wwPDB EM Validation Summary Report

Oct 30, 2024 – 02:08 PM JST

PDB ID	:	8ZFM
EMDB ID	:	EMD-60065
Title	:	Caenorhabditis elegans ACR-23 in betaine bound state
Authors	:	Chen, Q.F.; Liu, F.L.; Li, T.Y.; Gong, H.H.; Guo, F.; Liu, S.
Deposited on	:	2024-05-08
Resolution	:	2.96 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

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

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

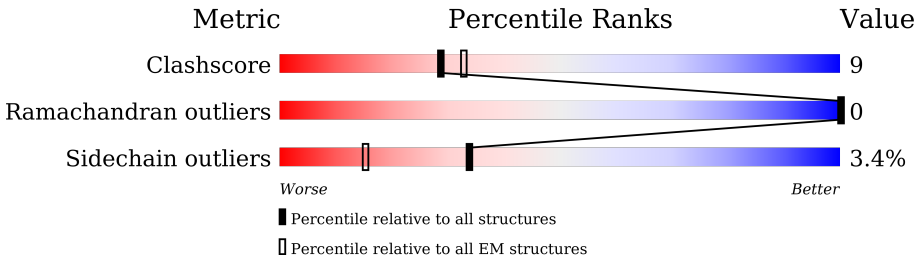
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	620	50% 15% 34%
1	B	620	51% 14% • 34%
1	C	620	51% 14% • 34%
1	D	620	51% 15% • 34%
1	E	620	51% 15% • 34%
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	50% 50%
2	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	J	2	50% 50%
2	K	2	50% 50%
2	L	2	50% 50%
2	M	2	50% 50%
2	N	2	50% 50%
2	O	2	50% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17120 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 Betaine receptor acr-23,Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	412	Total	C	N	O	S	0	0
			3344	2188	538	597	21		
1	A	412	Total	C	N	O	S	0	0
			3344	2188	538	597	21		
1	B	412	Total	C	N	O	S	0	0
			3344	2188	538	597	21		
1	C	412	Total	C	N	O	S	0	0
			3344	2188	538	597	21		
1	E	412	Total	C	N	O	S	0	0
			3344	2188	538	597	21		

There are 220 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP G5EG88
D	?	-	VAL	deletion	UNP G5EG88
D	?	-	ASN	deletion	UNP G5EG88
D	?	-	PRO	deletion	UNP G5EG88
D	?	-	PHE	deletion	UNP G5EG88
D	?	-	THR	deletion	UNP G5EG88
D	?	-	ASN	deletion	UNP G5EG88
D	?	-	PHE	deletion	UNP G5EG88
D	?	-	CYS	deletion	UNP G5EG88
D	?	-	ASN	deletion	UNP G5EG88
D	?	-	VAL	deletion	UNP G5EG88
D	385B	MET	-	linker	UNP G5EG88
D	385C	ALA	-	linker	UNP G5EG88
D	385D	GLU	-	linker	UNP G5EG88
D	385E	ALA	-	linker	UNP G5EG88
D	385F	GLY	-	linker	UNP G5EG88
D	385G	ALA	-	linker	UNP G5EG88
D	385H	MET	-	linker	UNP G5EG88
D	385O	TRP	MET	conflict	UNP P0ABE7
D	389F	ILE	HIS	conflict	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	389J	LEU	-	linker	UNP P0ABE7
D	389K	SER	-	linker	UNP P0ABE7
D	535	LEU	-	expression tag	UNP G5EG88
D	536	GLU	-	expression tag	UNP G5EG88
D	537	GLY	-	expression tag	UNP G5EG88
D	538	THR	-	expression tag	UNP G5EG88
D	539	LYS	-	expression tag	UNP G5EG88
D	540	LEU	-	expression tag	UNP G5EG88
D	541	VAL	-	expression tag	UNP G5EG88
D	542	PRO	-	expression tag	UNP G5EG88
D	543	ARG	-	expression tag	UNP G5EG88
D	544	GLY	-	expression tag	UNP G5EG88
D	545	SER	-	expression tag	UNP G5EG88
D	546	SER	-	expression tag	UNP G5EG88
D	547	SER	-	expression tag	UNP G5EG88
D	548	GLY	-	expression tag	UNP G5EG88
D	549	TRP	-	expression tag	UNP G5EG88
D	550	SER	-	expression tag	UNP G5EG88
D	551	HIS	-	expression tag	UNP G5EG88
D	552	PRO	-	expression tag	UNP G5EG88
D	553	GLN	-	expression tag	UNP G5EG88
D	554	PHE	-	expression tag	UNP G5EG88
D	555	GLU	-	expression tag	UNP G5EG88
D	556	LYS	-	expression tag	UNP G5EG88
A	?	-	SER	deletion	UNP G5EG88
A	?	-	VAL	deletion	UNP G5EG88
A	?	-	ASN	deletion	UNP G5EG88
A	?	-	PRO	deletion	UNP G5EG88
A	?	-	PHE	deletion	UNP G5EG88
A	?	-	THR	deletion	UNP G5EG88
A	?	-	ASN	deletion	UNP G5EG88
A	?	-	PHE	deletion	UNP G5EG88
A	?	-	CYS	deletion	UNP G5EG88
A	?	-	ASN	deletion	UNP G5EG88
A	?	-	VAL	deletion	UNP G5EG88
A	385B	MET	-	linker	UNP G5EG88
A	385C	ALA	-	linker	UNP G5EG88
A	385D	GLU	-	linker	UNP G5EG88
A	385E	ALA	-	linker	UNP G5EG88
A	385F	GLY	-	linker	UNP G5EG88
A	385G	ALA	-	linker	UNP G5EG88
A	385H	MET	-	linker	UNP G5EG88

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Chain	Residue	Modelled	Actual	Comment	Reference
A	385O	TRP	MET	conflict	UNP P0ABE7
A	389F	ILE	HIS	conflict	UNP P0ABE7
A	389J	LEU	-	linker	UNP P0ABE7
A	389K	SER	-	linker	UNP P0ABE7
A	535	LEU	-	expression tag	UNP G5EG88
A	536	GLU	-	expression tag	UNP G5EG88
A	537	GLY	-	expression tag	UNP G5EG88
A	538	THR	-	expression tag	UNP G5EG88
A	539	LYS	-	expression tag	UNP G5EG88
A	540	LEU	-	expression tag	UNP G5EG88
A	541	VAL	-	expression tag	UNP G5EG88
A	542	PRO	-	expression tag	UNP G5EG88
A	543	ARG	-	expression tag	UNP G5EG88
A	544	GLY	-	expression tag	UNP G5EG88
A	545	SER	-	expression tag	UNP G5EG88
A	546	SER	-	expression tag	UNP G5EG88
A	547	SER	-	expression tag	UNP G5EG88
A	548	GLY	-	expression tag	UNP G5EG88
A	549	TRP	-	expression tag	UNP G5EG88
A	550	SER	-	expression tag	UNP G5EG88
A	551	HIS	-	expression tag	UNP G5EG88
A	552	PRO	-	expression tag	UNP G5EG88
A	553	GLN	-	expression tag	UNP G5EG88
A	554	PHE	-	expression tag	UNP G5EG88
A	555	GLU	-	expression tag	UNP G5EG88
A	556	LYS	-	expression tag	UNP G5EG88
B	?	-	SER	deletion	UNP G5EG88
B	?	-	VAL	deletion	UNP G5EG88
B	?	-	ASN	deletion	UNP G5EG88
B	?	-	PRO	deletion	UNP G5EG88
B	?	-	PHE	deletion	UNP G5EG88
B	?	-	THR	deletion	UNP G5EG88
B	?	-	ASN	deletion	UNP G5EG88
B	?	-	PHE	deletion	UNP G5EG88
B	?	-	CYS	deletion	UNP G5EG88
B	?	-	ASN	deletion	UNP G5EG88
B	?	-	VAL	deletion	UNP G5EG88
B	385B	MET	-	linker	UNP G5EG88
B	385C	ALA	-	linker	UNP G5EG88
B	385D	GLU	-	linker	UNP G5EG88
B	385E	ALA	-	linker	UNP G5EG88
B	385F	GLY	-	linker	UNP G5EG88

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Chain	Residue	Modelled	Actual	Comment	Reference
B	385G	ALA	-	linker	UNP G5EG88
B	385H	MET	-	linker	UNP G5EG88
B	385O	TRP	MET	conflict	UNP P0ABE7
B	389F	ILE	HIS	conflict	UNP P0ABE7
B	389J	LEU	-	linker	UNP P0ABE7
B	389K	SER	-	linker	UNP P0ABE7
B	535	LEU	-	expression tag	UNP G5EG88
B	536	GLU	-	expression tag	UNP G5EG88
B	537	GLY	-	expression tag	UNP G5EG88
B	538	THR	-	expression tag	UNP G5EG88
B	539	LYS	-	expression tag	UNP G5EG88
B	540	LEU	-	expression tag	UNP G5EG88
B	541	VAL	-	expression tag	UNP G5EG88
B	542	PRO	-	expression tag	UNP G5EG88
B	543	ARG	-	expression tag	UNP G5EG88
B	544	GLY	-	expression tag	UNP G5EG88
B	545	SER	-	expression tag	UNP G5EG88
B	546	SER	-	expression tag	UNP G5EG88
B	547	SER	-	expression tag	UNP G5EG88
B	548	GLY	-	expression tag	UNP G5EG88
B	549	TRP	-	expression tag	UNP G5EG88
B	550	SER	-	expression tag	UNP G5EG88
B	551	HIS	-	expression tag	UNP G5EG88
B	552	PRO	-	expression tag	UNP G5EG88
B	553	GLN	-	expression tag	UNP G5EG88
B	554	PHE	-	expression tag	UNP G5EG88
B	555	GLU	-	expression tag	UNP G5EG88
B	556	LYS	-	expression tag	UNP G5EG88
C	?	-	SER	deletion	UNP G5EG88
C	?	-	VAL	deletion	UNP G5EG88
C	?	-	ASN	deletion	UNP G5EG88
C	?	-	PRO	deletion	UNP G5EG88
C	?	-	PHE	deletion	UNP G5EG88
C	?	-	THR	deletion	UNP G5EG88
C	?	-	ASN	deletion	UNP G5EG88
C	?	-	PHE	deletion	UNP G5EG88
C	?	-	CYS	deletion	UNP G5EG88
C	?	-	ASN	deletion	UNP G5EG88
C	?	-	VAL	deletion	UNP G5EG88
C	385B	MET	-	linker	UNP G5EG88
C	385C	ALA	-	linker	UNP G5EG88
C	385D	GLU	-	linker	UNP G5EG88

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Chain	Residue	Modelled	Actual	Comment	Reference
C	385E	ALA	-	linker	UNP G5EG88
C	385F	GLY	-	linker	UNP G5EG88
C	385G	ALA	-	linker	UNP G5EG88
C	385H	MET	-	linker	UNP G5EG88
C	385O	TRP	MET	conflict	UNP P0ABE7
C	389F	ILE	HIS	conflict	UNP P0ABE7
C	389J	LEU	-	linker	UNP P0ABE7
C	389K	SER	-	linker	UNP P0ABE7
C	535	LEU	-	expression tag	UNP G5EG88
C	536	GLU	-	expression tag	UNP G5EG88
C	537	GLY	-	expression tag	UNP G5EG88
C	538	THR	-	expression tag	UNP G5EG88
C	539	LYS	-	expression tag	UNP G5EG88
C	540	LEU	-	expression tag	UNP G5EG88
C	541	VAL	-	expression tag	UNP G5EG88
C	542	PRO	-	expression tag	UNP G5EG88
C	543	ARG	-	expression tag	UNP G5EG88
C	544	GLY	-	expression tag	UNP G5EG88
C	545	SER	-	expression tag	UNP G5EG88
C	546	SER	-	expression tag	UNP G5EG88
C	547	SER	-	expression tag	UNP G5EG88
C	548	GLY	-	expression tag	UNP G5EG88
C	549	TRP	-	expression tag	UNP G5EG88
C	550	SER	-	expression tag	UNP G5EG88
C	551	HIS	-	expression tag	UNP G5EG88
C	552	PRO	-	expression tag	UNP G5EG88
C	553	GLN	-	expression tag	UNP G5EG88
C	554	PHE	-	expression tag	UNP G5EG88
C	555	GLU	-	expression tag	UNP G5EG88
C	556	LYS	-	expression tag	UNP G5EG88
E	?	-	SER	deletion	UNP G5EG88
E	?	-	VAL	deletion	UNP G5EG88
E	?	-	ASN	deletion	UNP G5EG88
E	?	-	PRO	deletion	UNP G5EG88
E	?	-	PHE	deletion	UNP G5EG88
E	?	-	THR	deletion	UNP G5EG88
E	?	-	ASN	deletion	UNP G5EG88
E	?	-	PHE	deletion	UNP G5EG88
E	?	-	CYS	deletion	UNP G5EG88
E	?	-	ASN	deletion	UNP G5EG88
E	?	-	VAL	deletion	UNP G5EG88
E	385B	MET	-	linker	UNP G5EG88

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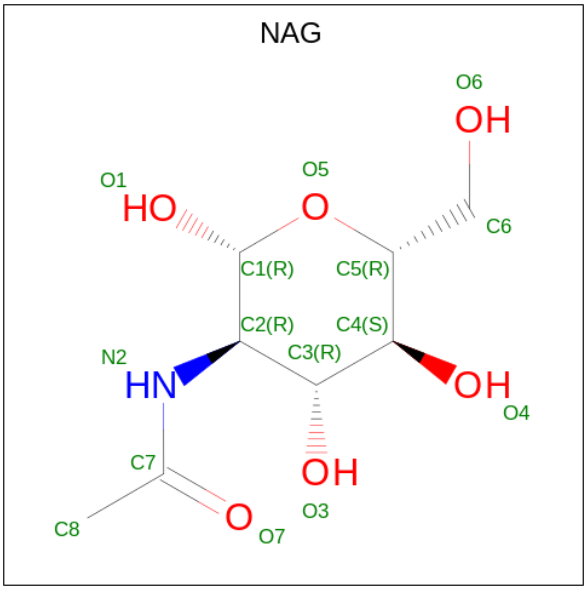
Chain	Residue	Modelled	Actual	Comment	Reference
E	385C	ALA	-	linker	UNP G5EG88
E	385D	GLU	-	linker	UNP G5EG88
E	385E	ALA	-	linker	UNP G5EG88
E	385F	GLY	-	linker	UNP G5EG88
E	385G	ALA	-	linker	UNP G5EG88
E	385H	MET	-	linker	UNP G5EG88
E	385O	TRP	MET	conflict	UNP P0ABE7
E	389F	ILE	HIS	conflict	UNP P0ABE7
E	389J	LEU	-	linker	UNP P0ABE7
E	389K	SER	-	linker	UNP P0ABE7
E	535	LEU	-	expression tag	UNP G5EG88
E	536	GLU	-	expression tag	UNP G5EG88
E	537	GLY	-	expression tag	UNP G5EG88
E	538	THR	-	expression tag	UNP G5EG88
E	539	LYS	-	expression tag	UNP G5EG88
E	540	LEU	-	expression tag	UNP G5EG88
E	541	VAL	-	expression tag	UNP G5EG88
E	542	PRO	-	expression tag	UNP G5EG88
E	543	ARG	-	expression tag	UNP G5EG88
E	544	GLY	-	expression tag	UNP G5EG88
E	545	SER	-	expression tag	UNP G5EG88
E	546	SER	-	expression tag	UNP G5EG88
E	547	SER	-	expression tag	UNP G5EG88
E	548	GLY	-	expression tag	UNP G5EG88
E	549	TRP	-	expression tag	UNP G5EG88
E	550	SER	-	expression tag	UNP G5EG88
E	551	HIS	-	expression tag	UNP G5EG88
E	552	PRO	-	expression tag	UNP G5EG88
E	553	GLN	-	expression tag	UNP G5EG88
E	554	PHE	-	expression tag	UNP G5EG88
E	555	GLU	-	expression tag	UNP G5EG88
E	556	LYS	-	expression tag	UNP G5EG88

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

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

- Molecule 3 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
3	D	1	Total C N O 14 8 1 5	0

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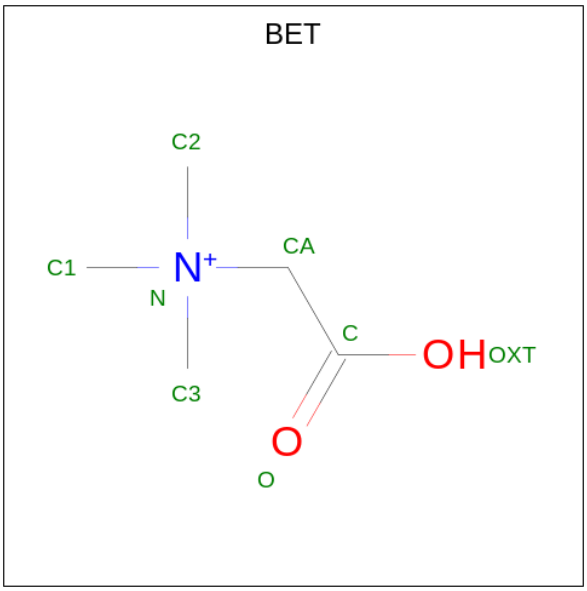
Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C N O 14 8 1 5	0
3	B	1	Total C N O 14 8 1 5	0
3	C	1	Total C N O 14 8 1 5	0
3	E	1	Total C N O 14 8 1 5	0

- Molecule 4 is TRIMETHYL GLYCINE (three-letter code: BET) (formula: $C_5H_{12}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C N O 8 5 1 2	0
4	A	1	Total C N O 8 5 1 2	0
4	B	1	Total C N O 8 5 1 2	0
4	C	1	Total C N O 8 5 1 2	0
4	E	1	Total C N O 8 5 1 2	0

- Molecule 5 is water.

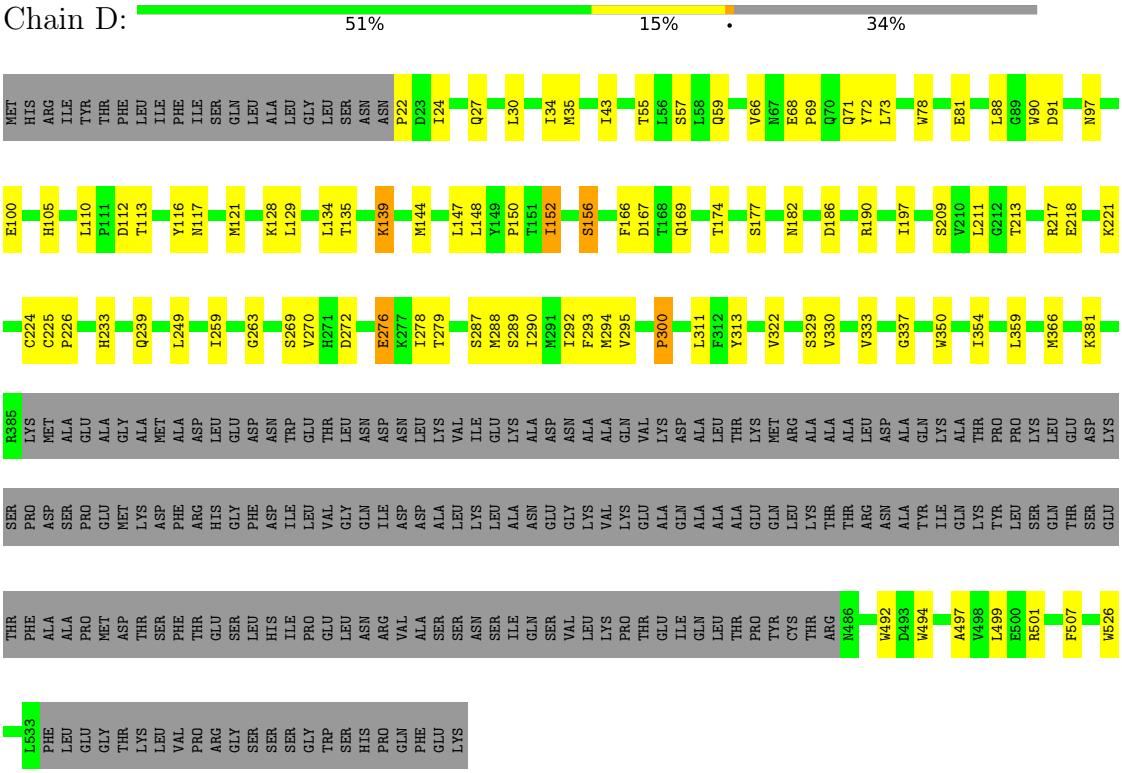
Mol	Chain	Residues	Atoms	AltConf
5	D	2	Total O 2 2	0
5	A	2	Total O 2 2	0
5	B	2	Total O 2 2	0
5	C	2	Total O 2 2	0
5	E	2	Total O 2 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

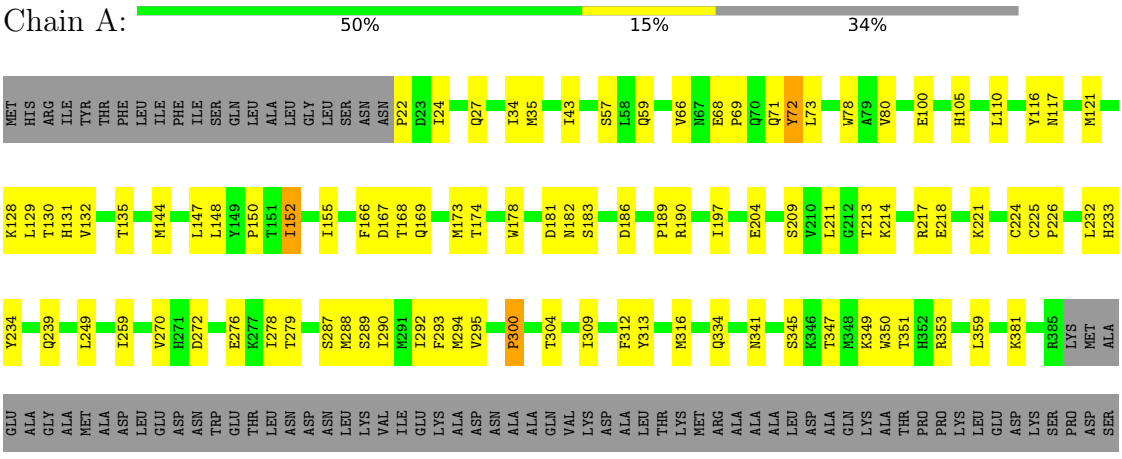
• Molecule 1: Betaine receptor acr-23,Soluble cytochrome b562

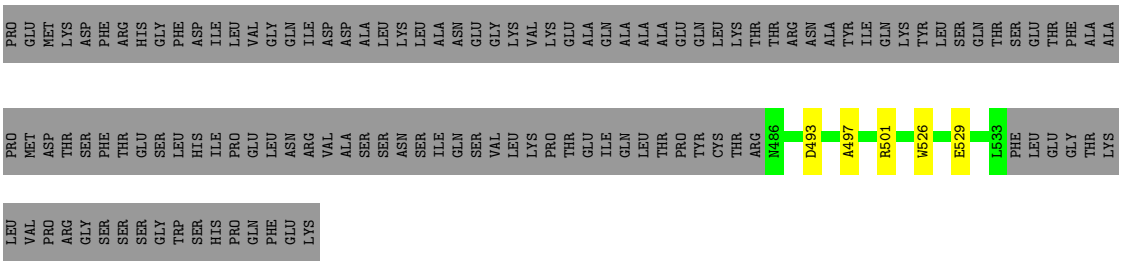
Chain D:



• Molecule 1: Betaine receptor acr-23,Soluble cytochrome b562

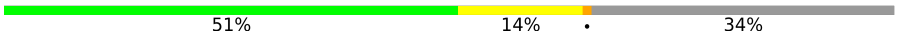
Chain A:

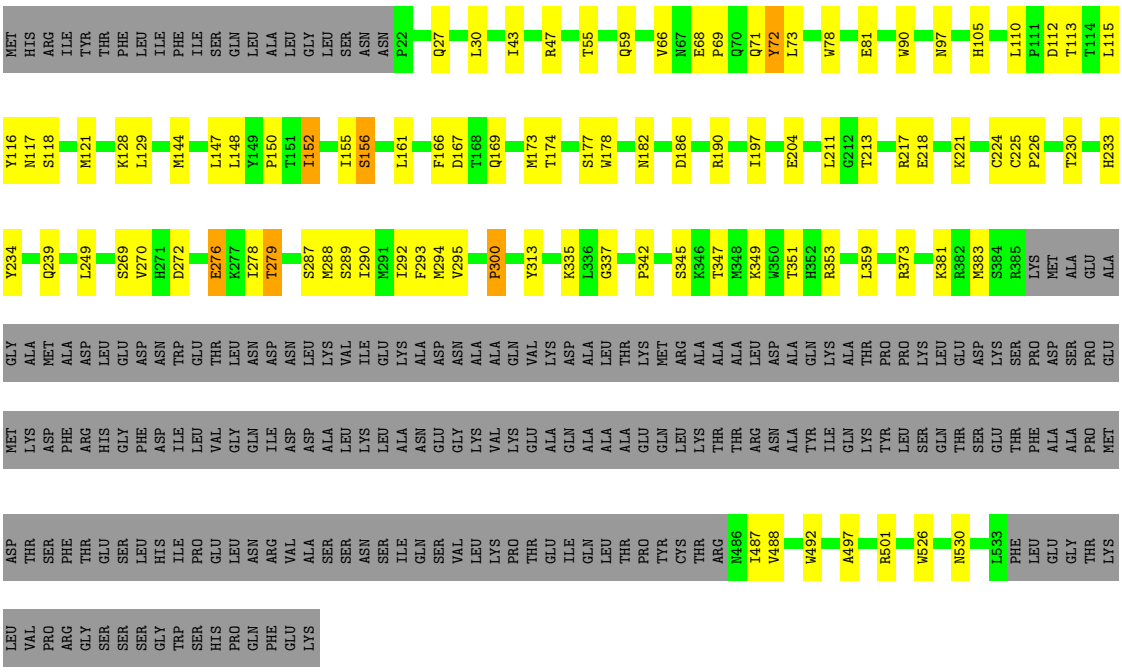




• Molecule 1: Betaine receptor acr-23,Soluble cytochrome b562

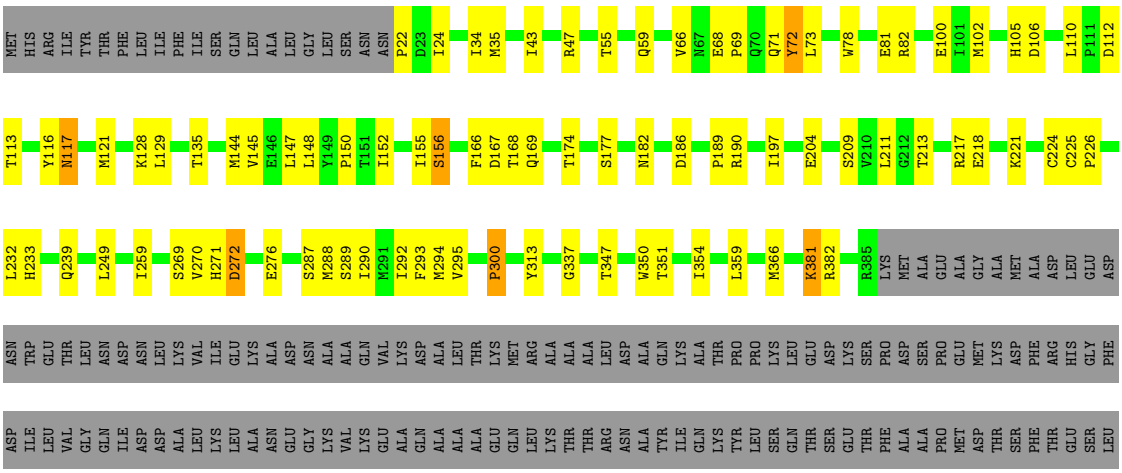
Chain B:

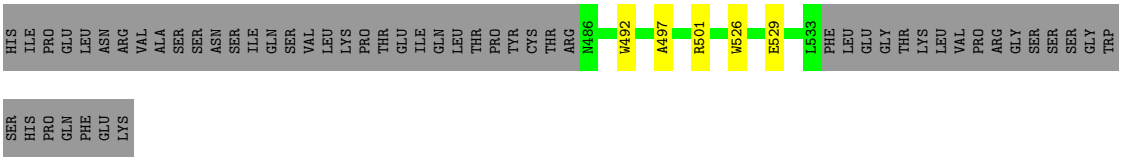




• Molecule 1: Betaine receptor acr-23,Soluble cytochrome b562

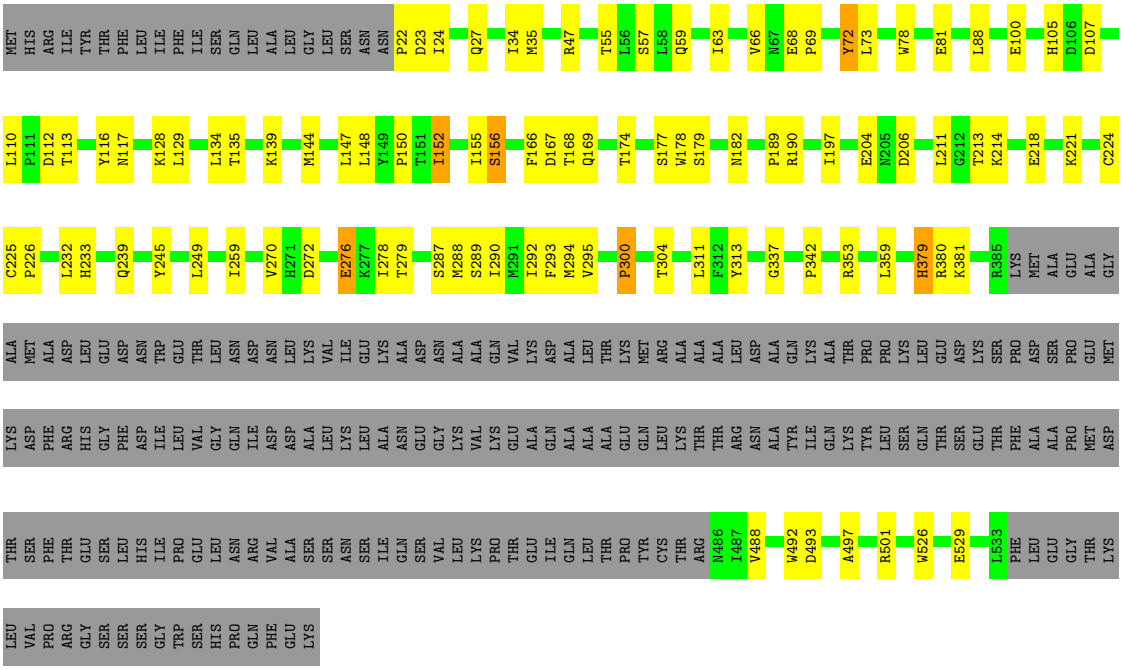
Chain C:





• Molecule 1: Betaine receptor acr-23,Soluble cytochrome b562

Chain E:



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

Chain F:

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

Chain G:

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

Chain H:

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

Chain I:

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

Chain J:

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

Chain K:

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

Chain L:

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

Chain M:

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

Chain N:

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

Chain O:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	214366	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.00, 50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k), GATAN K2 BASE (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	1/3431 (0.0%)	0.52	0/4668
1	B	0.41	1/3431 (0.0%)	0.52	0/4668
1	C	0.41	1/3431 (0.0%)	0.52	0/4668
1	D	0.41	1/3431 (0.0%)	0.52	0/4668
1	E	0.39	1/3431 (0.0%)	0.52	0/4668
All	All	0.41	5/17155 (0.0%)	0.52	0/23340

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	PRO	C-N	9.41	1.55	1.34
1	C	300	PRO	C-N	9.02	1.54	1.34
1	D	300	PRO	C-N	8.16	1.52	1.34
1	A	300	PRO	C-N	7.54	1.51	1.34
1	E	300	PRO	C-N	5.80	1.47	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3381	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3344	0	3381	71	0
1	C	3344	0	3381	63	0
1	D	3344	0	3381	71	0
1	E	3344	0	3381	75	0
2	F	28	0	25	1	0
2	G	28	0	25	2	0
2	H	28	0	25	1	0
2	I	28	0	25	2	0
2	J	28	0	25	1	0
2	K	28	0	25	2	0
2	L	28	0	25	1	0
2	M	28	0	25	2	0
2	N	28	0	25	1	0
2	O	28	0	25	2	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	1	0
3	E	14	0	13	0	0
4	A	8	0	11	3	0
4	B	8	0	11	2	0
4	C	8	0	11	1	0
4	D	8	0	11	2	0
4	E	8	0	11	2	0
5	A	2	0	0	1	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	1	0
5	E	2	0	0	0	0
All	All	17120	0	17275	316	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 9.

The worst 5 of 316 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:B:290:ILE:CG2	1:C:293:PHE:HE2	1.87	0.88
1:D:293:PHE:HE2	1:E:290:ILE:CG2	1.87	0.87
1:C:290:ILE:CG2	1:E:293:PHE:HE2	1.87	0.87
1:A:290:ILE:CG2	1:B:293:PHE:HE2	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ILE:CG2	1:A:293:PHE:HE2	1.87	0.86

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	408/620 (66%)	397 (97%)	11 (3%)	0	100	100
1	B	408/620 (66%)	398 (98%)	10 (2%)	0	100	100
1	C	408/620 (66%)	395 (97%)	13 (3%)	0	100	100
1	D	408/620 (66%)	397 (97%)	11 (3%)	0	100	100
1	E	408/620 (66%)	396 (97%)	12 (3%)	0	100	100
All	All	2040/3100 (66%)	1983 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	375/551 (68%)	361 (96%)	14 (4%)	29	54
1	B	375/551 (68%)	363 (97%)	12 (3%)	34	59
1	C	375/551 (68%)	360 (96%)	15 (4%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	375/551 (68%)	366 (98%)	9 (2%)	44	68
1	E	375/551 (68%)	361 (96%)	14 (4%)	29	54
All	All	1875/2755 (68%)	1811 (97%)	64 (3%)	34	57

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	204	GLU
1	E	276	GLU
1	B	72	TYR
1	B	47	ARG
1	E	287	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	530	ASN
1	A	39	GLN
1	B	530	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)

20 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	F	1	1,2	14,14,15	0.42	0	17,19,21	1.30	2 (11%)
2	NAG	F	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	G	1	1,2	14,14,15	0.26	0	17,19,21	0.46	0
2	NAG	G	2	2	14,14,15	0.43	0	17,19,21	1.25	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.41	0	17,19,21	1.29	2 (11%)
2	NAG	H	2	2	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	I	1	1,2	14,14,15	0.27	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.42	0	17,19,21	1.26	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.41	0	17,19,21	1.29	2 (11%)
2	NAG	J	2	2	14,14,15	0.24	0	17,19,21	0.42	0
2	NAG	K	1	1,2	14,14,15	0.27	0	17,19,21	0.48	0
2	NAG	K	2	2	14,14,15	0.42	0	17,19,21	1.25	1 (5%)
2	NAG	L	1	1,2	14,14,15	0.40	0	17,19,21	1.28	2 (11%)
2	NAG	L	2	2	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	M	1	1,2	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	M	2	2	14,14,15	0.41	0	17,19,21	1.25	1 (5%)
2	NAG	N	1	1,2	14,14,15	0.40	0	17,19,21	1.29	2 (11%)
2	NAG	N	2	2	14,14,15	0.22	0	17,19,21	0.43	0
2	NAG	O	1	1,2	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	O	2	2	14,14,15	0.43	0	17,19,21	1.25	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
2	NAG	F	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	3/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	3/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	NAG	C2-N2-C7	4.40	129.16	122.90
2	O	2	NAG	C2-N2-C7	4.36	129.11	122.90
2	G	2	NAG	C2-N2-C7	4.36	129.11	122.90
2	M	2	NAG	C2-N2-C7	4.35	129.10	122.90
2	K	2	NAG	C2-N2-C7	4.34	129.08	122.90

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6

There are no ring outliers.

15 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1	NAG	1	0
2	O	1	NAG	1	0
2	H	1	NAG	1	0
2	F	1	NAG	1	0
2	G	2	NAG	2	0
2	K	2	NAG	2	0
2	G	1	NAG	1	0

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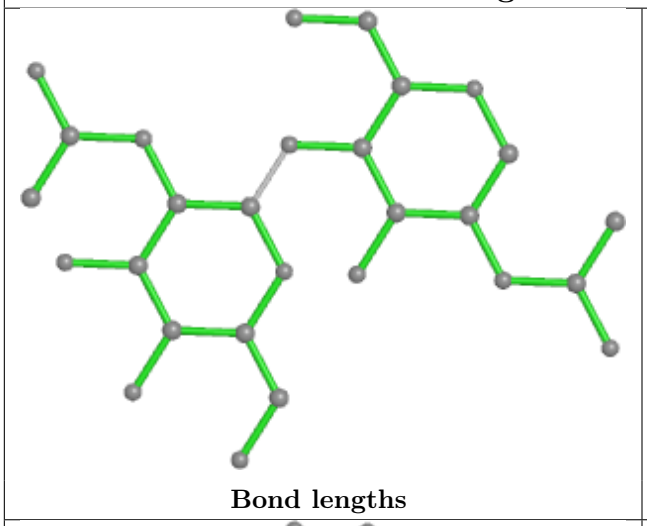
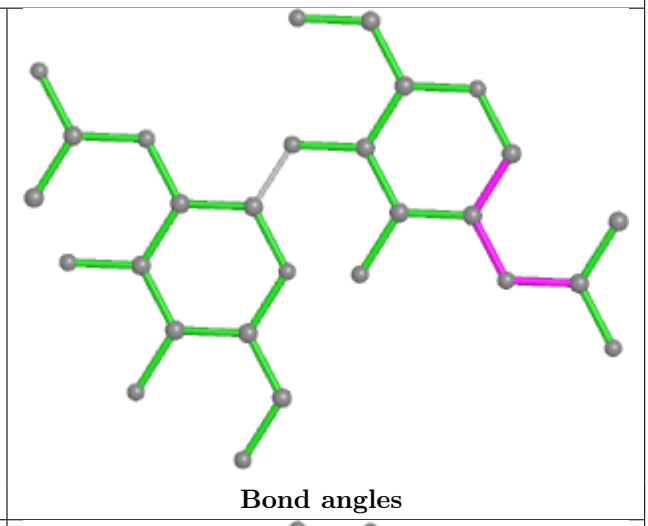
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	1	0
2	N	1	NAG	1	0
2	M	1	NAG	1	0
2	I	1	NAG	1	0
2	O	2	NAG	2	0
2	I	2	NAG	2	0
2	M	2	NAG	2	0
2	L	1	NAG	1	0

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

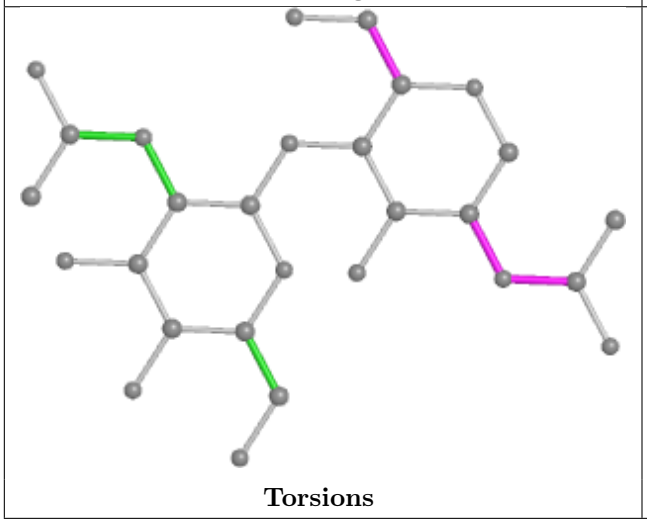
Oligosaccharide Chain F



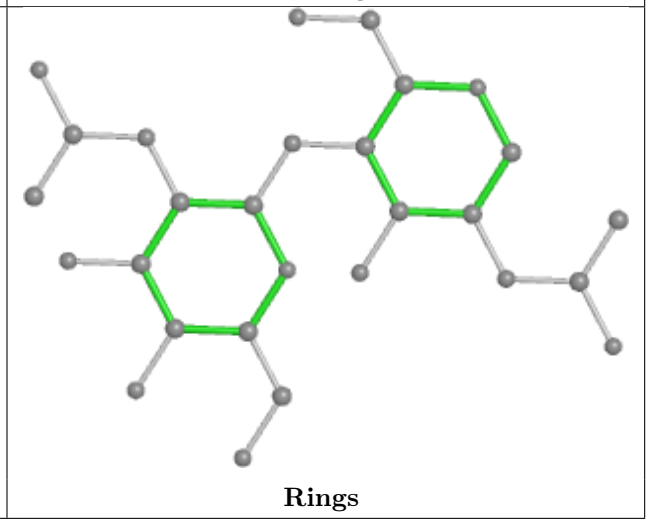
Bond lengths



Bond angles

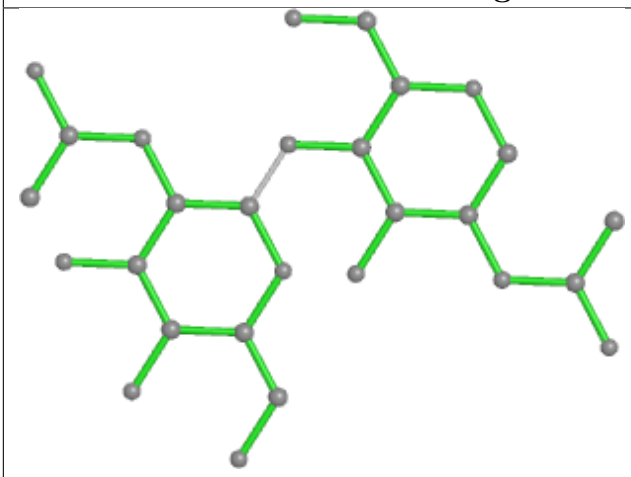


Torsions

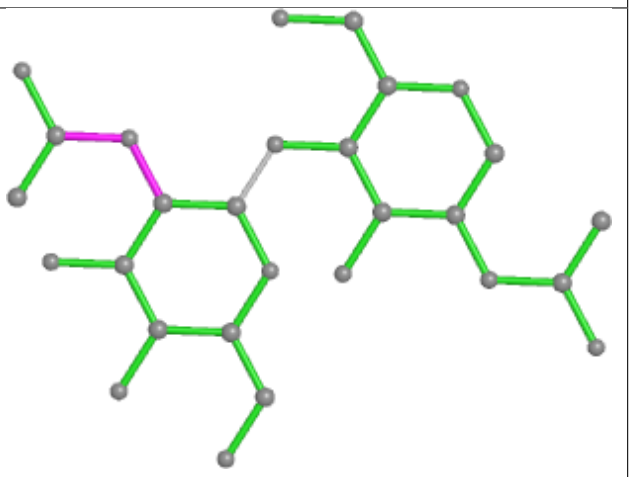


Rings

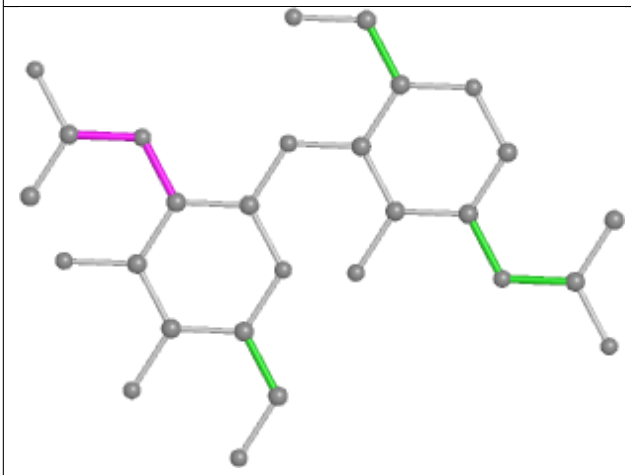
Oligosaccharide Chain G



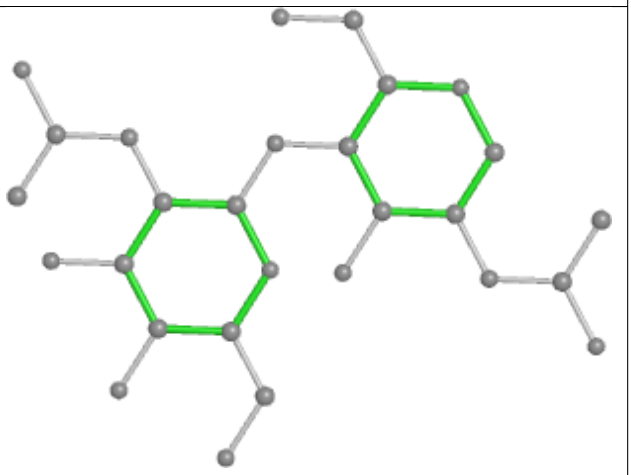
Bond lengths



Bond angles

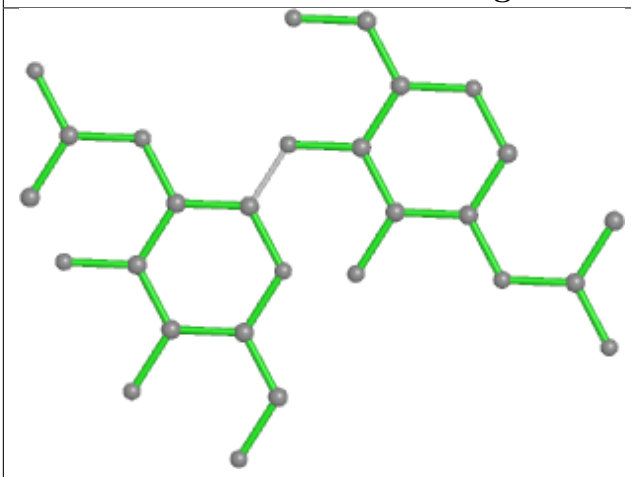


Torsions

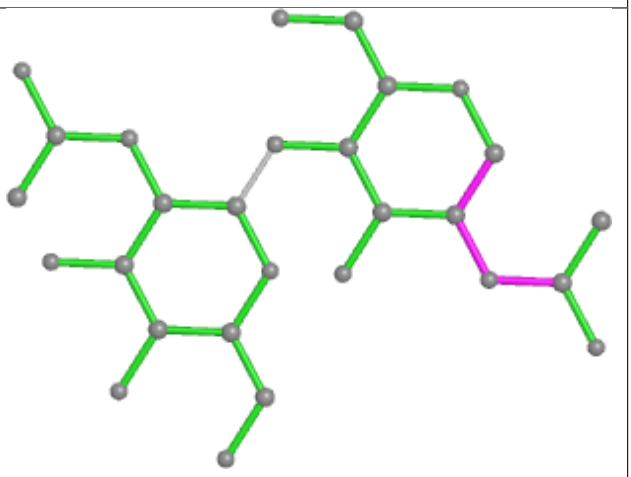


Rings

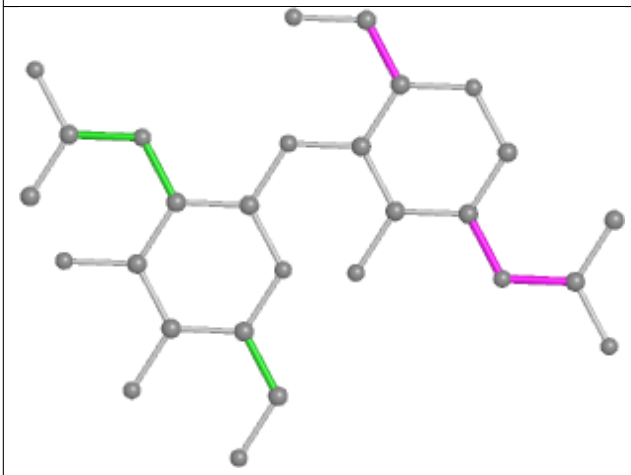
Oligosaccharide Chain H



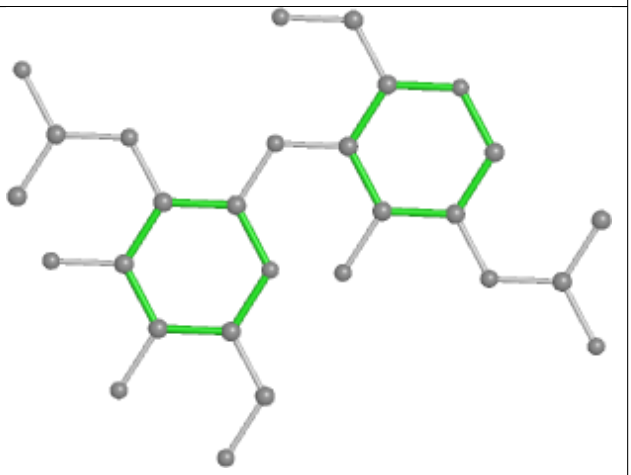
Bond lengths



Bond angles

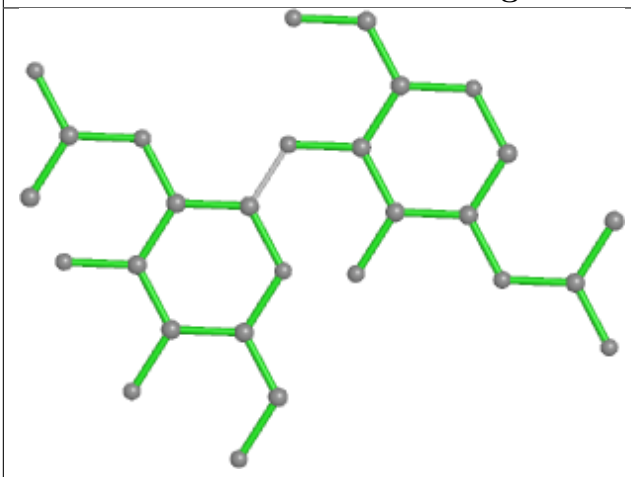


Torsions

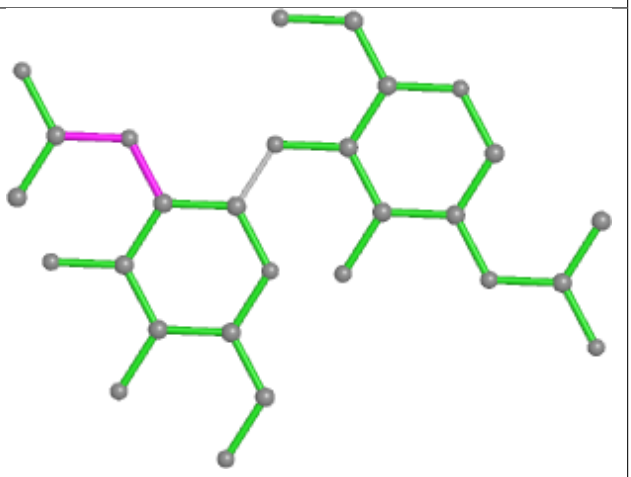


Rings

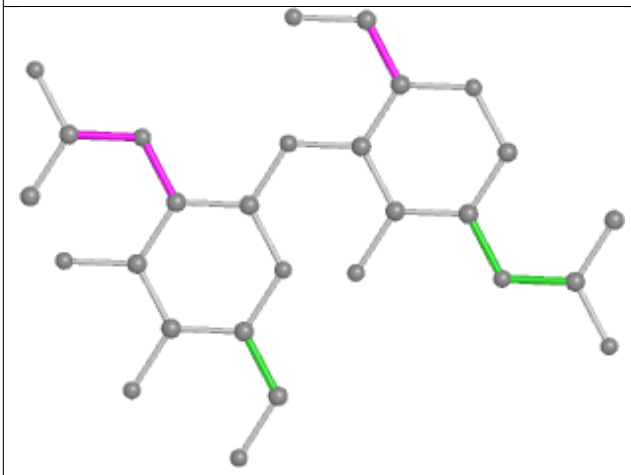
Oligosaccharide Chain I



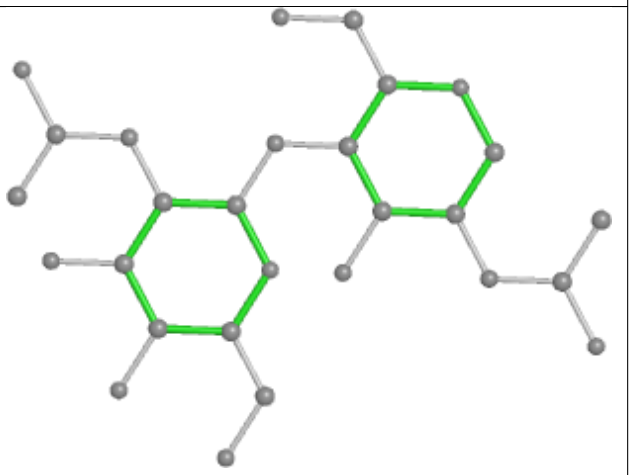
Bond lengths



Bond angles

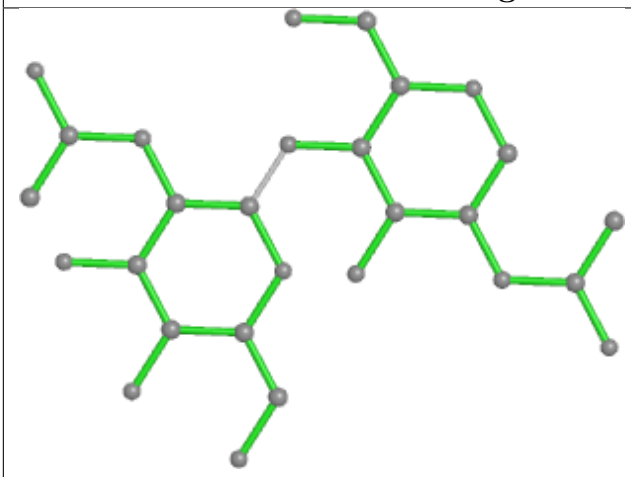


Torsions

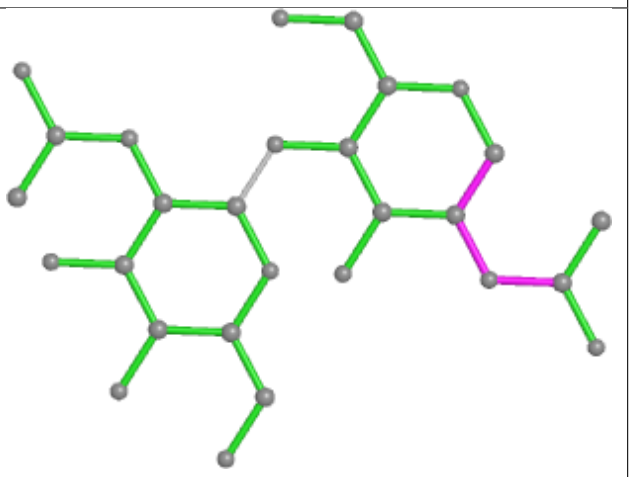


Rings

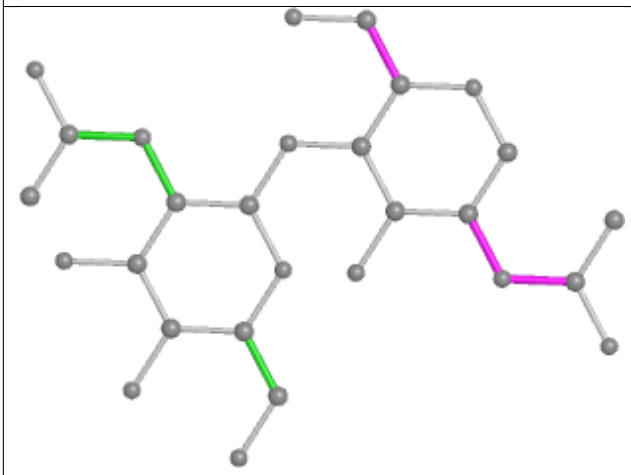
Oligosaccharide Chain J



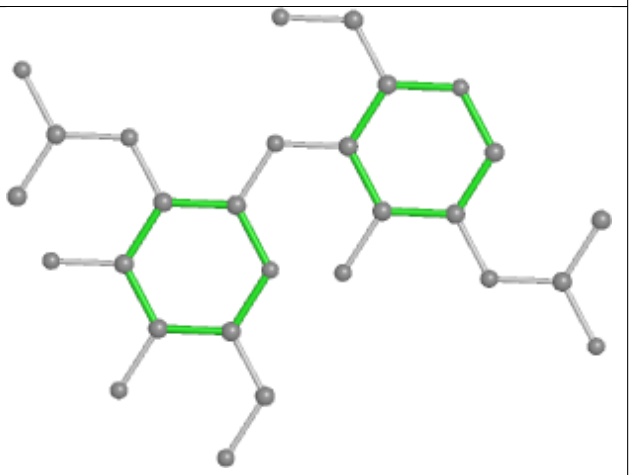
Bond lengths



Bond angles

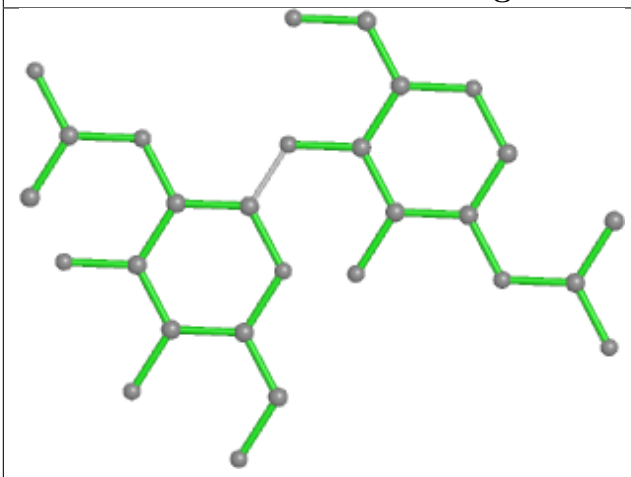


Torsions



Rings

Oligosaccharide Chain K



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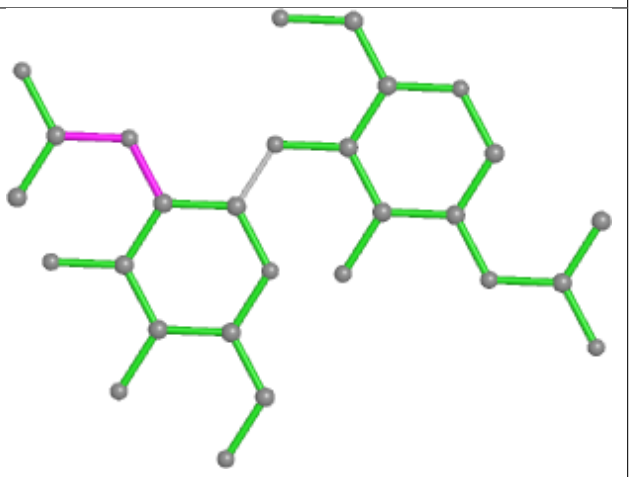
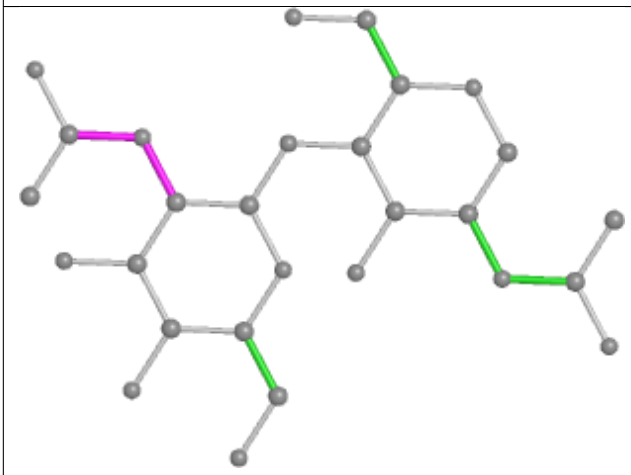
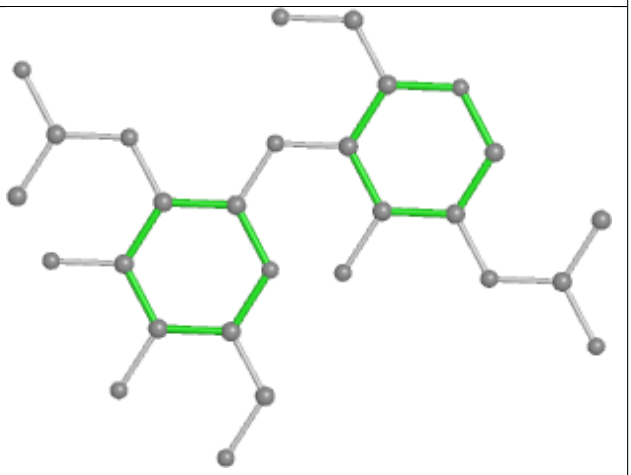


Bond angles

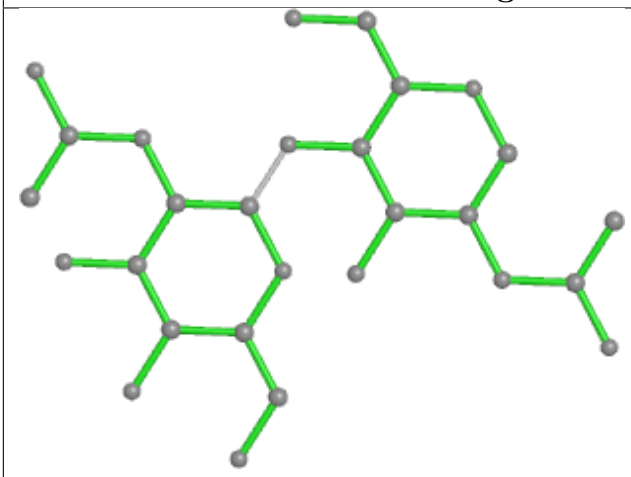


Torsions

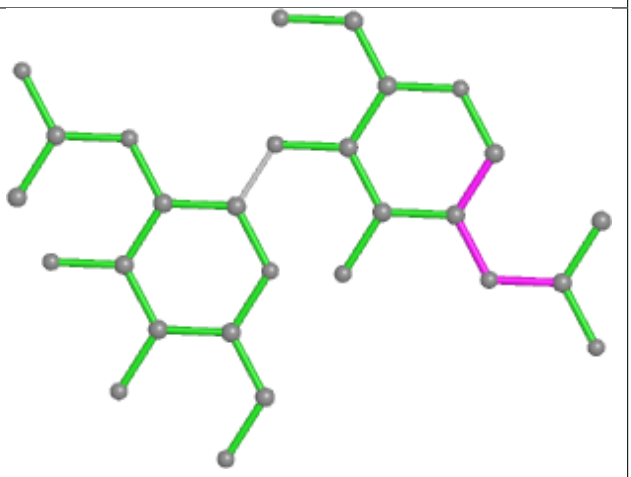


Rings

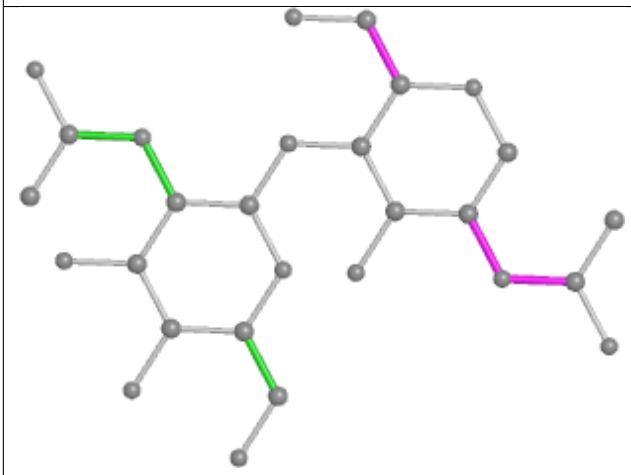
Oligosaccharide Chain L



Bond lengths



Bond angles



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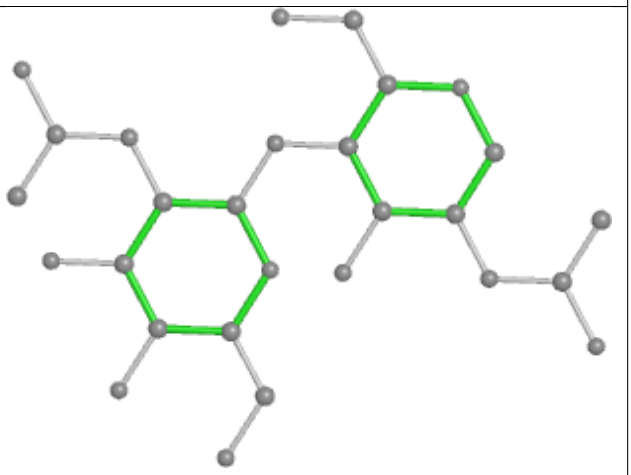
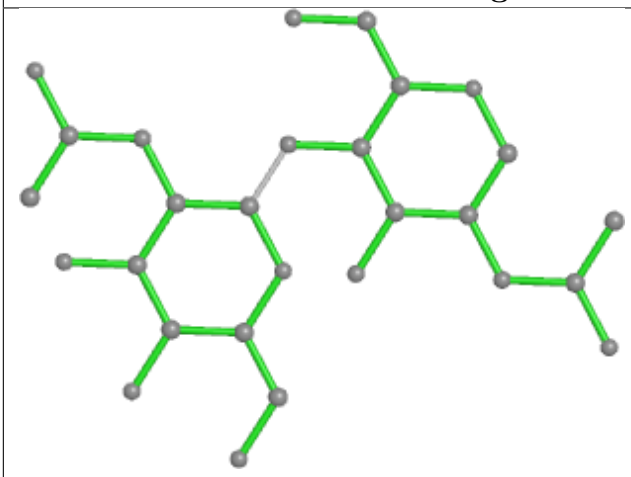


Rings

Oligosaccharide Chain M



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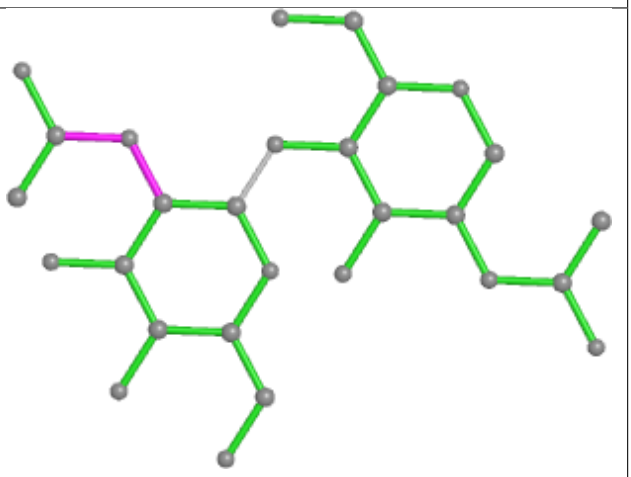

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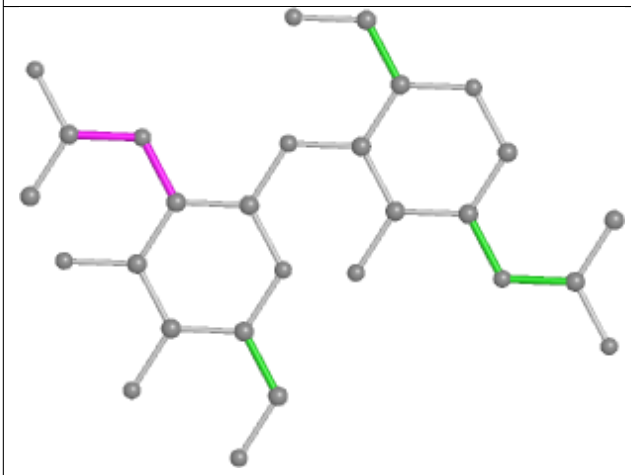

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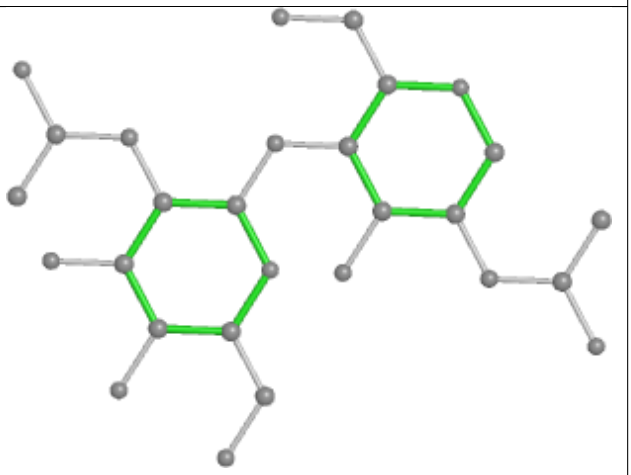
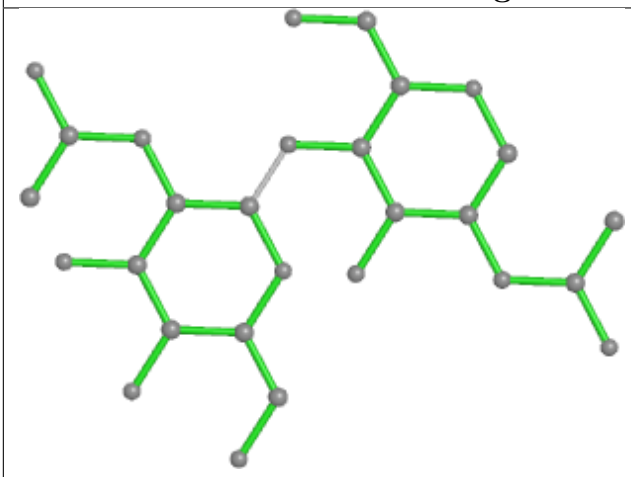
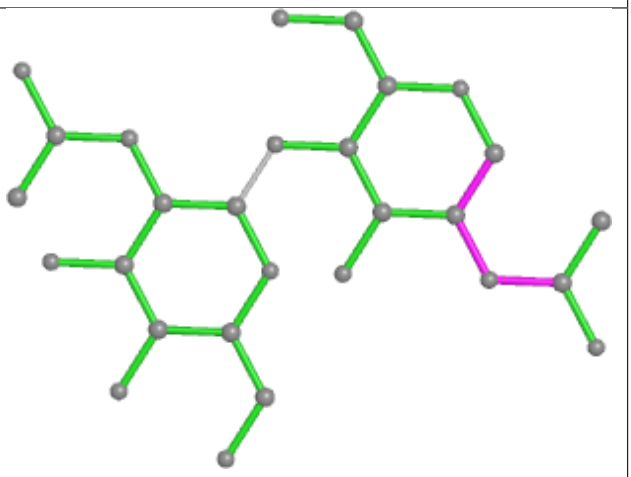


Rings

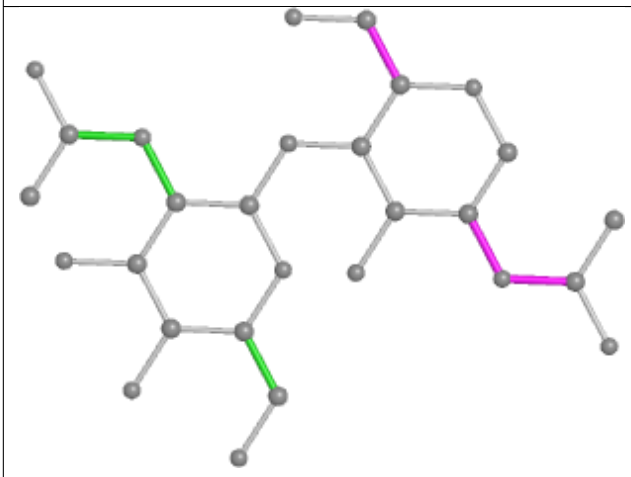
Oligosaccharide Chain N



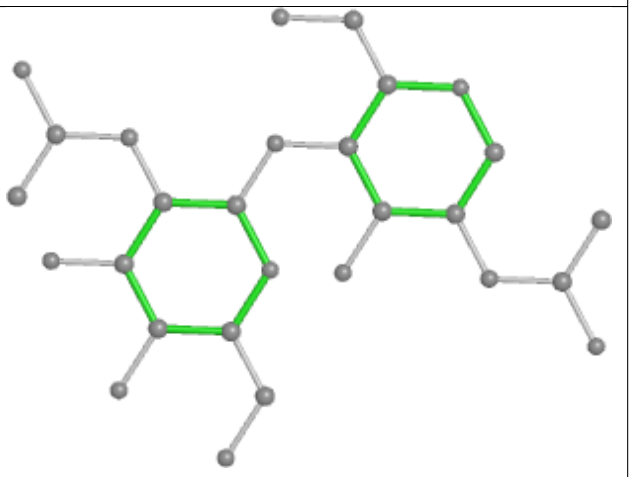
Bond lengths



Bond angles

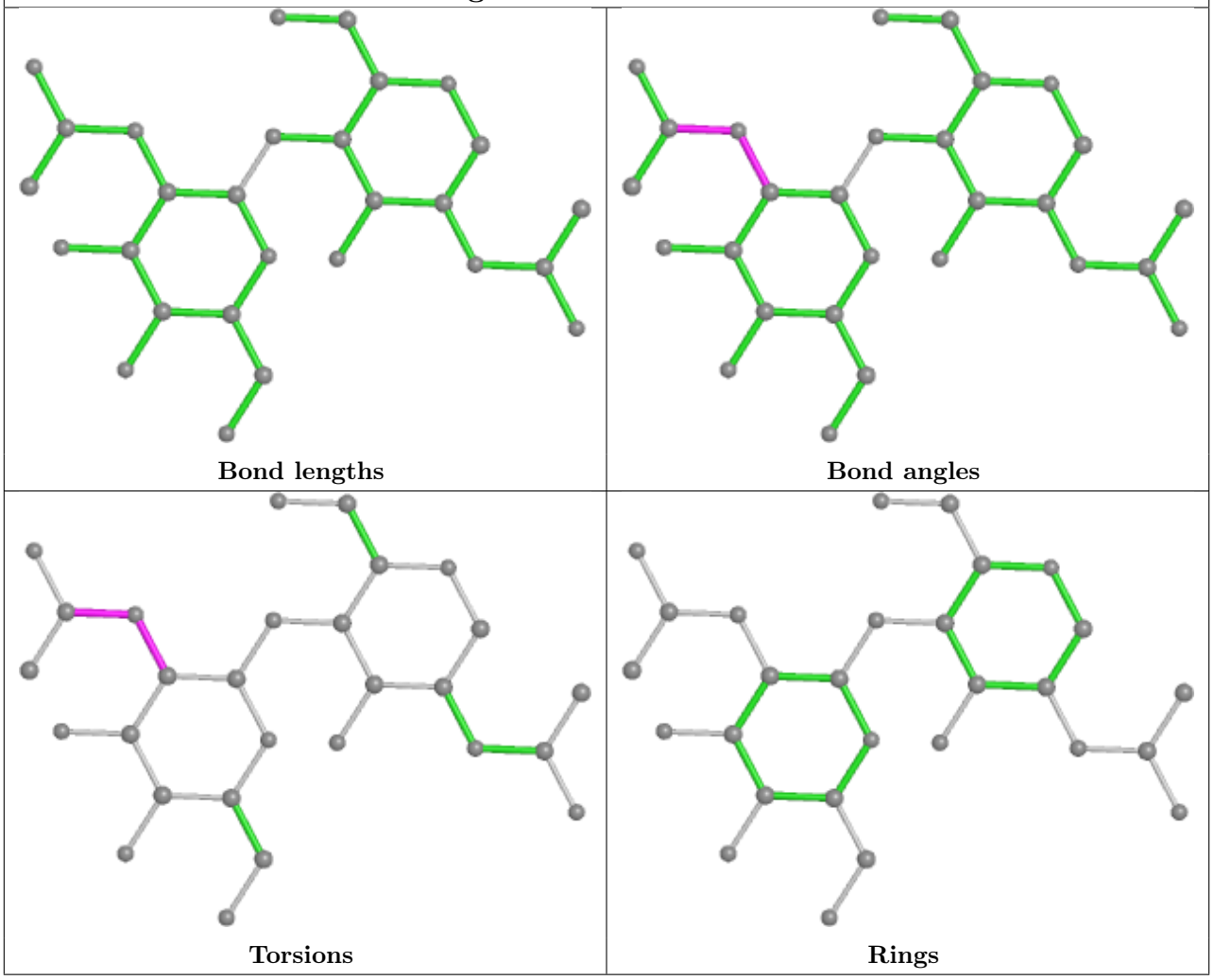


Torsions



Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	BET	E	602	-	7,7,7	1.08	0	10,10,10	1.03	1 (10%)
3	NAG	E	601	1	14,14,15	0.68	0	17,19,21	1.02	1 (5%)
4	BET	D	602	-	7,7,7	1.04	0	10,10,10	1.26	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BET	B	602	-	7,7,7	1.05	0	10,10,10	1.26	1 (10%)
4	BET	C	602	-	7,7,7	1.05	0	10,10,10	1.27	1 (10%)
3	NAG	D	601	1	14,14,15	0.18	0	17,19,21	0.43	0
3	NAG	B	601	1	14,14,15	1.14	1 (7%)	17,19,21	0.73	0
4	BET	A	602	-	7,7,7	1.05	0	10,10,10	1.25	1 (10%)
3	NAG	A	601	1	14,14,15	0.35	0	17,19,21	0.52	0
3	NAG	C	601	1	14,14,15	0.27	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BET	E	602	-	-	2/5/5/5	-
3	NAG	E	601	1	-	2/6/23/26	0/1/1/1
4	BET	D	602	-	-	2/5/5/5	-
4	BET	B	602	-	-	2/5/5/5	-
4	BET	C	602	-	-	2/5/5/5	-
3	NAG	D	601	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	1/6/23/26	0/1/1/1
4	BET	A	602	-	-	2/5/5/5	-
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	C	601	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	NAG	O5-C1	-3.89	1.37	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	601	NAG	C1-O5-C5	3.56	117.01	112.19
4	C	602	BET	C-CA-N	2.34	119.55	116.34
4	D	602	BET	C-CA-N	2.32	119.52	116.34
4	A	602	BET	C-CA-N	2.27	119.45	116.34
4	B	602	BET	C-CA-N	2.25	119.43	116.34

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	602	BET	O-C-CA-N
4	D	602	BET	OXT-C-CA-N
4	A	602	BET	O-C-CA-N
4	A	602	BET	OXT-C-CA-N
4	B	602	BET	O-C-CA-N

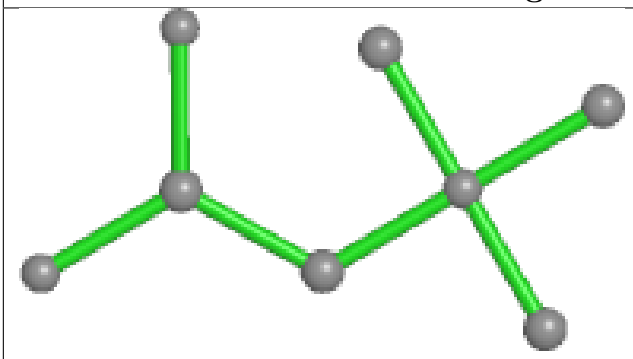
There are no ring outliers.

6 monomers are involved in 11 short contacts:

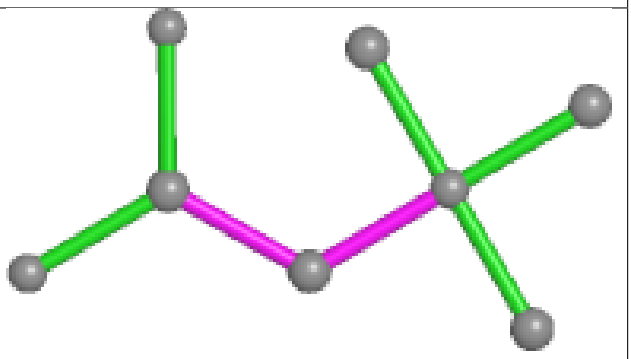
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	602	BET	2	0
4	D	602	BET	2	0
4	B	602	BET	2	0
4	C	602	BET	1	0
3	D	601	NAG	1	0
4	A	602	BET	3	0

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

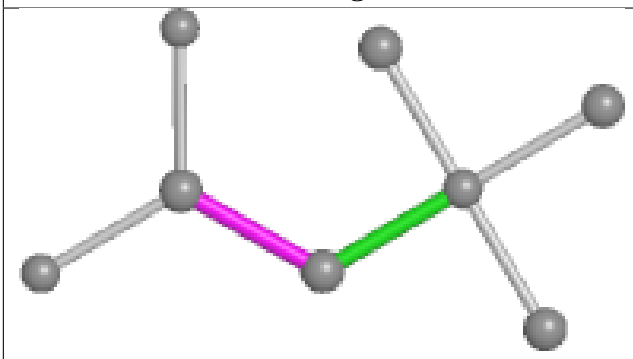
Ligand BET E 602



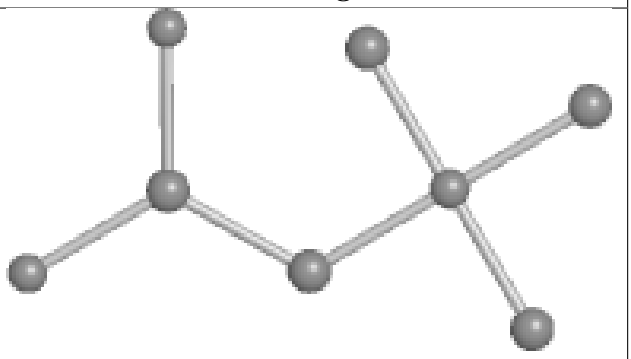
Bond lengths



Bond angles

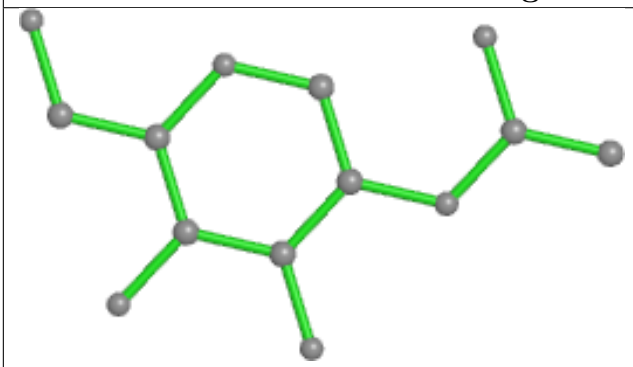


Torsions



Rings

Ligand NAG E 601



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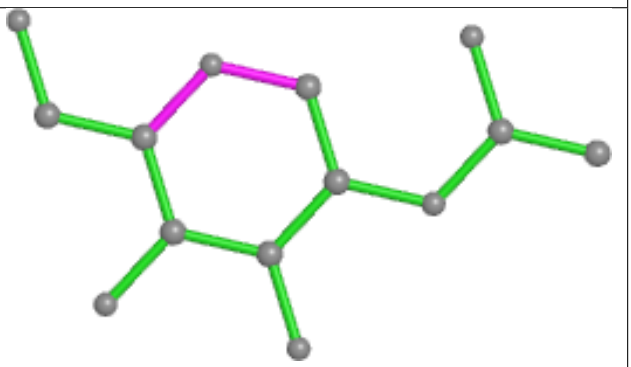

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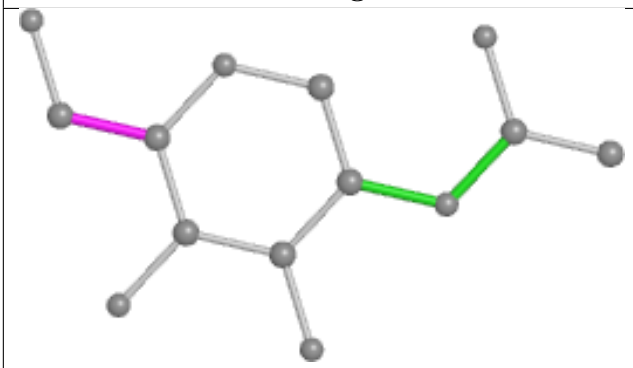
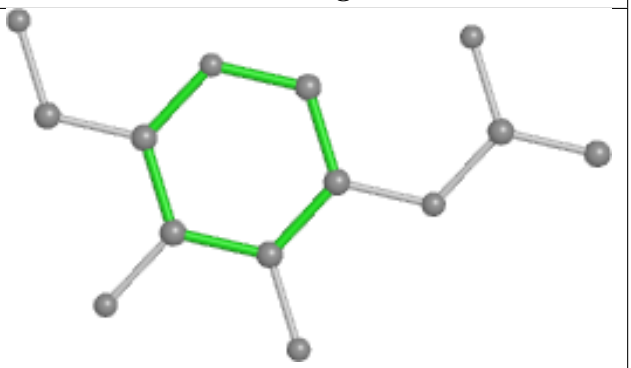
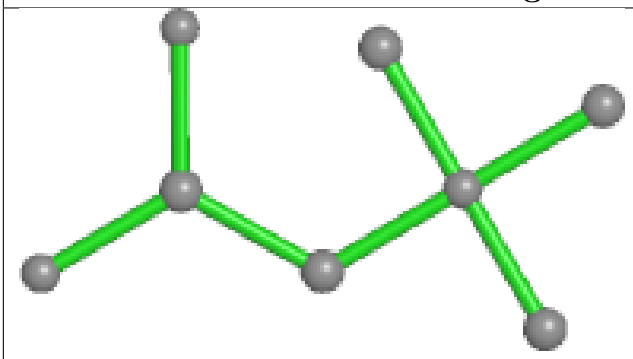


Torsions

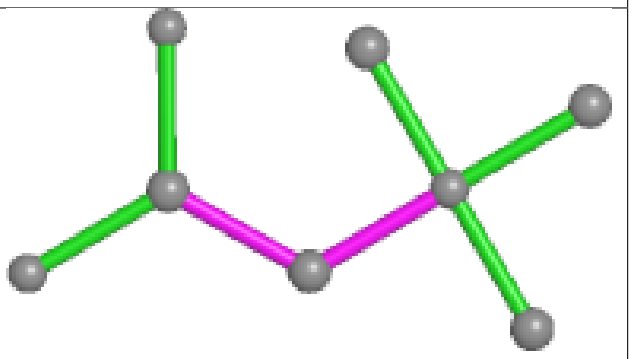


Rings

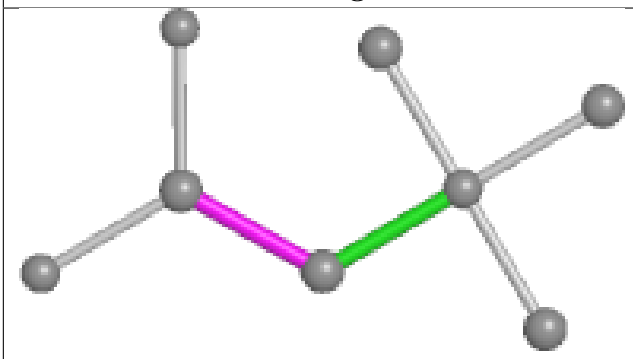
Ligand BET D 602



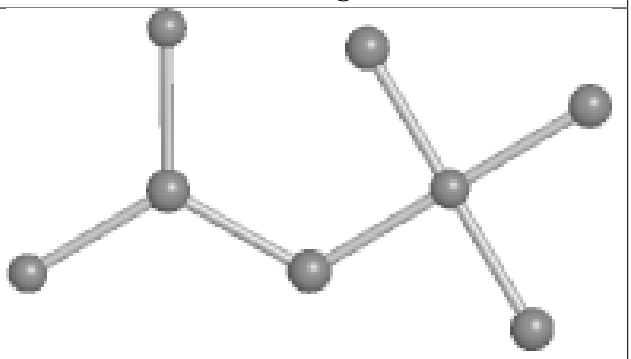
Bond lengths



Bond angles

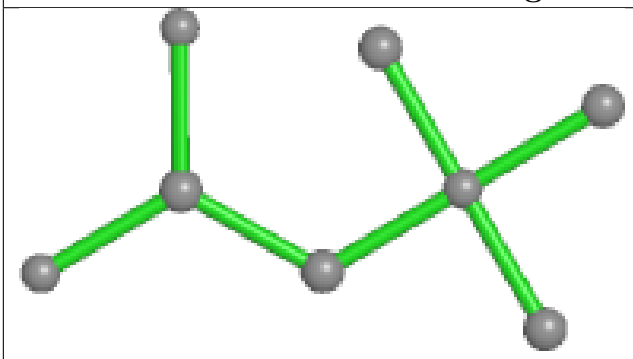


Torsions

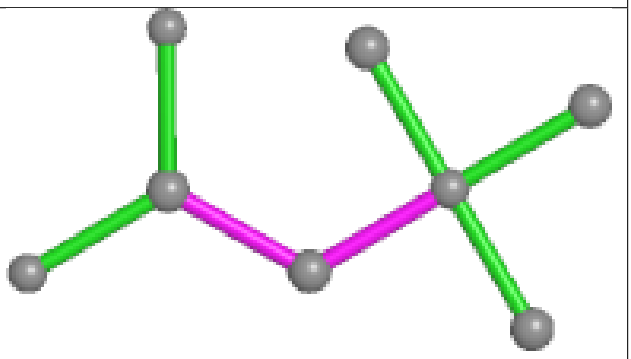


Rings

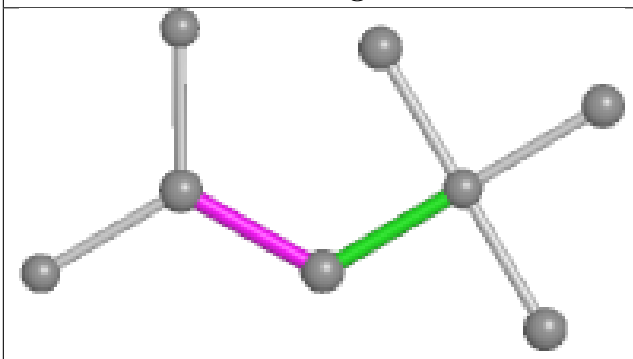
Ligand BET B 602



Bond lengths



Bond angles



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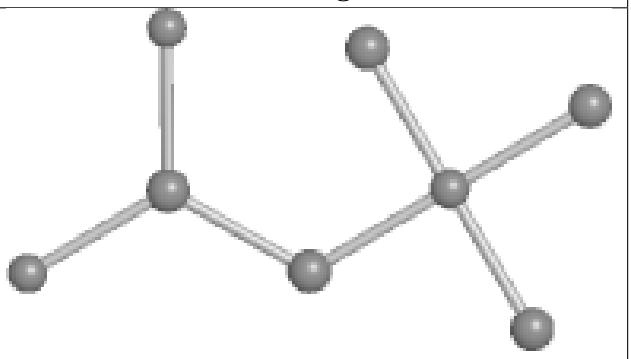
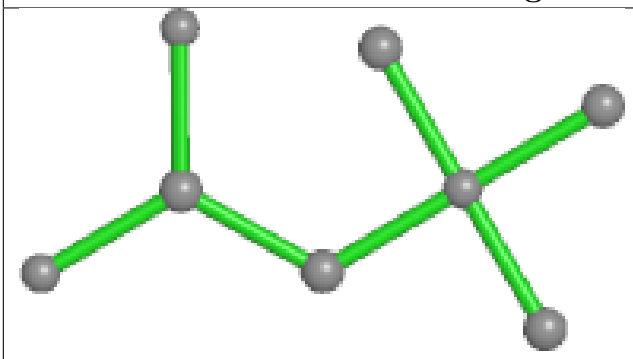
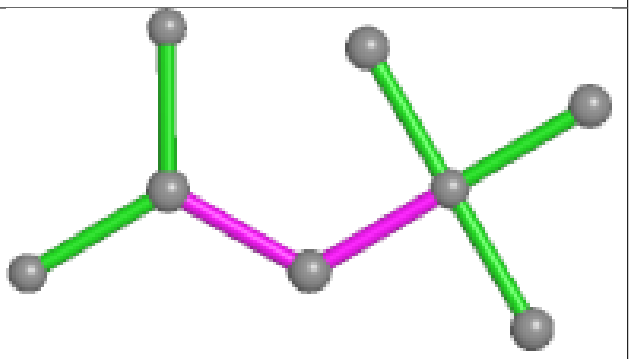


Rings

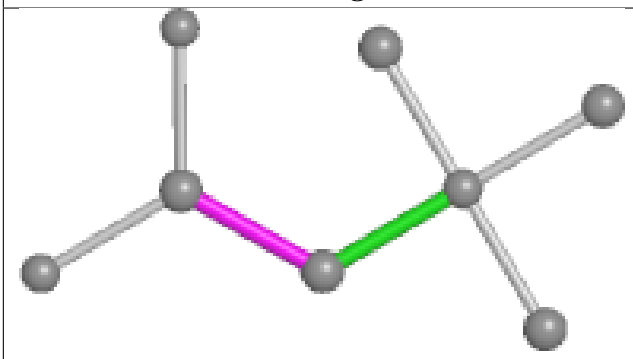
Ligand BET C 602



Bond lengths



Bond angles



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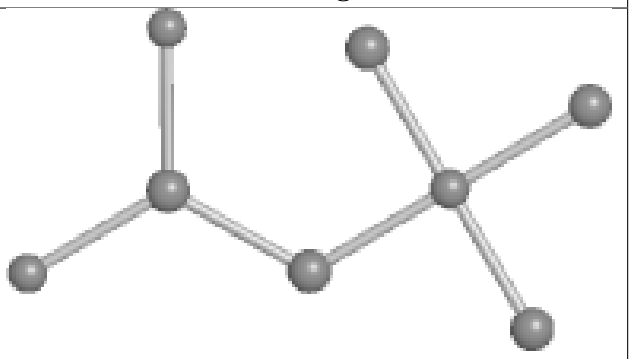
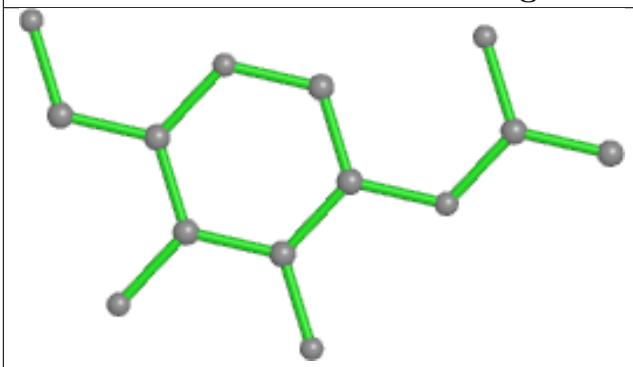
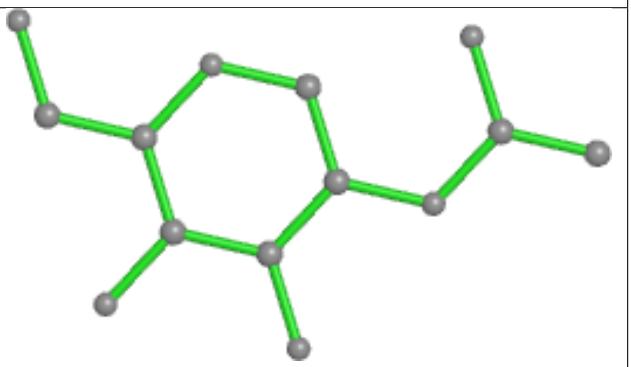


Rings

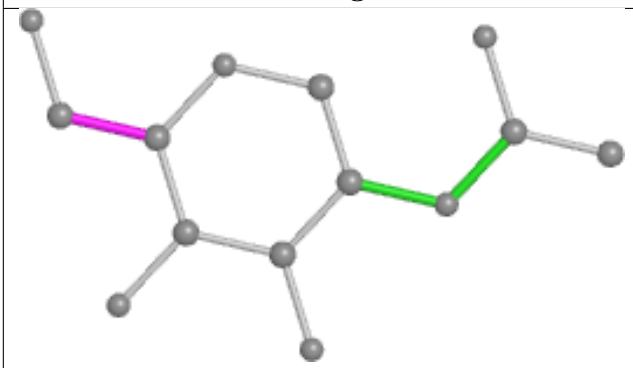
Ligand NAG D 601



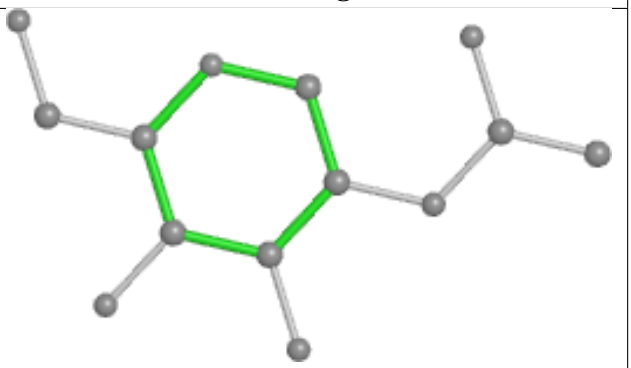
Bond lengths



Bond angles

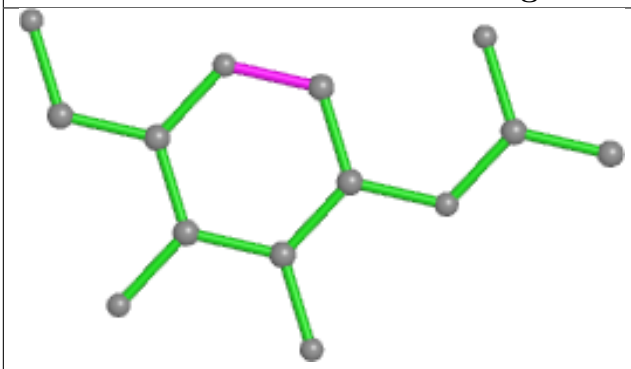


Torsions



Rings

Ligand NAG B 601



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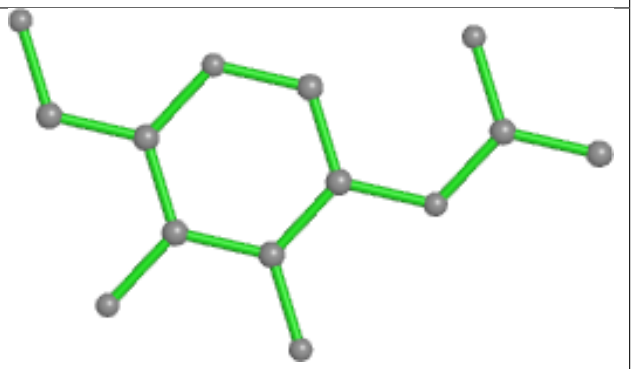

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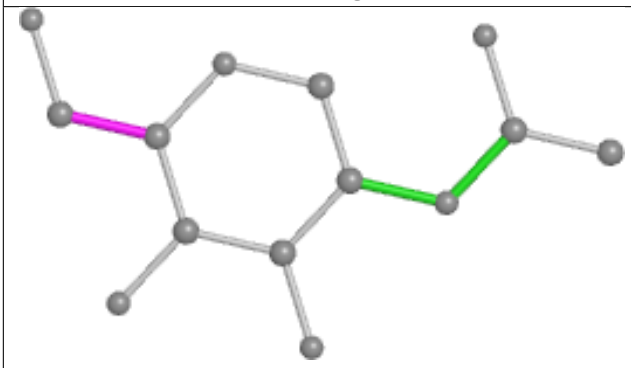

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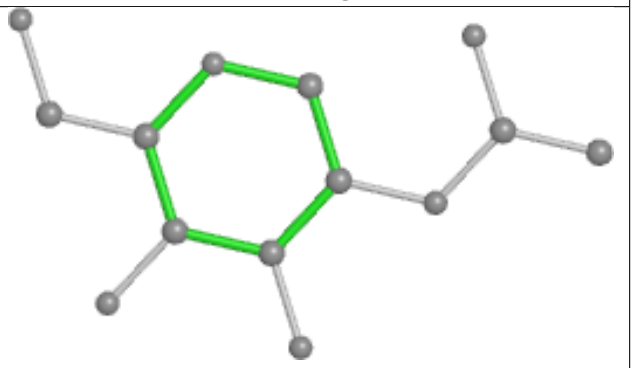
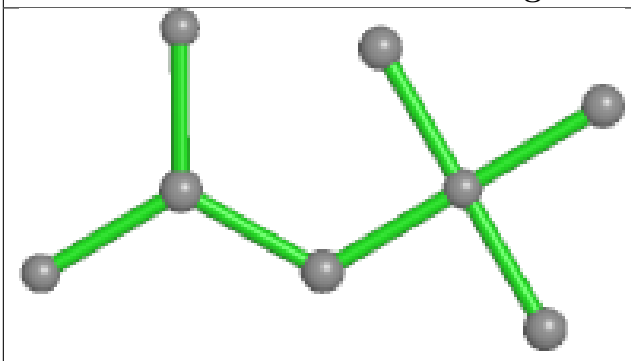


Rings

Ligand BET A 602



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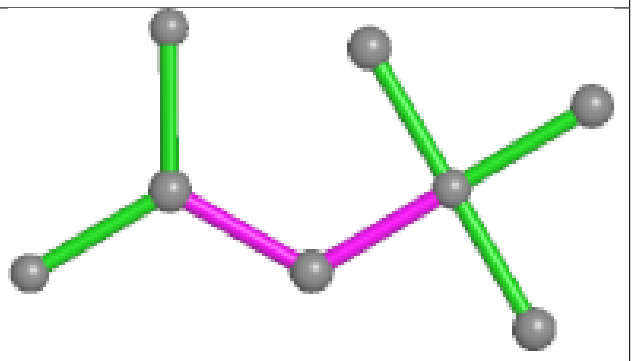

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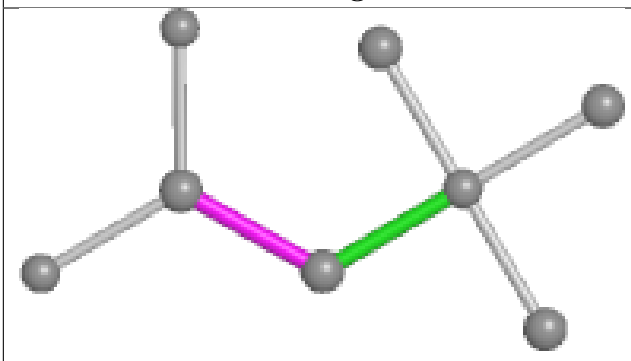

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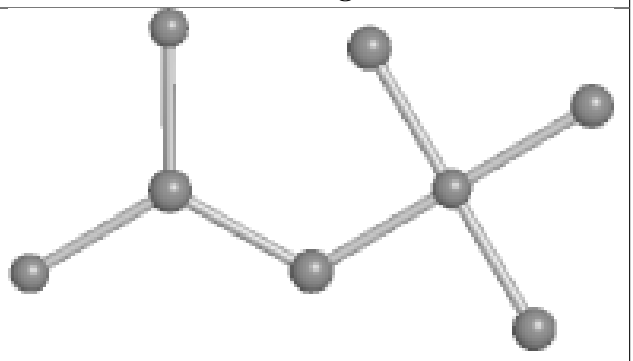
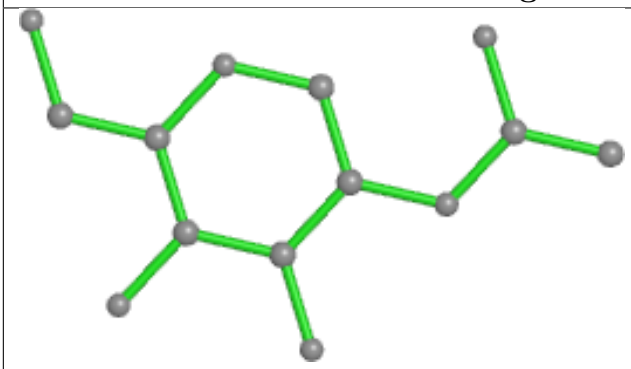


Rings

Ligand NAG A 601



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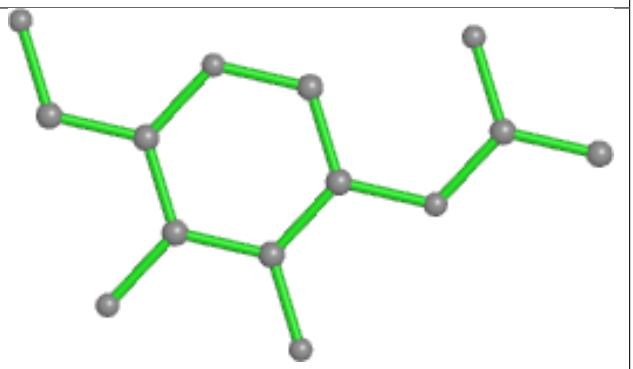
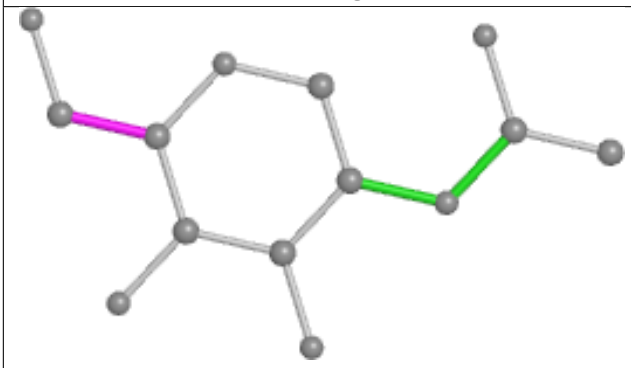


Bond angles



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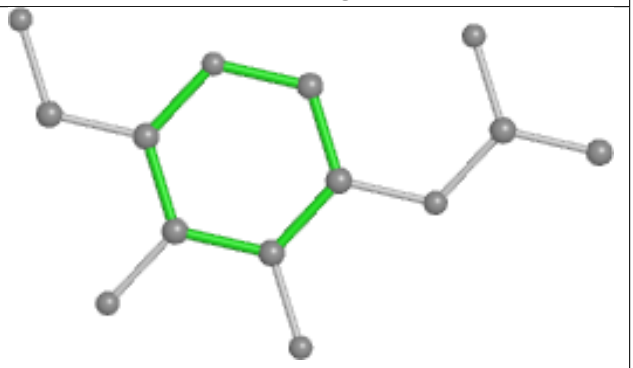
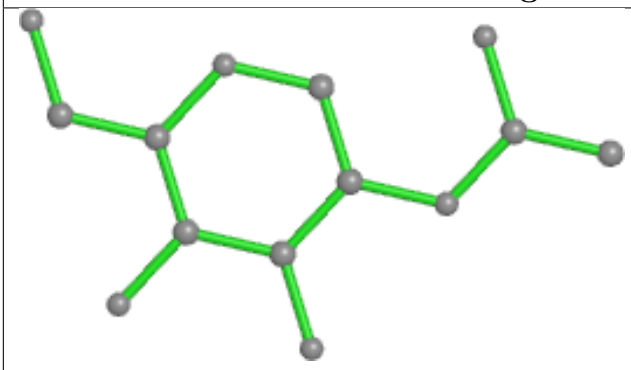


Rings

Ligand NAG C 601



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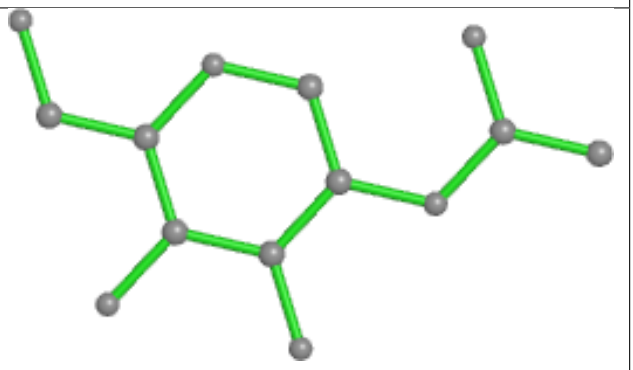
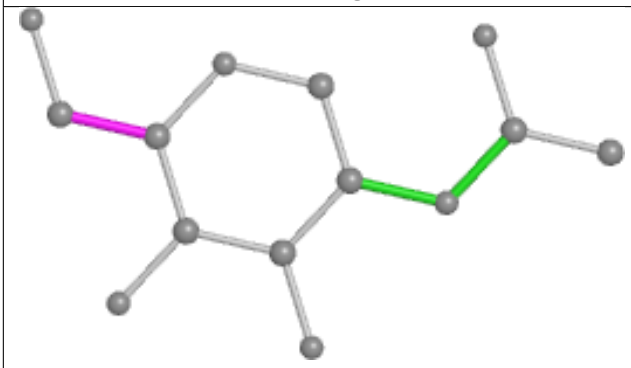


Bond angles



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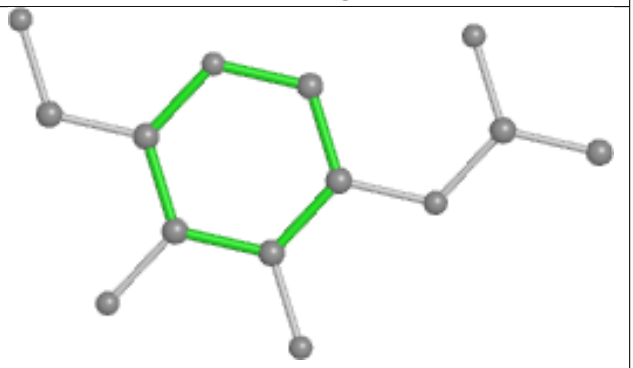

Rings

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.