	0	14361	290	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (290) 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:E:362:ASN:HD22	1:E:371:THR:HA	0.94	1.06
1:C:362:ASN:ND2	1:C:371:THR:HA	1.71	1.05
1:E:362:ASN:ND2	1:E:371:THR:HA	1.73	1.02
1:C:367:ASP:O	1:C:369:GLU:N	1.96	0.99
1:E:362:ASN:HD22	1:E:371:THR:CA	1.75	0.98
1:E:363:SER:HB3	1:E:467:ARG:NH1	1.78	0.98
1:A:363:SER:H	1:A:467:ARG:HH12	1.25	0.84
1:C:362:ASN:ND2	1:C:371:THR:CA	2.45	0.79
1:E:363:SER:CB	1:E:467:ARG:NH1	2.47	0.77
1:A:363:SER:H	1:A:467:ARG:NH1	1.83	0.77
1:E:362:ASN:ND2	1:E:371:THR:O	2.20	0.75
5:A:609:NAG:O7	5:A:609:NAG:O3	2.05	0.73
5:C:609:NAG:O7	5:C:609:NAG:O3	2.06	0.73
1:A:362:ASN:OD1	1:A:468:PRO:HG2	1.90	0.72
1:C:362:ASN:ND2	1:C:370:VAL:O	2.24	0.70
5:E:609:NAG:O7	5:E:609:NAG:O3	2.07	0.70
1:E:249:HIS:HD1	1:E:484:TYR:HH	1.37	0.69
1:C:249:HIS:HD1	1:C:484:TYR:HH	1.40	0.66
1:A:249:HIS:HD1	1:A:484:TYR:HH	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LEU:HD21	2:D:619:LEU:HD12	1.78	0.65
1:A:363:SER:N	1:A:467:ARG:NH1	2.45	0.65
2:B:565:LEU:HD11	1:C:427:ARG:HH22	1.62	0.65
1:C:367:ASP:O	1:C:368:LEU:C	2.36	0.63
1:A:264:SER:O	1:A:287:GLN:NE2	2.32	0.63
1:A:34:LEU:HD21	2:B:619:LEU:HD12	1.80	0.62
1:A:199:SER:HA	1:E:312:GLY:H	1.64	0.62
2:D:648:GLU:HA	2:D:652:GLN:HE21	1.65	0.62
2:F:648:GLU:HA	2:F:652:GLN:HE21	1.65	0.62
1:A:363:SER:N	1:A:467:ARG:HH12	1.97	0.62
2:F:529:THR:HG23	2:F:532:ALA:H	1.65	0.62
1:A:73:ALA:HB1	1:A:76:PRO:HB3	1.82	0.61
2:D:529:THR:HG23	2:D:532:ALA:H	1.65	0.61
2:B:648:GLU:HA	2:B:652:GLN:HE21	1.65	0.61
1:E:264:SER:O	1:E:287:GLN:NE2	2.32	0.61
2:B:529:THR:HG23	2:B:532:ALA:H	1.65	0.61
1:C:264:SER:O	1:C:287:GLN:NE2	2.32	0.61
1:C:73:ALA:HB1	1:C:76:PRO:HB3	1.82	0.60
1:E:73:ALA:HB1	1:E:76:PRO:HB3	1.82	0.60
1:A:301:ASN:HD22	1:A:322:ILE:HG13	1.67	0.60
1:C:300:ASN:HD21	1:C:326:ARG:H	1.50	0.60
1:E:361:ALA:O	1:E:467:ARG:NH1	2.35	0.60
1:A:276:ASN:ND2	1:A:278:THR:OG1	2.35	0.60
1:C:312:GLY:H	1:E:199:SER:HA	1.65	0.60
1:E:300:ASN:HD21	1:E:326:ARG:H	1.50	0.59
1:C:362:ASN:HD22	1:C:371:THR:C	2.05	0.59
1:A:361:ALA:O	1:A:467:ARG:NH1	2.35	0.59
1:A:192:ARG:NH1	1:A:193:LEU:O	2.36	0.59
1:A:300:ASN:HD21	1:A:326:ARG:H	1.50	0.59
1:C:301:ASN:HD22	1:C:322:ILE:HG13	1.67	0.59
1:C:192:ARG:NH1	1:C:193:LEU:O	2.36	0.58
1:A:277:ILE:O	1:A:454:ARG:NH2	2.35	0.58
1:E:301:ASN:HD22	1:E:322:ILE:HG13	1.67	0.58
1:C:276:ASN:ND2	1:C:278:THR:OG1	2.35	0.58
1:E:276:ASN:ND2	1:E:278:THR:OG1	2.35	0.58
1:E:192:ARG:NH1	1:E:193:LEU:O	2.36	0.58
1:C:277:ILE:O	1:C:454:ARG:NH2	2.35	0.57
2:D:610:TRP:NE1	2:D:616:ASN:OD1	2.36	0.57
1:E:363:SER:HB3	1:E:467:ARG:CZ	2.35	0.57
1:E:34:LEU:HD21	2:F:619:LEU:HD12	1.85	0.57
1:E:273:ARG:NH1	1:E:287:GLN:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:ASP:O	1:E:370:VAL:HG22	2.05	0.56
1:E:277:ILE:O	1:E:454:ARG:NH2	2.35	0.56
2:B:559:PRO:HB3	2:B:579:ARG:HH22	1.71	0.56
1:A:489:ILE:O	2:B:585:ARG:NH2	2.38	0.56
1:A:63:THR:OG1	1:A:64:GLU:N	2.39	0.56
2:D:553:SER:HA	2:D:556:LEU:HB2	1.87	0.56
2:B:553:SER:HA	2:B:556:LEU:HB2	1.87	0.56
2:D:559:PRO:HB3	2:D:579:ARG:HH22	1.71	0.56
2:F:559:PRO:HB3	2:F:579:ARG:HH22	1.71	0.56
1:A:273:ARG:NH1	1:A:287:GLN:OE1	2.38	0.55
1:C:71:THR:HG21	2:D:571:TRP:HE1	1.72	0.55
1:C:273:ARG:NH1	1:C:287:GLN:OE1	2.38	0.55
1:A:197:ASN:O	1:E:308:ARG:NH1	2.39	0.55
1:A:70:ALA:HB2	1:A:213:ILE:HD11	1.89	0.55
1:A:300:ASN:ND2	1:A:324:ASP:O	2.40	0.55
1:C:63:THR:OG1	1:C:64:GLU:N	2.39	0.55
1:E:300:ASN:ND2	1:E:324:ASP:O	2.40	0.55
2:B:552:GLN:HB2	2:D:588:ARG:HH21	1.71	0.54
1:E:70:ALA:HB2	1:E:213:ILE:HD11	1.89	0.54
1:C:70:ALA:HB2	1:C:213:ILE:HD11	1.89	0.54
1:A:92:GLU:HA	1:A:238:PRO:HA	1.90	0.54
1:A:312:GLY:H	1:C:199:SER:HA	1.72	0.54
2:F:553:SER:HA	2:F:556:LEU:HB2	1.87	0.54
1:E:489:ILE:O	2:F:585:ARG:NH2	2.40	0.54
1:C:300:ASN:ND2	1:C:324:ASP:O	2.40	0.54
2:B:610:TRP:NE1	2:B:616:ASN:OD1	2.36	0.53
1:C:308:ARG:NH1	1:E:197:ASN:O	2.41	0.53
1:E:63:THR:OG1	1:E:64:GLU:N	2.39	0.53
1:A:167:LEU:O	1:A:318:THR:OG1	2.27	0.53
1:C:385:ASN:HB3	1:C:415:PRO:HG2	1.91	0.53
3:M:2:NAG:HO3	3:M:3:BMA:HO2	1.57	0.53
1:E:92:GLU:HA	1:E:238:PRO:HA	1.90	0.52
1:A:308:ARG:NH1	1:C:197:ASN:O	2.42	0.52
1:A:385:ASN:HB3	1:A:415:PRO:HG2	1.91	0.52
1:C:92:GLU:HA	1:C:238:PRO:HA	1.90	0.52
1:E:357:ILE:HD13	1:E:464:GLU:HB3	1.92	0.52
2:D:529:THR:O	2:D:533:ALA:N	2.43	0.52
2:F:529:THR:O	2:F:533:ALA:N	2.43	0.52
1:A:298:ARG:NH2	1:A:439:GLY:O	2.43	0.52
1:C:298:ARG:NH2	1:C:439:GLY:O	2.43	0.52
1:E:298:ARG:NH2	1:E:439:GLY:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:545:LEU:HG	2:D:591:GLN:HE21	1.74	0.52
2:B:529:THR:O	2:B:533:ALA:N	2.43	0.52
1:C:167:LEU:O	1:C:318:THR:OG1	2.27	0.52
1:E:362:ASN:ND2	1:E:371:THR:CA	2.52	0.52
2:F:610:TRP:NE1	2:F:616:ASN:OD1	2.36	0.51
1:C:362:ASN:HD22	1:C:371:THR:CA	2.22	0.51
1:E:385:ASN:HB3	1:E:415:PRO:HG2	1.91	0.51
1:A:231:LYS:NZ	1:A:269:GLU:OE2	2.44	0.51
1:A:357:ILE:HD13	1:A:464:GLU:HB3	1.92	0.51
1:C:80:ASN:O	1:C:82:GLN:NE2	2.44	0.51
1:E:363:SER:HB3	1:E:467:ARG:HH12	1.70	0.51
1:E:167:LEU:O	1:E:318:THR:OG1	2.27	0.51
1:C:357:ILE:HD13	1:C:464:GLU:HB3	1.92	0.50
2:F:638:TYR:HA	2:F:641:LEU:HD13	1.93	0.50
2:B:530:MET:HA	2:B:533:ALA:HB3	1.94	0.50
1:A:80:ASN:O	1:A:82:GLN:NE2	2.44	0.50
1:C:386:THR:HG22	1:C:414:LEU:HD13	1.94	0.50
2:D:530:MET:HA	2:D:533:ALA:HB3	1.94	0.50
1:E:71:THR:HG21	2:F:571:TRP:HE1	1.77	0.50
1:E:80:ASN:O	1:E:82:GLN:NE2	2.44	0.50
1:E:231:LYS:NZ	1:E:269:GLU:OE2	2.44	0.50
1:E:137:ASN:HB2	1:E:325:ILE:HB	1.94	0.49
2:B:638:TYR:HA	2:B:641:LEU:HD13	1.93	0.49
1:C:423:ASN:ND2	1:C:427:ARG:O	2.46	0.49
1:E:384:CYS:HA	1:E:416:CYS:HA	1.94	0.49
1:A:136:ASN:ND2	1:A:137:ASN:OD1	2.43	0.49
1:A:137:ASN:HB2	1:A:325:ILE:HB	1.94	0.49
1:A:386:THR:HG22	1:A:414:LEU:HD13	1.94	0.49
1:C:77:THR:OG1	1:C:78:ASP:N	2.45	0.49
2:D:565:LEU:HD11	1:E:427:ARG:HH22	1.78	0.49
2:D:638:TYR:HA	2:D:641:LEU:HD13	1.93	0.49
1:A:77:THR:OG1	1:A:78:ASP:N	2.45	0.49
1:E:74:CYS:SG	1:E:75:VAL:N	2.85	0.49
1:E:423:ASN:ND2	1:E:427:ARG:O	2.46	0.49
1:E:77:THR:OG1	1:E:78:ASP:N	2.45	0.49
2:B:533:ALA:O	2:B:536:THR:OG1	2.24	0.49
1:E:132:THR:HG23	1:E:148:ASN:HB3	1.95	0.49
1:A:423:ASN:ND2	1:A:427:ARG:O	2.46	0.49
1:C:384:CYS:HA	1:C:416:CYS:HA	1.94	0.49
1:E:386:THR:HG22	1:E:414:LEU:HD13	1.94	0.49
2:F:530:MET:HA	2:F:533:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:635:ILE:O	2:F:639:THR:OG1	2.31	0.48
1:A:132:THR:HG23	1:A:148:ASN:HB3	1.95	0.48
1:C:132:THR:HG23	1:C:148:ASN:HB3	1.95	0.48
1:C:358:ILE:HG23	1:C:392:SER:HB2	1.95	0.48
1:C:137:ASN:HB2	1:C:325:ILE:HB	1.94	0.48
1:E:136:ASN:ND2	1:E:137:ASN:OD1	2.43	0.48
1:C:74:CYS:SG	1:C:75:VAL:N	2.85	0.48
2:D:529:THR:HA	2:D:627:THR:HA	1.96	0.48
2:D:635:ILE:O	2:D:639:THR:OG1	2.31	0.48
2:B:529:THR:HA	2:B:627:THR:HA	1.96	0.48
1:E:358:ILE:HG23	1:E:392:SER:HB2	1.95	0.48
1:C:333:SER:HG	1:C:336:THR:HG1	1.60	0.48
1:A:358:ILE:HG23	1:A:392:SER:HB2	1.95	0.48
1:A:384:CYS:HA	1:A:416:CYS:HA	1.94	0.48
1:E:132:THR:O	1:E:148:ASN:N	2.35	0.48
2:F:529:THR:HA	2:F:627:THR:HA	1.96	0.48
1:A:74:CYS:SG	1:A:75:VAL:N	2.85	0.47
1:A:231:LYS:HE2	1:A:267:GLU:HG3	1.96	0.47
1:C:231:LYS:NZ	1:C:269:GLU:OE2	2.44	0.47
2:B:647:GLU:O	2:B:652:GLN:NE2	2.47	0.47
2:B:635:ILE:O	2:B:639:THR:OG1	2.31	0.47
2:B:651:ASN:HA	2:B:655:LYS:HG2	1.96	0.47
2:D:647:GLU:O	2:D:652:GLN:NE2	2.47	0.47
2:B:547:GLY:HA2	2:B:550:GLN:HG2	1.97	0.47
2:F:647:GLU:O	2:F:652:GLN:NE2	2.47	0.47
1:A:198:THR:OG1	1:A:199:SER:N	2.48	0.47
1:C:132:THR:O	1:C:148:ASN:N	2.36	0.47
1:C:231:LYS:HE2	1:C:267:GLU:HG3	1.96	0.47
5:C:609:NAG:HO3	5:C:609:NAG:C7	2.21	0.47
5:E:609:NAG:HO3	5:E:609:NAG:C7	2.19	0.47
2:D:547:GLY:HA2	2:D:550:GLN:HG2	1.97	0.47
1:A:40:TYR:HE2	2:B:545:LEU:HD13	1.80	0.47
1:A:349:ARG:HD3	1:A:354:ASN:HB3	1.96	0.47
1:E:259:LEU:HB2	1:E:373:HIS:CD2	2.50	0.46
1:A:347:GLN:HA	1:A:350:LYS:HG3	1.97	0.46
1:C:136:ASN:ND2	1:C:137:ASN:OD1	2.43	0.46
2:D:638:TYR:HD1	2:D:641:LEU:HD22	1.81	0.46
1:E:347:GLN:HA	1:E:350:LYS:HG3	1.97	0.46
1:E:198:THR:OG1	1:E:199:SER:N	2.48	0.46
1:E:362:ASN:ND2	1:E:371:THR:C	2.68	0.46
1:C:349:ARG:HD3	1:C:354:ASN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:172:ASP:N	1:E:172:ASP:OD1	2.49	0.46
1:E:231:LYS:HE2	1:E:267:GLU:HG3	1.96	0.46
2:F:651:ASN:HA	2:F:655:LYS:HG2	1.96	0.46
1:E:262:ASN:ND2	3:M:1:NAG:O7	2.49	0.46
1:A:262:ASN:ND2	3:G:1:NAG:O7	2.49	0.46
2:F:547:GLY:HA2	2:F:550:GLN:HG2	1.97	0.46
1:A:259:LEU:HB2	1:A:373:HIS:CD2	2.50	0.46
1:C:259:LEU:HB2	1:C:373:HIS:CD2	2.50	0.46
1:C:347:GLN:HA	1:C:350:LYS:HG3	1.97	0.46
2:D:651:ASN:HA	2:D:655:LYS:HG2	1.96	0.46
1:A:479:SER:OG	1:A:480:GLU:OE1	2.34	0.46
1:C:262:ASN:ND2	3:J:1:NAG:O7	2.49	0.46
1:C:479:SER:OG	1:C:480:GLU:OE1	2.34	0.46
1:E:479:SER:OG	1:E:480:GLU:OE1	2.34	0.46
1:C:229:LYS:HE3	1:C:229:LYS:HB2	1.78	0.45
1:C:361:ALA:O	1:C:362:ASN:C	2.54	0.45
1:E:212:PRO:HG2	1:E:254:VAL:HG12	1.99	0.45
1:C:308:ARG:HE	1:C:308:ARG:HB3	1.64	0.45
1:E:349:ARG:HD3	1:E:354:ASN:HB3	1.97	0.45
1:C:212:PRO:HG2	1:C:254:VAL:HG12	1.99	0.45
1:C:363:SER:O	1:C:371:THR:HG22	2.15	0.45
1:A:332:VAL:O	1:A:412:ILE:N	2.39	0.45
2:B:524:GLY:HA3	2:B:542:ARG:HE	1.81	0.45
1:C:198:THR:OG1	1:C:199:SER:N	2.48	0.45
1:E:311:PRO:O	1:E:313:GLN:N	2.48	0.45
1:E:332:VAL:O	1:E:412:ILE:N	2.39	0.45
2:F:524:GLY:HA3	2:F:542:ARG:HE	1.82	0.45
1:A:172:ASP:OD1	1:A:172:ASP:N	2.49	0.45
1:A:212:PRO:HG2	1:A:254:VAL:HG12	1.99	0.45
1:A:427:ARG:HH22	2:F:565:LEU:HD11	1.82	0.45
1:C:172:ASP:OD1	1:C:172:ASP:N	2.49	0.45
2:F:592:LEU:HD23	2:F:592:LEU:HA	1.85	0.45
1:A:39:TYR:N	1:A:493:GLY:O	2.47	0.44
2:D:524:GLY:HA3	2:D:542:ARG:HE	1.82	0.44
1:A:311:PRO:O	1:A:313:GLN:N	2.48	0.44
2:F:638:TYR:HD1	2:F:641:LEU:HD22	1.81	0.44
2:B:638:TYR:HD1	2:B:641:LEU:HD22	1.81	0.44
1:C:366:GLY:HA3	1:C:370:VAL:HG21	1.99	0.44
2:B:588:ARG:HH21	2:F:552:GLN:HB2	1.83	0.44
2:D:533:ALA:O	2:D:536:THR:OG1	2.24	0.44
1:A:50:THR:O	1:A:103:GLN:NE2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:PHE:H	5:C:606:NAG:H81	1.83	0.44
2:F:533:ALA:O	2:F:536:THR:OG1	2.24	0.44
1:E:40:TYR:HE2	2:F:545:LEU:HD13	1.82	0.43
1:E:229:LYS:HE3	1:E:229:LYS:HB2	1.78	0.43
1:A:141:ASP:H	1:A:145:GLU:HG2	1.84	0.43
1:A:390:PHE:H	5:A:606:NAG:H81	1.83	0.43
1:E:141:ASP:H	1:E:145:GLU:HG2	1.83	0.43
1:A:71:THR:HG21	2:B:571:TRP:HE1	1.83	0.43
1:E:492:LEU:HD12	1:E:492:LEU:HA	1.89	0.43
1:E:50:THR:O	1:E:103:GLN:NE2	2.48	0.43
1:C:332:VAL:O	1:C:412:ILE:N	2.39	0.43
1:C:414:LEU:HD23	1:C:414:LEU:HA	1.92	0.43
1:A:333:SER:OG	1:A:336:THR:OG1	2.34	0.43
1:E:333:SER:HG	1:E:336:THR:HG1	1.63	0.43
1:E:390:PHE:H	5:E:606:NAG:H81	1.83	0.43
1:A:362:ASN:OD1	1:A:468:PRO:CG	2.64	0.42
1:C:40:TYR:HE2	2:D:545:LEU:HD13	1.84	0.42
1:E:108:ILE:HD13	1:E:108:ILE:HA	1.87	0.42
2:D:530:MET:O	2:D:534:SER:N	2.53	0.42
2:D:566:LEU:HD23	2:D:566:LEU:HA	1.90	0.42
1:C:136:ASN:ND2	1:C:323:GLY:O	2.53	0.42
1:C:489:ILE:O	2:D:585:ARG:NH2	2.53	0.42
2:F:611:ASN:OD1	2:F:613:SER:N	2.50	0.42
1:C:311:PRO:O	1:C:313:GLN:N	2.48	0.42
1:A:261:LEU:HD23	1:A:447:ILE:HG23	2.02	0.42
1:E:308:ARG:HE	1:E:308:ARG:HB3	1.64	0.42
3:I:1:NAG:H4	3:I:2:NAG:H83	2.02	0.42
3:O:1:NAG:H4	3:O:2:NAG:H83	2.02	0.42
2:B:530:MET:O	2:B:534:SER:N	2.53	0.42
1:E:261:LEU:HD23	1:E:447:ILE:HG23	2.02	0.42
3:L:1:NAG:H4	3:L:2:NAG:H83	2.02	0.42
2:B:591:GLN:HE21	2:F:545:LEU:HG	1.83	0.41
1:A:308:ARG:HE	1:A:308:ARG:HB3	1.63	0.41
2:D:611:ASN:OD1	2:D:613:SER:N	2.50	0.41
1:E:136:ASN:ND2	1:E:323:GLY:O	2.53	0.41
1:C:141:ASP:H	1:C:145:GLU:HG2	1.83	0.41
1:A:136:ASN:ND2	1:A:323:GLY:O	2.53	0.41
2:F:581:LEU:HD23	2:F:581:LEU:HA	1.89	0.41
1:A:501:ARG:NE	2:B:605:CYS:O	2.32	0.41
5:A:609:NAG:HO3	5:A:609:NAG:C7	2.22	0.41
1:C:258:GLN:HG3	1:C:468:PRO:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:547:GLY:HA2	2:D:550:GLN:HE21	1.85	0.41
1:E:259:LEU:HD22	1:E:447:ILE:HG21	2.03	0.41
1:E:307:ILE:N	1:E:315:PHE:O	2.45	0.41
2:B:547:GLY:HA2	2:B:550:GLN:HE21	1.85	0.41
2:F:530:MET:O	2:F:534:SER:N	2.53	0.41
1:C:259:LEU:HD22	1:C:447:ILE:HG21	2.03	0.41
1:C:273:ARG:HB2	1:C:285:LEU:HB2	2.02	0.41
1:E:258:GLN:HG3	1:E:468:PRO:HB2	2.03	0.41
2:F:547:GLY:HA2	2:F:550:GLN:HE21	1.85	0.41
2:D:562:GLN:H	2:D:562:GLN:HG2	1.69	0.41
1:A:273:ARG:HB2	1:A:285:LEU:HB2	2.02	0.40
2:D:545:LEU:HG	2:F:591:GLN:HE21	1.84	0.40
1:E:111:LEU:HD23	1:E:111:LEU:HA	1.91	0.40
2:B:660:LEU:HD12	2:B:660:LEU:HA	1.97	0.40
1:A:132:THR:O	1:A:148:ASN:N	2.36	0.40
1:A:345:VAL:HA	1:A:348:LEU:HB2	2.04	0.40
1:A:35:TRP:CD1	1:A:500:LYS:HG3	2.57	0.40
1:A:259:LEU:HD22	1:A:447:ILE:HG21	2.03	0.40
1:C:35:TRP:CD1	1:C:500:LYS:HG3	2.56	0.40
1:C:50:THR:O	1:C:103:GLN:NE2	2.48	0.40
1:C:261:LEU:HD23	1:C:447:ILE:HG23	2.02	0.40
1:C:268:GLU:OE1	1:C:289:ASN:ND2	2.52	0.40
1:C:345:VAL:HA	1:C:348:LEU:HB2	2.04	0.40
1:E:273:ARG:HB2	1:E:285:LEU:HB2	2.02	0.40
1:E:345:VAL:HA	1:E:348:LEU:HB2	2.04	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	430/474 (91%)	382 (89%)	47 (11%)	1 (0%)	47 79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	430/474 (91%)	382 (89%)	46 (11%)	2 (0%)	29	67
1	E	430/474 (91%)	383 (89%)	46 (11%)	1 (0%)	47	79
2	B	148/212 (70%)	129 (87%)	19 (13%)	0	100	100
2	D	148/212 (70%)	129 (87%)	19 (13%)	0	100	100
2	F	148/212 (70%)	129 (87%)	19 (13%)	0	100	100
All	All	1734/2058 (84%)	1534 (88%)	196 (11%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	368	LEU
1	A	263	GLY
1	C	263	GLY
1	E	263	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	393/422 (93%)	389 (99%)	4 (1%)	76	86
1	C	393/422 (93%)	389 (99%)	4 (1%)	76	86
1	E	393/422 (93%)	389 (99%)	4 (1%)	76	86
2	B	121/182 (66%)	119 (98%)	2 (2%)	60	78
2	D	121/182 (66%)	119 (98%)	2 (2%)	60	78
2	F	121/182 (66%)	119 (98%)	2 (2%)	60	78
All	All	1542/1812 (85%)	1524 (99%)	18 (1%)	72	83

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	274	SER

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Mol	Chain	Res	Type
1	A	326	ARG
1	A	447	ILE
2	B	568	LEU
2	B	636	SER
1	C	59	ARG
1	C	274	SER
1	C	326	ARG
1	C	447	ILE
2	D	568	LEU
2	D	636	SER
1	E	59	ARG
1	E	274	SER
1	E	326	ARG
1	E	447	ILE
2	F	568	LEU
2	F	636	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	262	ASN
1	A	276	ASN
1	A	295	ASN
1	A	300	ASN
1	A	373	HIS
1	A	423	ASN
2	B	550	GLN
2	B	652	GLN
1	C	99	ASN
1	C	262	ASN
1	C	276	ASN
1	C	295	ASN
1	C	300	ASN
1	C	373	HIS
1	C	423	ASN
2	D	550	GLN
2	D	652	GLN
2	D	656	ASN
1	E	99	ASN
1	E	262	ASN
1	E	276	ASN

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Mol	Chain	Res	Type
1	E	295	ASN
1	E	300	ASN
1	E	362	ASN
1	E	373	HIS
1	E	423	ASN
2	F	550	GLN
2	F	652	GLN
2	F	656	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 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	G	1	1,3	14,14,15	0.19	0	17,19,21	0.59	0
3	NAG	G	2	3	14,14,15	0.50	0	17,19,21	1.08	2 (11%)
3	BMA	G	3	3	11,11,12	1.18	1 (9%)	15,15,17	1.14	1 (6%)
4	NAG	H	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	H	2	4	14,14,15	0.46	0	17,19,21	0.42	0
3	NAG	I	1	1,3	14,14,15	0.22	0	17,19,21	0.66	0
3	NAG	I	2	3	14,14,15	0.76	1 (7%)	17,19,21	0.76	1 (5%)
3	BMA	I	3	3	11,11,12	0.75	0	15,15,17	0.81	0
3	NAG	J	1	1,3	14,14,15	0.19	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	J	2	3	14,14,15	0.50	0	17,19,21	1.08	2 (11%)
3	BMA	J	3	3	11,11,12	1.18	1 (9%)	15,15,17	1.14	1 (6%)
4	NAG	K	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	K	2	4	14,14,15	0.44	0	17,19,21	0.41	0
3	NAG	L	1	1,3	14,14,15	0.22	0	17,19,21	0.66	0
3	NAG	L	2	3	14,14,15	0.75	1 (7%)	17,19,21	0.76	1 (5%)
3	BMA	L	3	3	11,11,12	0.75	0	15,15,17	0.82	0
3	NAG	M	1	1,3	14,14,15	0.19	0	17,19,21	0.59	0
3	NAG	M	2	3	14,14,15	0.48	0	17,19,21	1.08	2 (11%)
3	BMA	M	3	3	11,11,12	1.19	1 (9%)	15,15,17	1.14	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.86	1 (7%)	17,19,21	1.23	2 (11%)
4	NAG	N	2	4	14,14,15	0.44	0	17,19,21	0.42	0
3	NAG	O	1	1,3	14,14,15	0.21	0	17,19,21	0.66	0
3	NAG	O	2	3	14,14,15	0.77	1 (7%)	17,19,21	0.76	1 (5%)
3	BMA	O	3	3	11,11,12	0.75	0	15,15,17	0.82	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	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	BMA	J	3	3	-	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	BMA	L	3	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	0/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	3	BMA	C1-C2	3.35	1.59	1.52
3	G	3	BMA	C1-C2	3.32	1.59	1.52
3	J	3	BMA	C1-C2	3.32	1.59	1.52
4	H	1	NAG	O5-C1	-3.02	1.38	1.43
4	K	1	NAG	O5-C1	-3.01	1.38	1.43
4	N	1	NAG	O5-C1	-3.00	1.38	1.43
3	O	2	NAG	C1-C2	2.63	1.56	1.52
3	I	2	NAG	C1-C2	2.61	1.56	1.52
3	L	2	NAG	C1-C2	2.55	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	NAG	C2-N2-C7	3.17	127.42	122.90
4	K	1	NAG	C2-N2-C7	3.13	127.36	122.90
4	N	1	NAG	C2-N2-C7	3.11	127.33	122.90
3	J	2	NAG	C2-N2-C7	2.91	127.05	122.90
3	G	2	NAG	C2-N2-C7	2.90	127.03	122.90
3	M	2	NAG	C2-N2-C7	2.87	126.99	122.90
3	J	3	BMA	O2-C2-C3	-2.80	104.53	110.14
3	M	3	BMA	O2-C2-C3	-2.78	104.56	110.14
3	G	3	BMA	O2-C2-C3	-2.78	104.56	110.14
3	L	2	NAG	C1-O5-C5	2.20	115.17	112.19
3	I	2	NAG	C1-O5-C5	2.19	115.16	112.19
3	O	2	NAG	C1-O5-C5	2.17	115.13	112.19
3	J	2	NAG	C1-O5-C5	2.10	115.03	112.19
3	G	2	NAG	C1-O5-C5	2.09	115.02	112.19
3	M	2	NAG	C1-O5-C5	2.08	115.00	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	1	NAG	C3-C4-C5	2.08	113.94	110.24
4	N	1	NAG	C3-C4-C5	2.07	113.94	110.24
4	H	1	NAG	C3-C4-C5	2.06	113.91	110.24

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	L	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	I	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	J	3	BMA	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
3	L	3	BMA	C4-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	M	2	NAG	C3-C2-N2-C7
4	H	1	NAG	C3-C2-N2-C7
4	K	1	NAG	C3-C2-N2-C7
4	N	1	NAG	C3-C2-N2-C7
3	L	3	BMA	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6

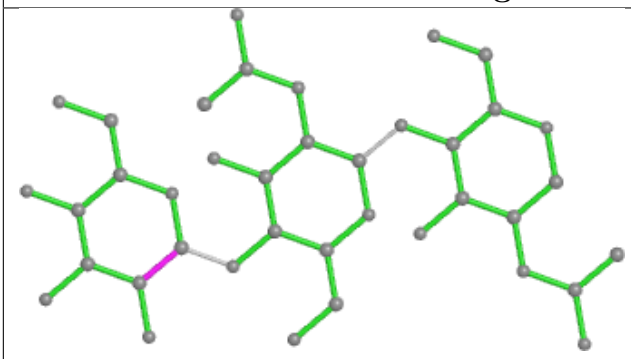
There are no ring outliers.

11 monomers are involved in 7 short contacts:

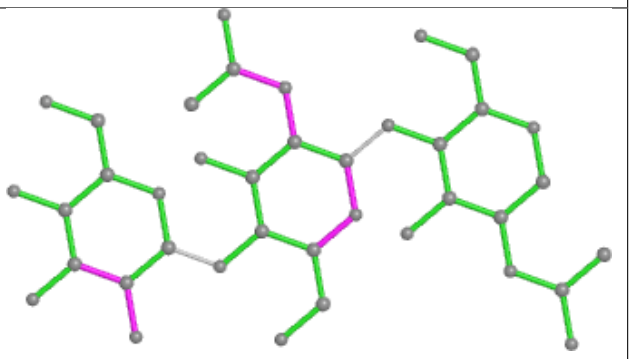
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2	NAG	1	0
3	M	1	NAG	1	0
3	G	1	NAG	1	0
3	M	3	BMA	1	0
3	I	2	NAG	1	0
3	O	1	NAG	1	0
3	I	1	NAG	1	0
3	L	2	NAG	1	0
3	O	2	NAG	1	0
3	L	1	NAG	1	0
3	J	1	NAG	1	0

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

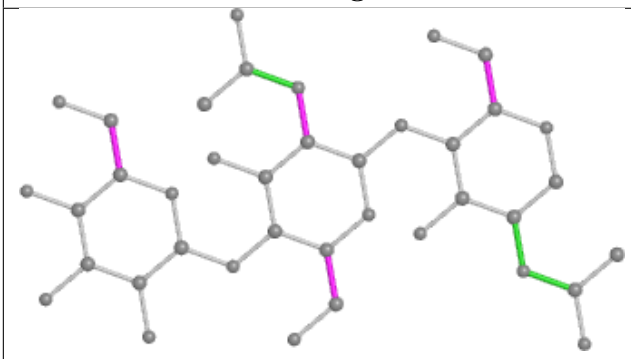
Oligosaccharide Chain G



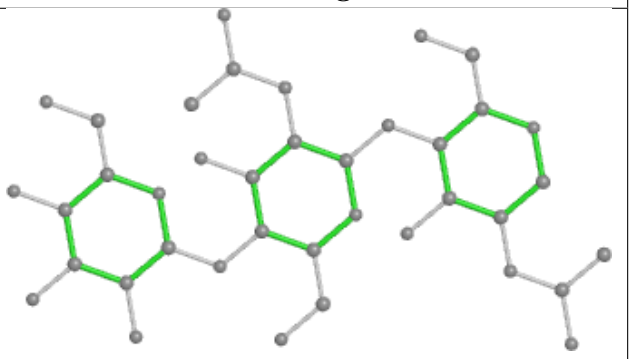
Bond lengths



Bond angles

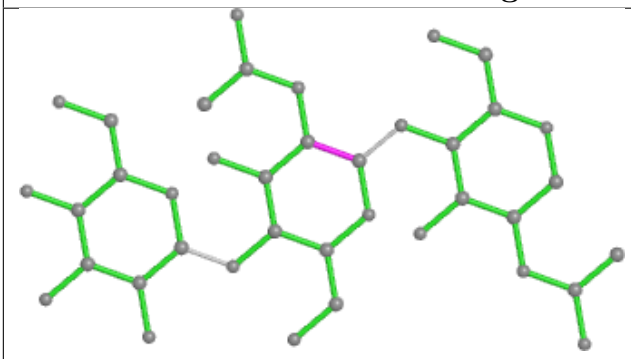


Torsions

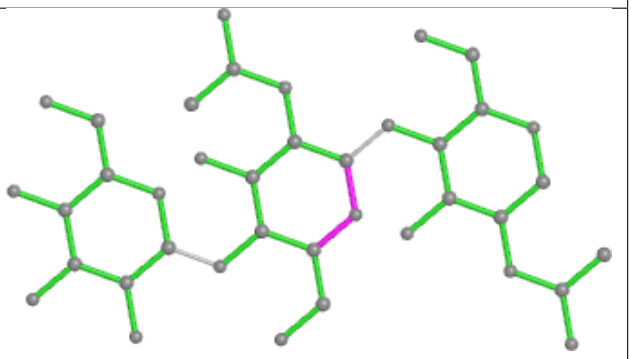


Rings

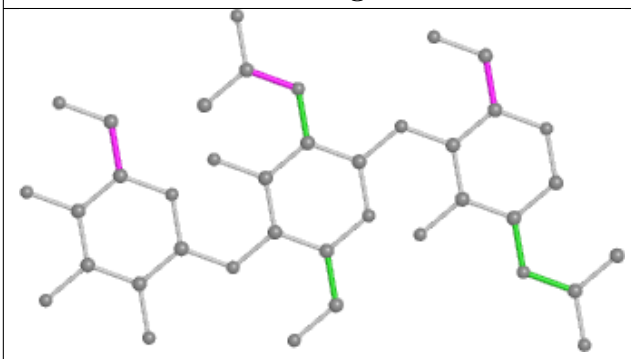
Oligosaccharide Chain I



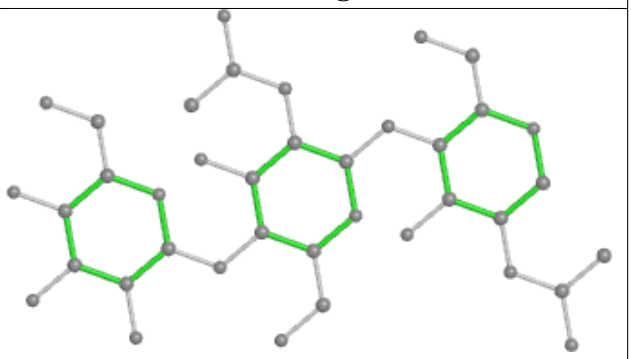
Bond lengths



Bond angles

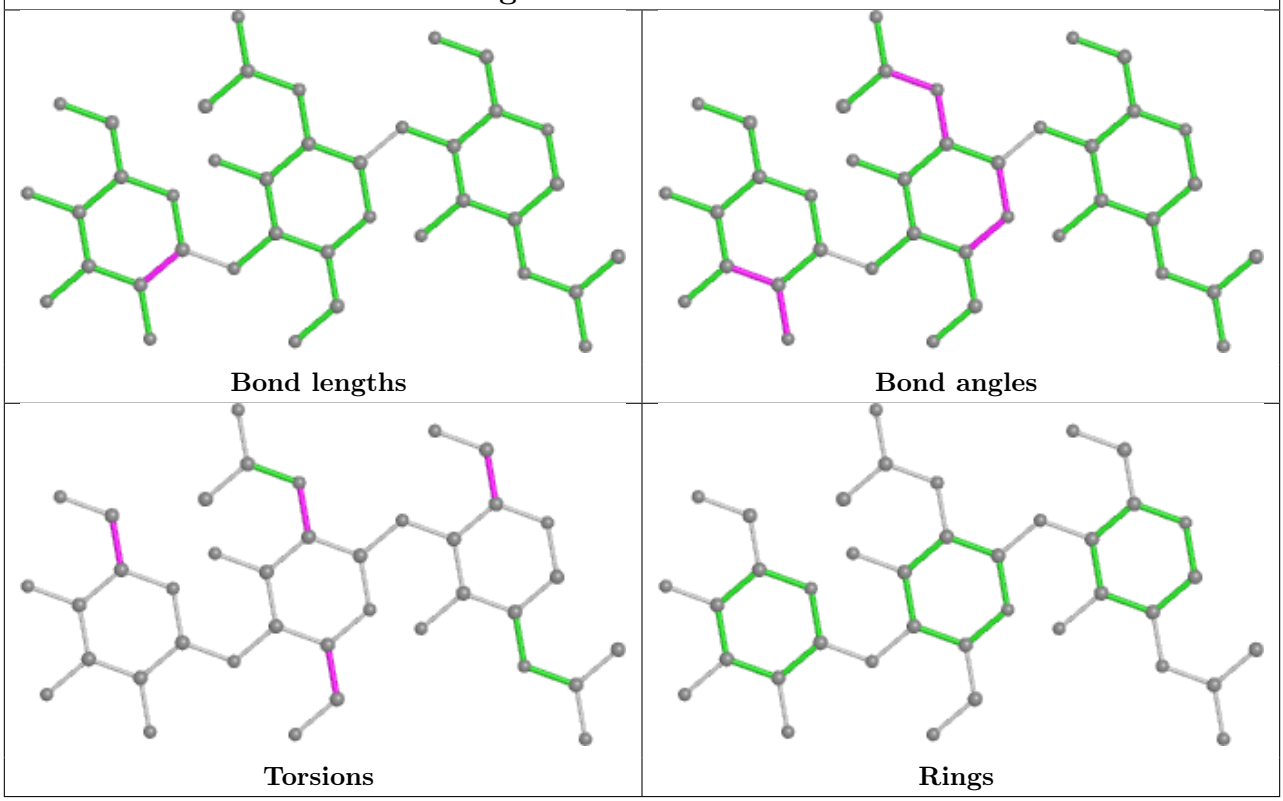


Torsions

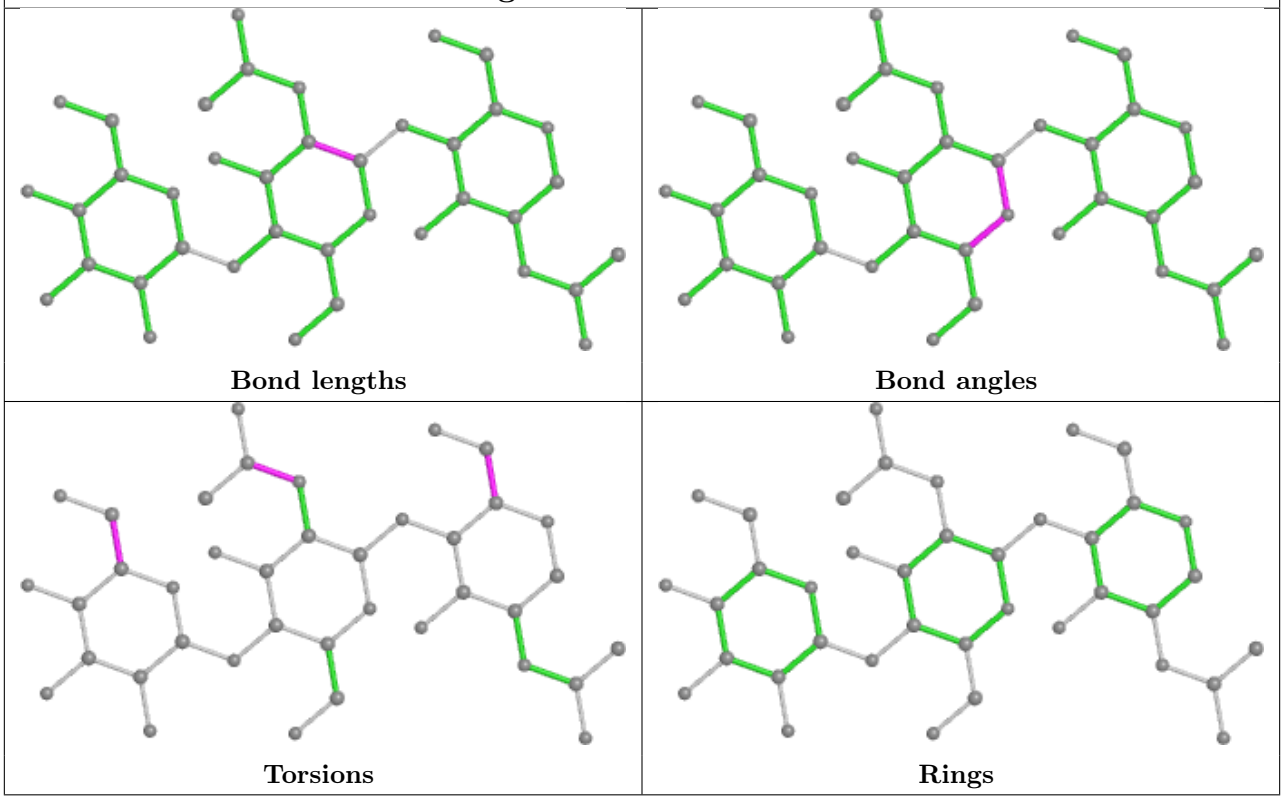


Rings

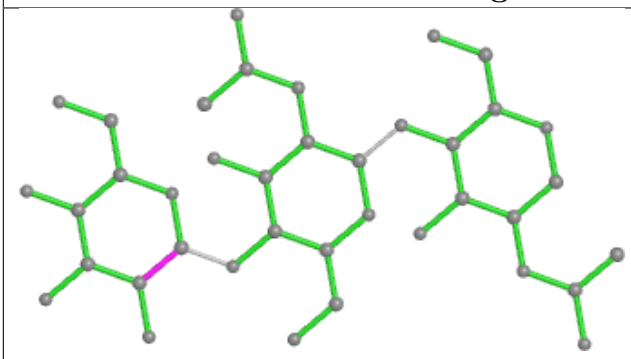
Oligosaccharide Chain J



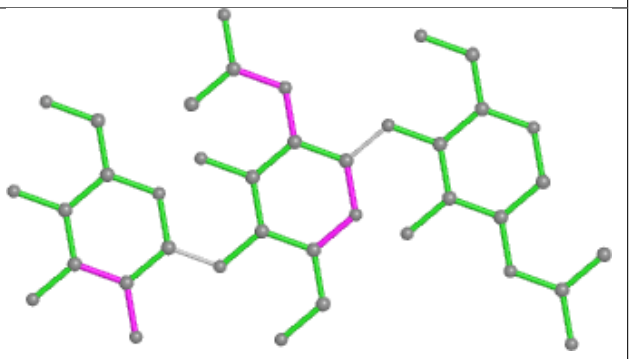
Oligosaccharide Chain L



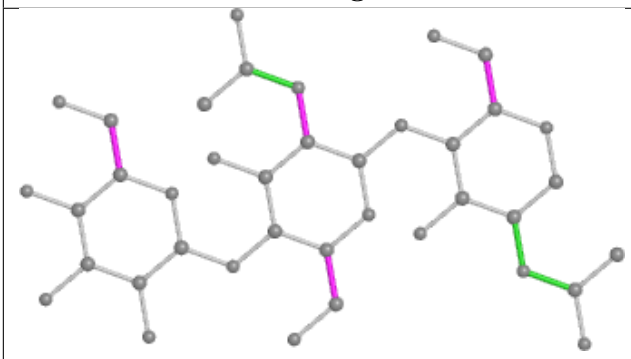
Oligosaccharide Chain M



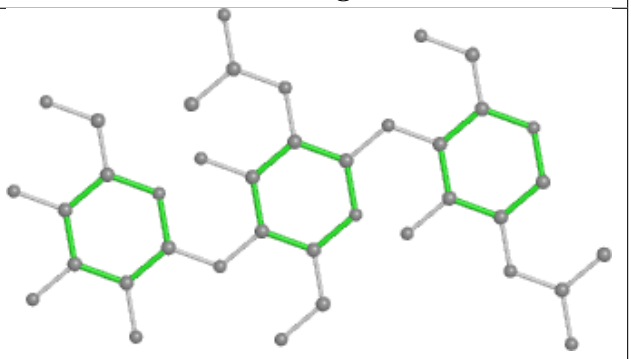
Bond lengths



Bond angles

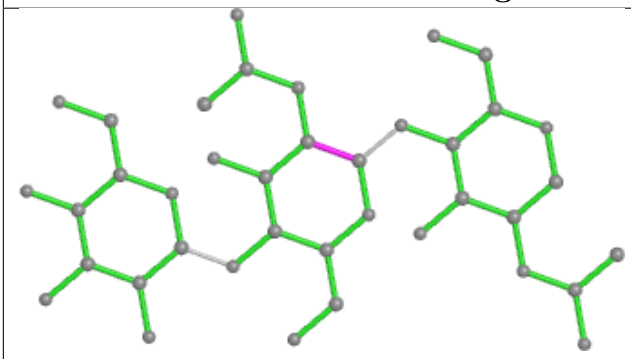


Torsions

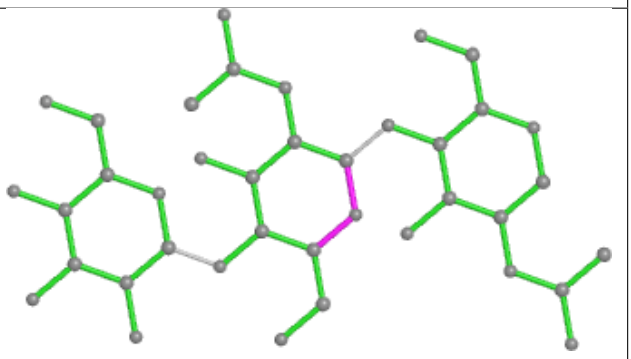


Rings

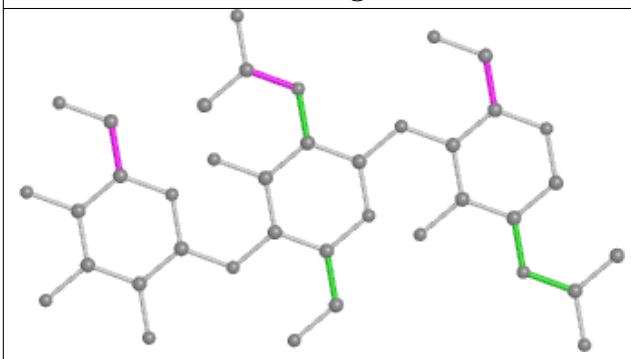
Oligosaccharide Chain O



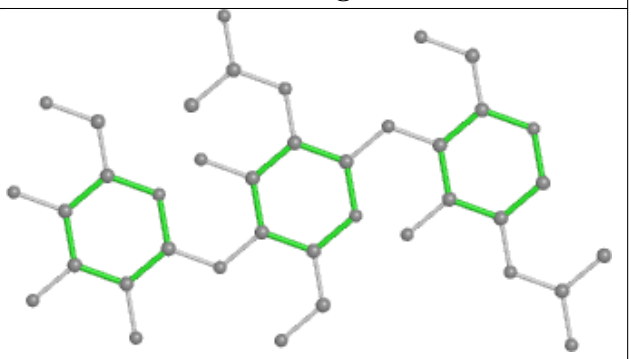
Bond lengths



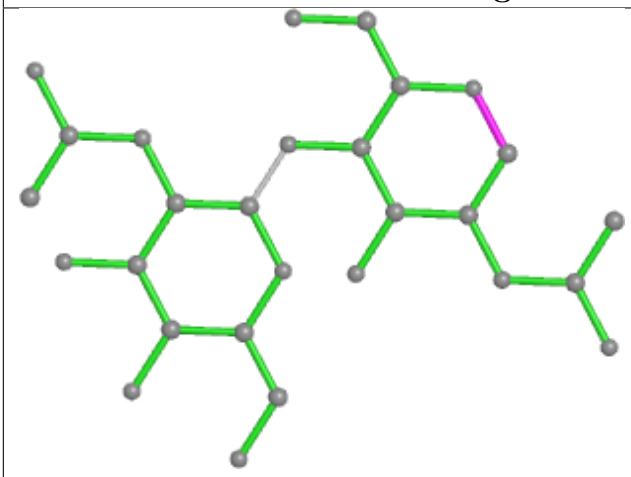
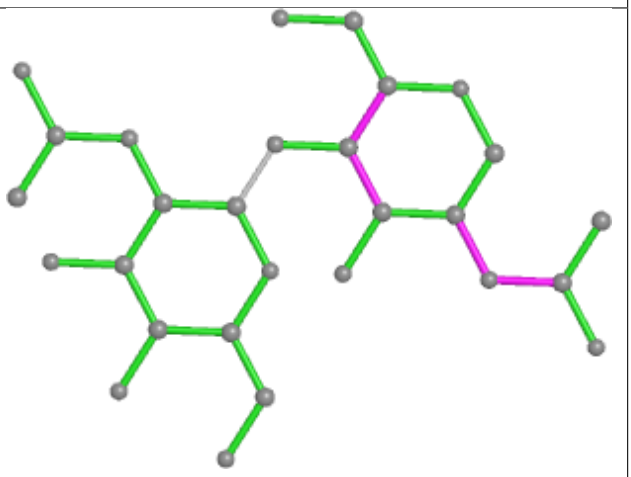
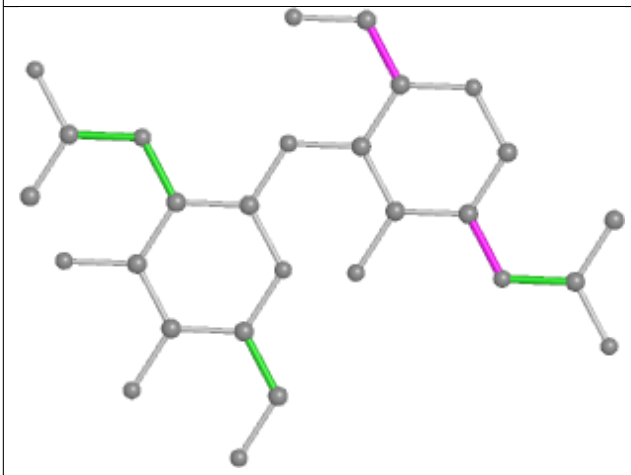
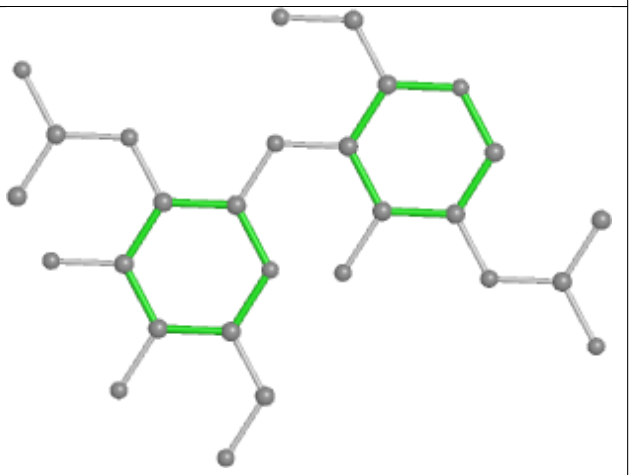
Bond angles

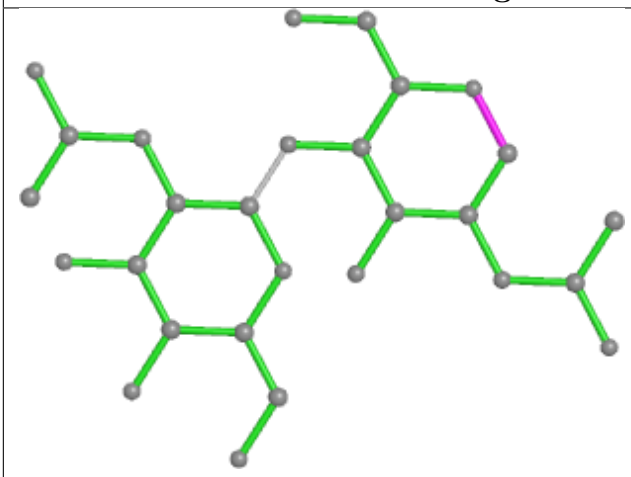
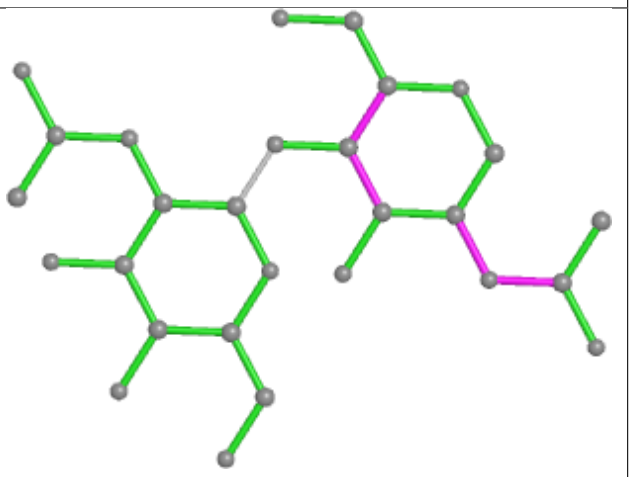
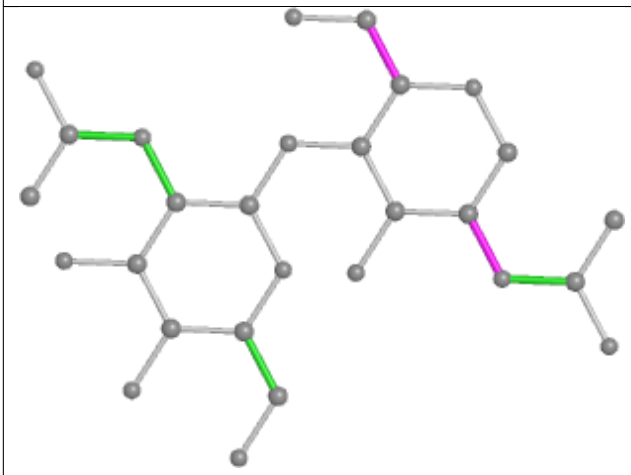
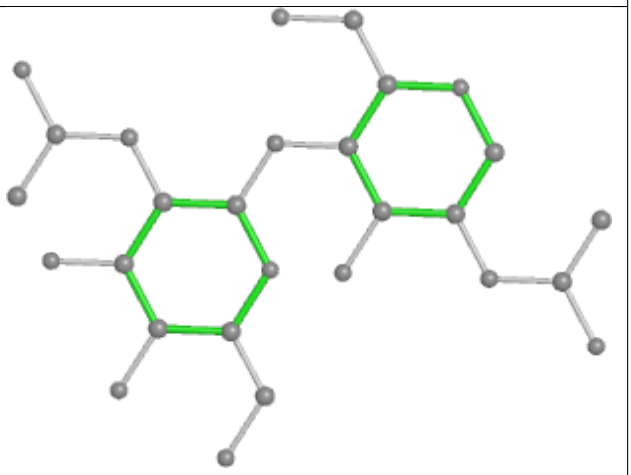


Torsions

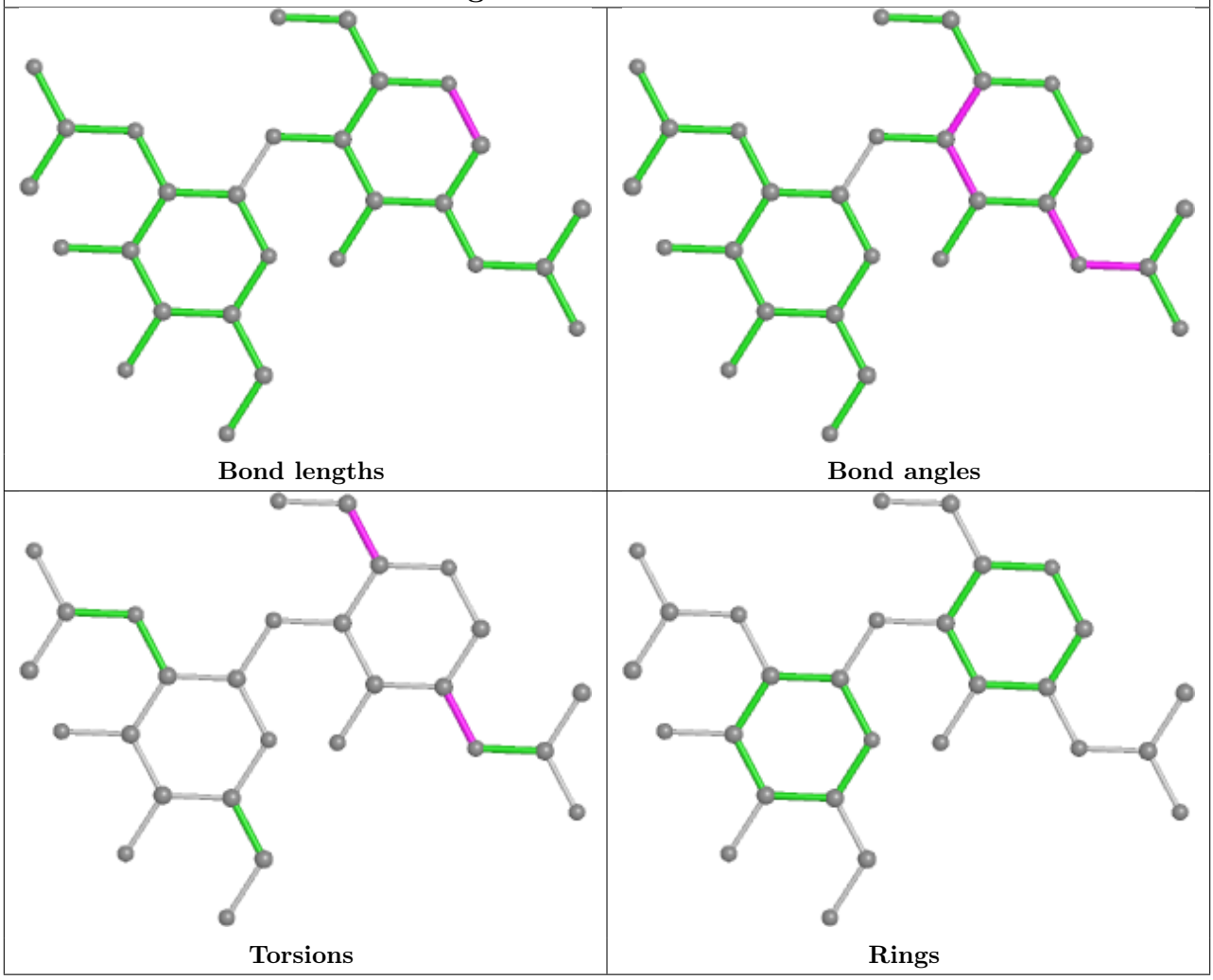


Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain K	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

36 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	C	609	1	14,14,15	0.28	0	17,19,21	0.84	0
5	NAG	A	607	1	14,14,15	0.58	0	17,19,21	0.46	0
5	NAG	A	601	1	14,14,15	0.31	0	17,19,21	0.83	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	F	802	2	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
5	NAG	D	803	2	14,14,15	0.68	0	17,19,21	2.24	3 (17%)
5	NAG	B	801	2	14,14,15	0.34	0	17,19,21	0.47	0
5	NAG	E	609	1	14,14,15	0.27	0	17,19,21	0.86	0
5	NAG	A	605	1	14,14,15	0.76	1 (7%)	17,19,21	2.26	4 (23%)
5	NAG	C	607	1	14,14,15	0.57	0	17,19,21	0.46	0
5	NAG	E	607	1	14,14,15	0.56	0	17,19,21	0.46	0
5	NAG	E	605	1	14,14,15	0.75	1 (7%)	17,19,21	2.26	4 (23%)
5	NAG	F	801	2	14,14,15	0.35	0	17,19,21	0.46	0
5	NAG	A	608	1	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	E	603	1	14,14,15	0.77	1 (7%)	17,19,21	2.25	4 (23%)
5	NAG	A	606	1	14,14,15	0.47	0	17,19,21	0.50	0
5	NAG	A	603	1	14,14,15	0.76	1 (7%)	17,19,21	2.26	4 (23%)
5	NAG	F	803	2	14,14,15	0.67	0	17,19,21	2.25	3 (17%)
5	NAG	C	606	1	14,14,15	0.46	0	17,19,21	0.50	0
5	NAG	A	604	1	14,14,15	0.25	0	17,19,21	0.56	0
5	NAG	E	606	1	14,14,15	0.47	0	17,19,21	0.49	0
5	NAG	C	601	1	14,14,15	0.31	0	17,19,21	0.83	1 (5%)
5	NAG	C	604	1	14,14,15	0.24	0	17,19,21	0.55	0
5	NAG	A	602	1	14,14,15	0.33	0	17,19,21	0.49	0
5	NAG	E	608	1	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	B	802	2	14,14,15	0.29	0	17,19,21	0.61	1 (5%)
5	NAG	C	605	1	14,14,15	0.75	1 (7%)	17,19,21	2.27	4 (23%)
5	NAG	A	609	1	14,14,15	0.27	0	17,19,21	0.82	0
5	NAG	D	802	2	14,14,15	0.29	0	17,19,21	0.61	1 (5%)
5	NAG	E	604	1	14,14,15	0.24	0	17,19,21	0.55	0
5	NAG	E	602	1	14,14,15	0.35	0	17,19,21	0.50	0
5	NAG	C	608	1	14,14,15	0.22	0	17,19,21	0.39	0
5	NAG	C	603	1	14,14,15	0.77	1 (7%)	17,19,21	2.26	4 (23%)
5	NAG	D	801	2	14,14,15	0.34	0	17,19,21	0.46	0
5	NAG	C	602	1	14,14,15	0.35	0	17,19,21	0.50	0
5	NAG	B	803	2	14,14,15	0.68	0	17,19,21	2.25	3 (17%)
5	NAG	E	601	1	14,14,15	0.31	0	17,19,21	0.82	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	609	1	-	5/6/23/26	0/1/1/1
5	NAG	A	607	1	-	1/6/23/26	0/1/1/1
5	NAG	A	601	1	-	4/6/23/26	0/1/1/1
5	NAG	F	802	2	-	2/6/23/26	0/1/1/1
5	NAG	D	803	2	-	5/6/23/26	0/1/1/1
5	NAG	B	801	2	-	2/6/23/26	0/1/1/1
5	NAG	E	609	1	-	5/6/23/26	0/1/1/1
5	NAG	A	605	1	-	4/6/23/26	0/1/1/1
5	NAG	C	607	1	-	1/6/23/26	0/1/1/1
5	NAG	E	607	1	-	1/6/23/26	0/1/1/1
5	NAG	E	605	1	-	4/6/23/26	0/1/1/1
5	NAG	F	801	2	-	2/6/23/26	0/1/1/1
5	NAG	A	608	1	-	2/6/23/26	0/1/1/1
5	NAG	E	603	1	-	3/6/23/26	0/1/1/1
5	NAG	A	606	1	-	1/6/23/26	0/1/1/1
5	NAG	A	603	1	-	3/6/23/26	0/1/1/1
5	NAG	F	803	2	-	5/6/23/26	0/1/1/1
5	NAG	C	606	1	-	1/6/23/26	0/1/1/1
5	NAG	A	604	1	-	2/6/23/26	0/1/1/1
5	NAG	E	606	1	-	1/6/23/26	0/1/1/1
5	NAG	C	601	1	-	4/6/23/26	0/1/1/1
5	NAG	C	604	1	-	2/6/23/26	0/1/1/1
5	NAG	A	602	1	-	2/6/23/26	0/1/1/1
5	NAG	E	608	1	-	2/6/23/26	0/1/1/1
5	NAG	B	802	2	-	2/6/23/26	0/1/1/1
5	NAG	C	605	1	-	4/6/23/26	0/1/1/1
5	NAG	A	609	1	-	5/6/23/26	0/1/1/1
5	NAG	D	802	2	-	2/6/23/26	0/1/1/1
5	NAG	E	604	1	-	2/6/23/26	0/1/1/1
5	NAG	E	602	1	-	2/6/23/26	0/1/1/1
5	NAG	C	608	1	-	2/6/23/26	0/1/1/1
5	NAG	C	603	1	-	3/6/23/26	0/1/1/1
5	NAG	D	801	2	-	2/6/23/26	0/1/1/1
5	NAG	C	602	1	-	2/6/23/26	0/1/1/1
5	NAG	B	803	2	-	5/6/23/26	0/1/1/1
5	NAG	E	601	1	-	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	603	NAG	C1-C2	2.26	1.55	1.52
5	C	603	NAG	C1-C2	2.24	1.55	1.52
5	A	603	NAG	C1-C2	2.20	1.55	1.52
5	A	605	NAG	C1-C2	2.16	1.55	1.52
5	C	605	NAG	C1-C2	2.12	1.55	1.52
5	E	605	NAG	C1-C2	2.10	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	803	NAG	C2-N2-C7	7.86	134.10	122.90
5	C	605	NAG	C2-N2-C7	7.85	134.08	122.90
5	F	803	NAG	C2-N2-C7	7.84	134.07	122.90
5	A	605	NAG	C2-N2-C7	7.83	134.05	122.90
5	E	605	NAG	C2-N2-C7	7.82	134.04	122.90
5	D	803	NAG	C2-N2-C7	7.82	134.04	122.90
5	C	603	NAG	C2-N2-C7	7.81	134.03	122.90
5	A	603	NAG	C2-N2-C7	7.80	134.00	122.90
5	E	603	NAG	C2-N2-C7	7.79	134.00	122.90
5	B	803	NAG	C1-C2-N2	3.77	116.93	110.49
5	F	803	NAG	C1-C2-N2	3.77	116.92	110.49
5	D	803	NAG	C1-C2-N2	3.76	116.91	110.49
5	E	605	NAG	C1-C2-N2	3.62	116.68	110.49
5	C	605	NAG	C1-C2-N2	3.60	116.64	110.49
5	A	605	NAG	C1-C2-N2	3.60	116.63	110.49
5	A	603	NAG	C1-C2-N2	3.57	116.59	110.49
5	C	603	NAG	C1-C2-N2	3.56	116.56	110.49
5	E	603	NAG	C1-C2-N2	3.55	116.55	110.49
5	C	601	NAG	C2-N2-C7	2.73	126.78	122.90
5	A	601	NAG	C2-N2-C7	2.69	126.74	122.90
5	E	601	NAG	C2-N2-C7	2.65	126.68	122.90
5	F	802	NAG	C1-O5-C5	2.20	115.18	112.19
5	C	603	NAG	C8-C7-N2	2.20	119.82	116.10
5	E	603	NAG	C8-C7-N2	2.19	119.80	116.10
5	A	603	NAG	C8-C7-N2	2.19	119.80	116.10
5	D	802	NAG	C1-O5-C5	2.18	115.15	112.19
5	B	802	NAG	C1-O5-C5	2.16	115.12	112.19
5	C	605	NAG	C1-O5-C5	2.16	115.11	112.19
5	D	803	NAG	C8-C7-N2	2.15	119.73	116.10
5	C	605	NAG	C8-C7-N2	2.14	119.73	116.10
5	A	603	NAG	C1-O5-C5	2.14	115.09	112.19
5	A	605	NAG	C1-O5-C5	2.14	115.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	605	NAG	C8-C7-N2	2.13	119.71	116.10
5	C	603	NAG	C1-O5-C5	2.13	115.08	112.19
5	E	603	NAG	C1-O5-C5	2.13	115.07	112.19
5	F	803	NAG	C8-C7-N2	2.12	119.68	116.10
5	E	605	NAG	C8-C7-N2	2.11	119.68	116.10
5	B	803	NAG	C8-C7-N2	2.10	119.66	116.10
5	E	605	NAG	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	609	NAG	C8-C7-N2-C2
5	C	609	NAG	O7-C7-N2-C2
5	E	609	NAG	C8-C7-N2-C2
5	E	609	NAG	O7-C7-N2-C2
5	B	802	NAG	O5-C5-C6-O6
5	D	802	NAG	O5-C5-C6-O6
5	F	802	NAG	O5-C5-C6-O6
5	A	604	NAG	C4-C5-C6-O6
5	C	604	NAG	C4-C5-C6-O6
5	E	604	NAG	C4-C5-C6-O6
5	A	609	NAG	C8-C7-N2-C2
5	A	609	NAG	O7-C7-N2-C2
5	B	801	NAG	O5-C5-C6-O6
5	B	803	NAG	O5-C5-C6-O6
5	D	801	NAG	O5-C5-C6-O6
5	D	803	NAG	O5-C5-C6-O6
5	F	801	NAG	O5-C5-C6-O6
5	F	803	NAG	O5-C5-C6-O6
5	A	601	NAG	C4-C5-C6-O6
5	B	802	NAG	C4-C5-C6-O6
5	C	601	NAG	C4-C5-C6-O6
5	D	802	NAG	C4-C5-C6-O6
5	E	601	NAG	C4-C5-C6-O6
5	F	802	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6
5	E	601	NAG	O5-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
5	C	602	NAG	O5-C5-C6-O6
5	E	602	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	608	NAG	C4-C5-C6-O6
5	C	608	NAG	C4-C5-C6-O6
5	E	608	NAG	C4-C5-C6-O6
5	A	603	NAG	C8-C7-N2-C2
5	A	603	NAG	O7-C7-N2-C2
5	A	605	NAG	C8-C7-N2-C2
5	A	605	NAG	O7-C7-N2-C2
5	B	803	NAG	C8-C7-N2-C2
5	B	803	NAG	O7-C7-N2-C2
5	C	603	NAG	C8-C7-N2-C2
5	C	603	NAG	O7-C7-N2-C2
5	C	605	NAG	C8-C7-N2-C2
5	C	605	NAG	O7-C7-N2-C2
5	D	803	NAG	C8-C7-N2-C2
5	D	803	NAG	O7-C7-N2-C2
5	E	603	NAG	C8-C7-N2-C2
5	E	603	NAG	O7-C7-N2-C2
5	E	605	NAG	C8-C7-N2-C2
5	E	605	NAG	O7-C7-N2-C2
5	F	803	NAG	C8-C7-N2-C2
5	F	803	NAG	O7-C7-N2-C2
5	B	801	NAG	C4-C5-C6-O6
5	D	801	NAG	C4-C5-C6-O6
5	F	801	NAG	C4-C5-C6-O6
5	A	608	NAG	O5-C5-C6-O6
5	C	608	NAG	O5-C5-C6-O6
5	E	608	NAG	O5-C5-C6-O6
5	A	604	NAG	O5-C5-C6-O6
5	C	604	NAG	O5-C5-C6-O6
5	E	604	NAG	O5-C5-C6-O6
5	B	803	NAG	C4-C5-C6-O6
5	D	803	NAG	C4-C5-C6-O6
5	F	803	NAG	C4-C5-C6-O6
5	A	609	NAG	C1-C2-N2-C7
5	E	609	NAG	C1-C2-N2-C7
5	C	609	NAG	C1-C2-N2-C7
5	A	601	NAG	C1-C2-N2-C7
5	C	601	NAG	C1-C2-N2-C7
5	E	601	NAG	C1-C2-N2-C7
5	C	606	NAG	O5-C5-C6-O6
5	E	606	NAG	O5-C5-C6-O6
5	A	606	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	609	NAG	O5-C5-C6-O6
5	E	609	NAG	O5-C5-C6-O6
5	C	609	NAG	O5-C5-C6-O6
5	A	607	NAG	O5-C5-C6-O6
5	C	607	NAG	O5-C5-C6-O6
5	E	607	NAG	O5-C5-C6-O6
5	C	602	NAG	C4-C5-C6-O6
5	E	602	NAG	C4-C5-C6-O6
5	A	602	NAG	C4-C5-C6-O6
5	A	605	NAG	C4-C5-C6-O6
5	C	605	NAG	C4-C5-C6-O6
5	E	605	NAG	C4-C5-C6-O6
5	A	603	NAG	C3-C2-N2-C7
5	C	603	NAG	C3-C2-N2-C7
5	E	603	NAG	C3-C2-N2-C7
5	A	601	NAG	C3-C2-N2-C7
5	A	605	NAG	C3-C2-N2-C7
5	A	609	NAG	C3-C2-N2-C7
5	B	803	NAG	C3-C2-N2-C7
5	C	601	NAG	C3-C2-N2-C7
5	C	605	NAG	C3-C2-N2-C7
5	C	609	NAG	C3-C2-N2-C7
5	D	803	NAG	C3-C2-N2-C7
5	E	601	NAG	C3-C2-N2-C7
5	E	605	NAG	C3-C2-N2-C7
5	E	609	NAG	C3-C2-N2-C7
5	F	803	NAG	C3-C2-N2-C7

There are no ring outliers.

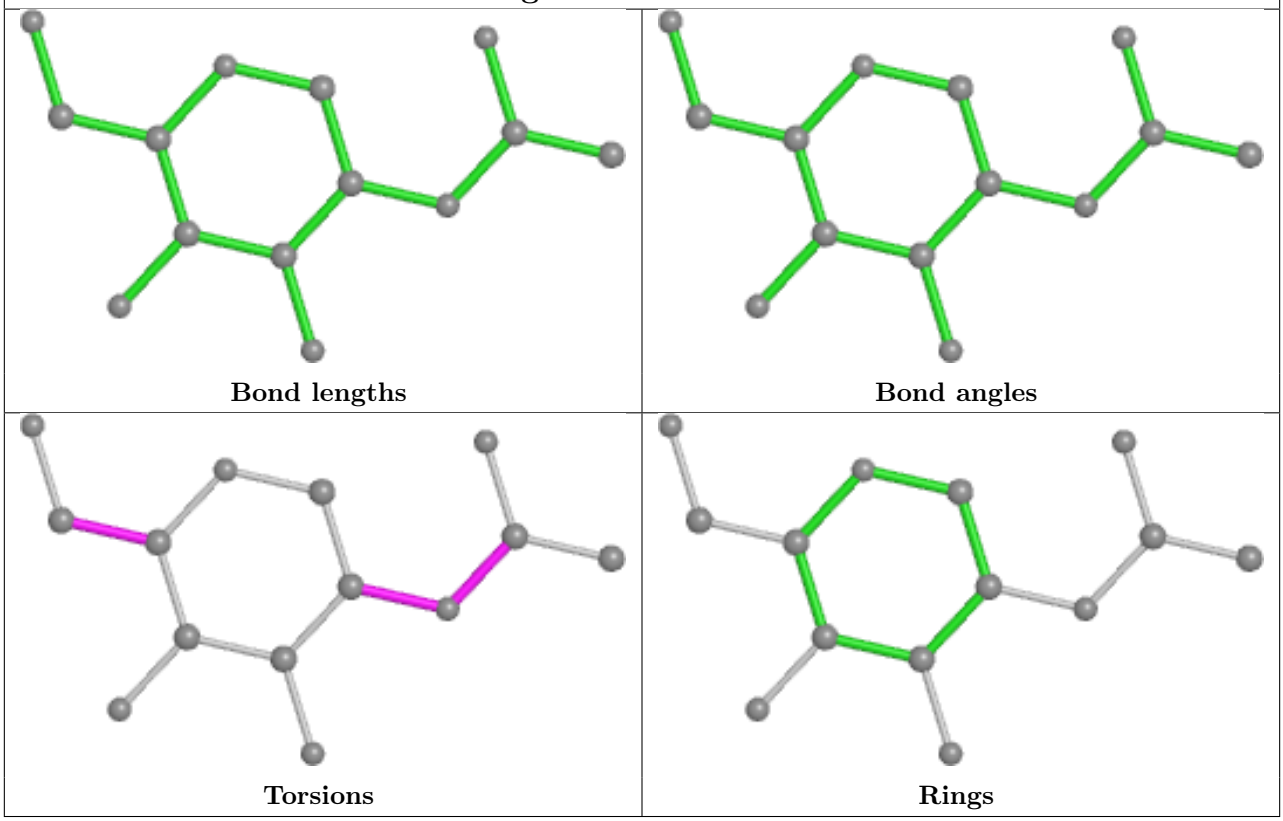
6 monomers are involved in 9 short contacts:

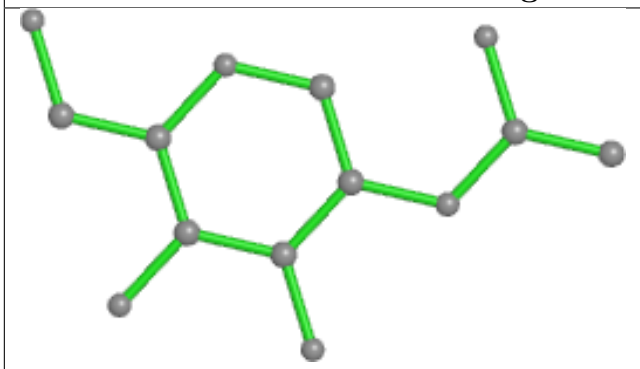
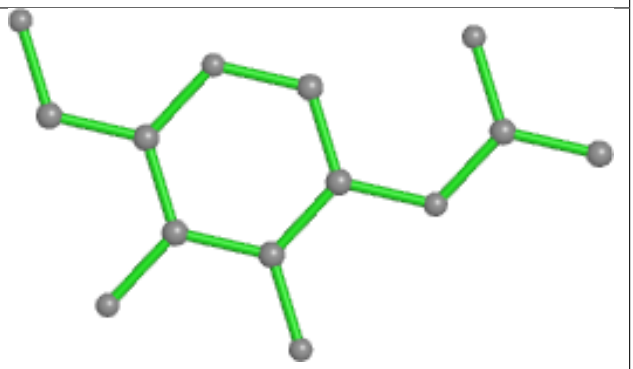
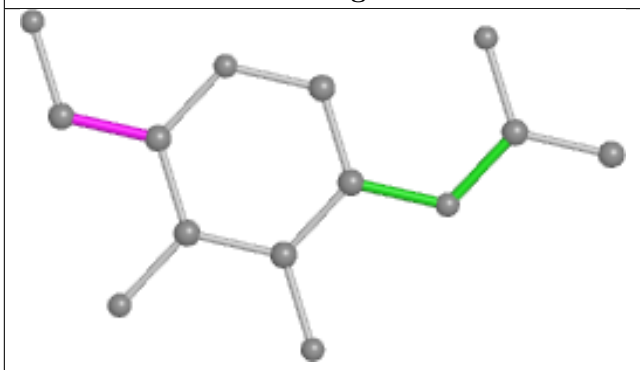
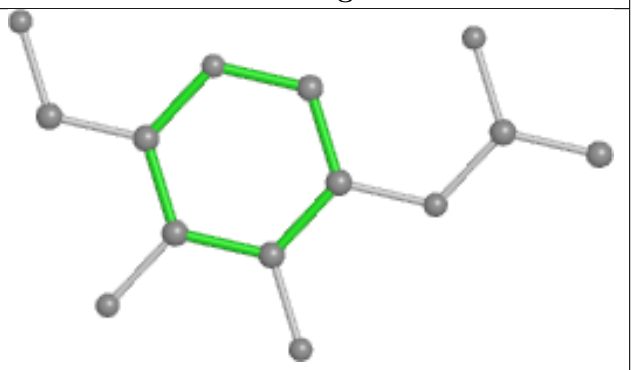
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	609	NAG	2	0
5	E	609	NAG	2	0
5	A	606	NAG	1	0
5	C	606	NAG	1	0
5	E	606	NAG	1	0
5	A	609	NAG	2	0

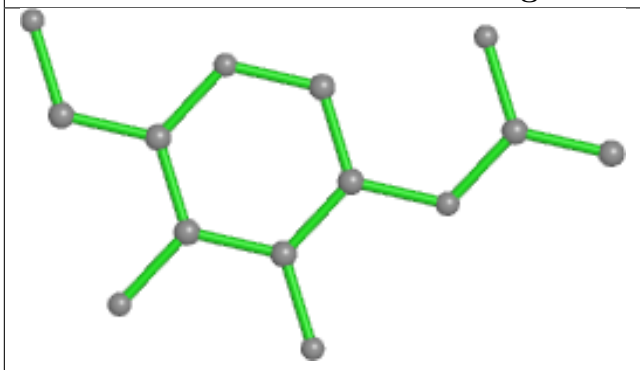
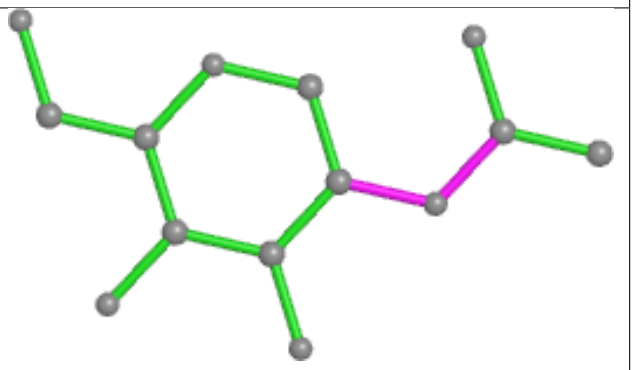
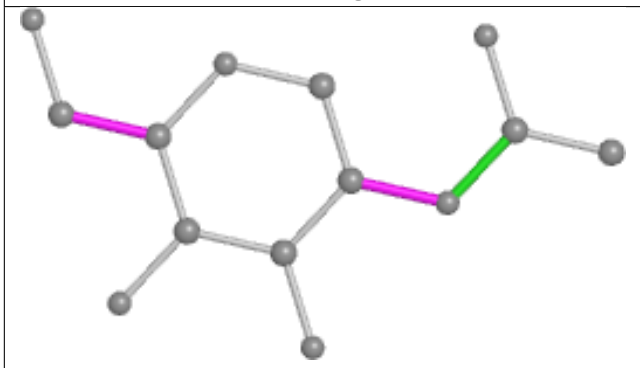
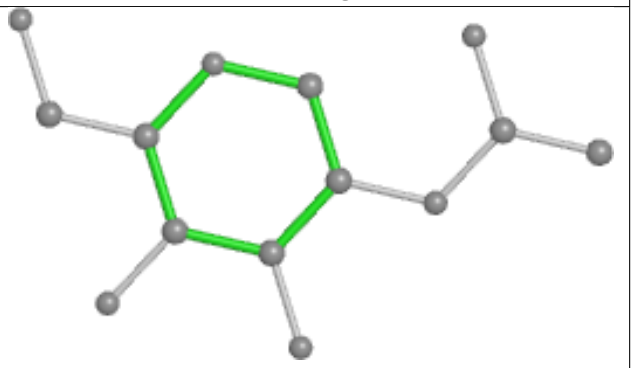
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

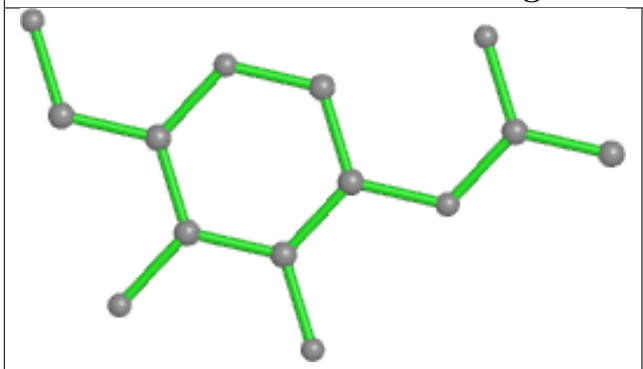
Ligand NAG C 609



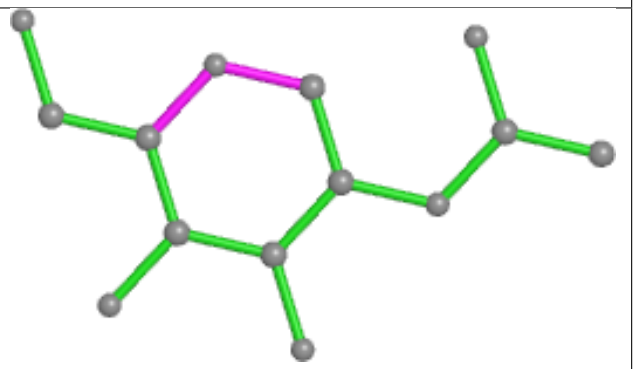
Ligand NAG A 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

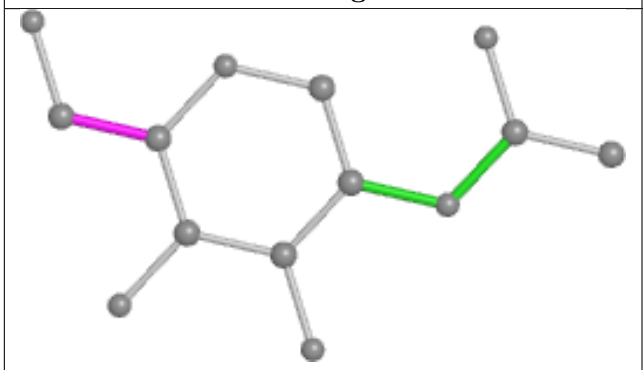
Ligand NAG F 802



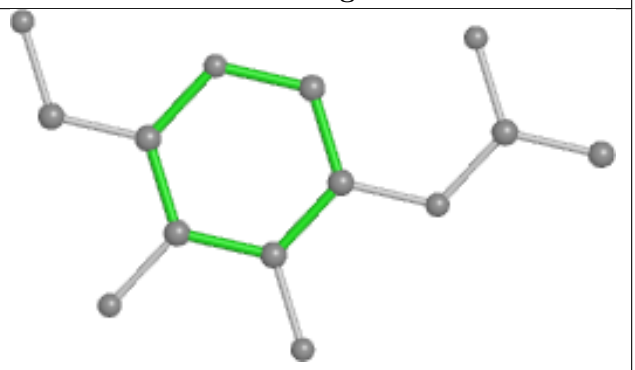
Bond lengths



Bond angles

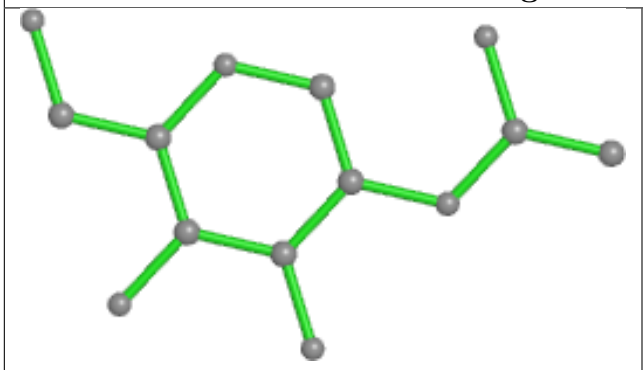


Torsions

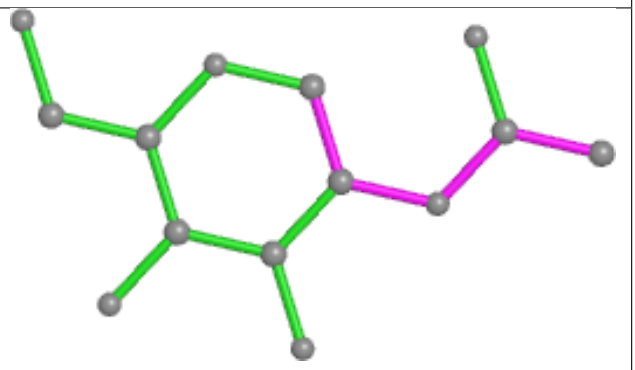


Rings

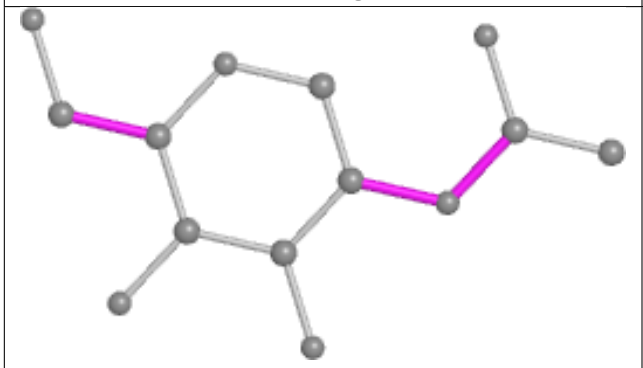
Ligand NAG D 803



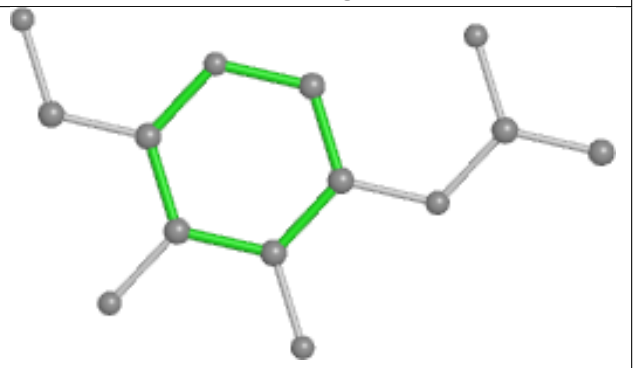
Bond lengths



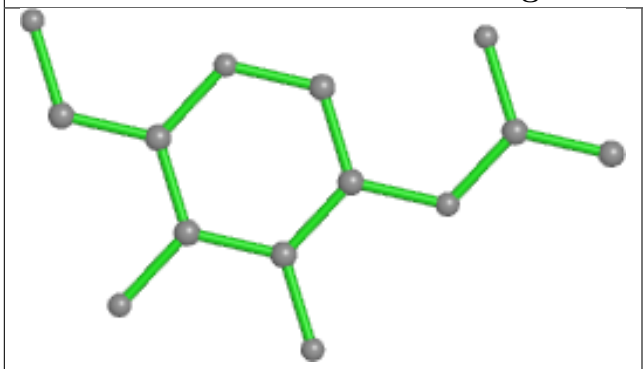
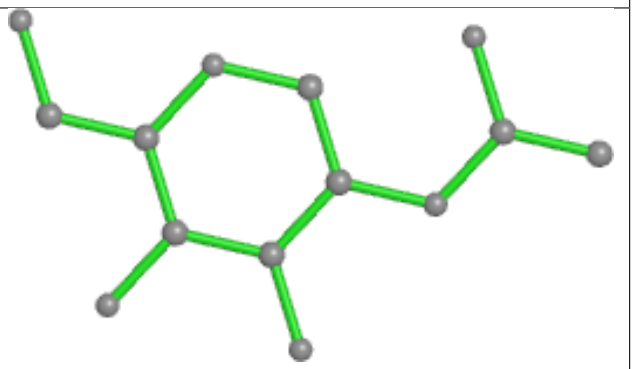
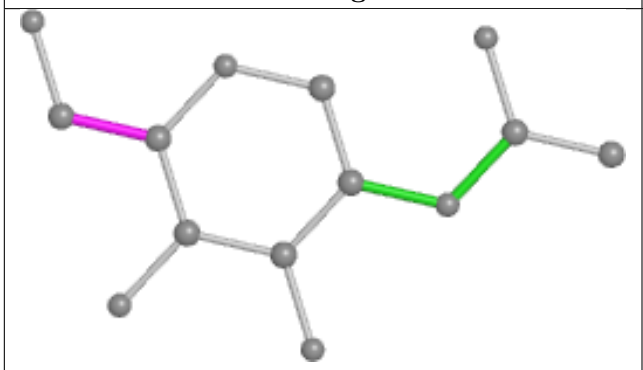
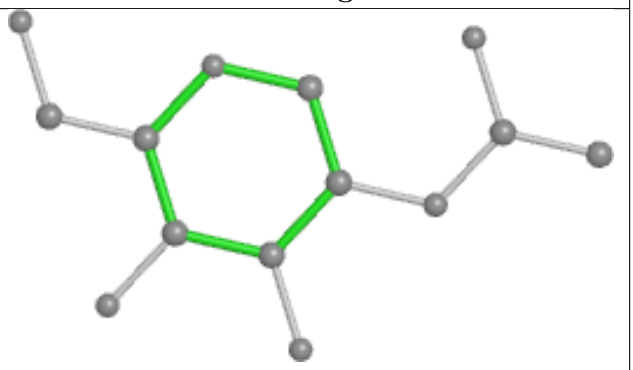
Bond angles



Torsions



Rings

Ligand NAG B 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

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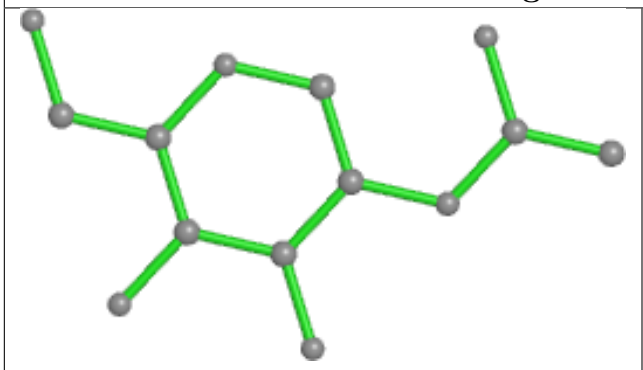
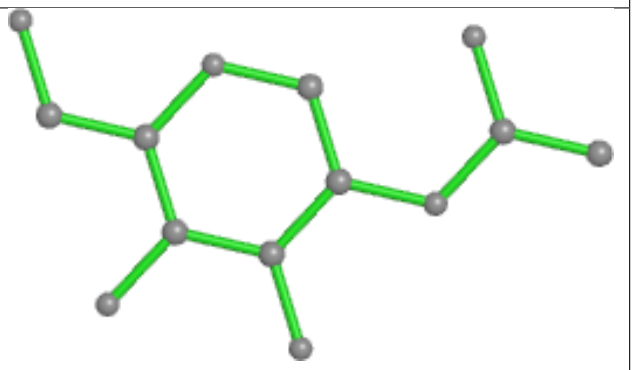
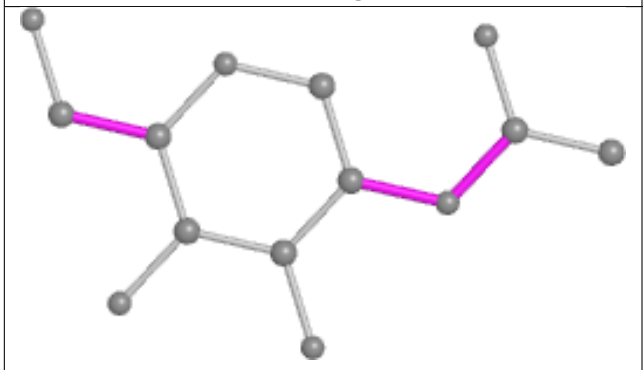
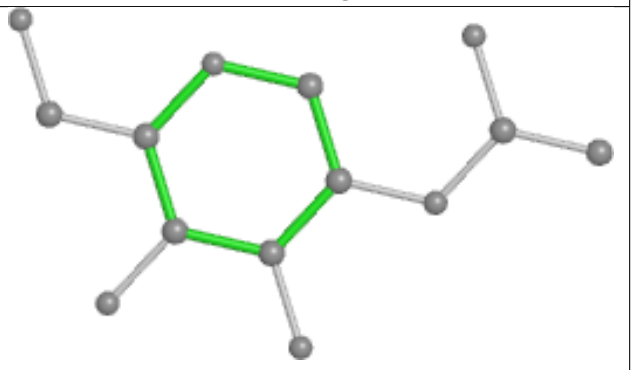
 Bond lengths	 Bond angles
 Torsions	 Rings

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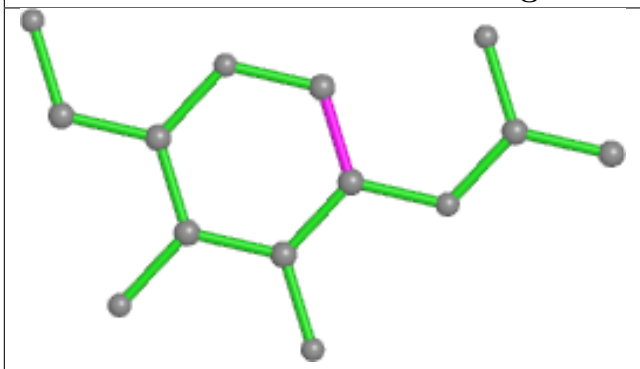
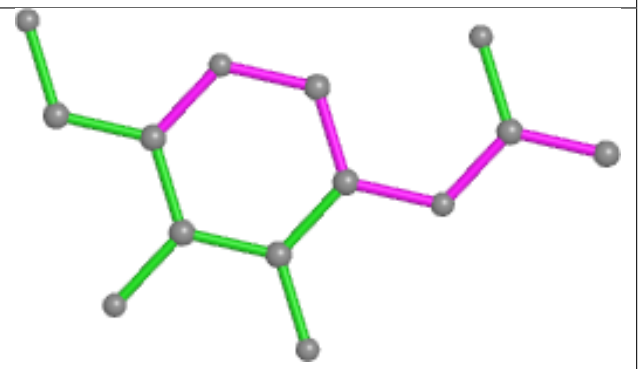
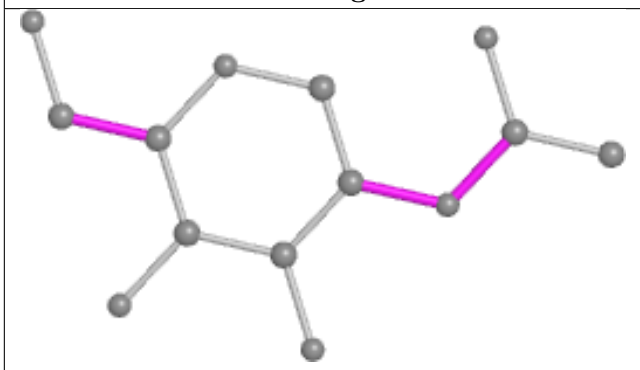
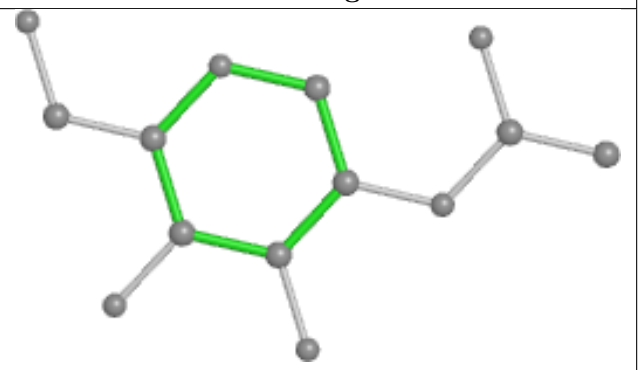
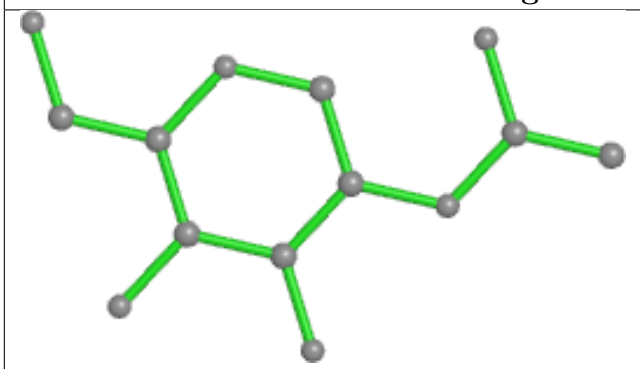
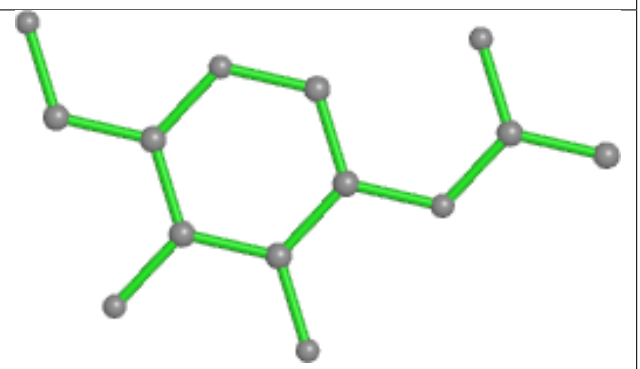
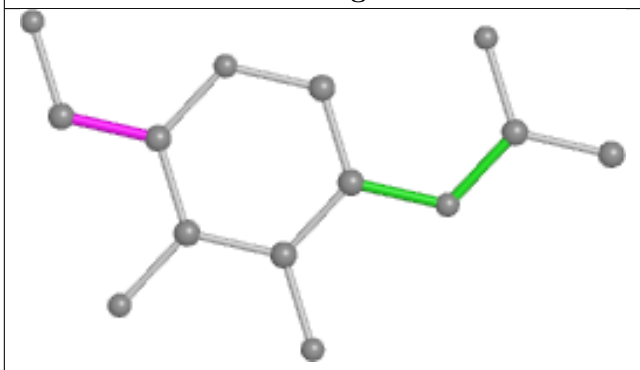
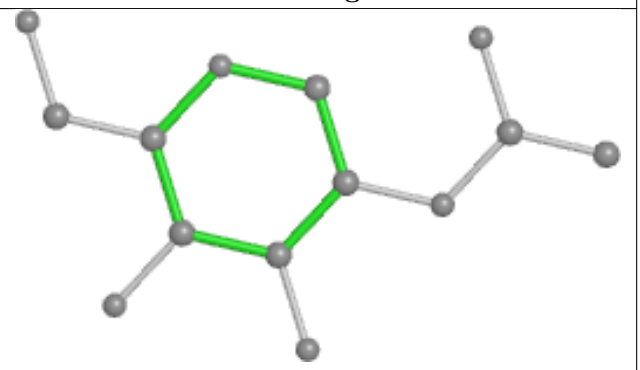
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 607	
 Bond lengths	 Bond angles
 Torsions	 Rings

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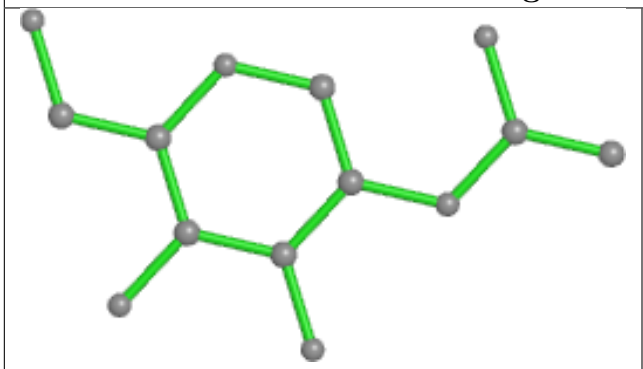
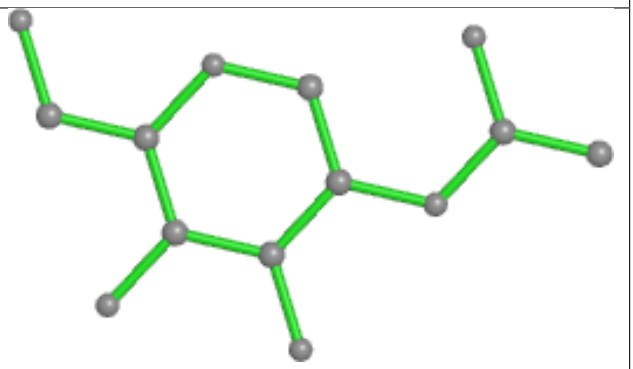
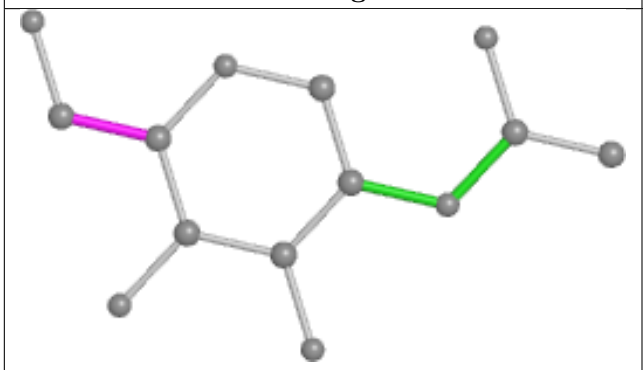
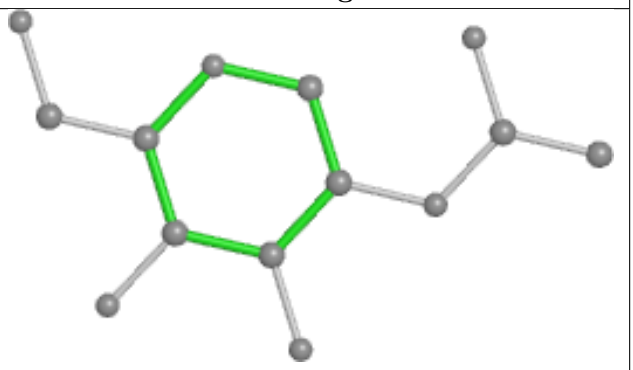
 Bond lengths	 Bond angles
 Torsions	 Rings

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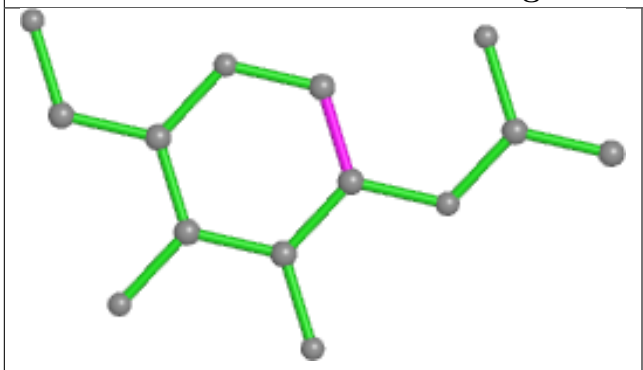
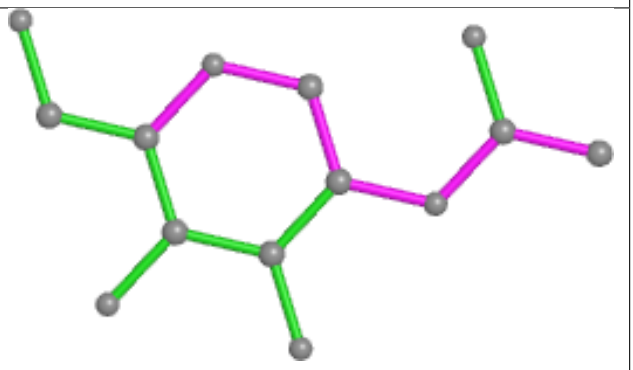
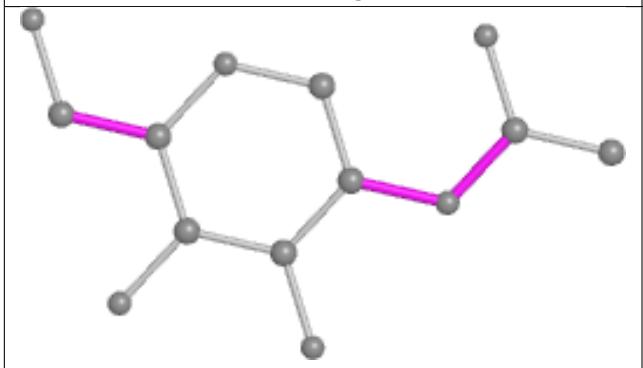
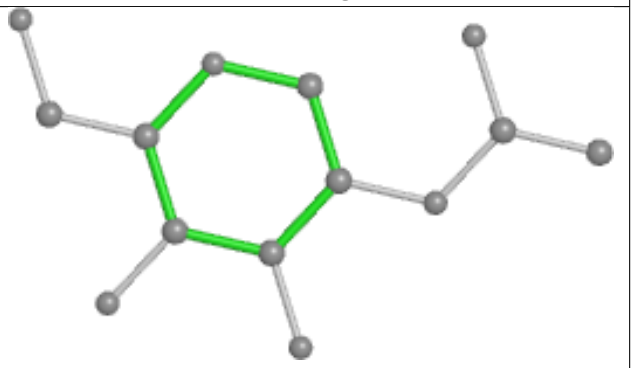
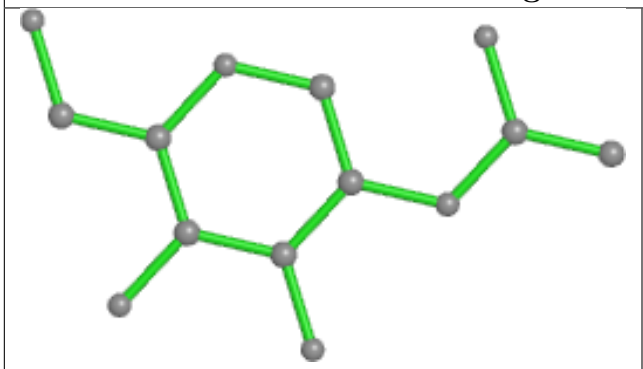
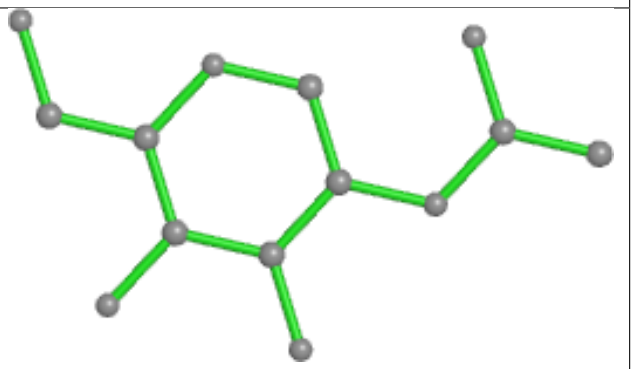
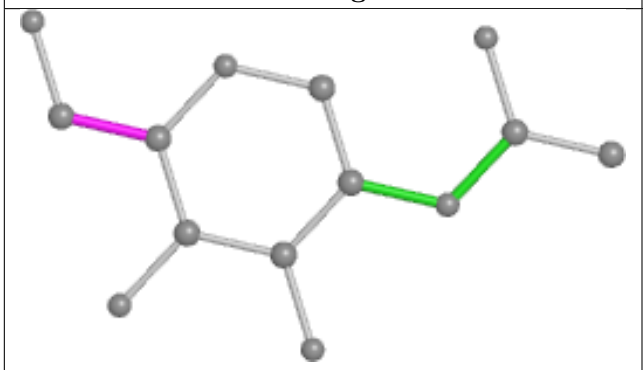
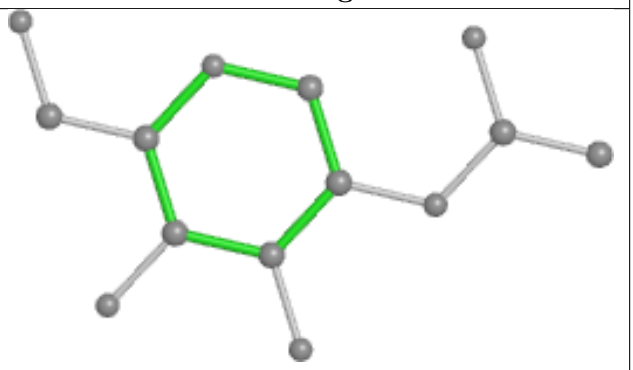
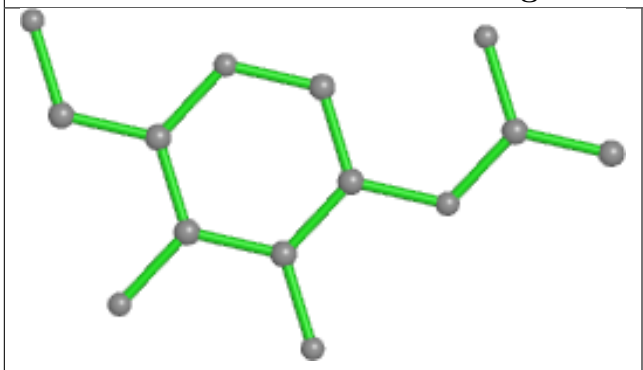
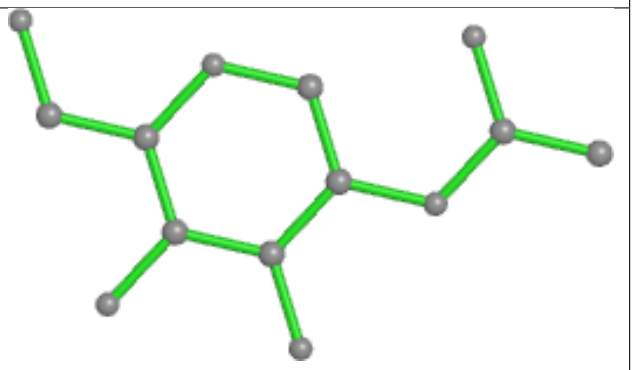
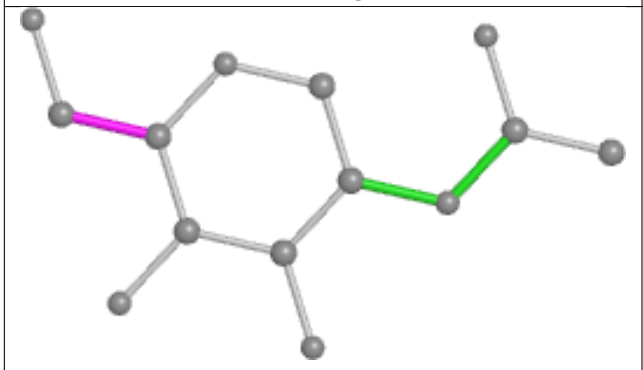
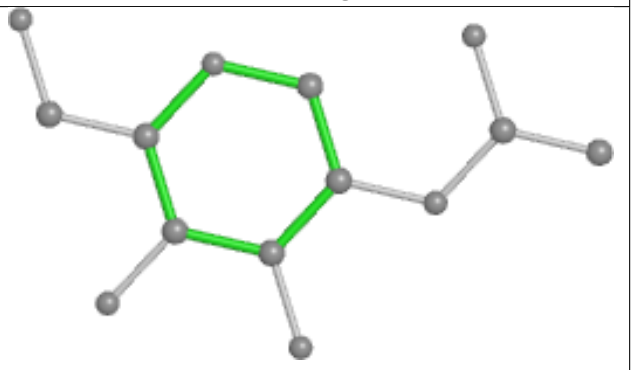
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG F 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

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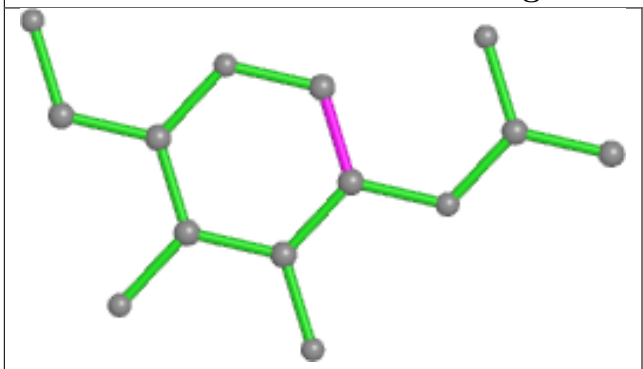
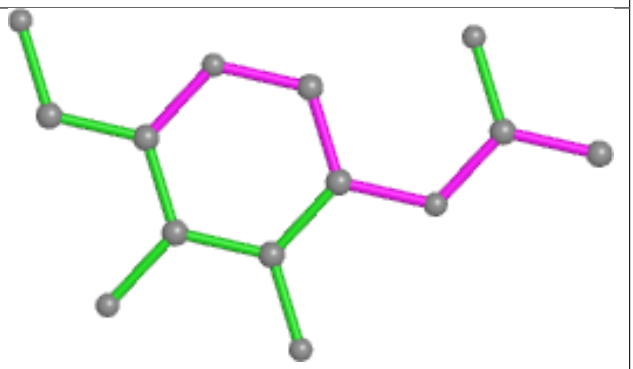
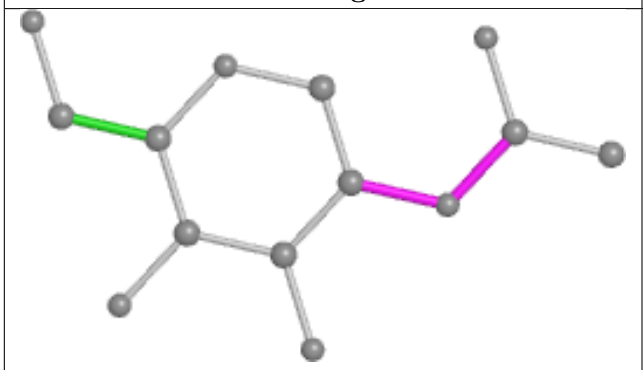
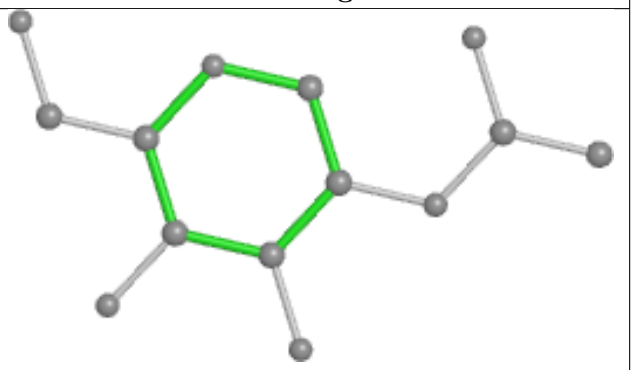
 Bond lengths	 Bond angles
 Torsions	 Rings

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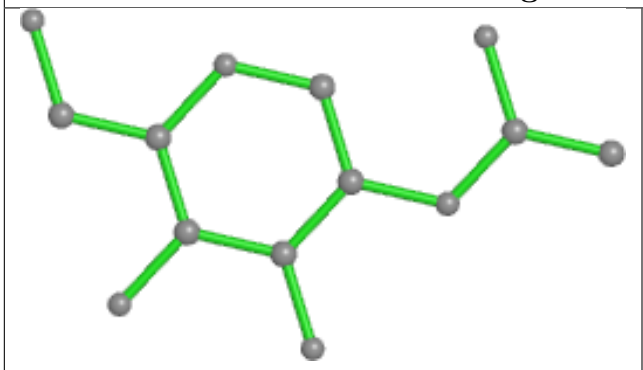
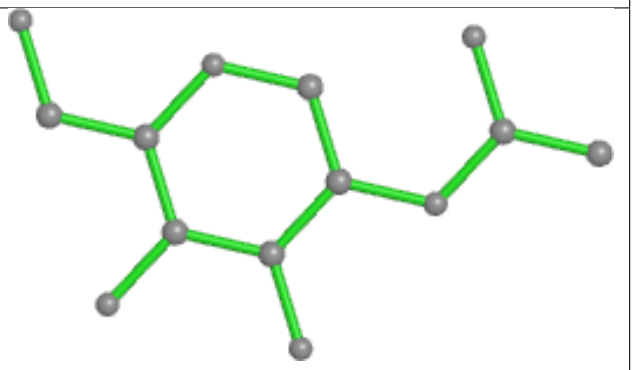
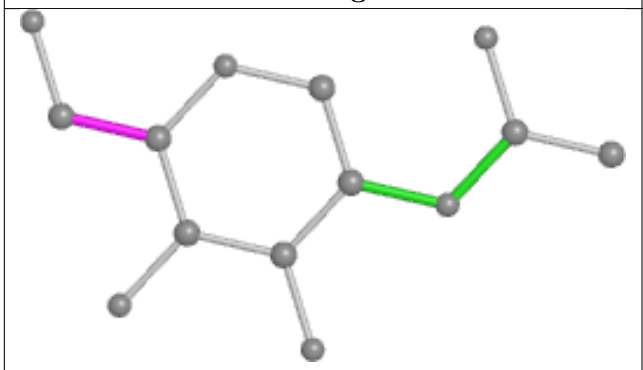
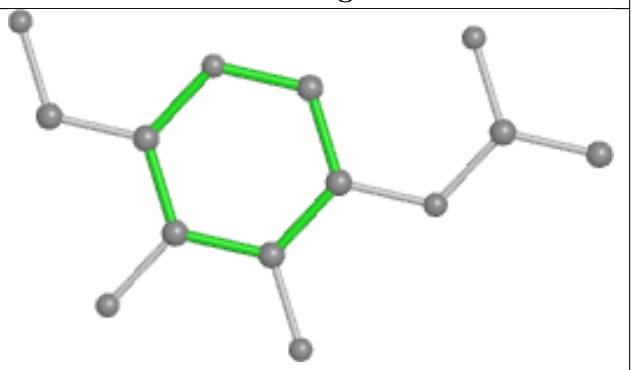
 Bond lengths	 Bond angles
 Torsions	 Rings

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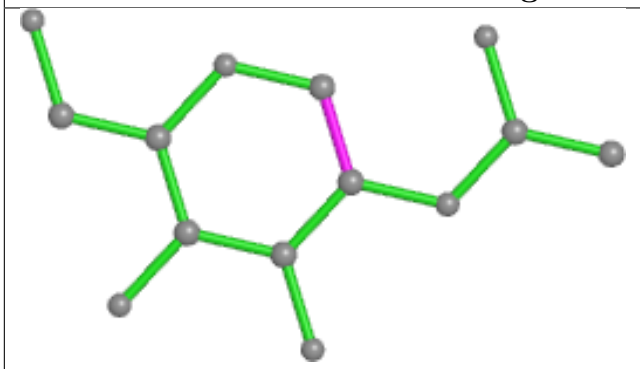
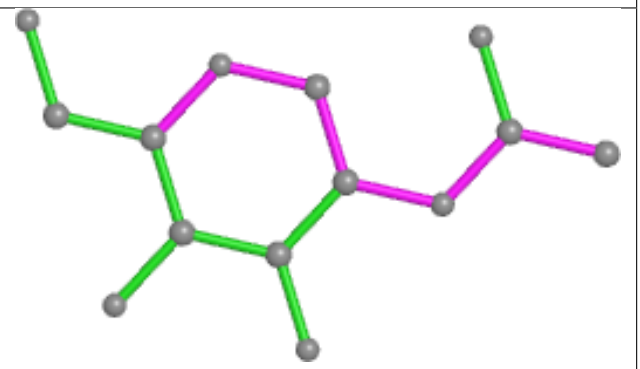
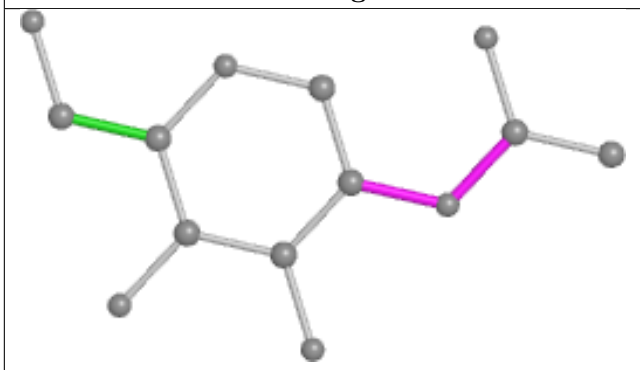
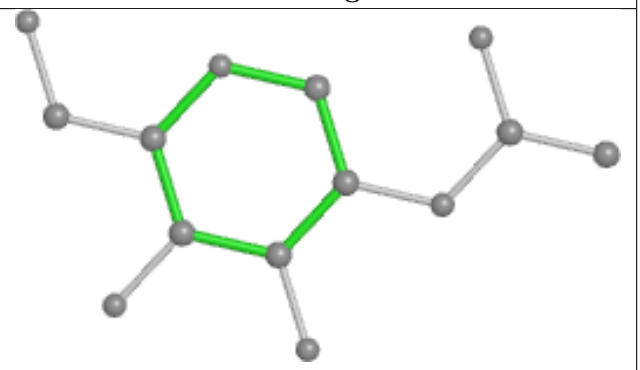
 Bond lengths	 Bond angles
 Torsions	 Rings

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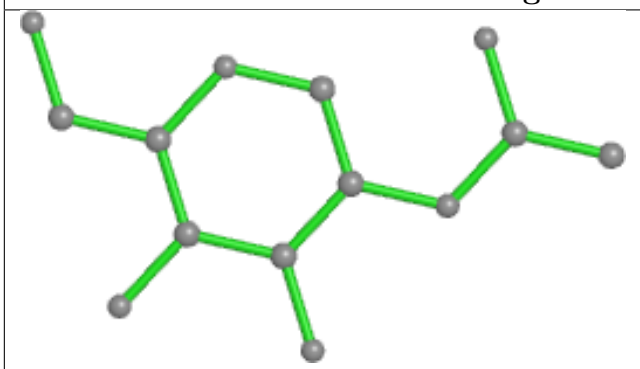
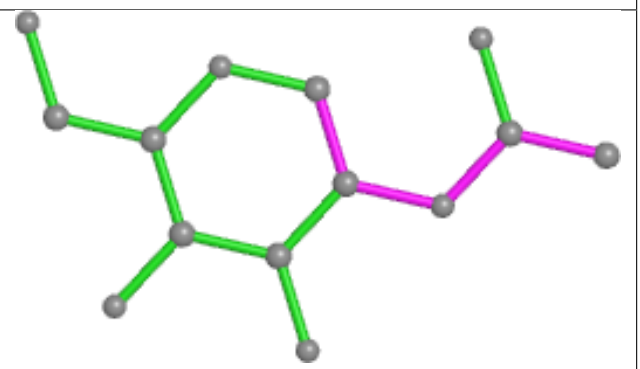
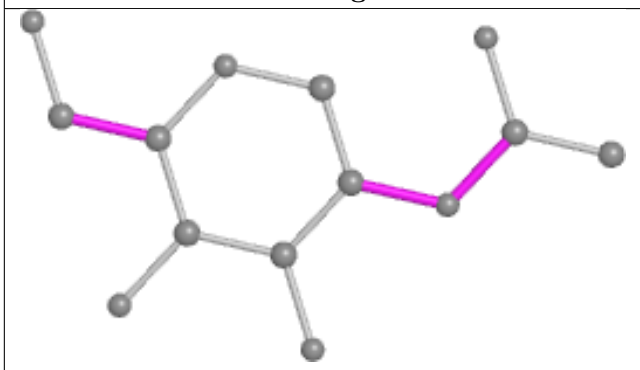
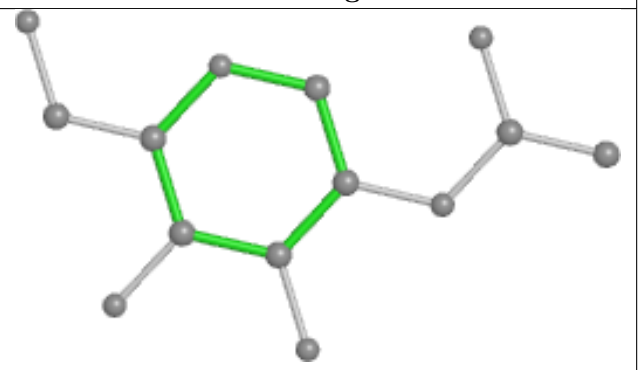
 Bond lengths	 Bond angles
 Torsions	 Rings

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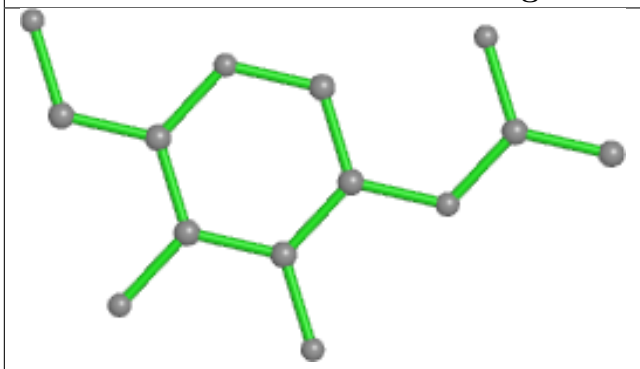
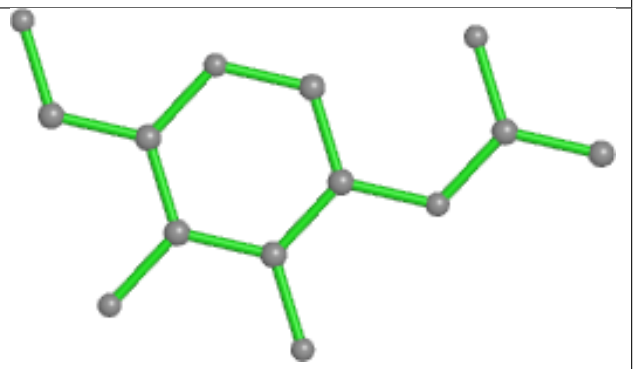
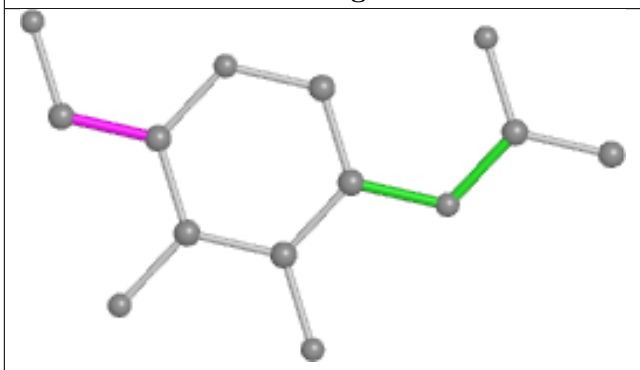
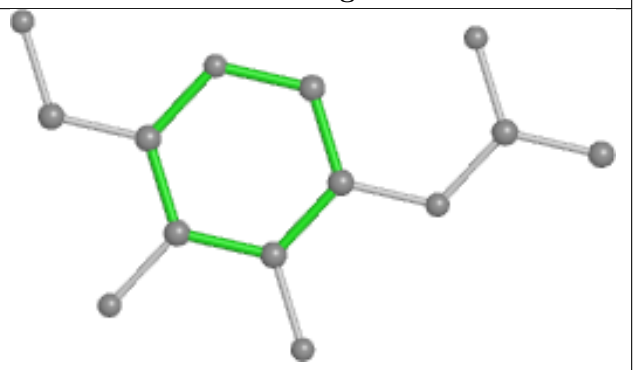
 Bond lengths	 Bond angles
 Torsions	 Rings

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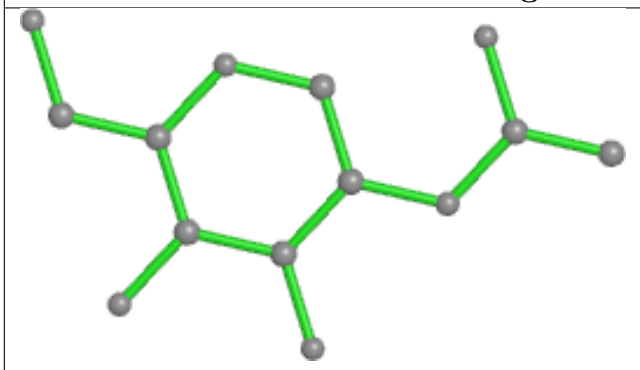
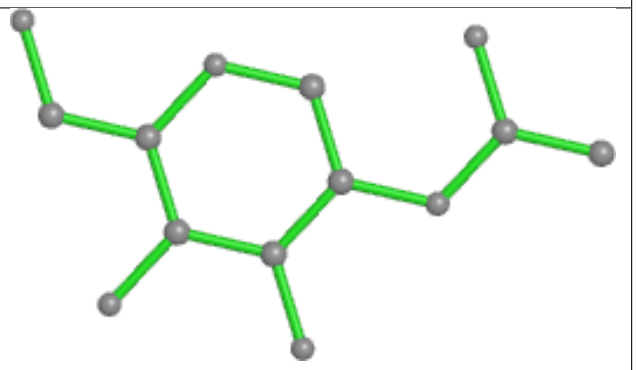
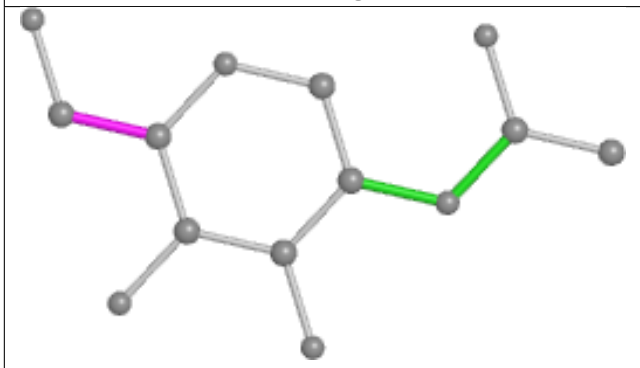
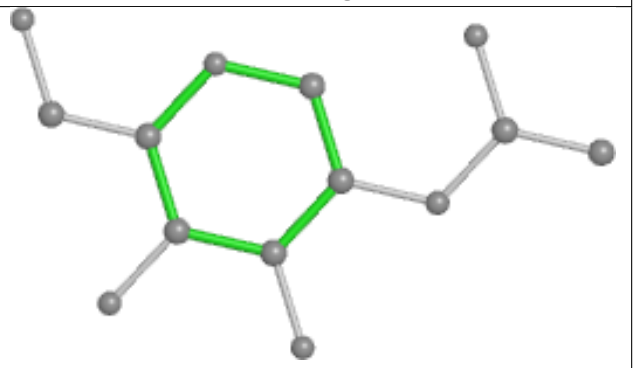
 Bond lengths	 Bond angles
 Torsions	 Rings

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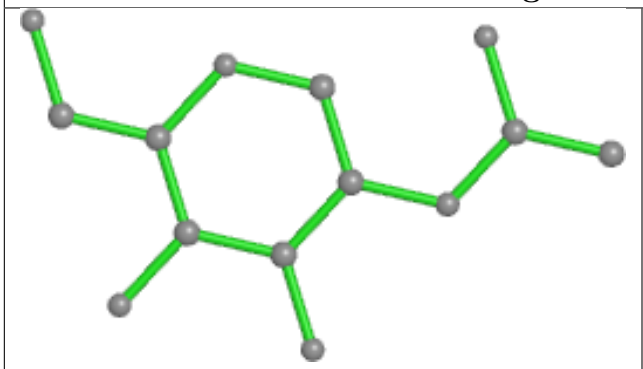
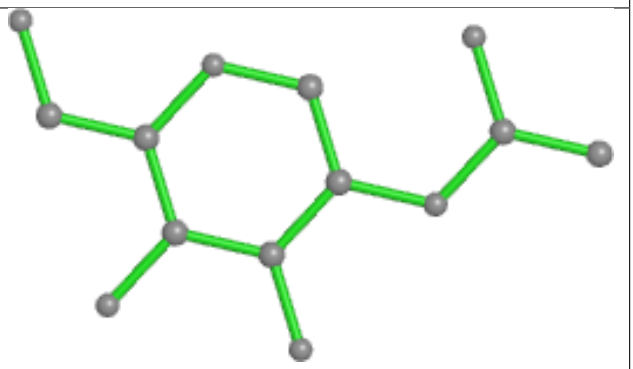
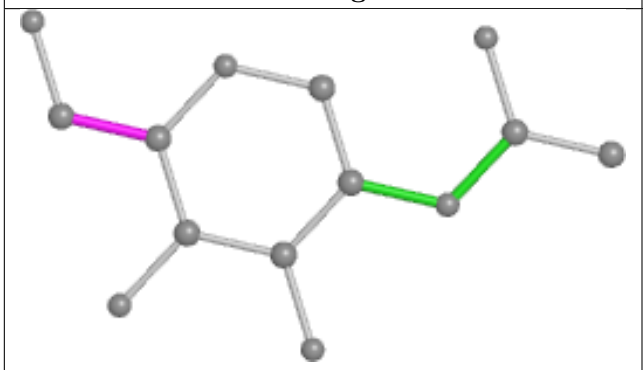
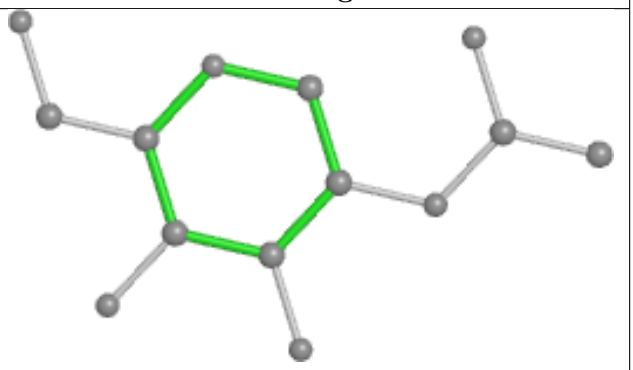
 Bond lengths	 Bond angles
 Torsions	 Rings

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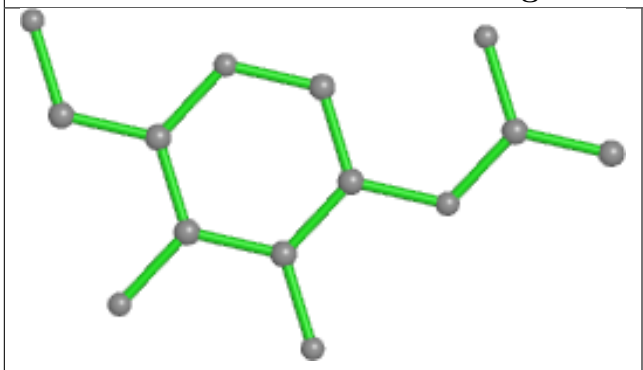
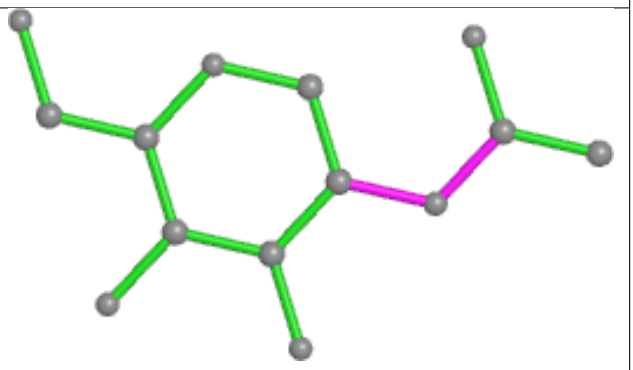
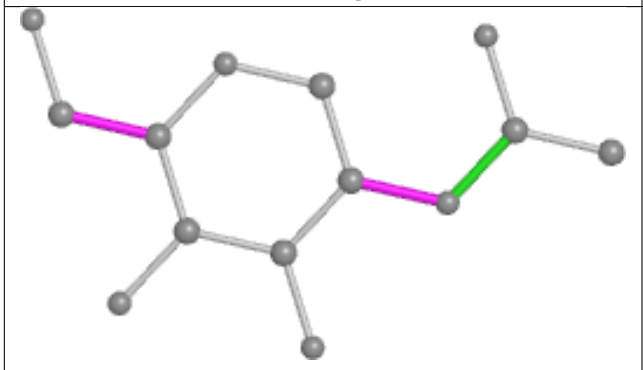
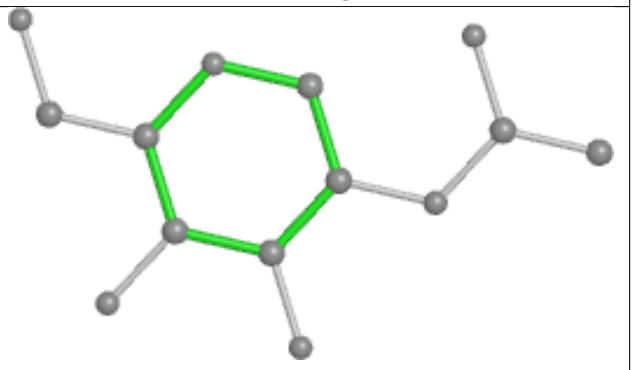
 Bond lengths	 Bond angles
 Torsions	 Rings

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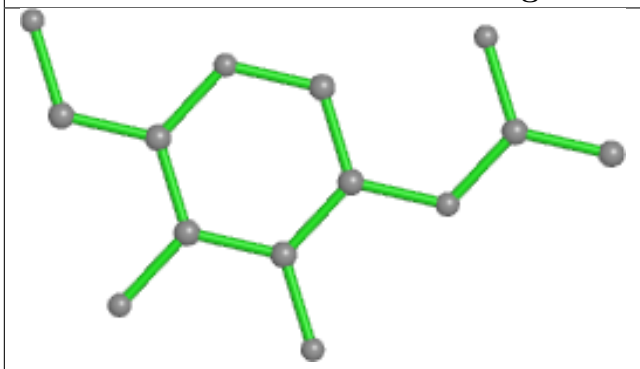
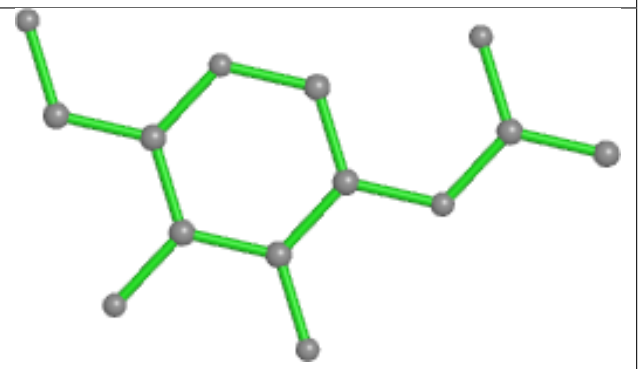
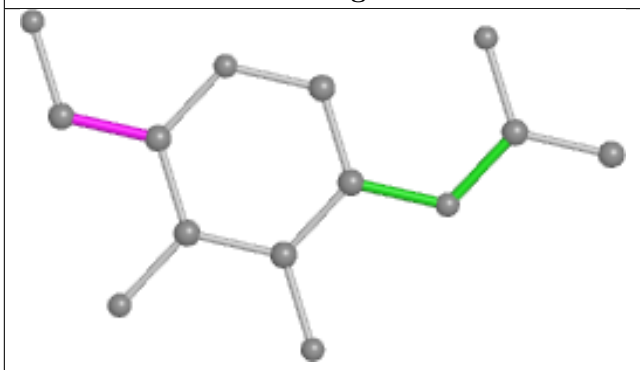
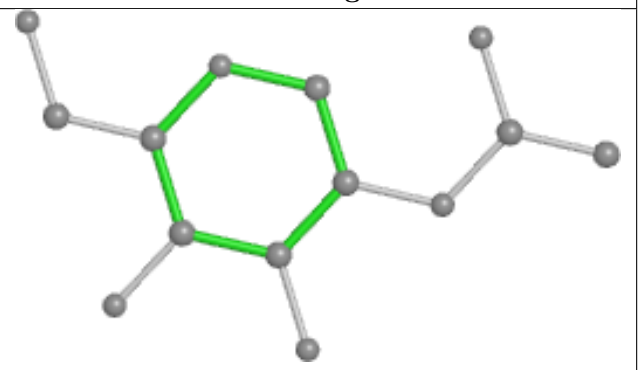
 Bond lengths	 Bond angles
 Torsions	 Rings

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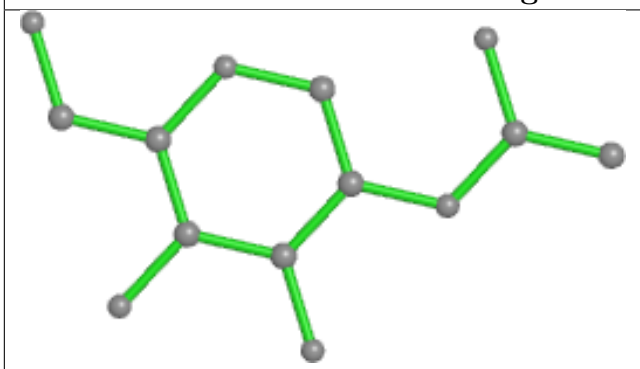
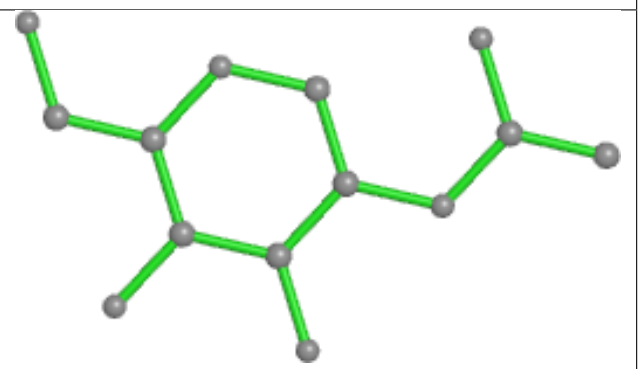
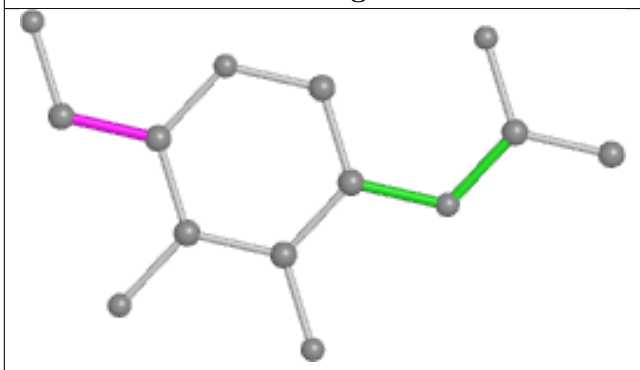
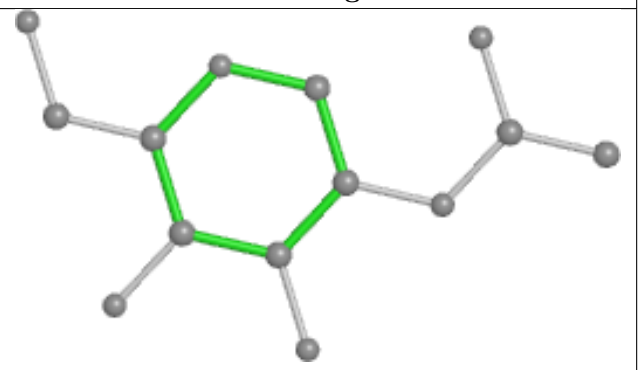
 Bond lengths	 Bond angles
 Torsions	 Rings

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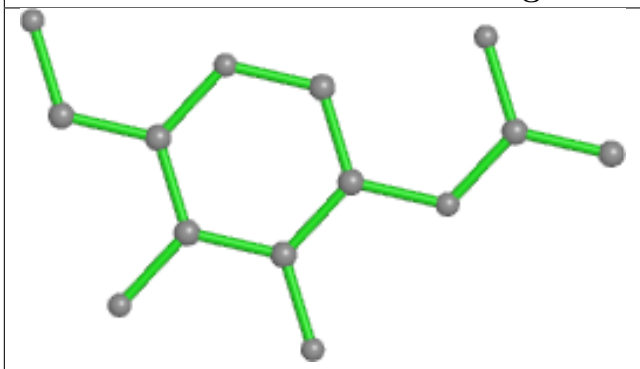
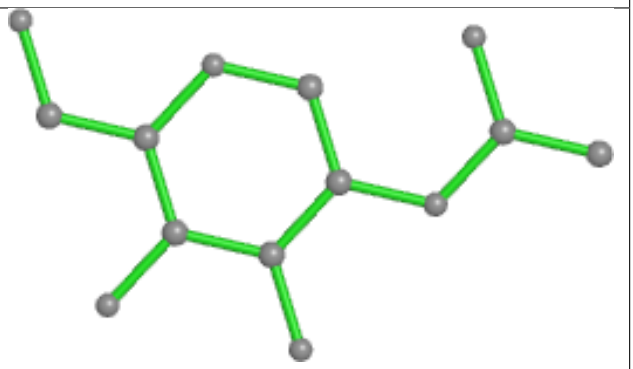
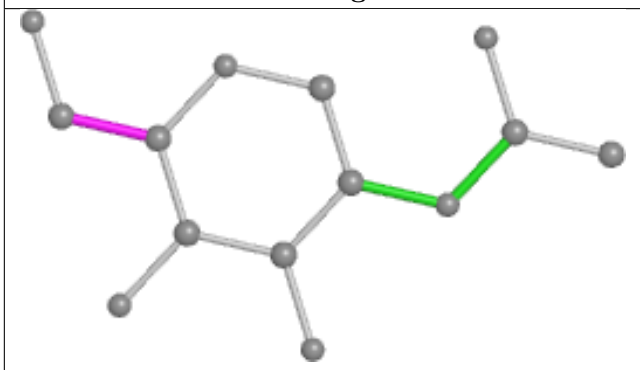
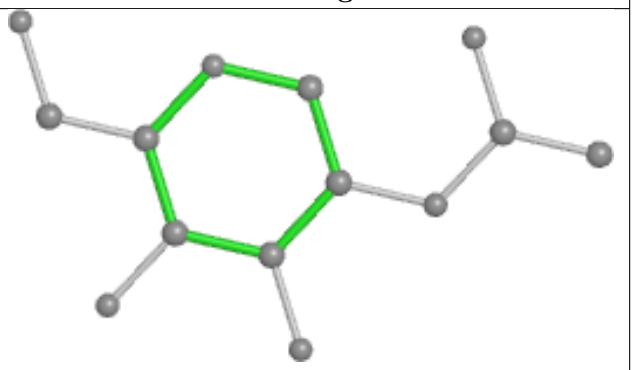
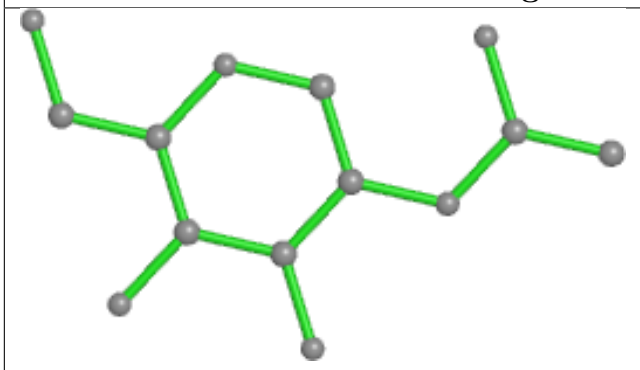
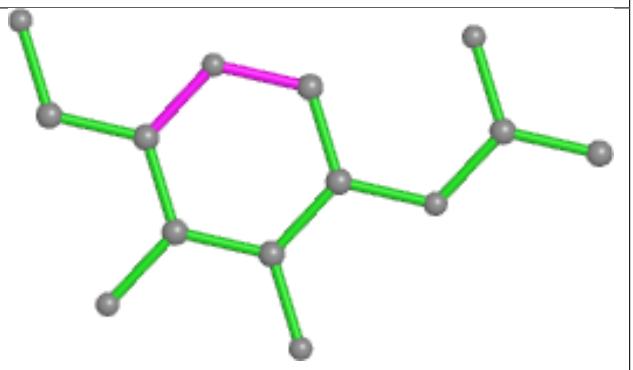
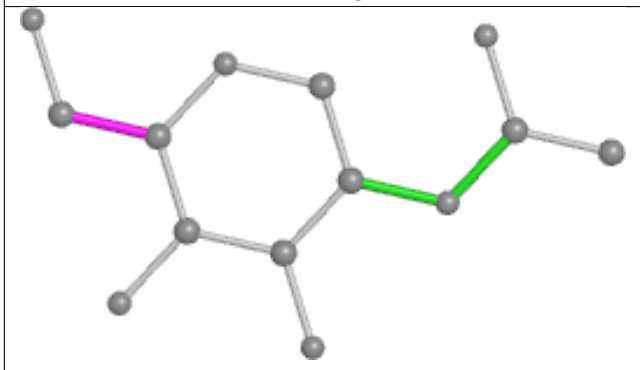
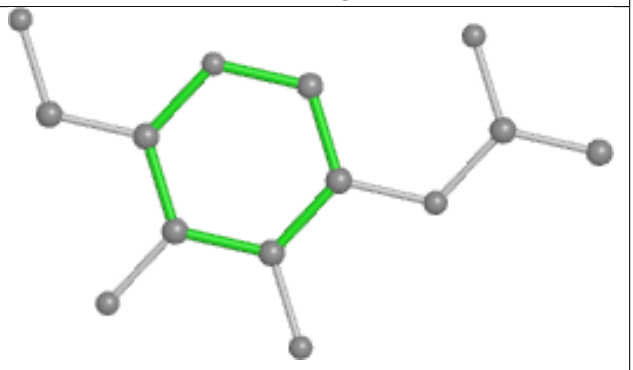
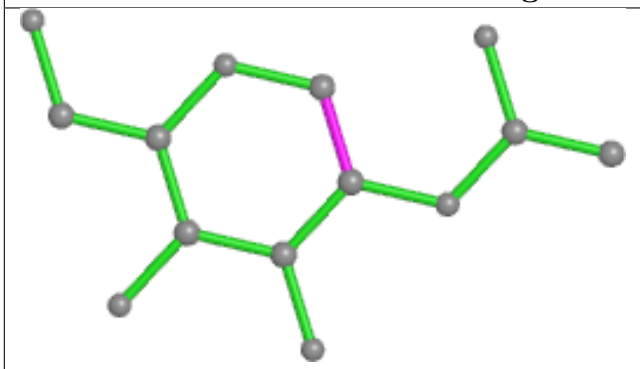
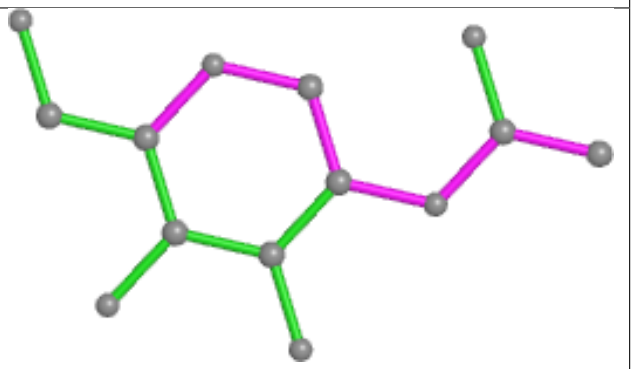
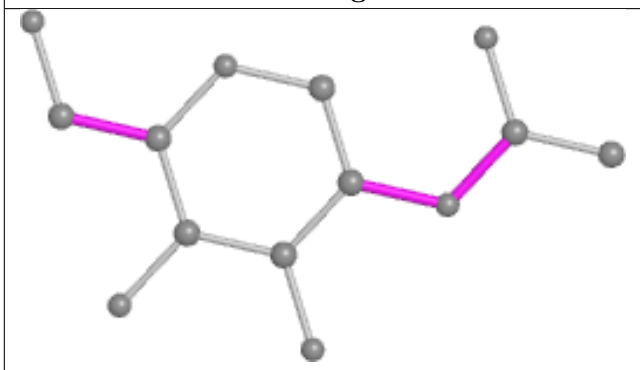
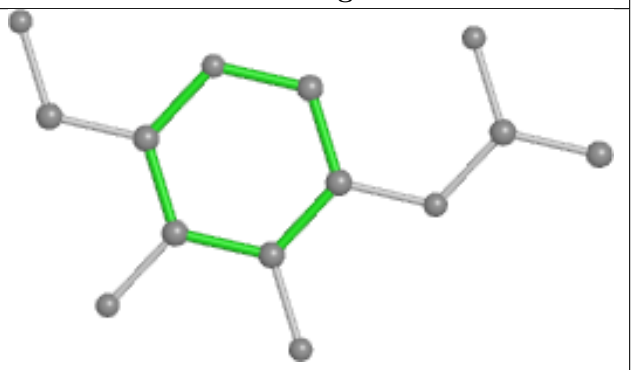
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 605	
 Bond lengths	 Bond angles
 Torsions	 Rings

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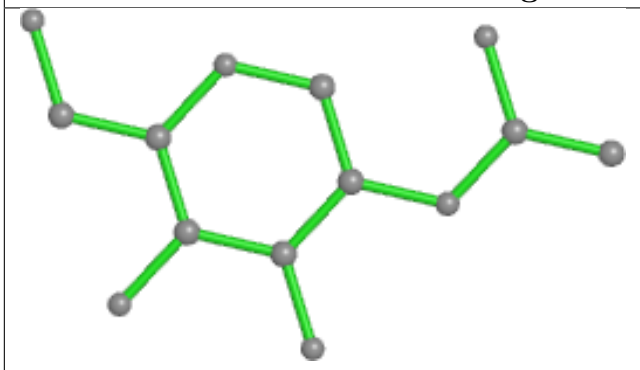
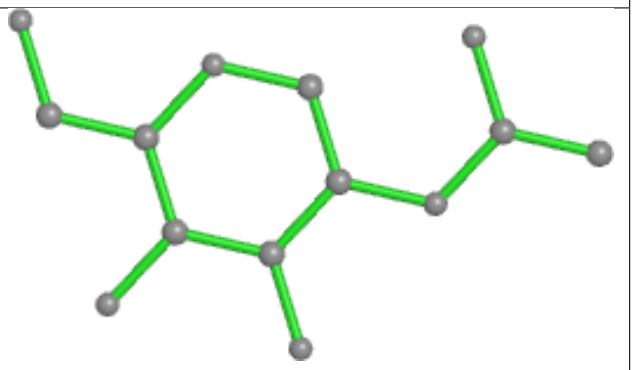
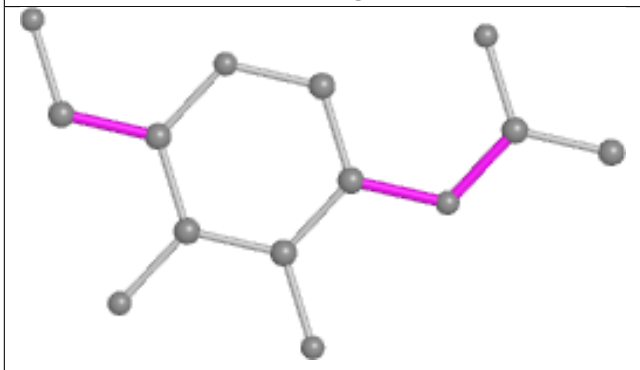
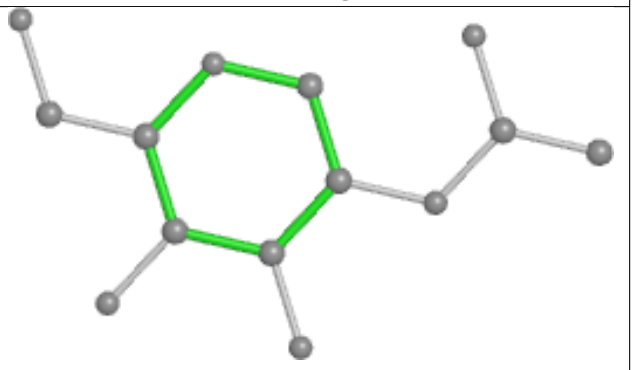
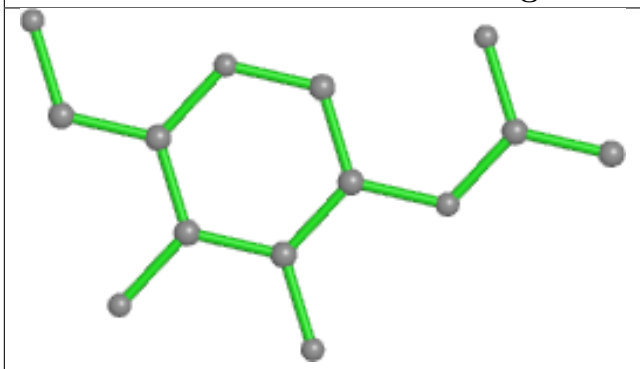
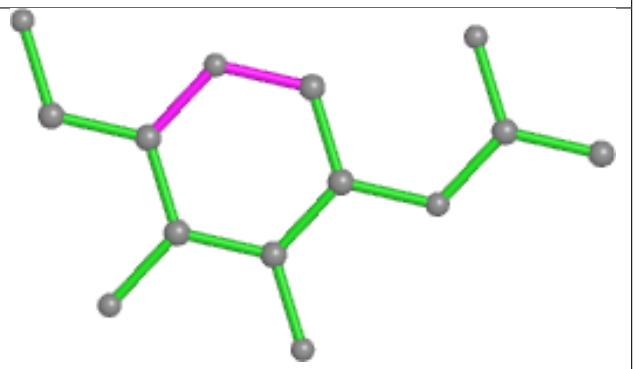
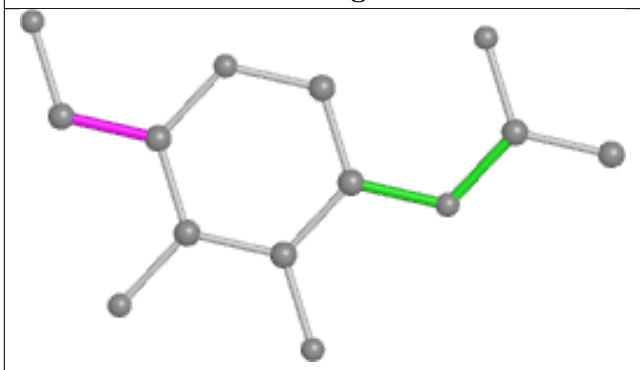
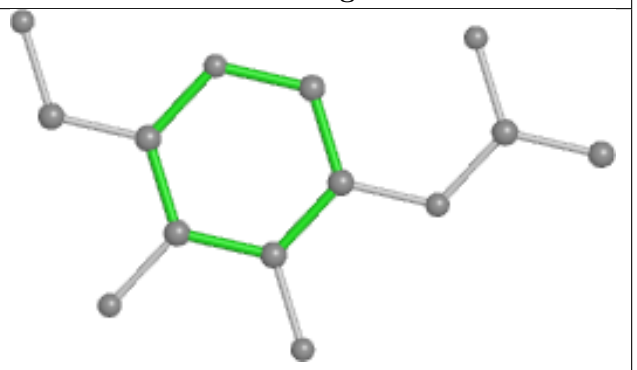
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG D 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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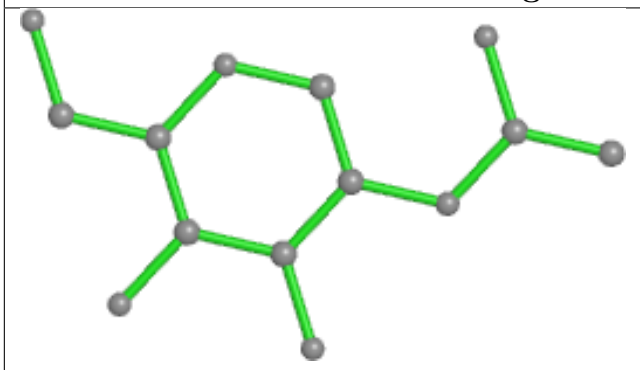
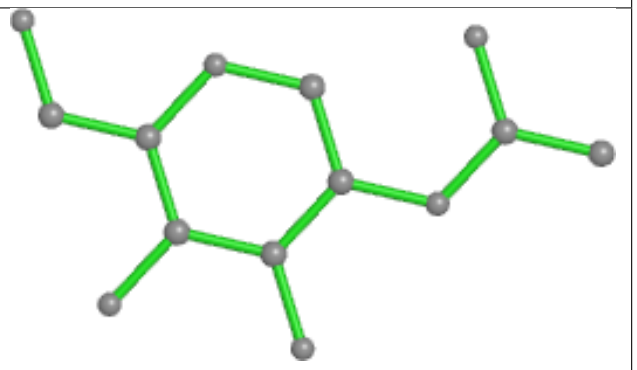
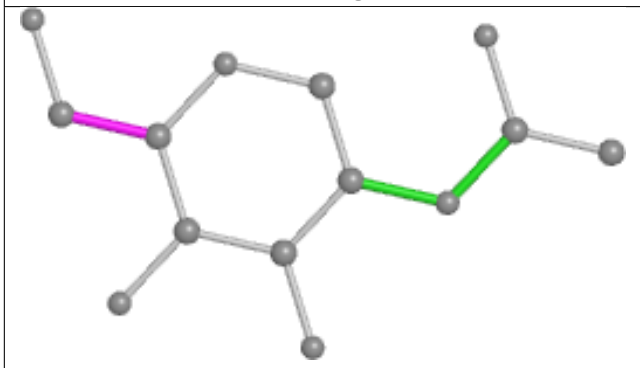
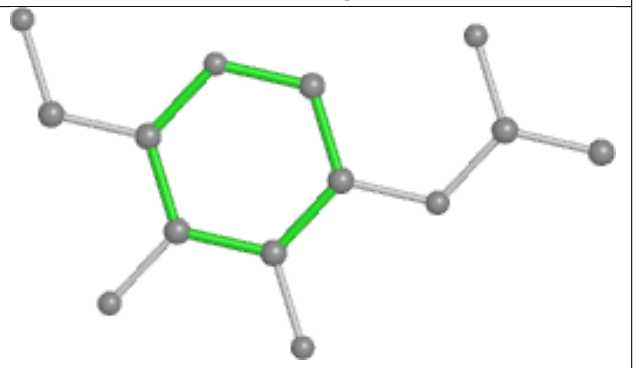
 Bond lengths	 Bond angles
 Torsions	 Rings

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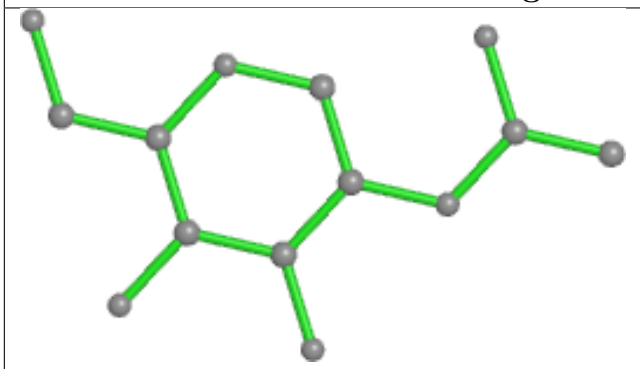
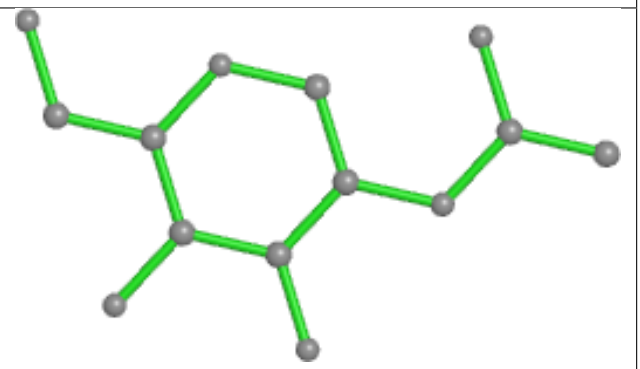
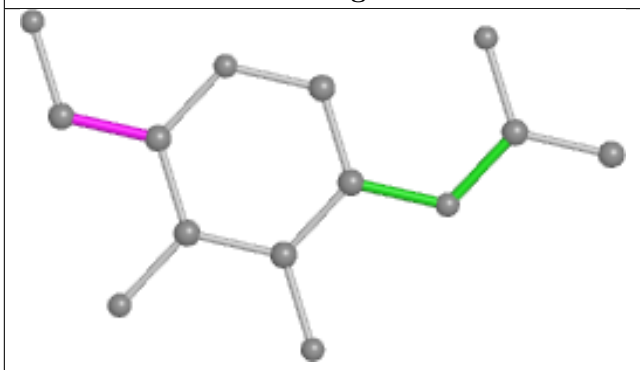
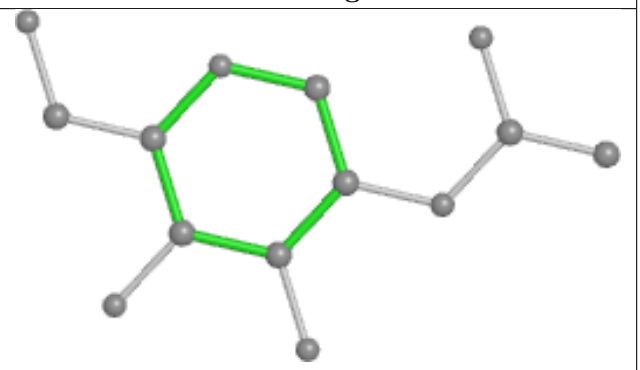
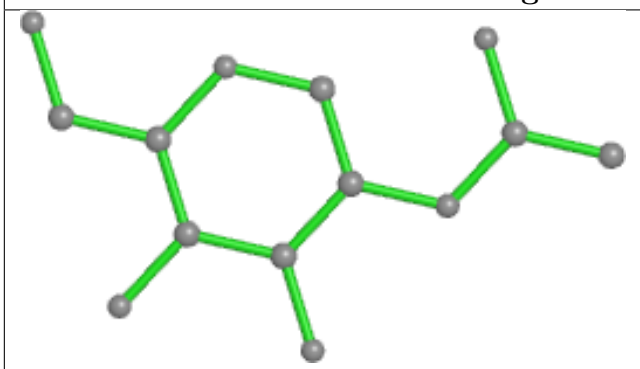
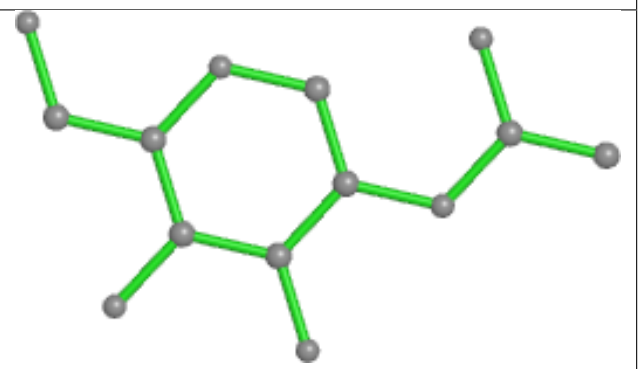
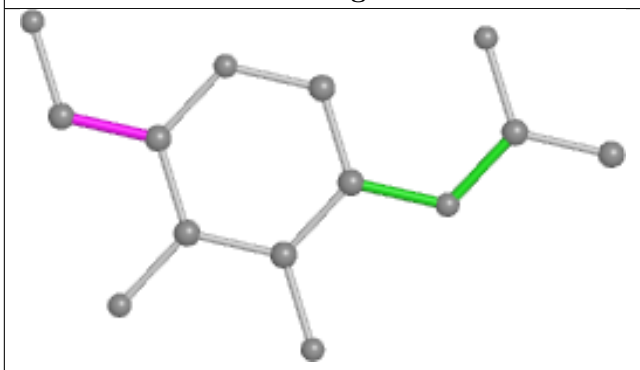
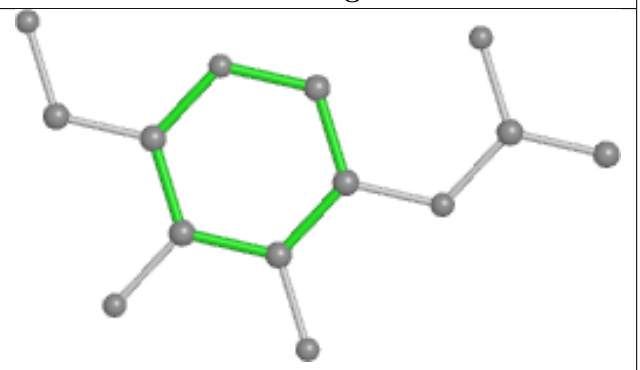
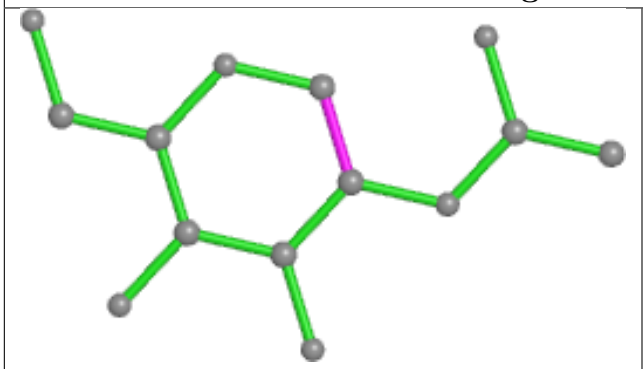
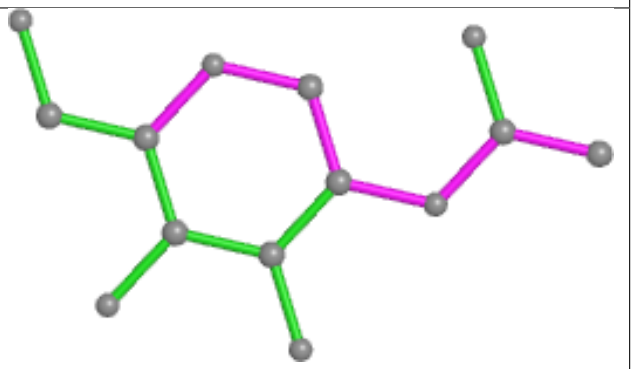
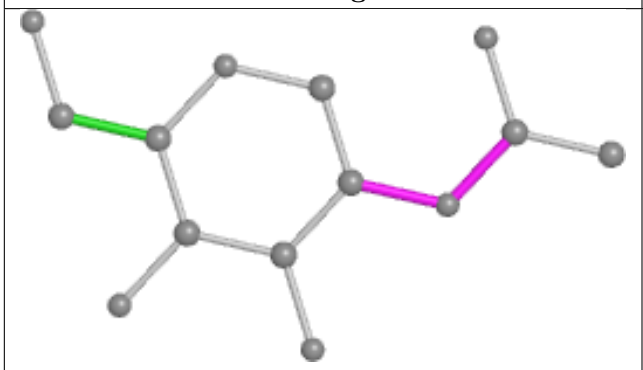
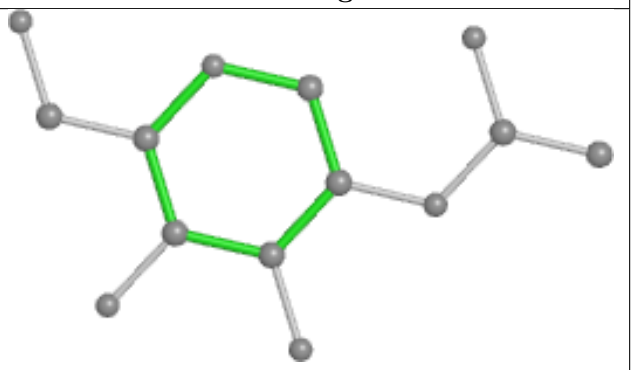
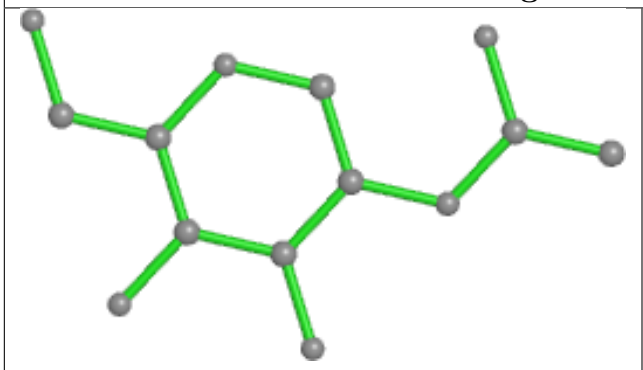
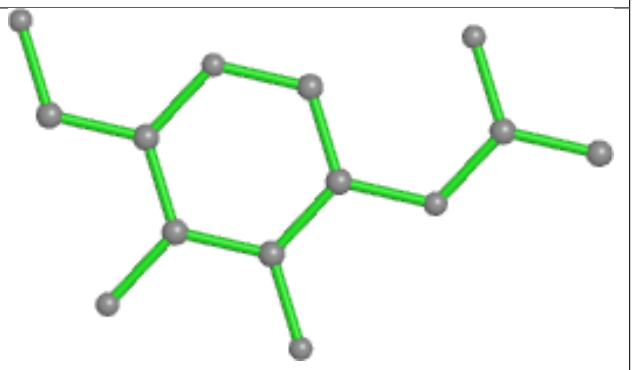
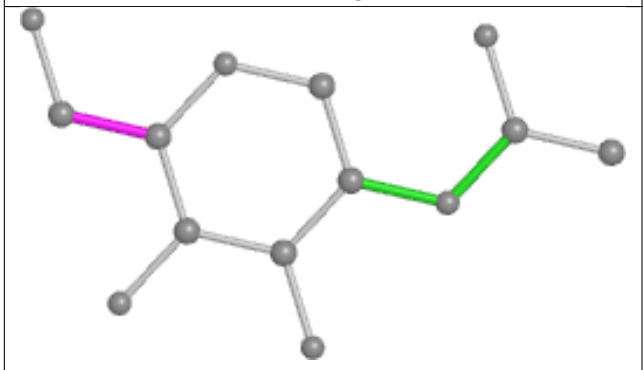
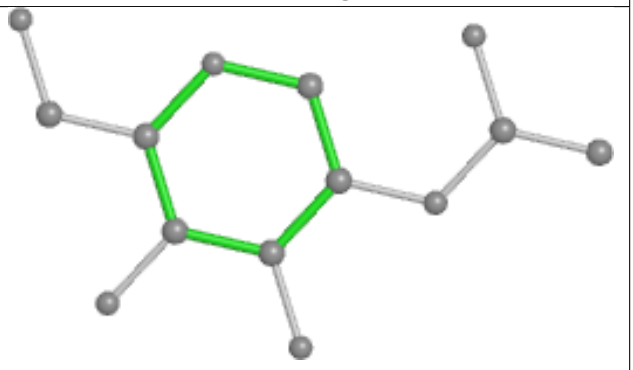
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG D 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

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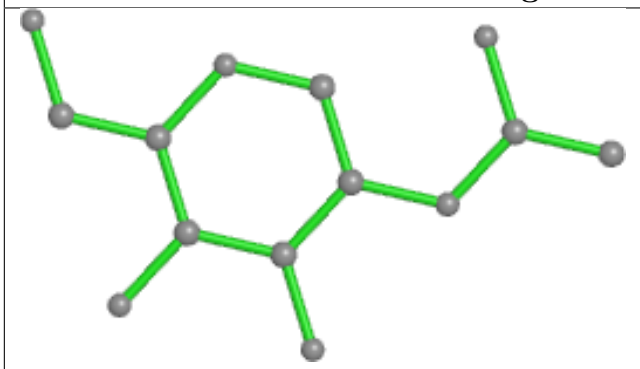
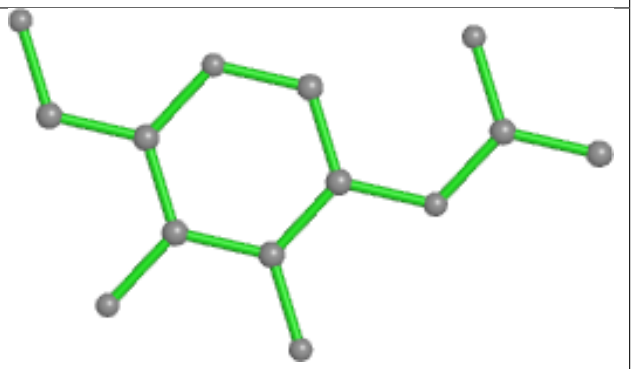
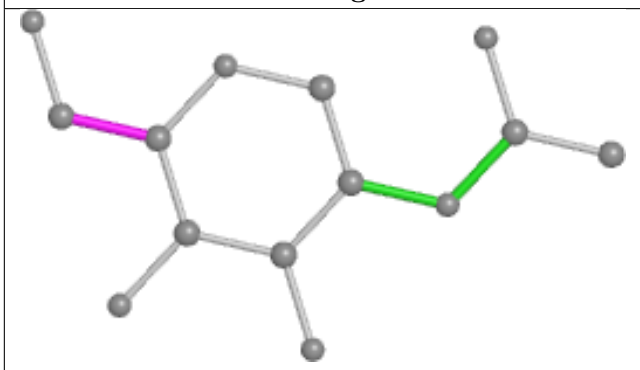
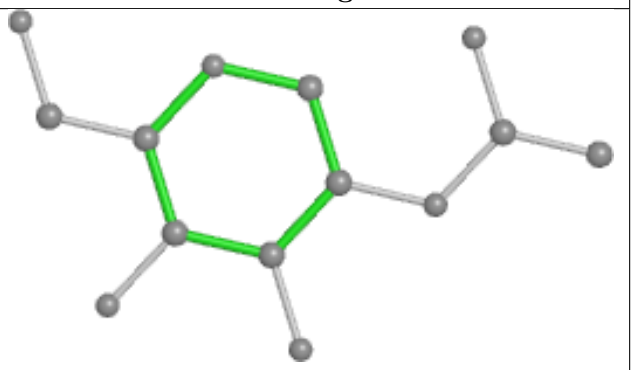
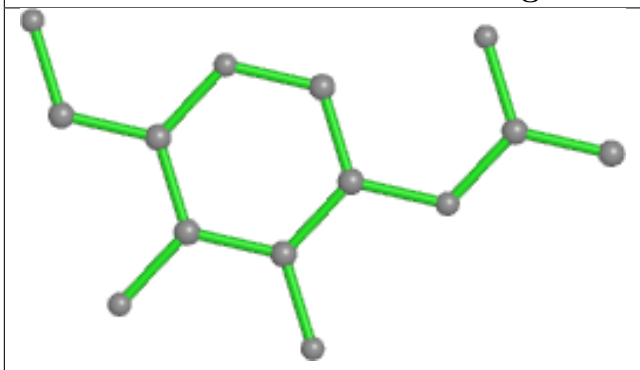
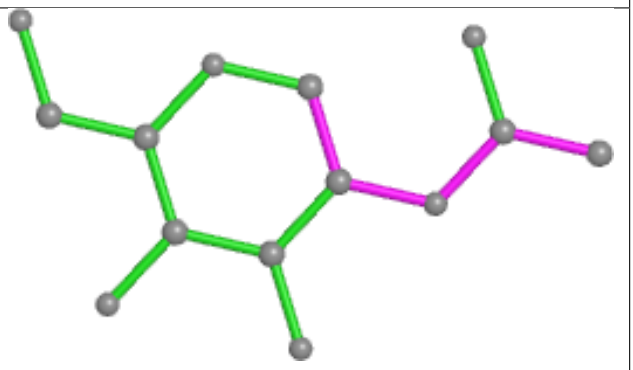
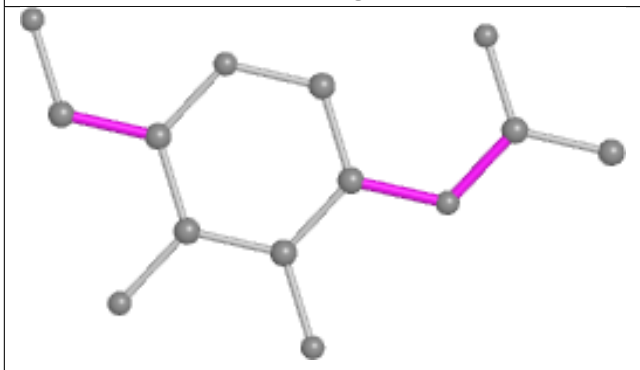
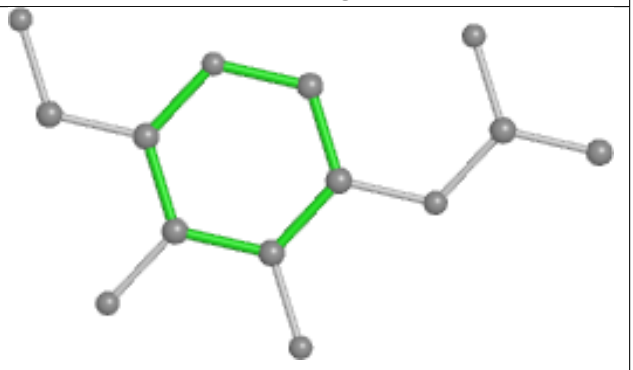
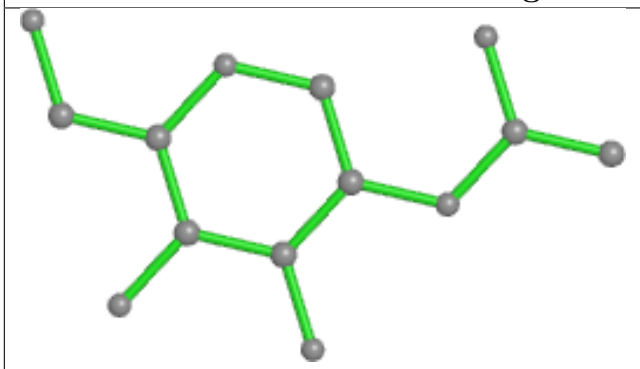
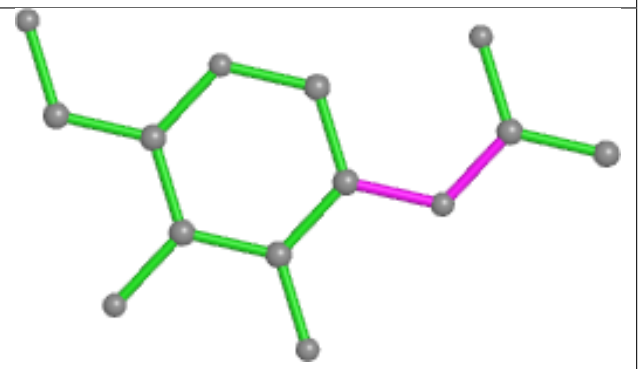
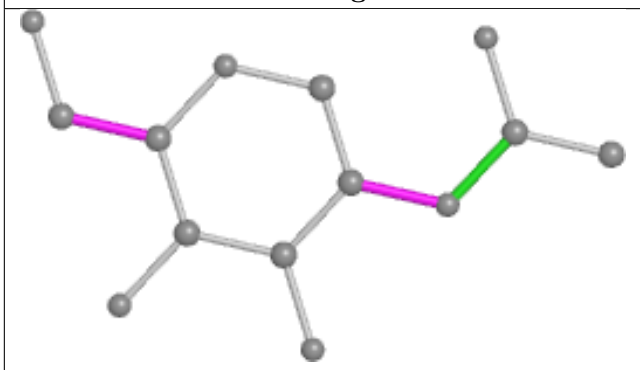
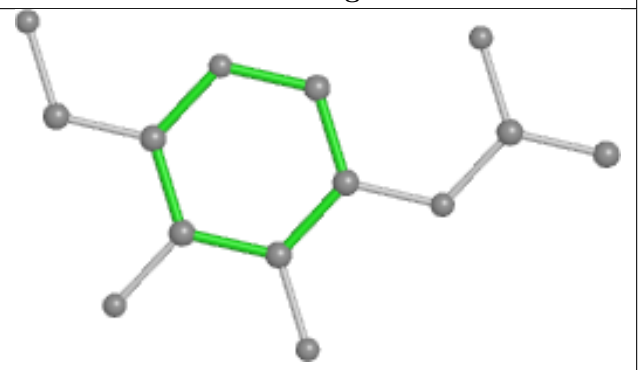
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG E 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

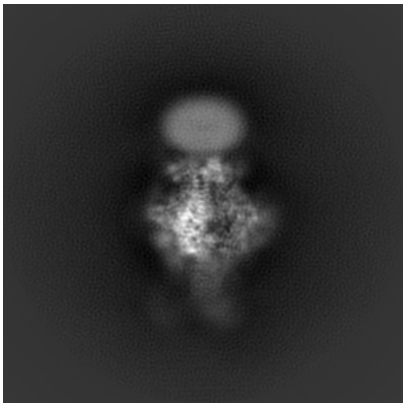
6 Map visualisation (i)

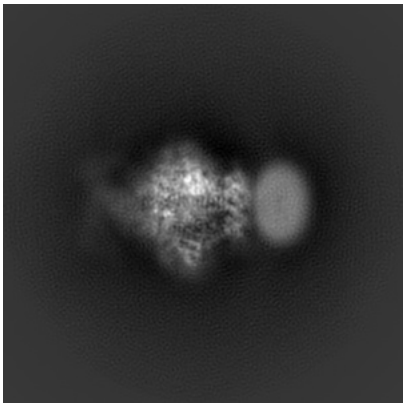
This section contains visualisations of the EMDB entry EMD-25022. These allow visual inspection of the internal detail of the map and identification of artifacts.

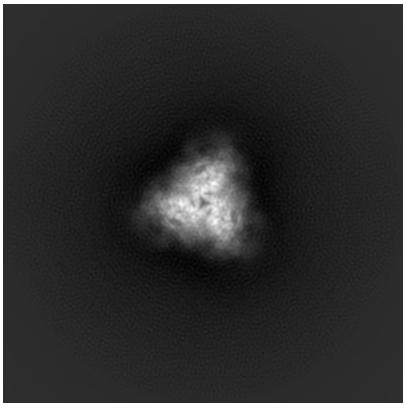
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

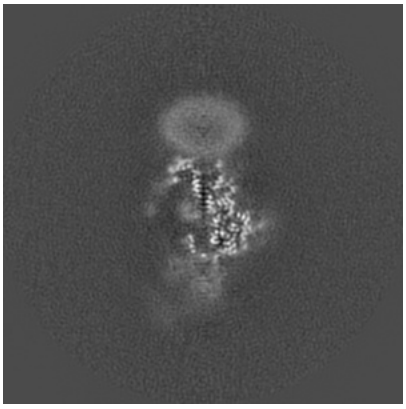

Y

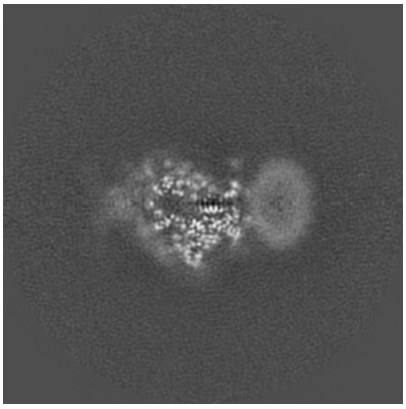

Z

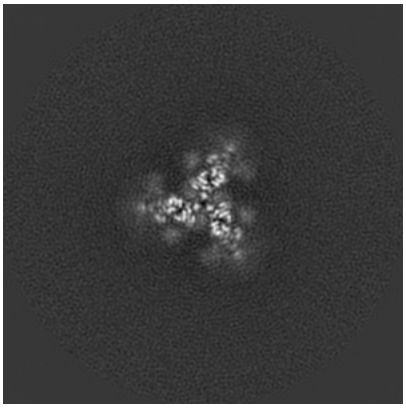
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 192

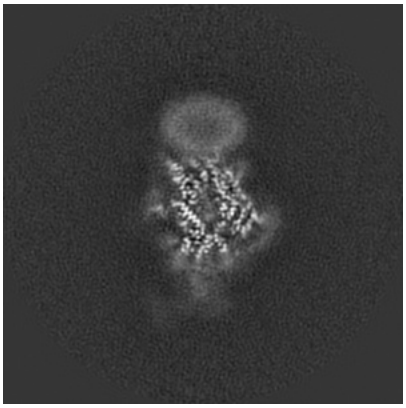

Y Index: 192


Z Index: 192

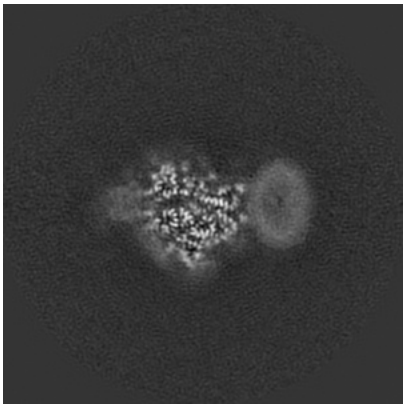
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

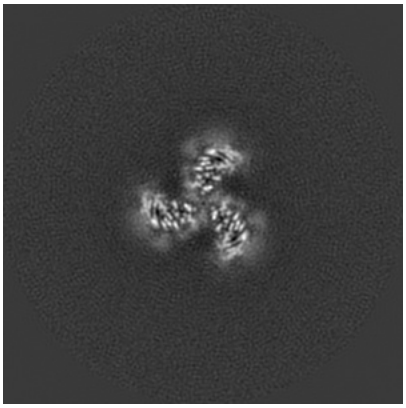
6.3.1 Primary map



X Index: 203



Y Index: 186

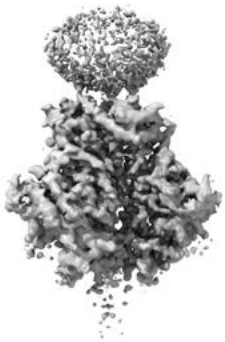


Z Index: 178

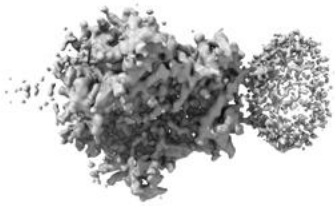
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

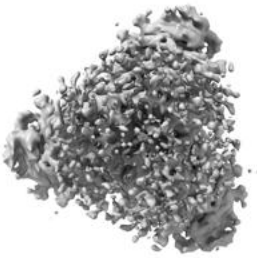
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0109. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

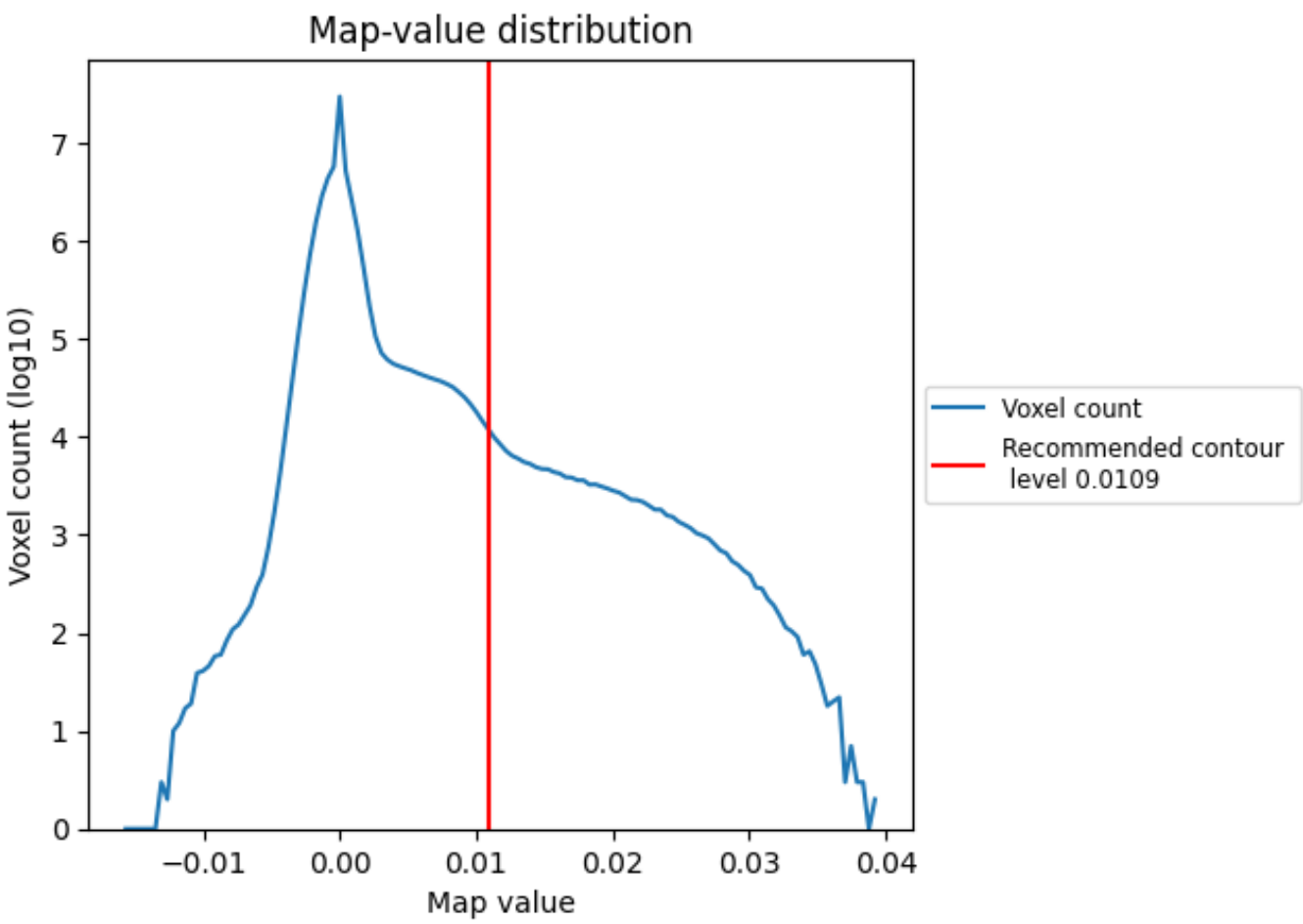
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

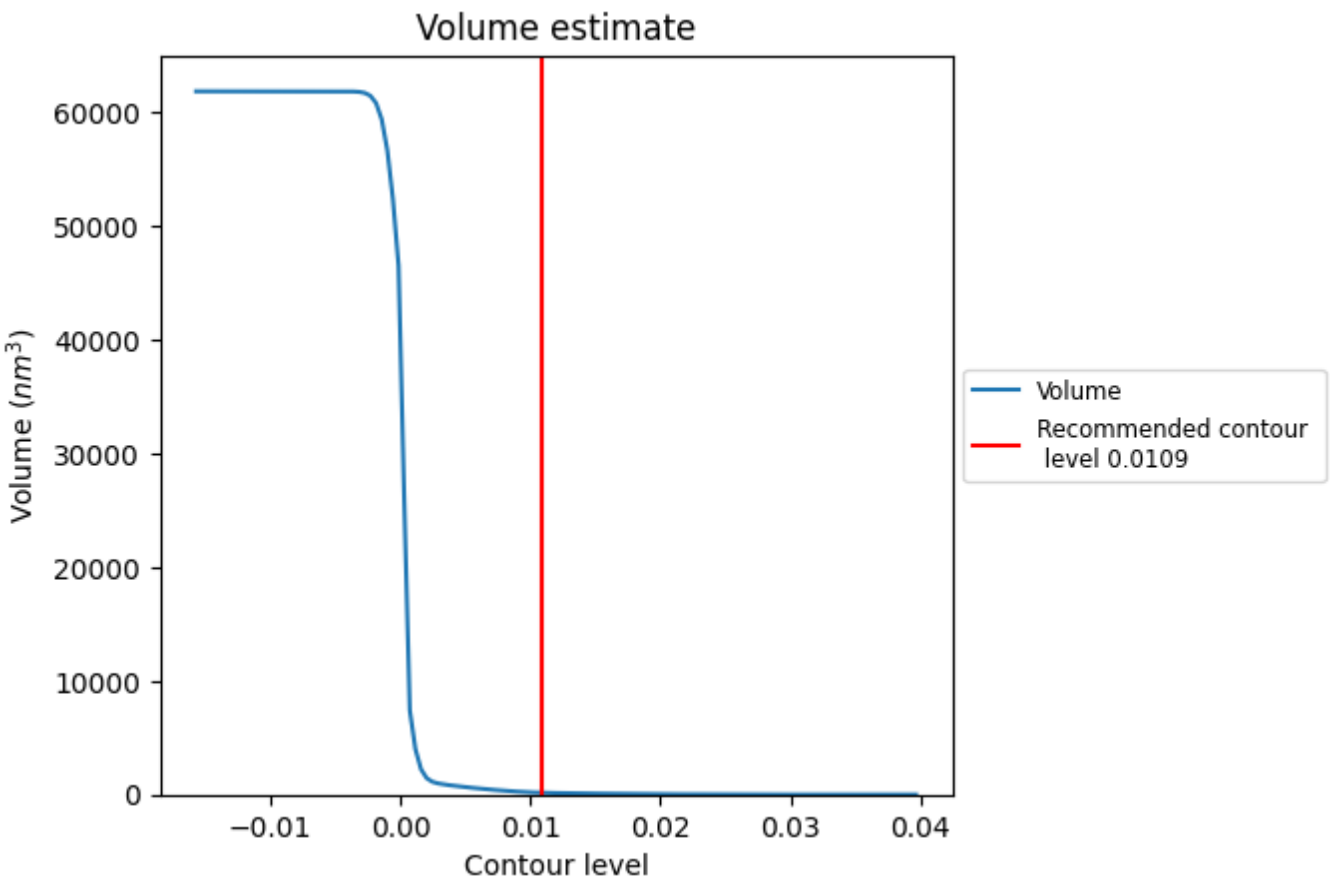
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

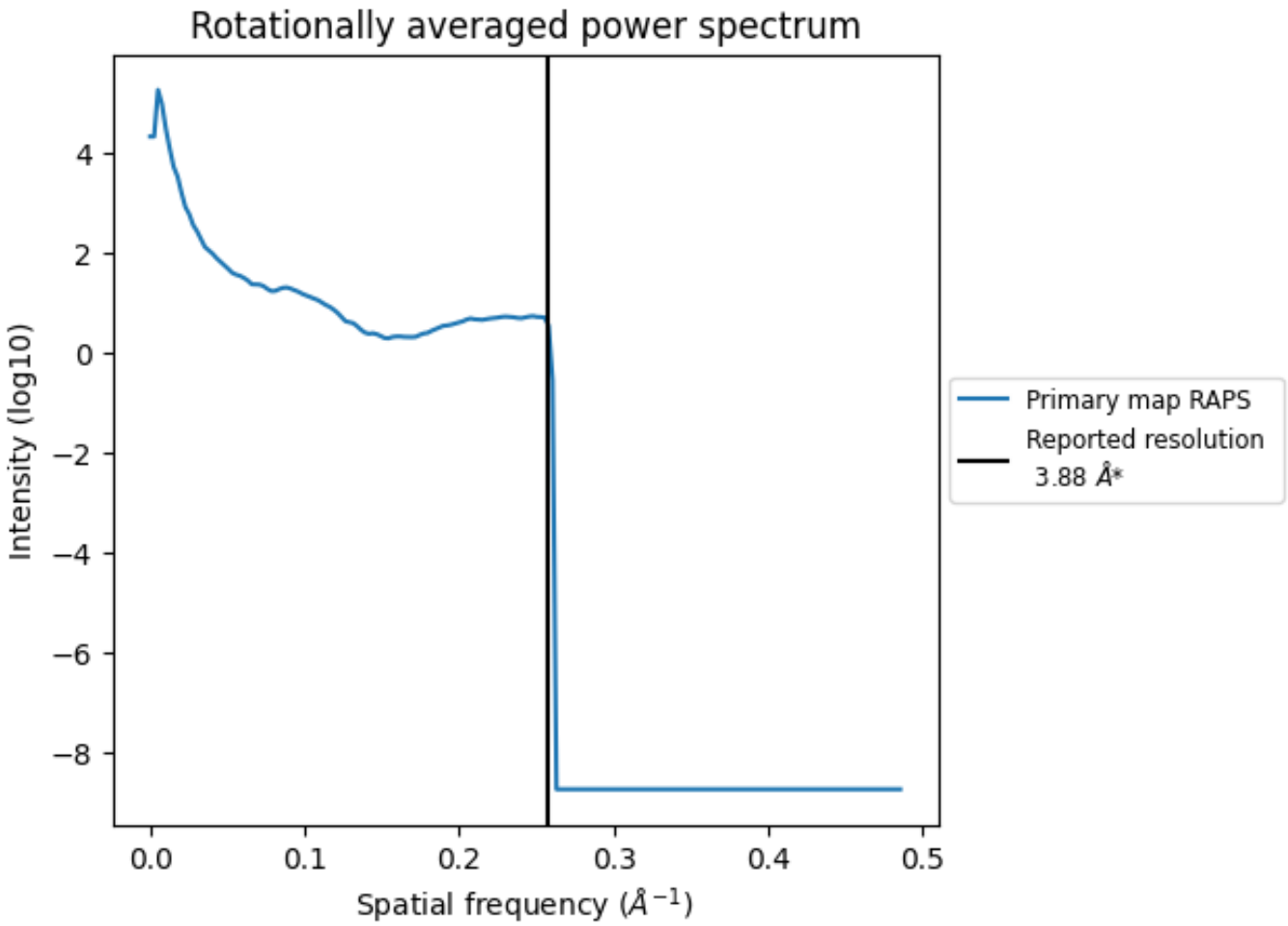
7.2 Volume estimate (i)



The volume at the recommended contour level is 161 nm^3; this corresponds to an approximate mass of 146 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.258 Å^{-1}

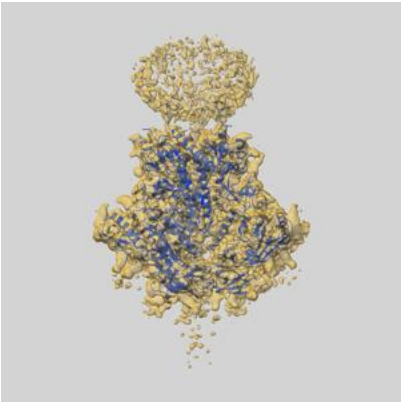
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

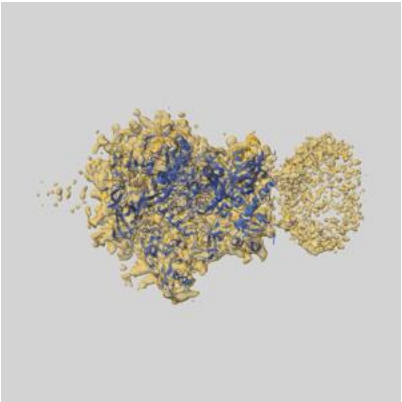
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25022 and PDB model 7SC5. Per-residue inclusion information can be found in section 3 on page 9.

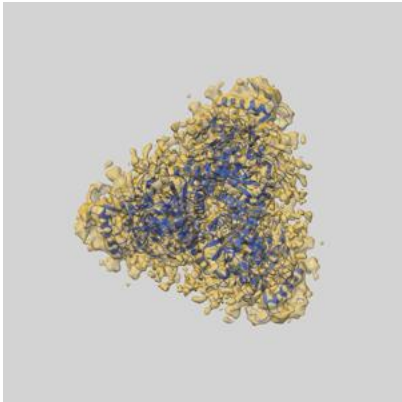
9.1 Map-model overlay (i)



X



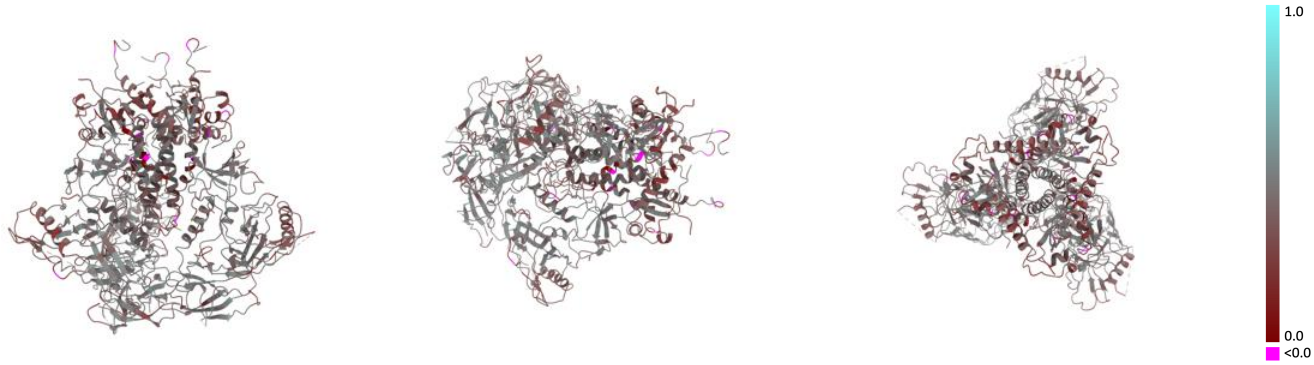
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0109 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

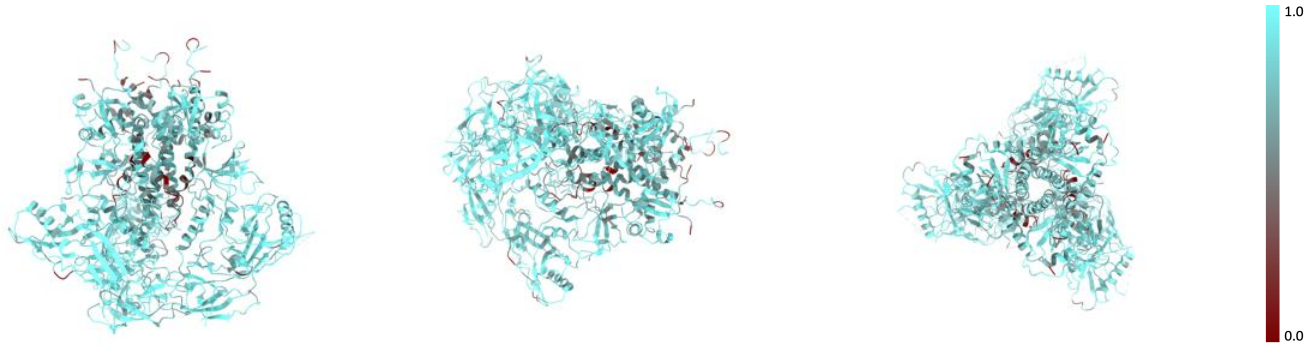
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

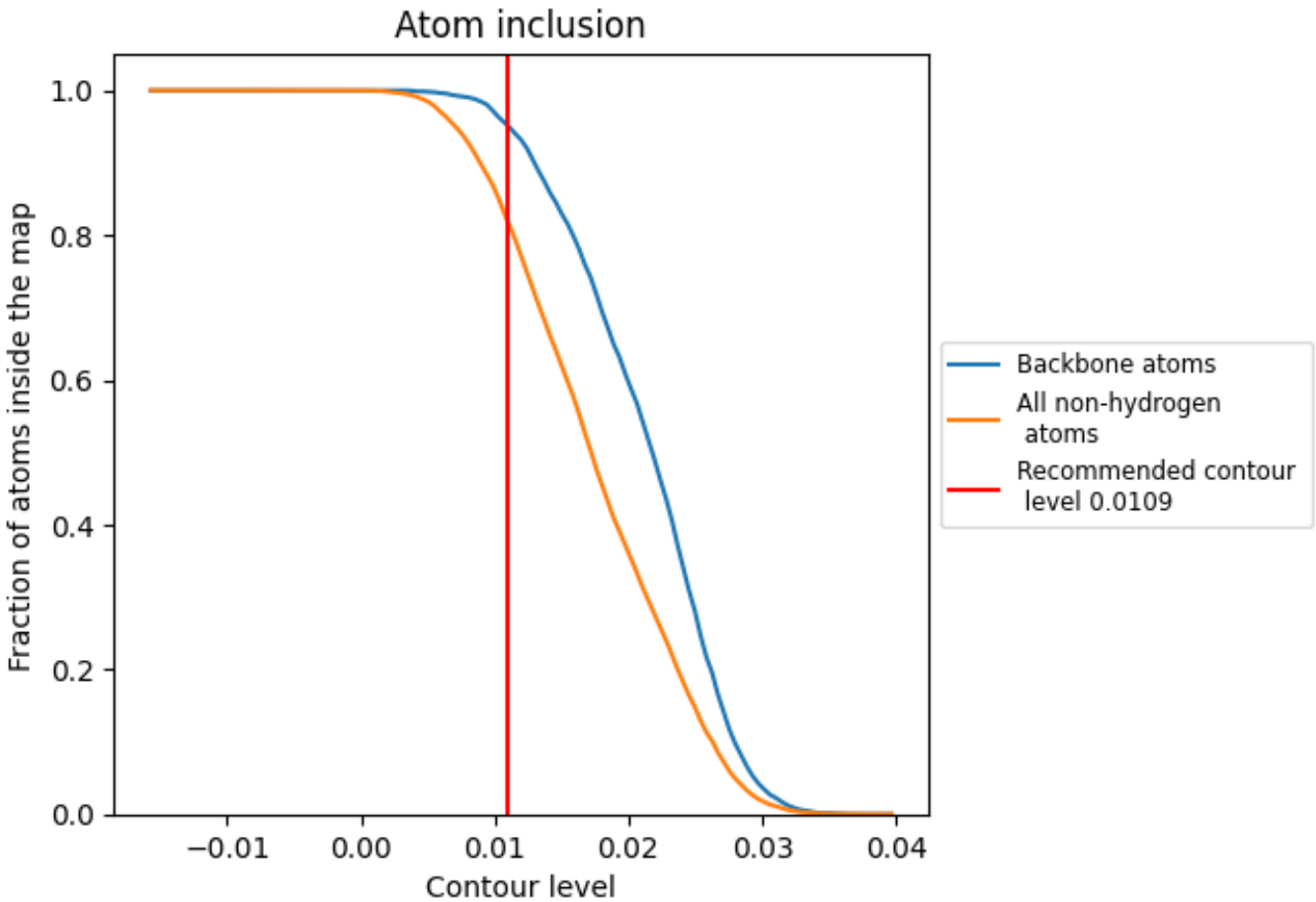
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0109).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0109) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8216	0.3940
A	0.8673	0.4190
B	0.7111	0.3280
C	0.8671	0.4200
D	0.7061	0.3280
E	0.8659	0.4200
F	0.7052	0.3270
G	0.8718	0.3520
H	0.6786	0.2850
I	0.2564	0.2230
J	0.8718	0.3500
K	0.6786	0.2790
L	0.2564	0.2170
M	0.8718	0.3580
N	0.6786	0.2910
O	0.2564	0.2300