wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2024 – 10:24 AM EDT

PDB ID	:	3U8N
Title	:	Crystal structure of the acetylcholine binding protein (AChBP) from Lymnaea stagnalis in complex with NS3950 (1-(6-bromo-5-ethoxypyridin-3-yl)-1,4-diaz epane)
Authors	:	Rohde, L.A.H.; Ahring, P.K.; Jensen, M.L.; Nielsen, E.O.; Peters, D.; Helgstrand, C.; Krintel, C.; Harpsoe, K.; Gajhede, M.; Kastrup, J.S.; Balle, T.
Deposited on	:	2011-10-17
Resolution	:	2.35 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

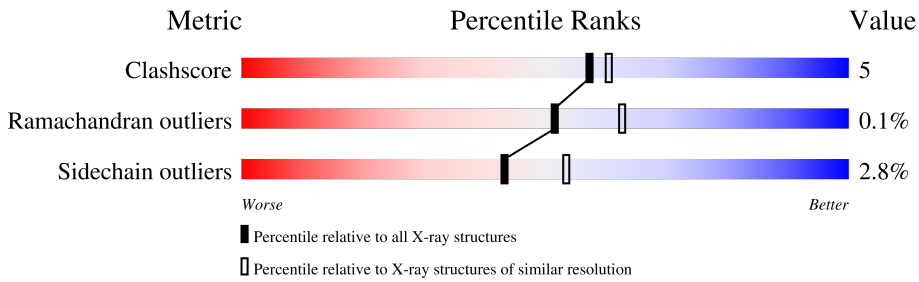
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	210	87% 10% •
1	B	210	83% 14% •
1	C	210	88% 9% •
1	D	210	85% 12% •
1	E	210	80% 15% • •
1	F	210	83% 13% • •
1	G	210	86% 9% • •
1	H	210	86% 9% • •

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Mol	Chain	Length	Quality of chain
1	I	210	85% 11% •
1	J	210	84% 11% • •
1	K	210	88% 9% •
1	L	210	83% 12% 5%
1	M	210	84% 12% •
1	N	210	84% 10% • 6%
1	O	210	85% 10% •
1	P	210	83% 14% •
1	Q	210	85% 12% •
1	R	210	83% 12% 5%
1	S	210	86% 10% •
1	T	210	84% 10% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34660 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	202	1616	1013	276	321	6	0	1	0
			Total	C	N	O	S			
1	B	203	1626	1018	278	323	7	0	2	0
			Total	C	N	O	S			
1	C	204	1635	1023	279	327	6	0	1	0
			Total	C	N	O	S			
1	D	205	1642	1027	280	328	7	0	2	0
			Total	C	N	O	S			
1	E	201	1625	1019	278	321	7	0	4	0
			Total	C	N	O	S			
1	F	204	1641	1027	284	324	6	0	2	0
			Total	C	N	O	S			
1	G	201	1609	1009	275	319	6	0	1	0
			Total	C	N	O	S			
1	H	201	1609	1009	275	319	6	0	1	0
			Total	C	N	O	S			
1	I	203	1637	1025	283	322	7	0	3	0
			Total	C	N	O	S			
1	J	201	1609	1009	275	319	6	0	1	0
			Total	C	N	O	S			
1	K	204	1633	1022	281	324	6	0	1	0
			Total	C	N	O	S			
1	L	200	1608	1009	274	318	7	0	2	0
			Total	C	N	O	S			
1	M	202	1628	1020	282	320	6	0	2	0
			Total	C	N	O	S			
1	N	198	1590	1000	272	311	7	0	2	0
			Total	C	N	O	S			
1	O	201	1609	1009	275	319	6	0	1	0
			Total	C	N	O	S			
1	P	203	1626	1018	280	322	6	0	1	0

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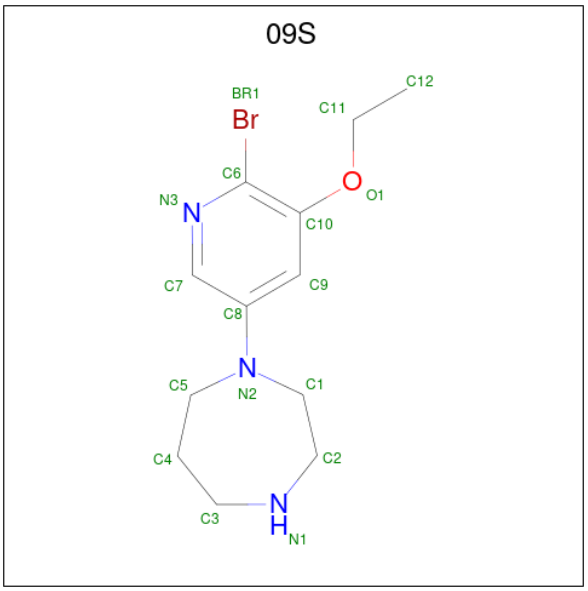
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	203	1626	1018	280	322	6	0	1	0
			Total	C	N	O	S			
1	R	200	1605	1007	274	318	6	0	1	0
			Total	C	N	O	S			
1	S	203	1629	1020	280	322	7	0	2	0
			Total	C	N	O	S			
1	T	201	1620	1016	278	319	7	0	3	0

- Molecule 2 is 1-(6-bromo-5-ethoxypyridin-3-yl)-1,4-diazepane (three-letter code: 09S) (formula: $C_{12}H_{18}BrN_3O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
2	A	1	17	1	12	3	1	0	0
			Total	Br	C	N	O		
2	B	1	17	1	12	3	1	0	0
			Total	Br	C	N	O		
2	C	1	17	1	12	3	1	0	0
			Total	Br	C	N	O		
2	D	1	17	1	12	3	1	0	0
			Total	Br	C	N	O		
2	E	1	17	1	12	3	1	0	0
			Total	Br	C	N	O		
2	F	1	17	1	12	3	1	0	0
			Total	Br	C	N	O		
2	G	1	17	1	12	3	1	0	0

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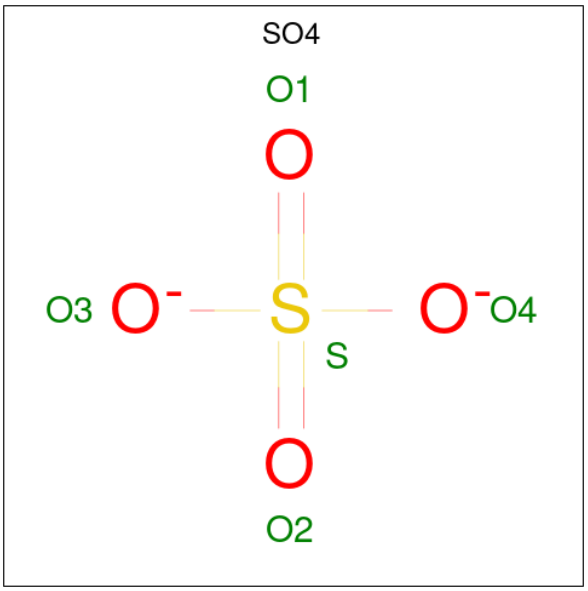
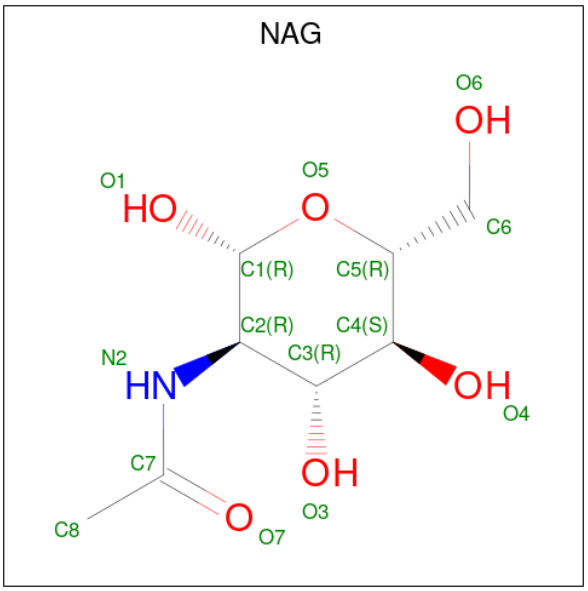
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
2	H	1	17	1	12	3	1	0	0
2	I	1	17	1	12	3	1	0	0
2	J	1	17	1	12	3	1	0	0
2	K	1	17	1	12	3	1	0	0
2	L	1	17	1	12	3	1	0	0
2	M	1	17	1	12	3	1	0	0
2	N	1	17	1	12	3	1	0	0
2	O	1	17	1	12	3	1	0	0
2	P	1	17	1	12	3	1	0	0
2	Q	1	17	1	12	3	1	0	0
2	R	1	17	1	12	3	1	0	0
2	S	1	17	1	12	3	1	0	0
2	T	1	17	1	12	3	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	H	1	5	4	1	0	0
3	N	1	5	4	1	0	0
3	P	1	5	4	1	0	0
3	P	1	5	4	1	0	0
3	S	1	5	4	1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	C	1	14	8	1	5	0	0
			Total	C	N	O		
4	G	1	14	8	1	5	0	0
			Total	C	N	O		
4	T	1	14	8	1	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	116	116	116	0	0
			Total	O		
5	B	130	130	130	0	0
			Total	O		
5	C	112	112	112	0	0
			Total	O		
5	D	118	118	118	0	0
			Total	O		
5	E	110	110	110	0	0
			Total	O		
5	F	79	79	79	0	0
			Total	O		
5	G	91	91	91	0	0
			Total	O		
5	H	77	77	77	0	0
			Total	O		
5	I	77	77	77	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	77	Total O 77 77	0	0
5	K	102	Total O 102 102	0	0
5	L	88	Total O 88 88	0	0
5	M	99	Total O 99 99	0	0
5	N	96	Total O 96 96	0	0
5	O	95	Total O 95 95	0	0
5	P	83	Total O 83 83	0	0
5	Q	69	Total O 69 69	0	0
5	R	80	Total O 80 80	0	0
5	S	68	Total O 68 68	0	0
5	T	58	Total O 58 58	0	0

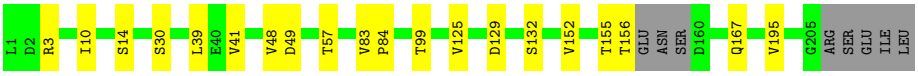
3 Residue-property plots (i)

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.

Note EDS failed to run properly.

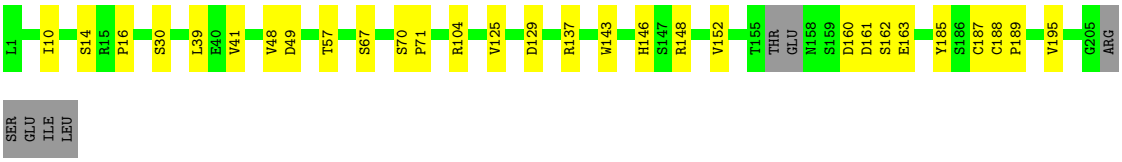
• Molecule 1: Acetylcholine-binding protein

Chain A:



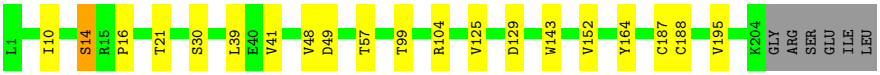
• Molecule 1: Acetylcholine-binding protein

Chain B:



• Molecule 1: Acetylcholine-binding protein

Chain C:

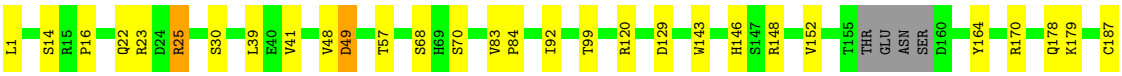


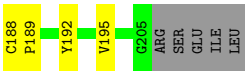
• Molecule 1: Acetylcholine-binding protein

Chain D:

• Molecule 1: Acetylcholine-binding protein

Chain E:





• Molecule 1: Acetylcholine-binding protein

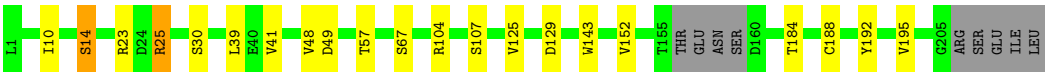
Chain F:

• Molecule 1: Acetylcholine-binding protein

Chain G:

• Molecule 1: Acetylcholine-binding protein

Chain H:



• Molecule 1: Acetylcholine-binding protein

Chain I:

• Molecule 1: Acetylcholine-binding protein

Chain J:

• Molecule 1: Acetylcholine-binding protein

Chain K:

• Molecule 1: Acetylcholine-binding protein

Chain L: 83% 12% 5%

L1 D2 R3 Q22 R25 P26 S30 L39 E40 V41 V48 D49 T57 V83 P84 V125 D129 W143 V152 T155 THR GLU ASN SER D160 Y168 S169 Q178 K179 Y185 S186 C187 C188 P189 V195 K204 GLY ARG SER GLU ILE LEU

• Molecule 1: Acetylcholine-binding protein

Chain M: 84% 12% •

L1 D2 R3 I10 S14 P20 D24 L39 E40 V41 V48 D49 S70 S80 L81 W82 V83 P84 K94 T99 R120 V125 D129 W143 V152 T155 THR GLU ASN SER D160 Y164 C188 V195 R206 SER GLU ILE LEU

• Molecule 1: Acetylcholine-binding protein

Chain N: 84% 10% • 6%

L1 I10 S14 R15 P16 S30 L39 E40 V41 V48 D49 T57 R61 S80 V125 D129 W143 H146 S147 R148 V152 T155 THR GLU ASN SER ASP ASP SER E163 C187 C188 P189 V195 G205 ARG SER GLU ILE LEU

• Molecule 1: Acetylcholine-binding protein

Chain O: 85% 10% •

L1 I10 R11 S14 R15 P16 Q22 S30 L39 E40 V41 V48 D49 T57 T99 V125 D129 W143 H146 S147 R148 V152 T155 THR GLU ASN SER D160 C187 C188 V195 G205 ARG SER GLU ILE LEU

• Molecule 1: Acetylcholine-binding protein

Chain P: 83% 14% •

L1 D2 R3 I10 S14 R15 P16 R23 D24 R25 P26 S30 L39 E40 V41 V48 D49 T57 S70 V74 T99 L112 V125 D129 W143 H146 S147 R148 V152 T155 THR GLU ASN SER D160 Y164 S182 V183 T184 C188

V195 S207 GLU ILE LEU

• Molecule 1: Acetylcholine-binding protein

Chain Q: 85% 12% •

L1 I10 S14 R15 P16 R23 D24 R25 L39 E40 V41 V48 D49 S67 S70 R104 S107 C123 D124 V125 D129 W143 V152 T155 THR GLU ASN S159 D160 E163 C187 C188 V195 R206 SER GLU ILE LEU

• Molecule 1: Acetylcholine-binding protein

Chain R: 83% 12% 5%

• Molecule 1: Acetylcholine-binding protein

Chain S:

• Molecule 1: Acetylcholine-binding protein

Chain T:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	239.12Å 73.11Å 271.84Å 90.00° 97.45° 90.00°	Depositor
Resolution (Å)	33.05 – 2.35	Depositor
% Data completeness (in resolution range)	95.3 (33.05-2.35)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.72 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.197 , 0.230	Depositor
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.539	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	34660	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 09S, 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	0/1654	0.53	0/2256
1	B	0.40	0/1667	0.54	0/2274
1	C	0.40	0/1674	0.54	0/2285
1	D	0.40	0/1684	0.53	0/2299
1	E	0.39	0/1672	0.52	0/2280
1	F	0.39	0/1682	0.54	0/2292
1	G	0.39	0/1647	0.53	0/2246
1	H	0.37	0/1647	0.53	0/2246
1	I	0.38	0/1681	0.52	0/2291
1	J	0.38	0/1647	0.52	0/2246
1	K	0.39	0/1671	0.52	0/2278
1	L	0.39	0/1649	0.51	0/2250
1	M	0.41	0/1669	0.54	0/2274
1	N	0.39	0/1631	0.51	0/2225
1	O	0.38	0/1647	0.52	0/2246
1	P	0.39	0/1664	0.53	0/2268
1	Q	0.38	0/1664	0.52	0/2268
1	R	0.37	0/1643	0.52	0/2241
1	S	0.37	0/1670	0.53	0/2277
1	T	0.38	0/1664	0.53	0/2269
All	All	0.39	0/33227	0.53	0/45311

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	155	THR	Peptide

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	1616	0	1568	14	0
1	B	1626	0	1577	18	0
1	C	1635	0	1582	13	0
1	D	1642	0	1591	18	0
1	E	1625	0	1583	28	0
1	F	1641	0	1599	24	1
1	G	1609	0	1560	15	0
1	H	1609	0	1561	14	1
1	I	1637	0	1597	13	0
1	J	1609	0	1561	16	0
1	K	1633	0	1586	15	0
1	L	1608	0	1563	20	0
1	M	1628	0	1587	18	0
1	N	1590	0	1553	16	0
1	O	1609	0	1561	16	0
1	P	1626	0	1579	26	0
1	Q	1626	0	1579	15	0
1	R	1605	0	1558	15	0
1	S	1629	0	1584	14	0
1	T	1620	0	1577	21	0
2	A	17	0	18	1	0
2	B	17	0	18	2	0
2	C	17	0	18	2	0
2	D	17	0	18	4	0
2	E	17	0	18	2	0
2	F	17	0	18	5	0
2	G	17	0	18	1	0
2	H	17	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	17	0	18	0	0
2	J	17	0	18	0	0
2	K	17	0	18	3	0
2	L	17	0	18	1	0
2	M	17	0	18	2	0
2	N	17	0	18	1	0
2	O	17	0	18	0	0
2	P	17	0	18	4	0
2	Q	17	0	18	1	0
2	R	17	0	18	3	0
2	S	17	0	18	0	0
2	T	17	0	18	5	0
3	A	5	0	0	1	0
3	H	5	0	0	0	0
3	N	5	0	0	0	0
3	P	10	0	0	0	0
3	S	5	0	0	0	0
4	C	14	0	13	0	0
4	G	14	0	13	0	0
4	T	14	0	13	2	0
5	A	116	0	0	3	0
5	B	130	0	0	2	0
5	C	112	0	0	0	0
5	D	118	0	0	2	0
5	E	110	0	0	2	0
5	F	79	0	0	3	0
5	G	91	0	0	3	0
5	H	77	0	0	2	0
5	I	77	0	0	0	0
5	J	77	0	0	2	0
5	K	102	0	0	3	0
5	L	88	0	0	1	0
5	M	99	0	0	2	0
5	N	96	0	0	0	0
5	O	95	0	0	3	0
5	P	83	0	0	3	0
5	Q	69	0	0	2	0
5	R	80	0	0	1	0
5	S	68	0	0	0	0
5	T	58	0	0	0	0
All	All	34660	0	31905	318	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 318 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:49:ASP:OD1	1:E:120[B]:ARG:HG2	1.52	1.07
1:T:49:ASP:OD1	1:T:120[B]:ARG:HG3	1.53	1.06
1:M:49:ASP:OD1	1:M:120[B]:ARG:HG2	1.58	1.04
1:I:49:ASP:OD1	1:I:120[B]:ARG:HG2	1.59	1.02
1:F:152:VAL:HG12	1:F:195:VAL:HG23	1.46	0.98

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:THR:OG1	1:H:184:THR:OG1[1_565]	2.05	0.15

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/210 (95%)	198 (100%)	1 (0%)	0	100	100
1	B	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	15	15
1	C	203/210 (97%)	202 (100%)	1 (0%)	0	100	100
1	D	205/210 (98%)	205 (100%)	0	0	100	100
1	E	201/210 (96%)	201 (100%)	0	0	100	100
1	F	202/210 (96%)	200 (99%)	2 (1%)	0	100	100
1	G	198/210 (94%)	198 (100%)	0	0	100	100
1	H	198/210 (94%)	198 (100%)	0	0	100	100
1	I	202/210 (96%)	201 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	198/210 (94%)	194 (98%)	4 (2%)	0	100	100
1	K	201/210 (96%)	200 (100%)	1 (0%)	0	100	100
1	L	198/210 (94%)	197 (100%)	1 (0%)	0	100	100
1	M	200/210 (95%)	199 (100%)	1 (0%)	0	100	100
1	N	196/210 (93%)	195 (100%)	1 (0%)	0	100	100
1	O	198/210 (94%)	197 (100%)	1 (0%)	0	100	100
1	P	200/210 (95%)	199 (100%)	1 (0%)	0	100	100
1	Q	200/210 (95%)	197 (98%)	3 (2%)	0	100	100
1	R	197/210 (94%)	196 (100%)	1 (0%)	0	100	100
1	S	201/210 (96%)	200 (100%)	1 (0%)	0	100	100
1	T	200/210 (95%)	200 (100%)	0	0	100	100
All	All	3998/4200 (95%)	3974 (99%)	22 (1%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	GLU
1	B	161	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/196 (96%)	185 (98%)	4 (2%)	53	65
1	B	191/196 (97%)	186 (97%)	5 (3%)	46	56
1	C	192/196 (98%)	184 (96%)	8 (4%)	30	36
1	D	193/196 (98%)	186 (96%)	7 (4%)	35	43
1	E	191/196 (97%)	184 (96%)	7 (4%)	34	42
1	F	192/196 (98%)	186 (97%)	6 (3%)	40	48
1	G	188/196 (96%)	182 (97%)	6 (3%)	39	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	188/196 (96%)	182 (97%)	6 (3%)	39	47
1	I	192/196 (98%)	187 (97%)	5 (3%)	46	56
1	J	188/196 (96%)	180 (96%)	8 (4%)	29	35
1	K	191/196 (97%)	184 (96%)	7 (4%)	34	42
1	L	189/196 (96%)	184 (97%)	5 (3%)	46	56
1	M	190/196 (97%)	186 (98%)	4 (2%)	53	65
1	N	186/196 (95%)	179 (96%)	7 (4%)	33	41
1	O	188/196 (96%)	183 (97%)	5 (3%)	44	55
1	P	190/196 (97%)	185 (97%)	5 (3%)	46	56
1	Q	190/196 (97%)	183 (96%)	7 (4%)	34	42
1	R	188/196 (96%)	181 (96%)	7 (4%)	34	42
1	S	191/196 (97%)	186 (97%)	5 (3%)	46	56
1	T	190/196 (97%)	183 (96%)	7 (4%)	34	42
All	All	3797/3920 (97%)	3676 (97%)	121 (3%)	43	47

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	39	LEU
1	S	49	ASP
1	L	129	ASP
1	S	39	LEU
1	T	129	ASP

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

Mol	Chain	Res	Type
1	A	200	ASN
1	G	200	ASN
1	S	69	HIS

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

29 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	09S	S	211	-	16,18,18	3.17	5 (31%)	16,23,23	1.47	3 (18%)
2	09S	O	211	-	16,18,18	3.22	2 (12%)	16,23,23	1.58	3 (18%)
2	09S	L	211	-	16,18,18	3.01	3 (18%)	16,23,23	1.37	3 (18%)
3	SO4	H	212	-	4,4,4	0.15	0	6,6,6	0.11	0
2	09S	A	211	-	16,18,18	3.26	3 (18%)	16,23,23	1.37	2 (12%)
2	09S	G	211	-	16,18,18	3.14	4 (25%)	16,23,23	1.67	3 (18%)
4	NAG	C	300	1	14,14,15	0.49	0	17,19,21	1.91	6 (35%)
3	SO4	S	212	-	4,4,4	0.11	0	6,6,6	0.14	0
2	09S	N	211	-	16,18,18	2.99	3 (18%)	16,23,23	1.47	2 (12%)
2	09S	E	211	-	16,18,18	3.02	4 (25%)	16,23,23	1.65	3 (18%)
4	NAG	G	301	1	14,14,15	0.59	0	17,19,21	1.30	2 (11%)
2	09S	F	211	-	16,18,18	3.39	4 (25%)	16,23,23	1.36	2 (12%)
2	09S	K	211	-	16,18,18	3.09	3 (18%)	16,23,23	1.47	2 (12%)
3	SO4	N	212	-	4,4,4	0.13	0	6,6,6	0.33	0
2	09S	Q	211	-	16,18,18	2.81	3 (18%)	16,23,23	1.73	3 (18%)
2	09S	D	211	-	16,18,18	3.05	4 (25%)	16,23,23	1.76	4 (25%)
2	09S	R	211	-	16,18,18	3.01	4 (25%)	16,23,23	1.55	3 (18%)
2	09S	T	211	-	16,18,18	3.04	3 (18%)	16,23,23	2.12	3 (18%)
2	09S	M	211	-	16,18,18	3.04	3 (18%)	16,23,23	1.56	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	212	-	4,4,4	0.12	0	6,6,6	0.22	0
2	09S	P	211	-	16,18,18	3.14	3 (18%)	16,23,23	1.59	2 (12%)
2	09S	H	211	-	16,18,18	3.01	3 (18%)	16,23,23	1.73	2 (12%)
3	SO4	P	213	-	4,4,4	0.16	0	6,6,6	0.09	0
2	09S	B	211	-	16,18,18	3.10	3 (18%)	16,23,23	1.32	2 (12%)
2	09S	J	211	-	16,18,18	3.21	4 (25%)	16,23,23	1.32	3 (18%)
2	09S	C	211	-	16,18,18	3.16	3 (18%)	16,23,23	1.37	2 (12%)
2	09S	I	211	-	16,18,18	3.08	3 (18%)	16,23,23	1.52	3 (18%)
4	NAG	T	212	1	14,14,15	0.44	0	17,19,21	1.49	5 (29%)
3	SO4	P	212	-	4,4,4	0.16	0	6,6,6	0.07	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
2	09S	S	211	-	-	0/7/16/16	0/2/2/2
2	09S	O	211	-	-	0/7/16/16	0/2/2/2
2	09S	L	211	-	-	1/7/16/16	0/2/2/2
2	09S	A	211	-	-	0/7/16/16	0/2/2/2
2	09S	G	211	-	-	0/7/16/16	0/2/2/2
4	NAG	C	300	1	-	2/6/23/26	0/1/1/1
2	09S	N	211	-	-	0/7/16/16	0/2/2/2
2	09S	E	211	-	-	0/7/16/16	0/2/2/2
4	NAG	G	301	1	-	0/6/23/26	0/1/1/1
2	09S	F	211	-	-	1/7/16/16	0/2/2/2
2	09S	K	211	-	-	1/7/16/16	0/2/2/2
2	09S	Q	211	-	-	0/7/16/16	0/2/2/2
2	09S	D	211	-	-	1/7/16/16	0/2/2/2
2	09S	R	211	-	-	0/7/16/16	0/2/2/2
2	09S	T	211	-	-	1/7/16/16	0/2/2/2
2	09S	M	211	-	-	0/7/16/16	0/2/2/2
2	09S	P	211	-	-	0/7/16/16	0/2/2/2
2	09S	H	211	-	-	1/7/16/16	0/2/2/2
2	09S	B	211	-	-	1/7/16/16	0/2/2/2
2	09S	J	211	-	-	2/7/16/16	0/2/2/2
2	09S	C	211	-	-	0/7/16/16	0/2/2/2
2	09S	I	211	-	-	0/7/16/16	0/2/2/2
4	NAG	T	212	1	-	0/6/23/26	0/1/1/1

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	211	09S	BR1-C6	-11.12	1.73	1.90
2	B	211	09S	BR1-C6	-11.07	1.73	1.90
2	F	211	09S	BR1-C6	-11.01	1.73	1.90
2	A	211	09S	BR1-C6	-10.97	1.73	1.90
2	O	211	09S	BR1-C6	-10.91	1.73	1.90

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	211	09S	C9-C8-C7	-5.11	115.43	119.48
2	T	211	09S	C9-C8-C7	-5.11	115.43	119.48
2	T	211	09S	O1-C10-C6	4.96	122.92	116.58
2	Q	211	09S	C9-C8-C7	-4.94	115.57	119.48
2	D	211	09S	C9-C8-C7	-4.51	115.91	119.48

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	300	NAG	C4-C5-C6-O6
2	K	211	09S	C12-C11-O1-C10
4	C	300	NAG	O5-C5-C6-O6
2	L	211	09S	C12-C11-O1-C10
2	F	211	09S	C12-C11-O1-C10

There are no ring outliers.

18 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	211	09S	1	0
2	A	211	09S	1	0
2	G	211	09S	1	0
2	N	211	09S	1	0
2	E	211	09S	2	0
2	F	211	09S	5	0
2	K	211	09S	3	0
2	Q	211	09S	1	0
2	D	211	09S	4	0
2	R	211	09S	3	0
2	T	211	09S	5	0

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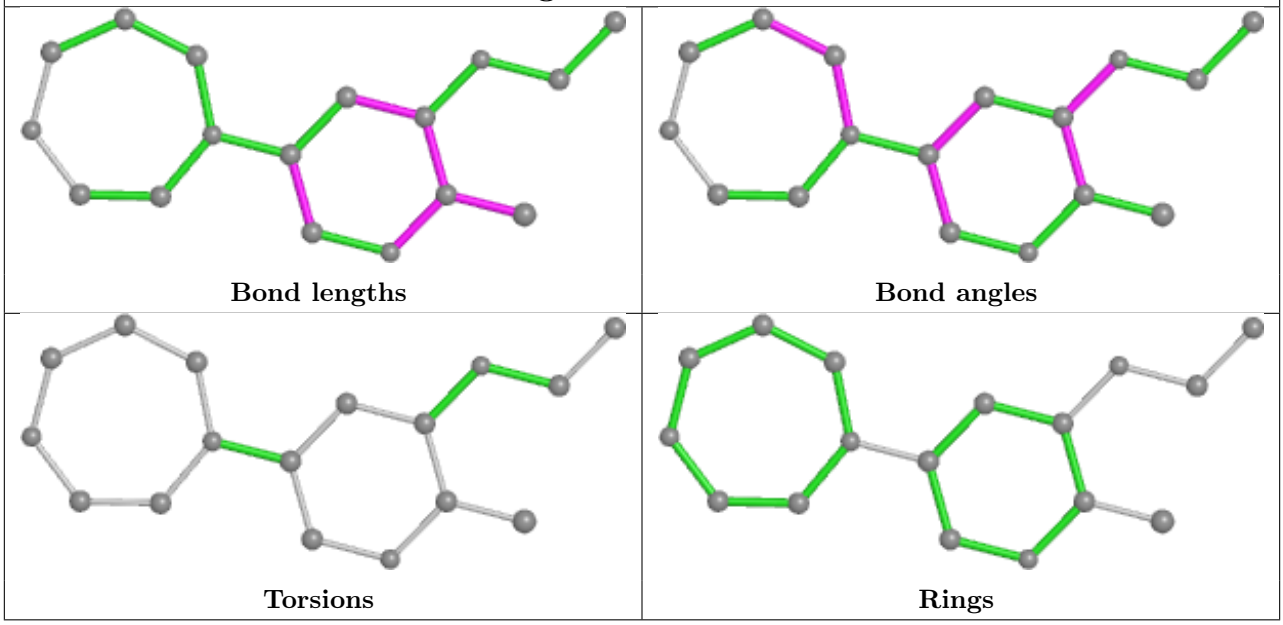
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	211	09S	2	0
3	A	212	SO4	1	0
2	P	211	09S	4	0
2	H	211	09S	2	0
2	B	211	09S	2	0
2	C	211	09S	2	0
4	T	212	NAG	2	0

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 09S S 211



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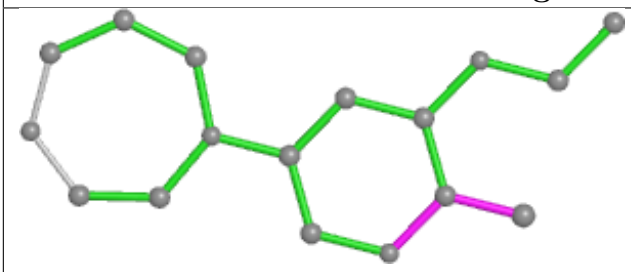
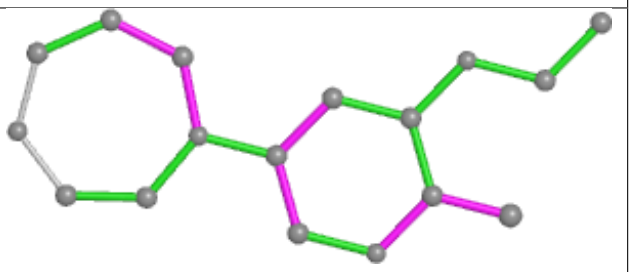
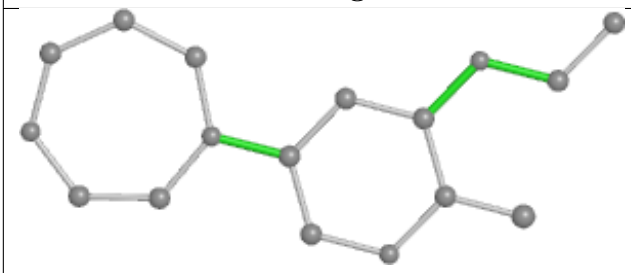


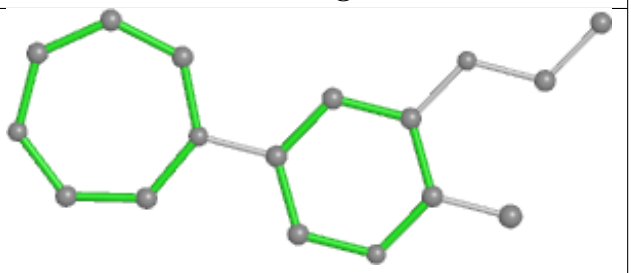
Bond lengths



Bond angles

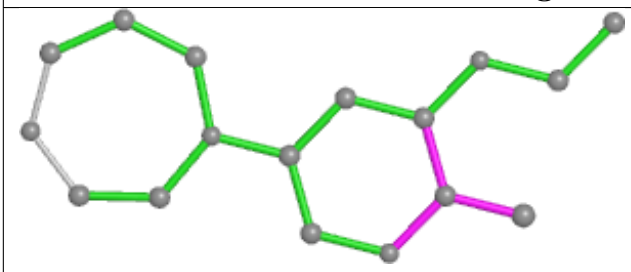


Torsions



Rings

Ligand 09S L 211



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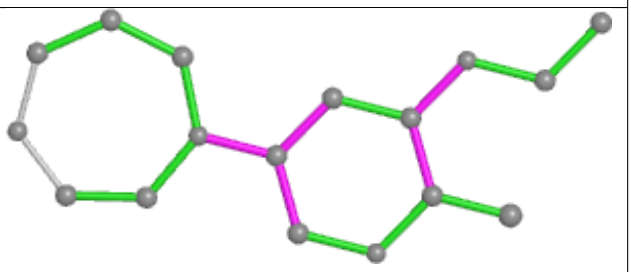

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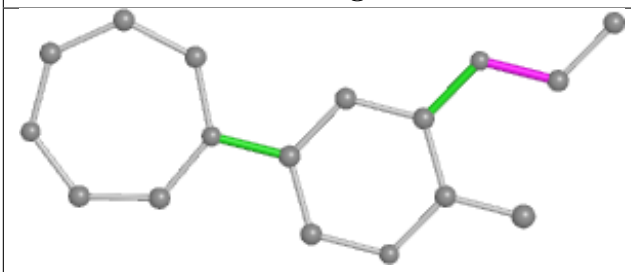

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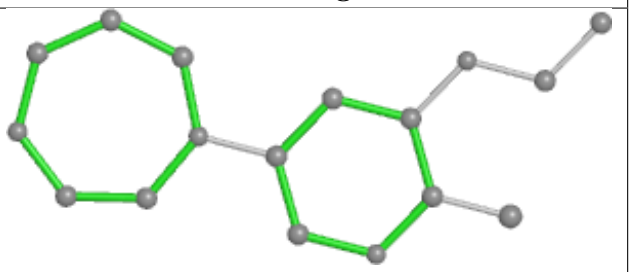
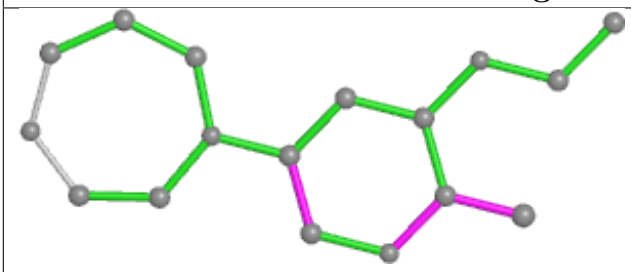


Rings

Ligand 09S A 211



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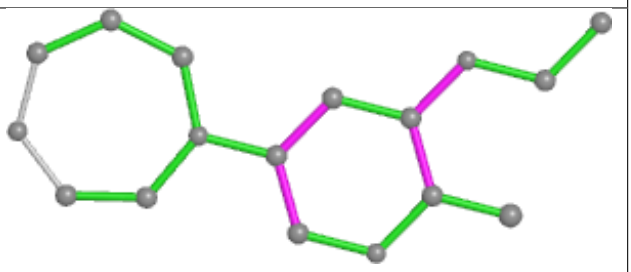
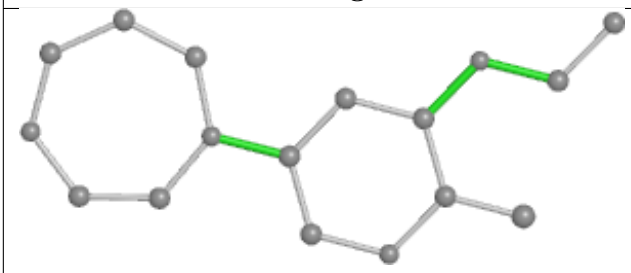


Bond angles



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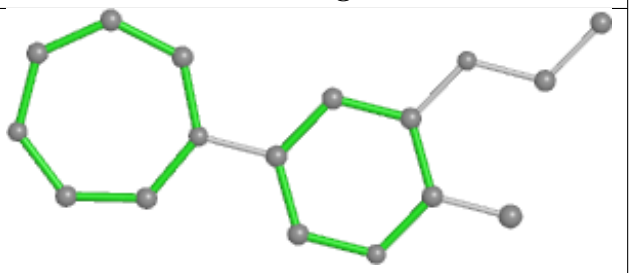
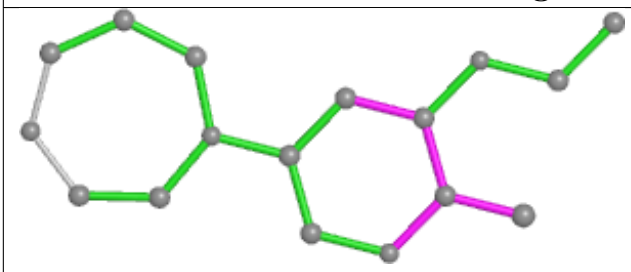


Rings

Ligand 09S G 211



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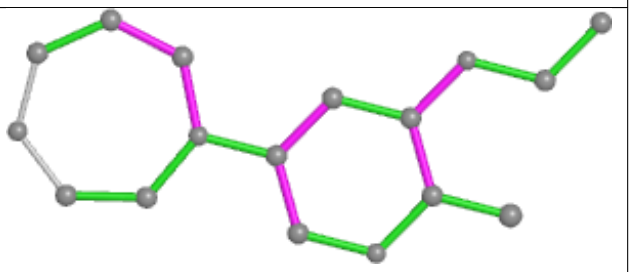
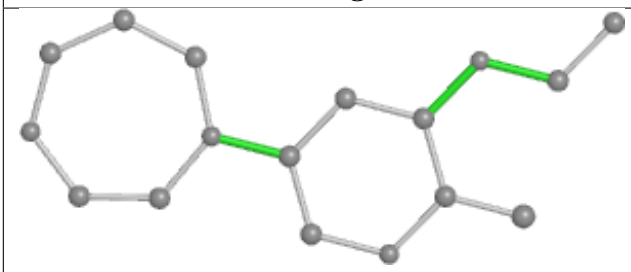
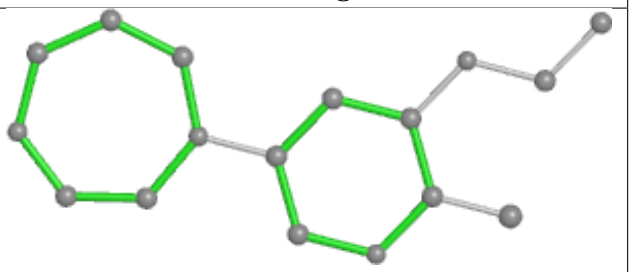


Bond angles

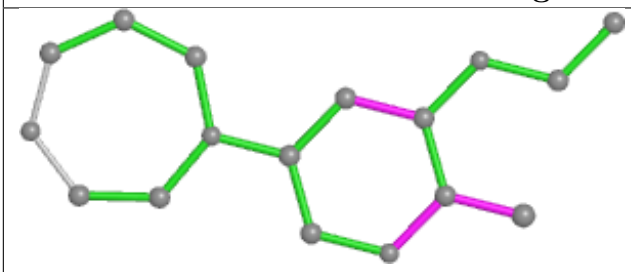


Torsions



Rings

Ligand 09S N 211



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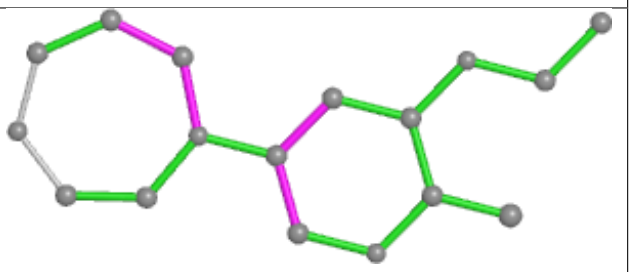

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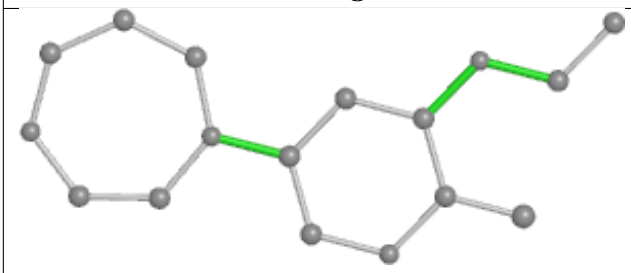

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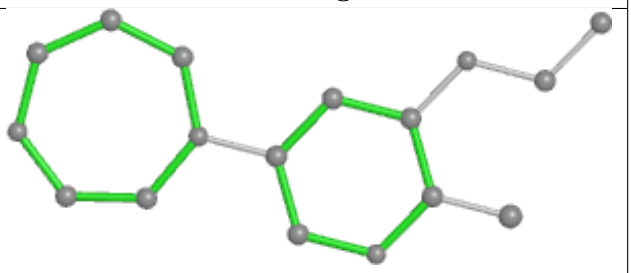
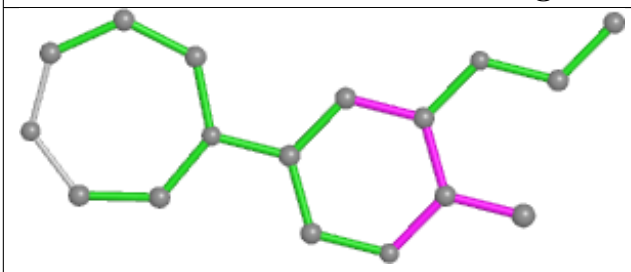


Rings

Ligand 09S E 211



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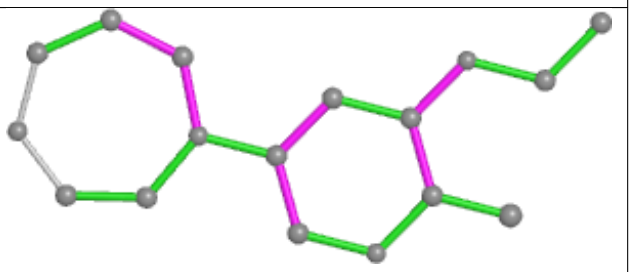

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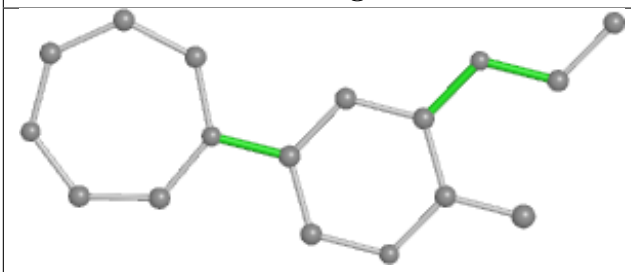

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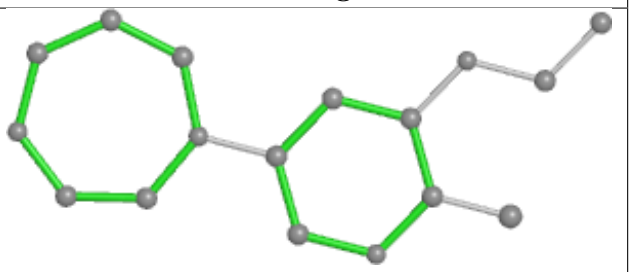

Rings

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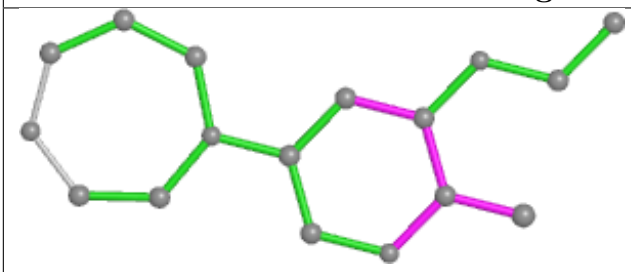

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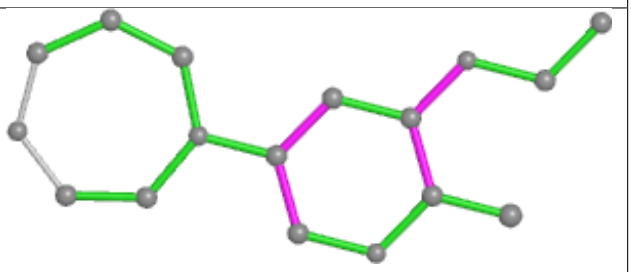

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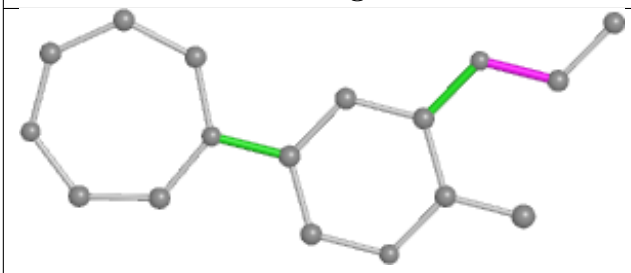

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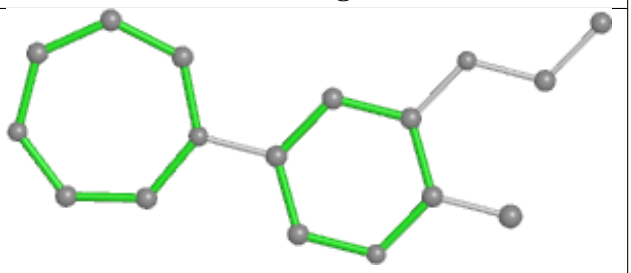

Rings

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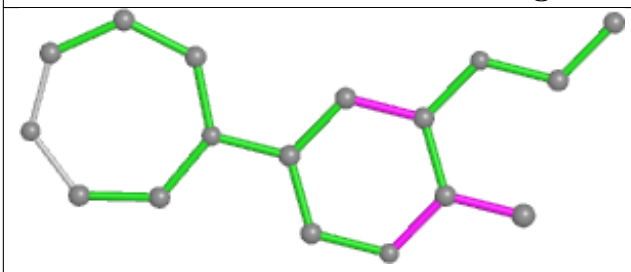

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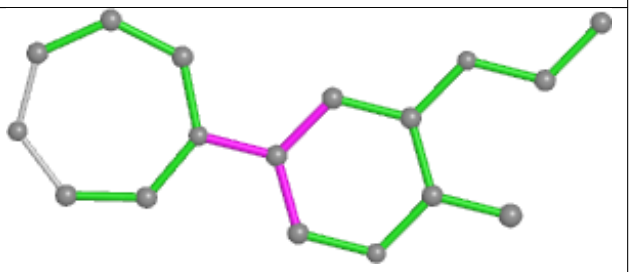

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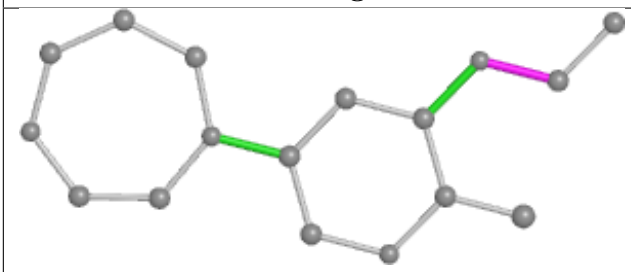

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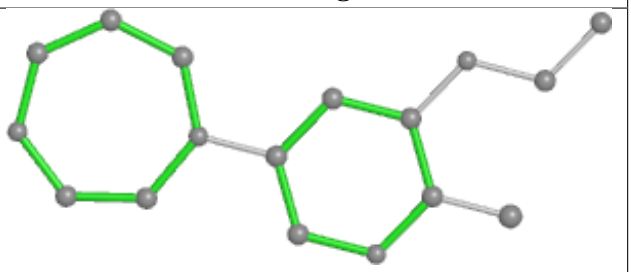

Rings

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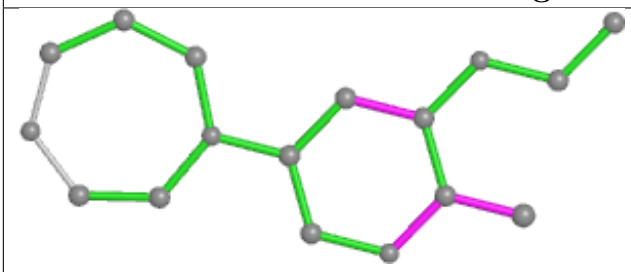

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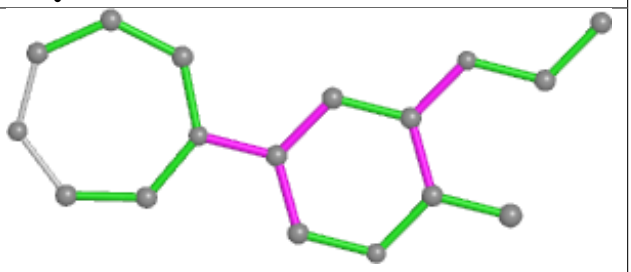

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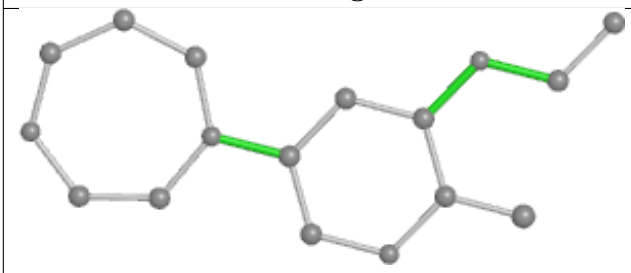

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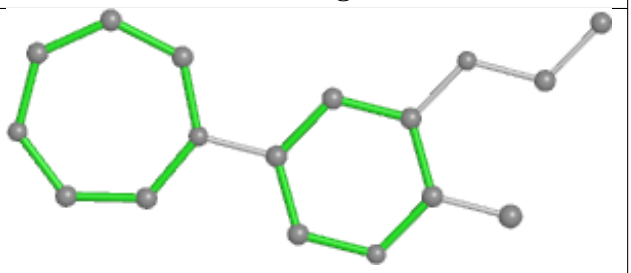

Rings

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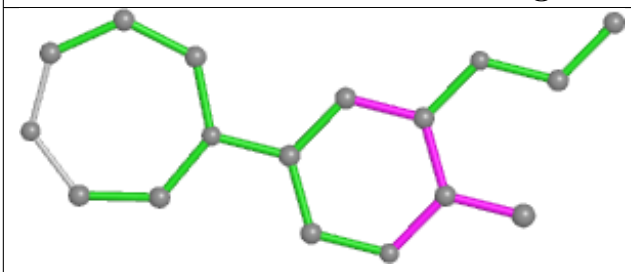

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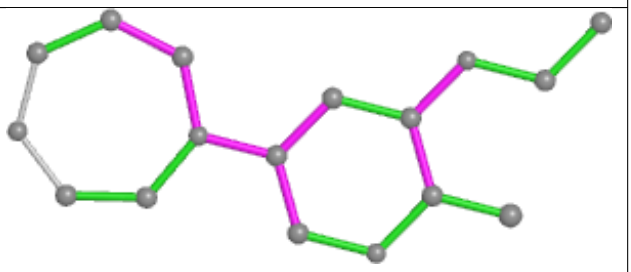

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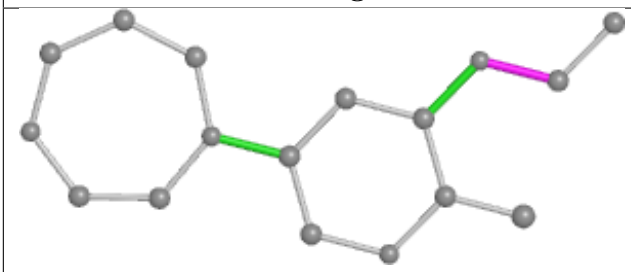

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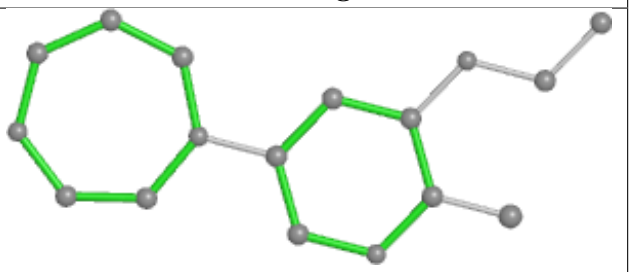

Rings

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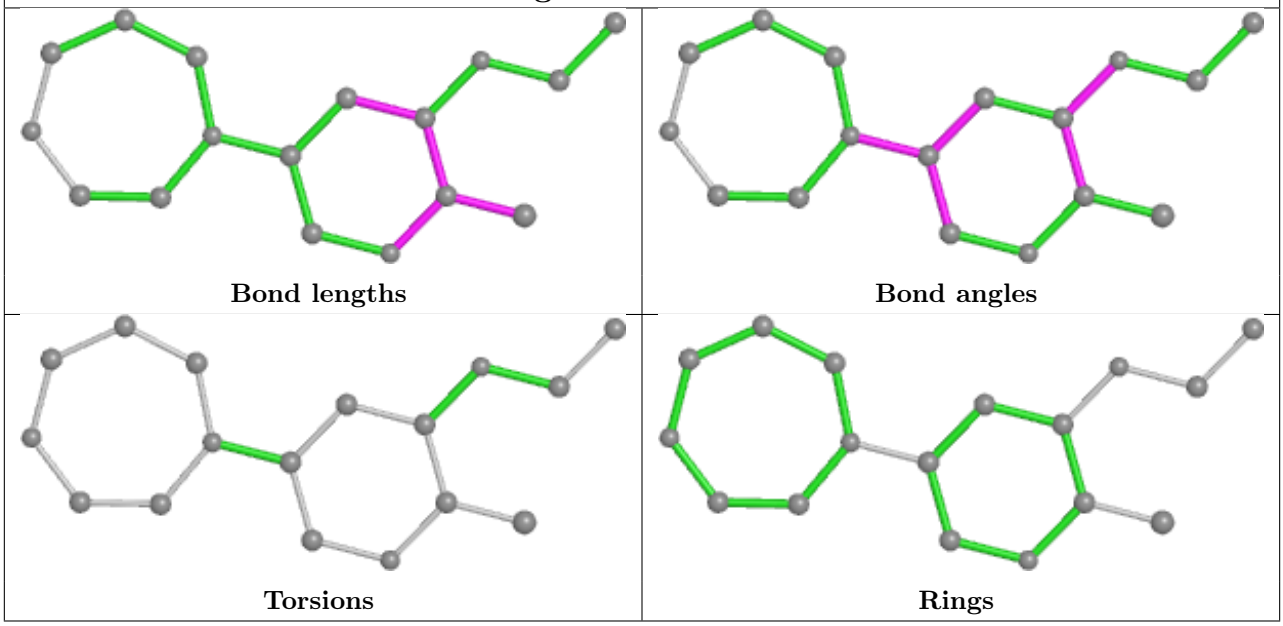

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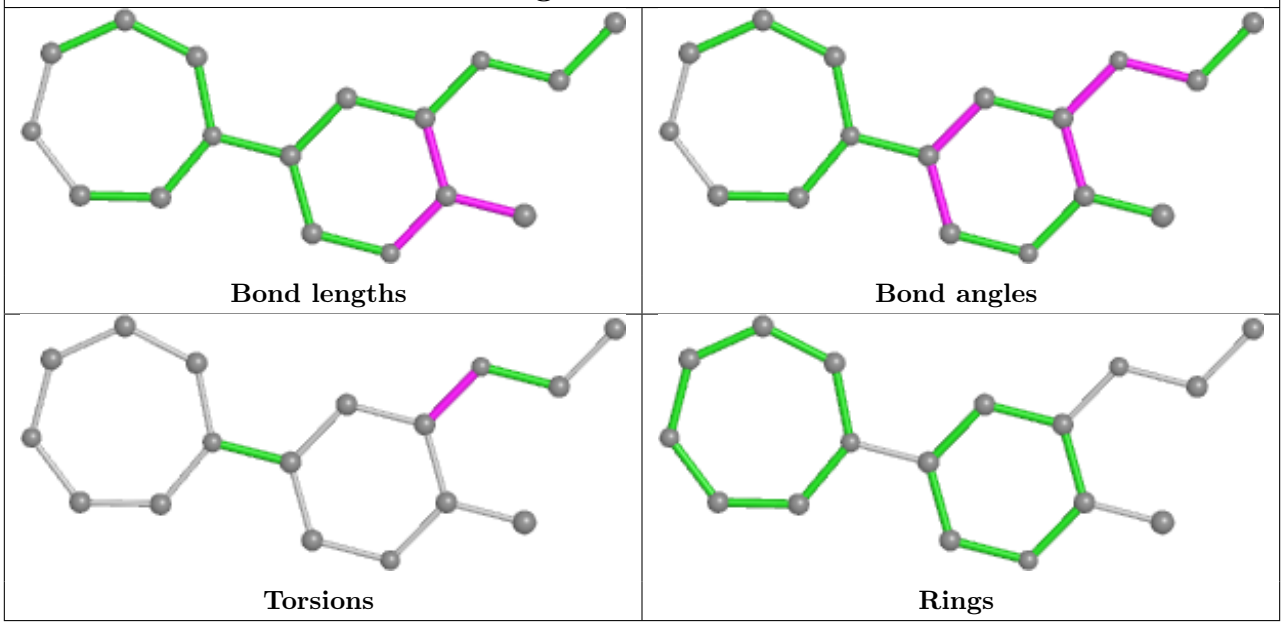

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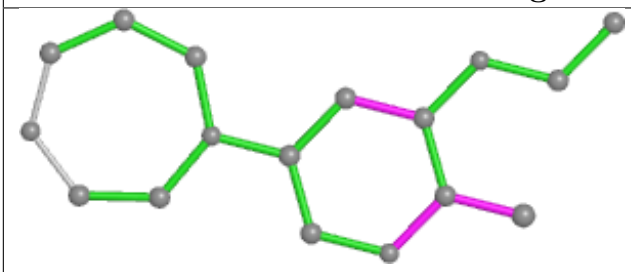

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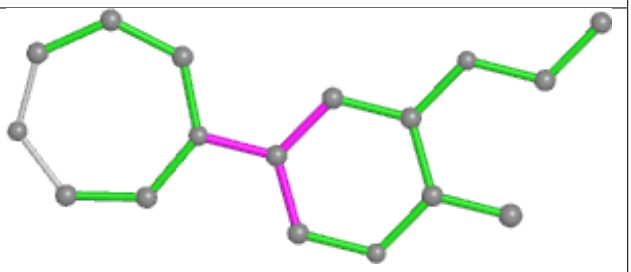
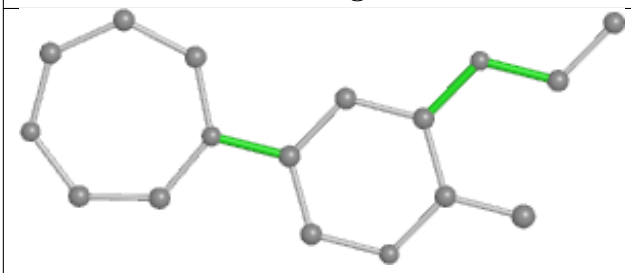


Bond angles



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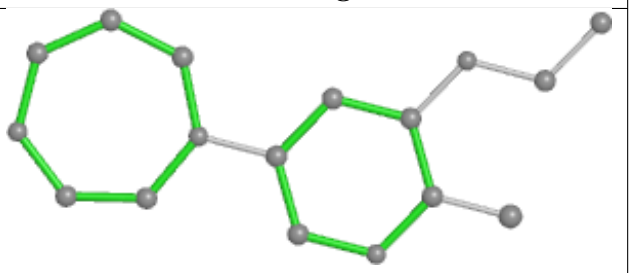
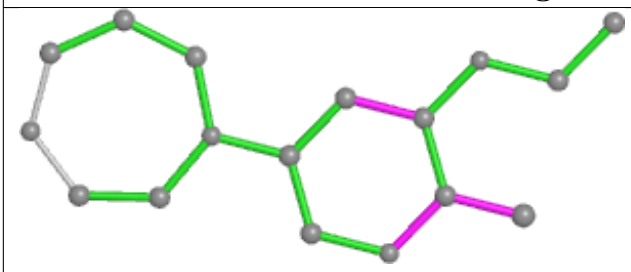


Rings

Ligand 09S P 211



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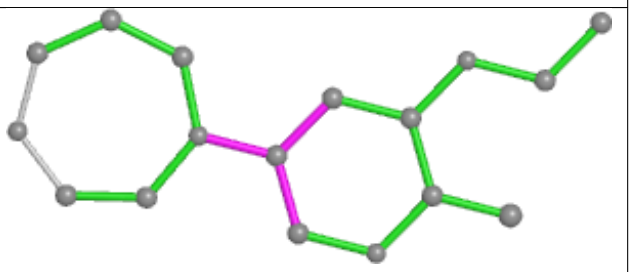

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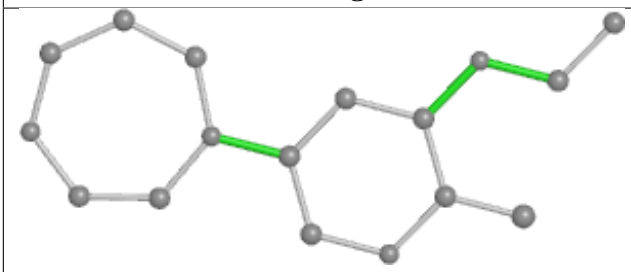

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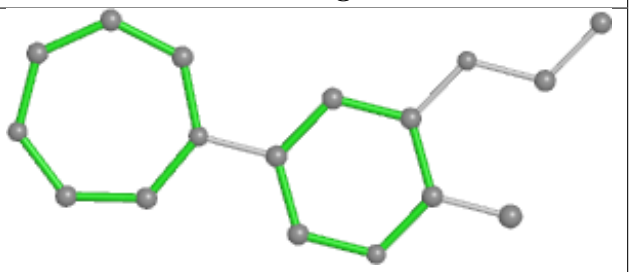

Rings

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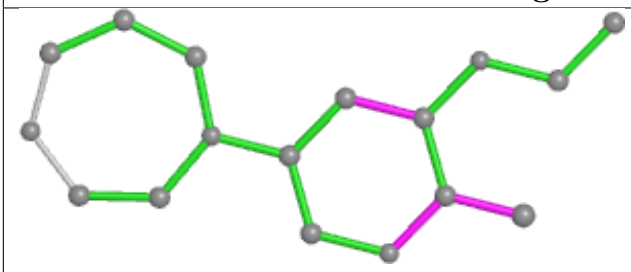

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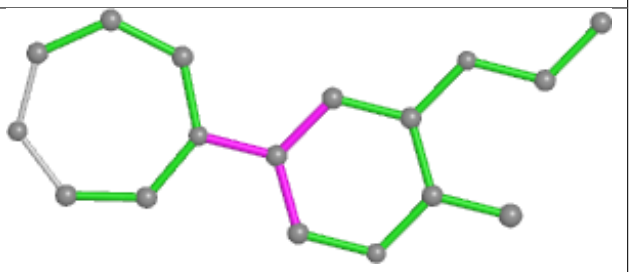

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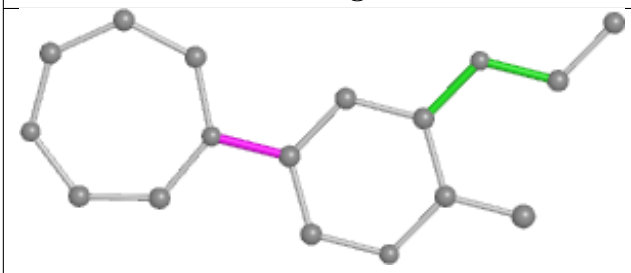

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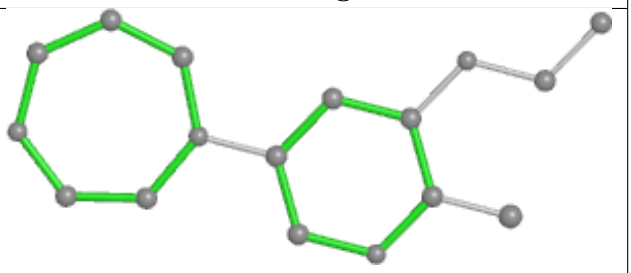
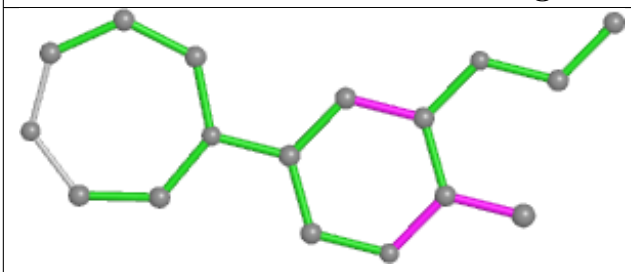


Rings

Ligand 09S B 211



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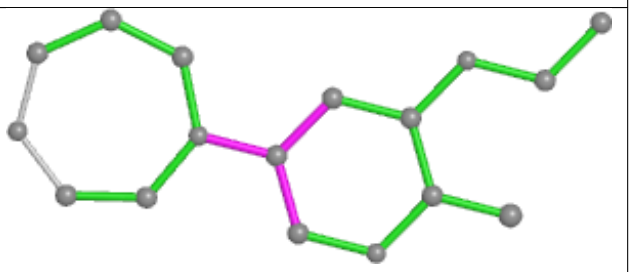

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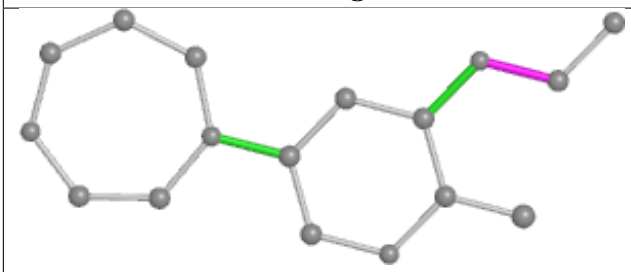

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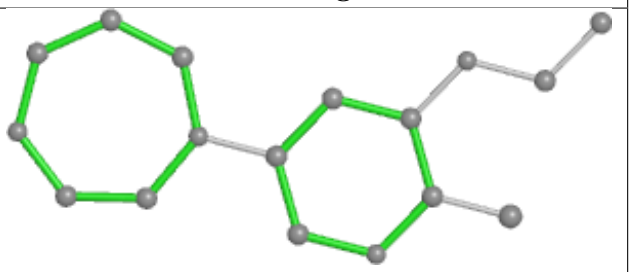
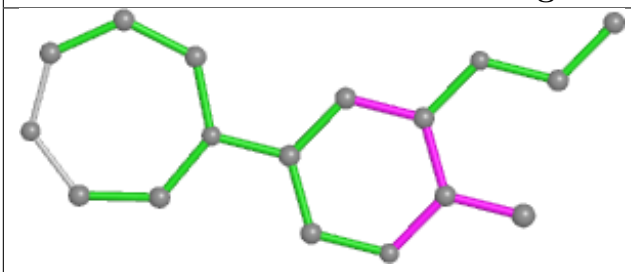


Rings

Ligand 09S J 211



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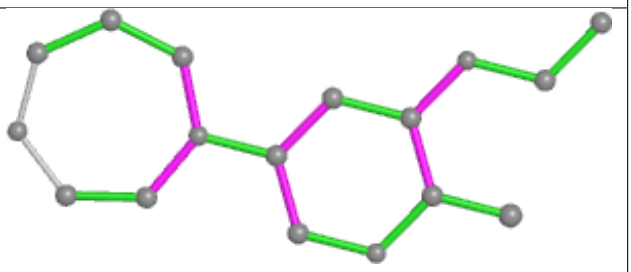

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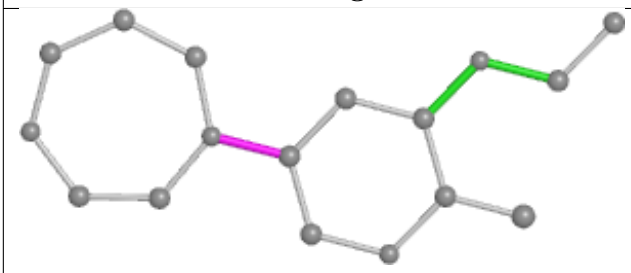

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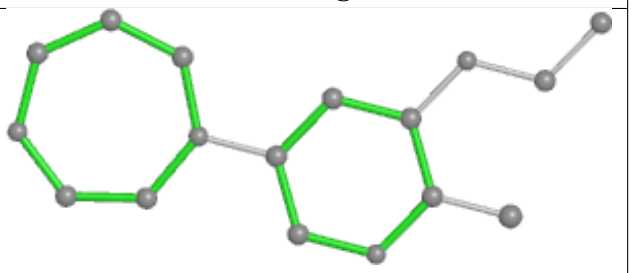
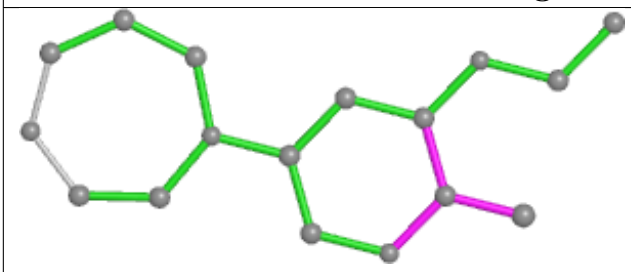


Rings

Ligand 09S C 211



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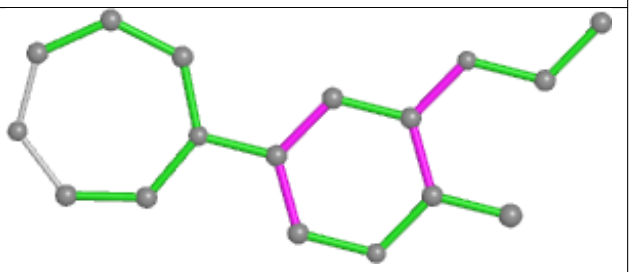
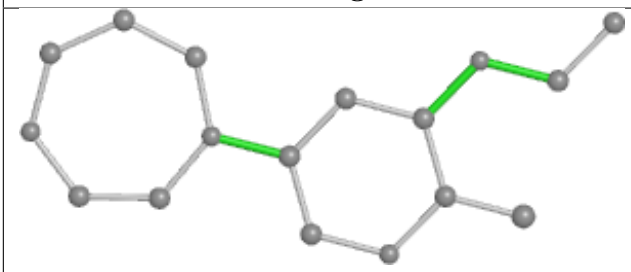


Bond angles



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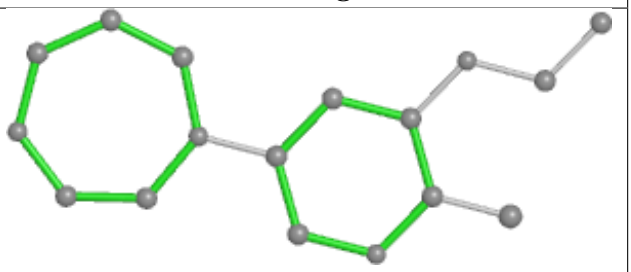

Rings

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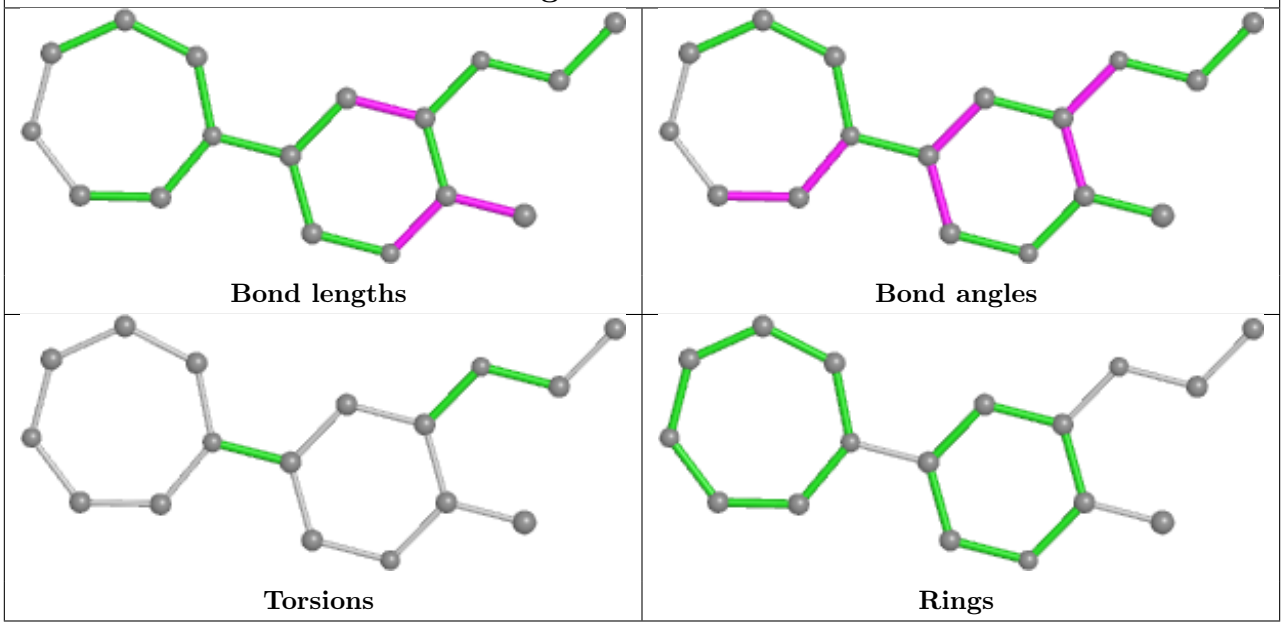

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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