Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 03:30 AM EDT

PDB ID	:	6VJK
Title	:	Streptavidin mutant M88 (N49C/A86C)
Authors	:	Marangoni, J.M.; Wu, S.C.; Fogen, D.; Wong, S.L.; Ng, K.K.S.
Deposited on	:	2020-01-16
Resolution	:	1.60 Å(reported)

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

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

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

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12685 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Streptavidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	0	0	0
			908	567	157	182	2			
1	B	118	Total	C	N	O	S	0	0	0
			879	548	152	177	2			
1	C	120	Total	C	N	O	S	0	0	0
			895	559	155	179	2			
1	D	123	Total	C	N	O	S	0	0	0
			917	572	158	185	2			
1	E	121	Total	C	N	O	S	0	0	0
			903	564	156	181	2			
1	F	123	Total	C	N	O	S	0	0	0
			917	572	158	185	2			
1	G	123	Total	C	N	O	S	0	0	0
			917	572	158	185	2			
1	H	123	Total	C	N	O	S	0	0	0
			917	572	158	185	2			
1	I	121	Total	C	N	O	S	0	0	0
			902	564	156	180	2			
1	J	119	Total	C	N	O	S	0	0	0
			890	556	154	178	2			
1	K	120	Total	C	N	O	S	0	0	0
			895	559	155	179	2			
1	L	119	Total	C	N	O	S	0	0	0
			886	553	153	178	2			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	MET	-	initiating methionine	UNP P22629
A	49	CYS	ASN	engineered mutation	UNP P22629
A	86	CYS	ALA	engineered mutation	UNP P22629
B	13	MET	-	initiating methionine	UNP P22629
B	49	CYS	ASN	engineered mutation	UNP P22629

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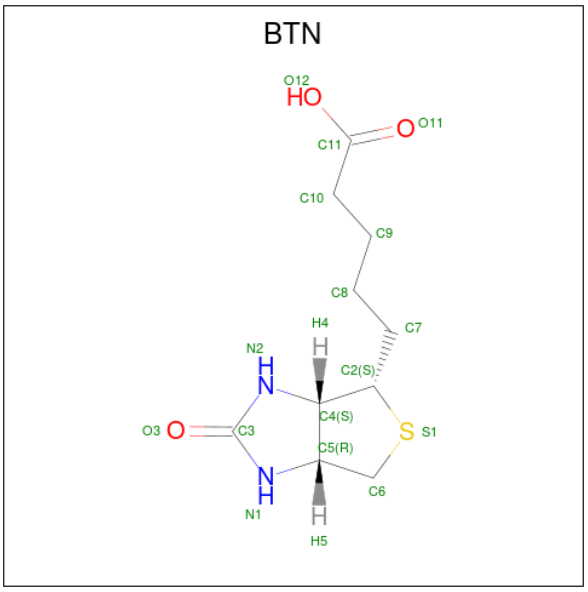
Chain	Residue	Modelled	Actual	Comment	Reference
B	86	CYS	ALA	engineered mutation	UNP P22629
C	13	MET	-	initiating methionine	UNP P22629
C	49	CYS	ASN	engineered mutation	UNP P22629
C	86	CYS	ALA	engineered mutation	UNP P22629
D	13	MET	-	initiating methionine	UNP P22629
D	49	CYS	ASN	engineered mutation	UNP P22629
D	86	CYS	ALA	engineered mutation	UNP P22629
E	13	MET	-	initiating methionine	UNP P22629
E	49	CYS	ASN	engineered mutation	UNP P22629
E	86	CYS	ALA	engineered mutation	UNP P22629
F	13	MET	-	initiating methionine	UNP P22629
F	49	CYS	ASN	engineered mutation	UNP P22629
F	86	CYS	ALA	engineered mutation	UNP P22629
G	13	MET	-	initiating methionine	UNP P22629
G	49	CYS	ASN	engineered mutation	UNP P22629
G	86	CYS	ALA	engineered mutation	UNP P22629
H	13	MET	-	initiating methionine	UNP P22629
H	49	CYS	ASN	engineered mutation	UNP P22629
H	86	CYS	ALA	engineered mutation	UNP P22629
I	13	MET	-	initiating methionine	UNP P22629
I	49	CYS	ASN	engineered mutation	UNP P22629
I	86	CYS	ALA	engineered mutation	UNP P22629
J	13	MET	-	initiating methionine	UNP P22629
J	49	CYS	ASN	engineered mutation	UNP P22629
J	86	CYS	ALA	engineered mutation	UNP P22629
K	13	MET	-	initiating methionine	UNP P22629
K	49	CYS	ASN	engineered mutation	UNP P22629
K	86	CYS	ALA	engineered mutation	UNP P22629
L	13	MET	-	initiating methionine	UNP P22629
L	49	CYS	ASN	engineered mutation	UNP P22629
L	86	CYS	ALA	engineered mutation	UNP P22629

- Molecule 2 is BIOTIN (three-letter code: BTN) (formula: $C_{10}H_{16}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	C	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	D	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	E	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	F	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	G	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	H	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	I	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	J	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	K	1	Total	C	N	O	S	0	0
			16	10	2	3	1		
2	L	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	154	Total O 154 154	0	0
3	B	145	Total O 145 145	0	0
3	C	150	Total O 150 150	0	0
3	D	120	Total O 120 120	0	0
3	E	159	Total O 159 159	0	0
3	F	171	Total O 171 171	0	0
3	G	116	Total O 116 116	0	0
3	H	154	Total O 154 154	0	0
3	I	127	Total O 127 127	0	0
3	J	121	Total O 121 121	0	0
3	K	132	Total O 132 132	0	0
3	L	118	Total O 118 118	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.26Å 79.55Å 281.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60	Depositor
% Data completeness (in resolution range)	98.5 (50.00-1.60)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.8.0135 2015/10/01	Depositor
R, R_{free}	0.184 , 0.215	Depositor
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.344	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12685	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

12 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	$\#\|Z\| > 2$
2	BTN	A	300	-	17,17,17	1.05	1 (5%)	23,23,23	1.24	2 (8%)
2	BTN	L	300	-	17,17,17	1.22	1 (5%)	23,23,23	1.30	2 (8%)
2	BTN	E	401	-	17,17,17	1.10	1 (5%)	23,23,23	1.14	2 (8%)
2	BTN	G	401	-	17,17,17	1.20	1 (5%)	23,23,23	1.10	2 (8%)
2	BTN	C	300	-	17,17,17	1.09	1 (5%)	23,23,23	1.14	1 (4%)
2	BTN	D	300	-	17,17,17	1.18	1 (5%)	23,23,23	1.06	1 (4%)
2	BTN	H	300	-	17,17,17	1.16	1 (5%)	23,23,23	1.08	2 (8%)
2	BTN	B	300	-	17,17,17	1.08	1 (5%)	23,23,23	1.15	1 (4%)
2	BTN	J	300	-	17,17,17	1.16	1 (5%)	23,23,23	1.16	1 (4%)
2	BTN	F	300	-	17,17,17	1.16	1 (5%)	23,23,23	1.05	1 (4%)
2	BTN	K	401	-	17,17,17	1.15	1 (5%)	23,23,23	0.90	1 (4%)
2	BTN	I	401	-	17,17,17	1.16	1 (5%)	23,23,23	1.05	1 (4%)

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	BTN	A	300	-	-	1/7/28/28	0/2/2/2
2	BTN	L	300	-	-	0/7/28/28	0/2/2/2
2	BTN	E	401	-	-	0/7/28/28	0/2/2/2
2	BTN	G	401	-	-	2/7/28/28	0/2/2/2
2	BTN	C	300	-	-	0/7/28/28	0/2/2/2
2	BTN	D	300	-	-	1/7/28/28	0/2/2/2
2	BTN	H	300	-	-	0/7/28/28	0/2/2/2
2	BTN	B	300	-	-	0/7/28/28	0/2/2/2
2	BTN	J	300	-	-	2/7/28/28	0/2/2/2
2	BTN	F	300	-	-	1/7/28/28	0/2/2/2
2	BTN	K	401	-	-	0/7/28/28	0/2/2/2
2	BTN	I	401	-	-	0/7/28/28	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	300	BTN	C2-S1	-3.65	1.76	1.82
2	D	300	BTN	C2-S1	-3.47	1.77	1.82
2	H	300	BTN	C2-S1	-3.45	1.77	1.82
2	J	300	BTN	C2-S1	-3.38	1.77	1.82
2	K	401	BTN	C2-S1	-3.36	1.77	1.82
2	G	401	BTN	C2-S1	-3.31	1.77	1.82
2	F	300	BTN	C2-S1	-3.29	1.77	1.82
2	B	300	BTN	C2-S1	-3.25	1.77	1.82
2	I	401	BTN	C2-S1	-3.19	1.77	1.82
2	C	300	BTN	C2-S1	-3.05	1.77	1.82
2	E	401	BTN	C2-S1	-3.03	1.77	1.82
2	A	300	BTN	C2-S1	-2.86	1.78	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	300	BTN	C6-C5-N1	-3.47	108.62	113.03
2	J	300	BTN	C6-C5-N1	-3.31	108.83	113.03
2	L	300	BTN	C6-C5-N1	-3.11	109.08	113.03
2	B	300	BTN	C6-C5-N1	-3.07	109.13	113.03
2	I	401	BTN	C6-C5-N1	-3.07	109.14	113.03
2	G	401	BTN	C6-C5-N1	-3.02	109.19	113.03
2	H	300	BTN	C6-C5-N1	-3.00	109.21	113.03
2	D	300	BTN	C6-C5-N1	-2.94	109.30	113.03
2	A	300	BTN	N2-C3-N1	2.72	111.31	108.76
2	E	401	BTN	C6-C5-N1	-2.68	109.62	113.03
2	F	300	BTN	C6-C5-N1	-2.60	109.73	113.03
2	E	401	BTN	N2-C3-N1	2.41	111.02	108.76
2	L	300	BTN	N2-C3-N1	2.31	110.93	108.76
2	A	300	BTN	C6-C5-N1	-2.27	110.14	113.03
2	H	300	BTN	N2-C3-N1	2.20	110.83	108.76
2	G	401	BTN	N2-C3-N1	2.11	110.74	108.76
2	K	401	BTN	N2-C3-N1	2.03	110.66	108.76

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	300	BTN	C9-C10-C11-O11
2	G	401	BTN	C9-C10-C11-O11
2	G	401	BTN	C9-C10-C11-O12
2	F	300	BTN	C9-C10-C11-O11

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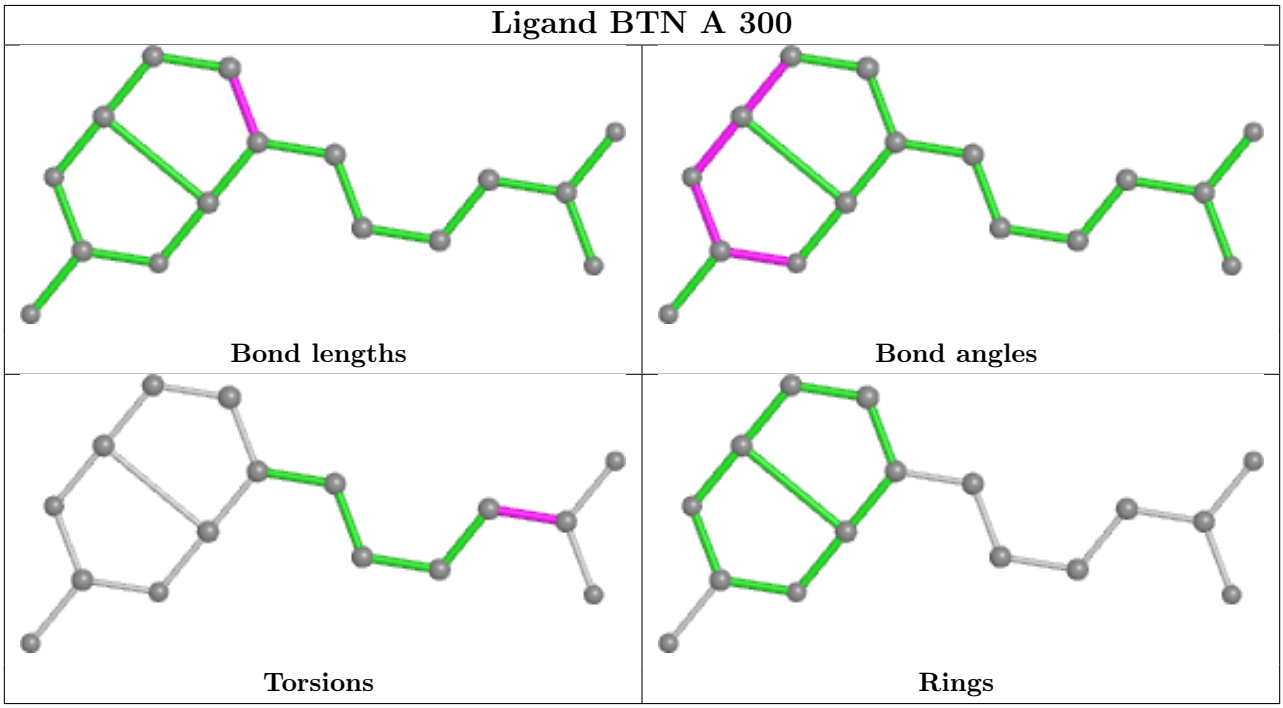
Mol	Chain	Res	Type	Atoms
2	J	300	BTN	C9-C10-C11-O12
2	A	300	BTN	C9-C10-C11-O11
2	D	300	BTN	C9-C10-C11-O11

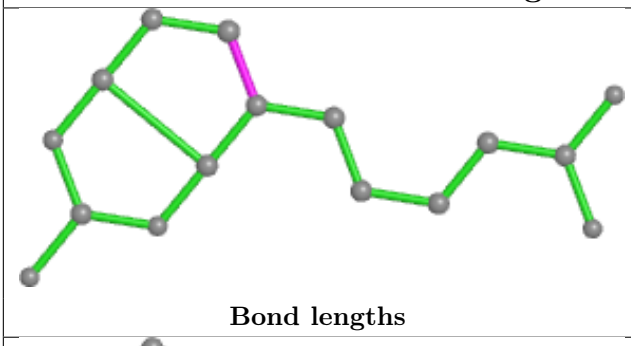
There are no ring outliers.

No monomer is involved in short contacts.

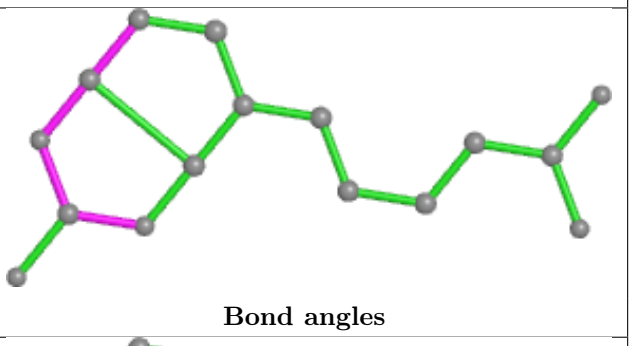
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



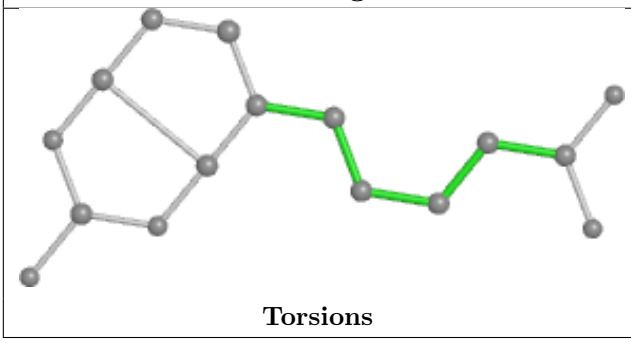
Ligand BTN L 300



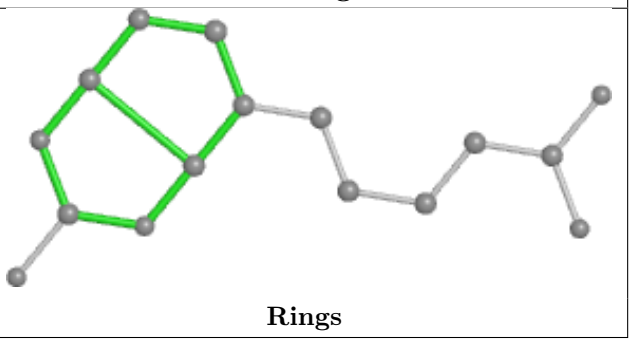
Bond lengths



Bond angles

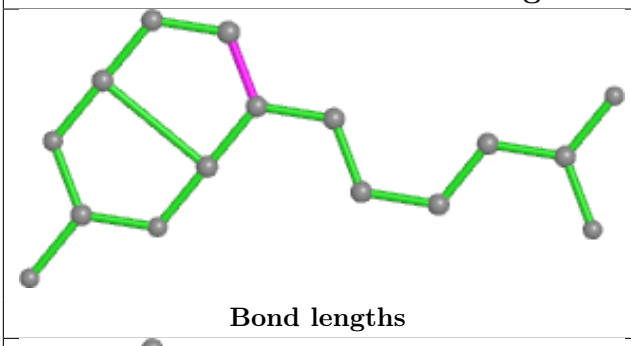


Torsions

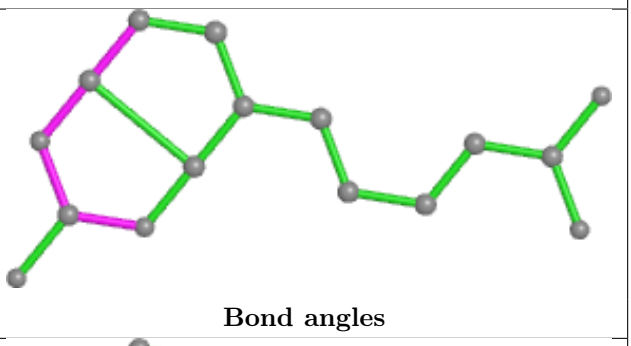


Rings

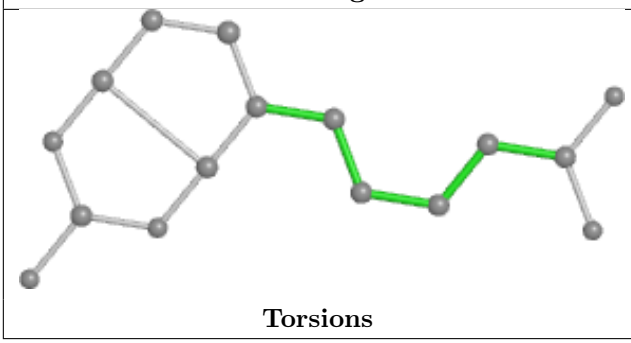
Ligand BTN E 401



Bond lengths



Bond angles



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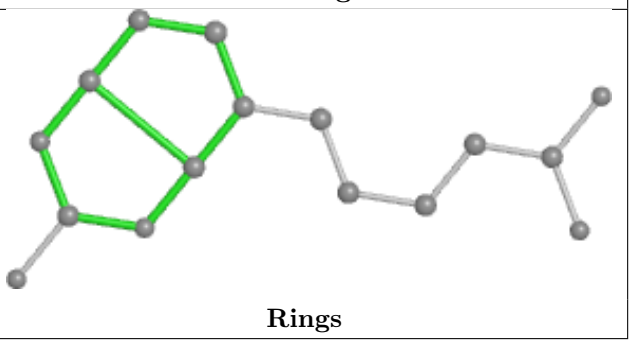
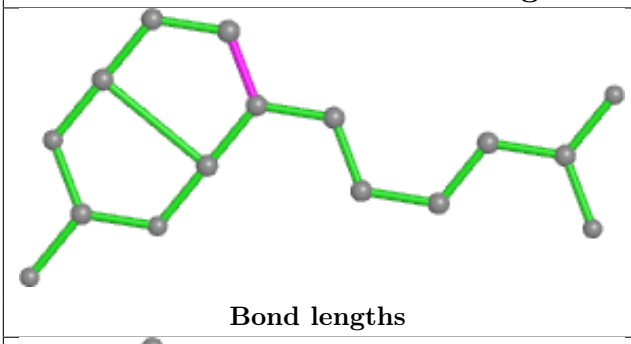
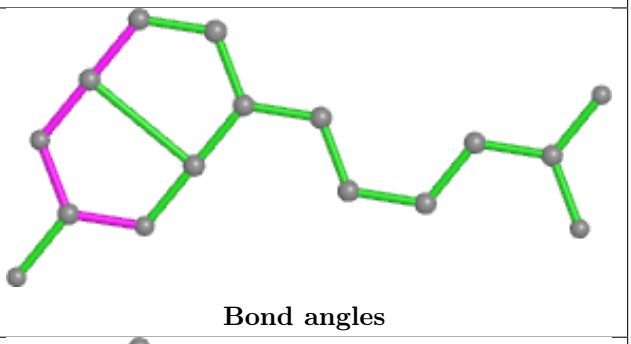


Rings

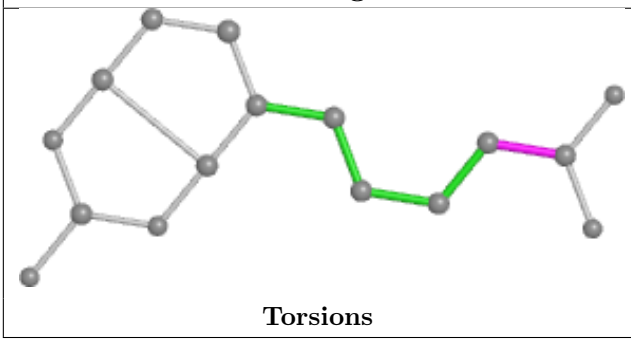
Ligand BTN G 401



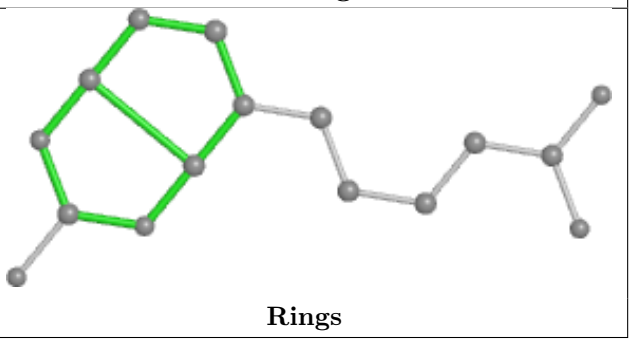
Bond lengths



Bond angles

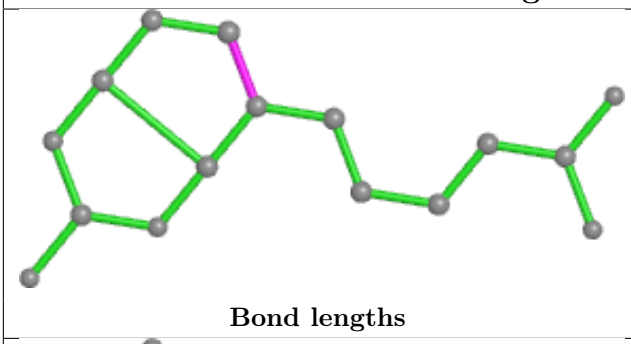


Torsions

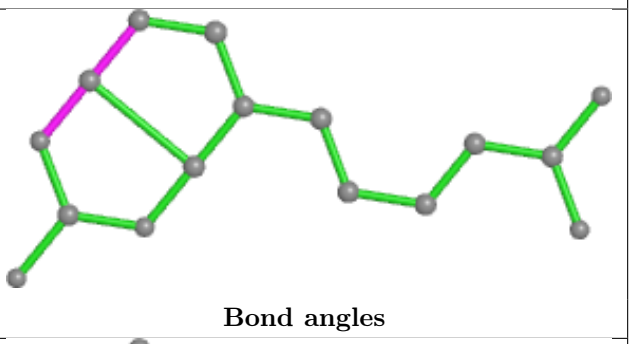


Rings

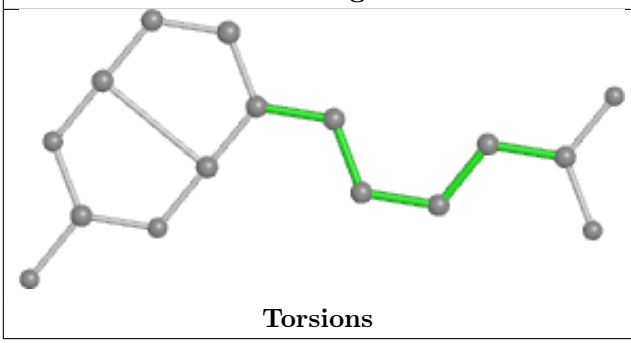
Ligand BTN C 300



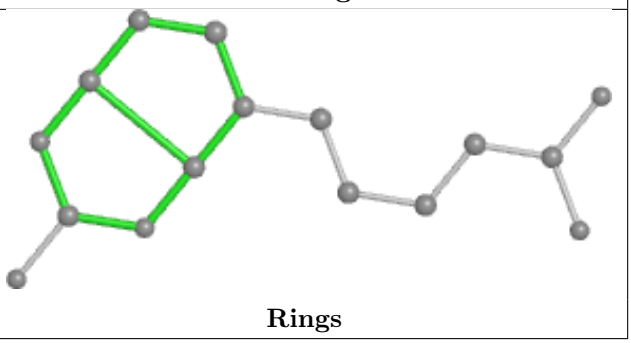
Bond lengths



Bond angles

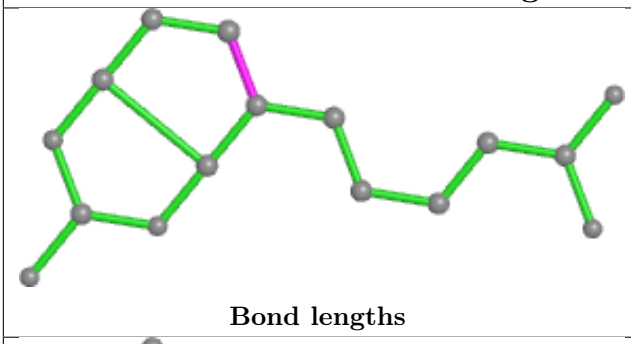


Torsions

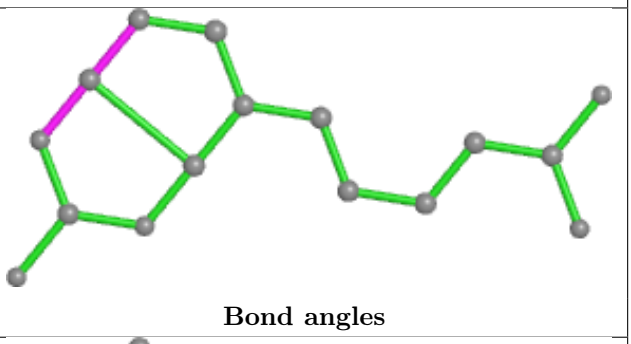


Rings

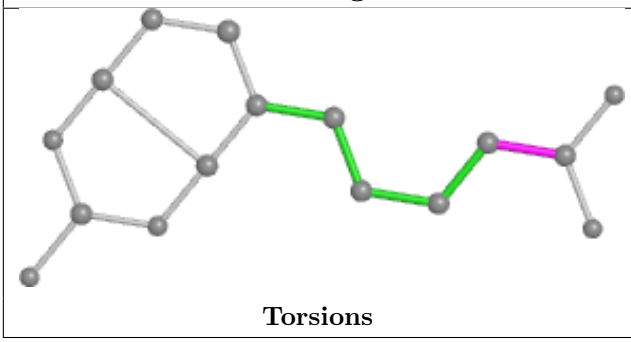
Ligand BTN D 300



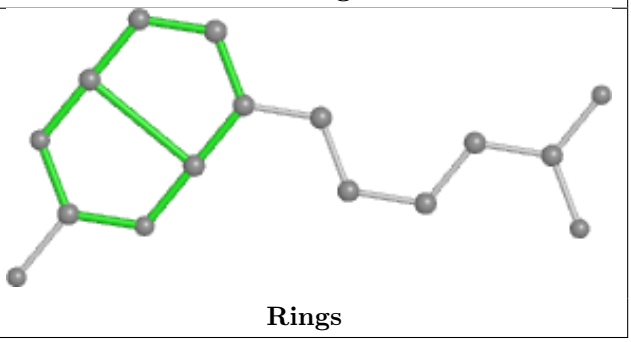
Bond lengths



Bond angles

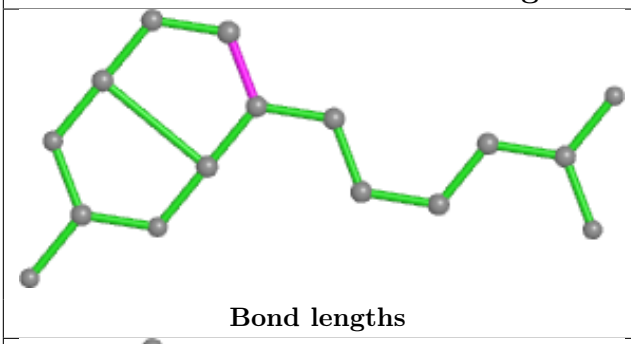


Torsions

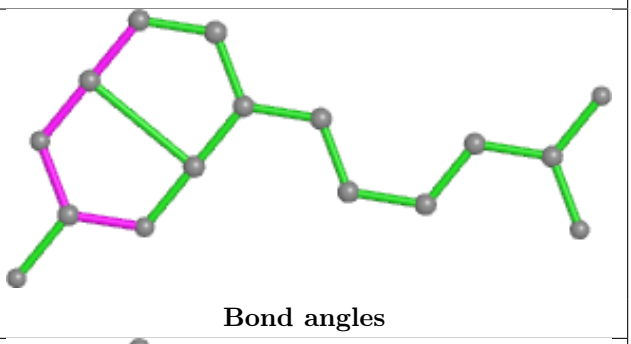


Rings

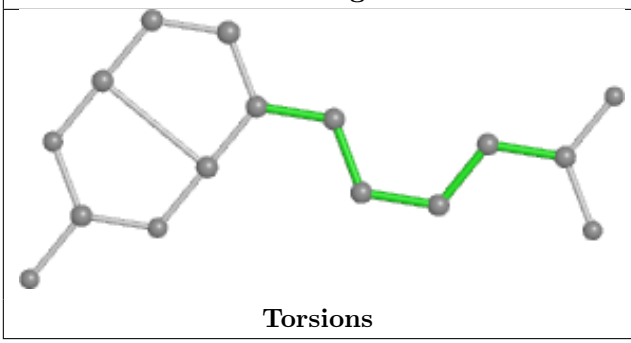
Ligand BTN H 300



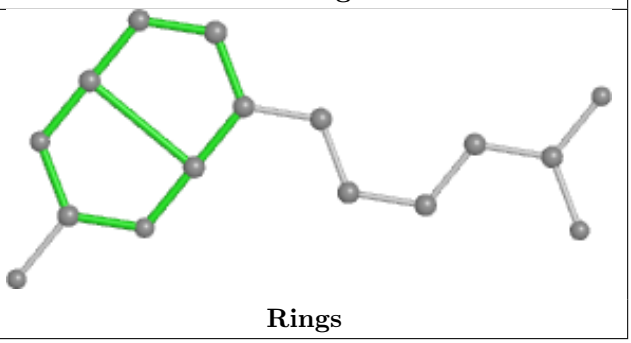
Bond lengths



Bond angles

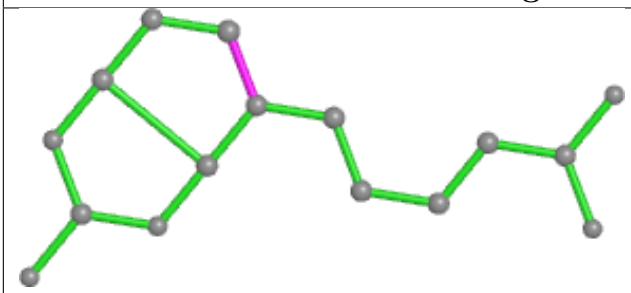


Torsions

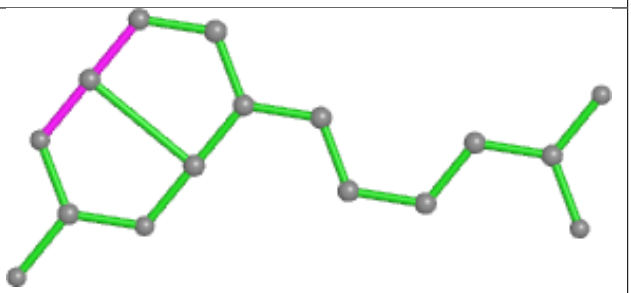


Rings

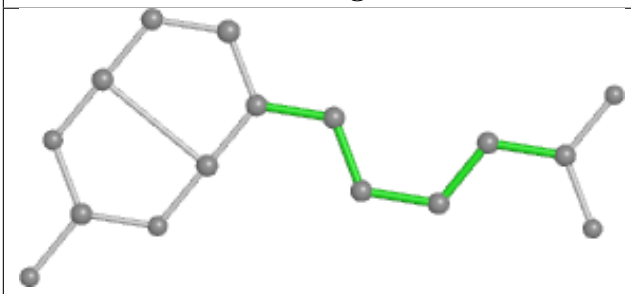
Ligand BTN B 300



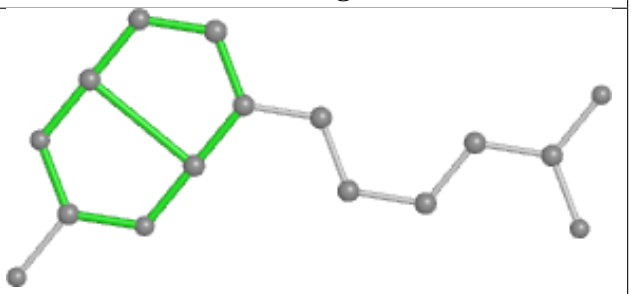
Bond lengths



Bond angles

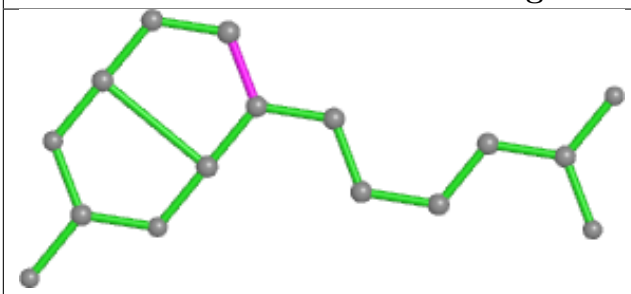


Torsions

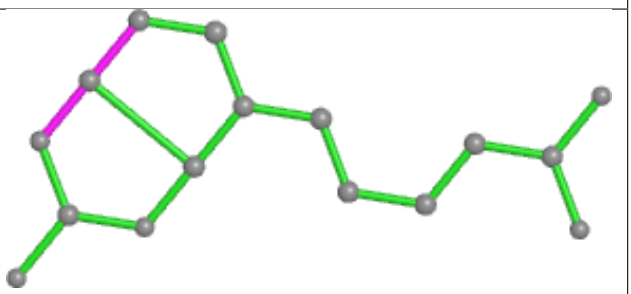


Rings

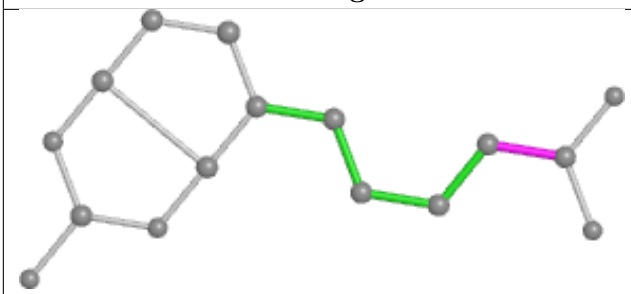
Ligand BTN J 300



Bond lengths



Bond angles



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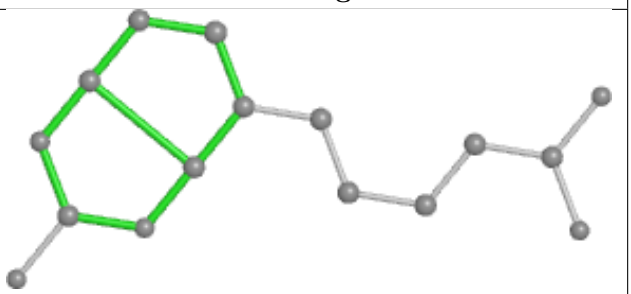
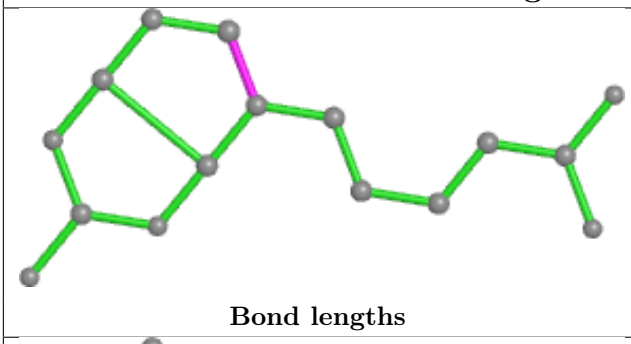
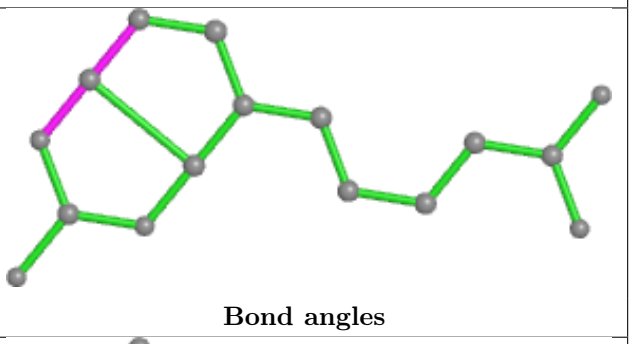


Rings

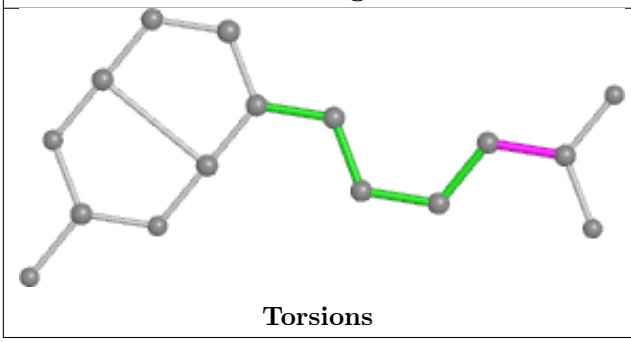
Ligand BTN F 300



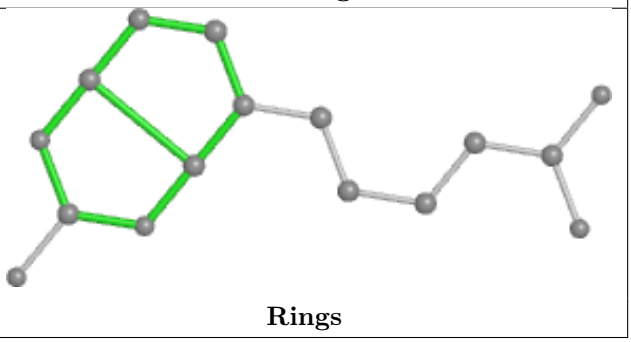
Bond lengths



Bond angles

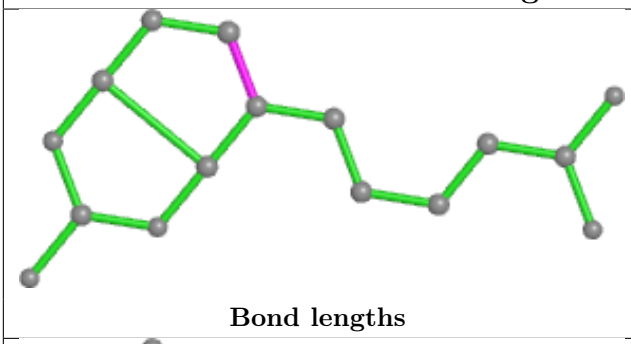


Torsions

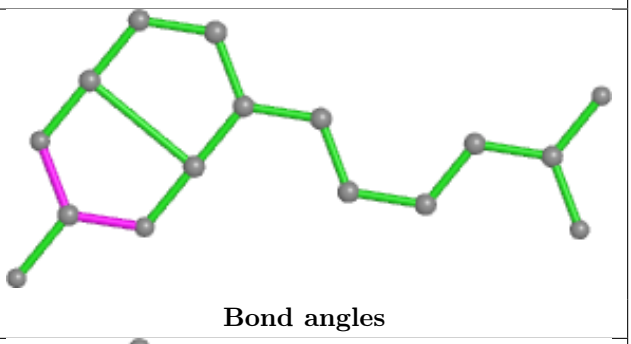


Rings

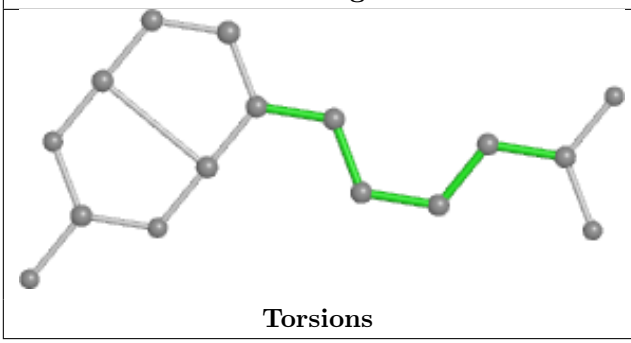
Ligand BTN K 401



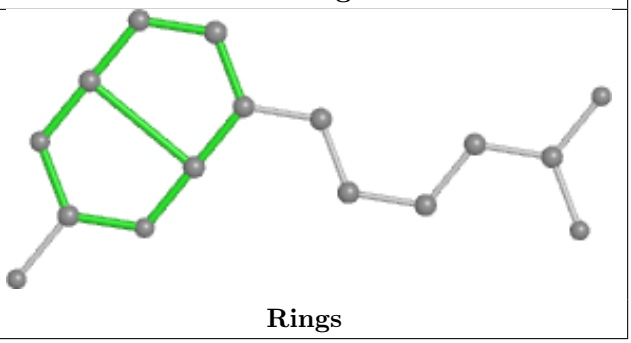
Bond lengths



Bond angles

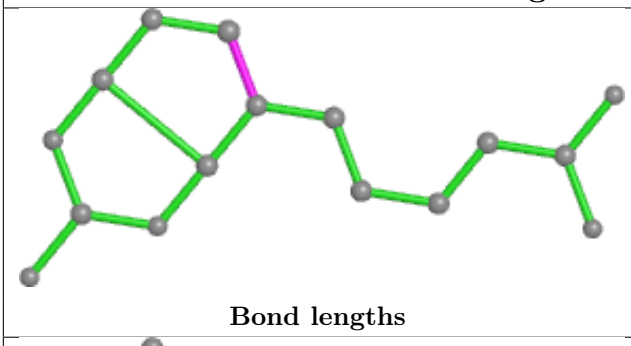


Torsions



Rings

Ligand BTN I 401



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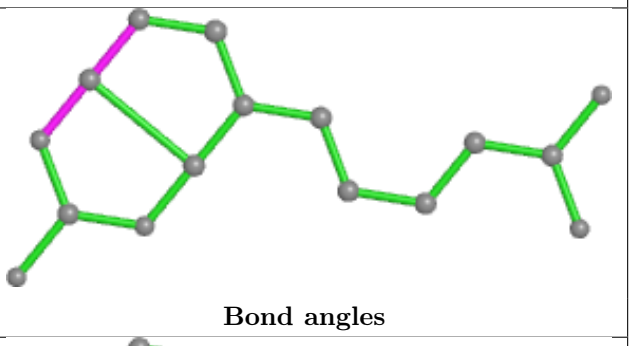
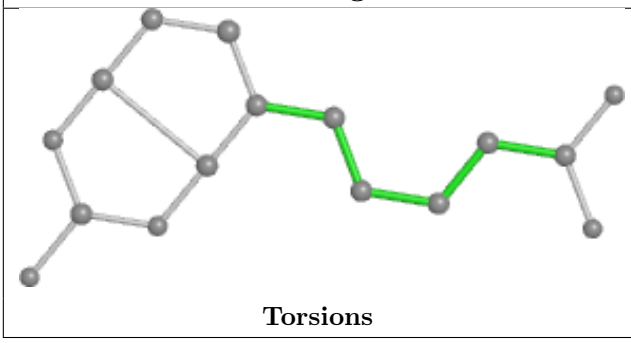
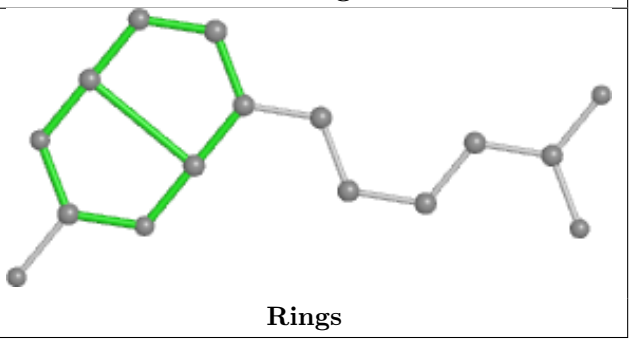


Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.