wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 03:43 pm GMT

PDB ID	:	4UM3
Title	:	Engineered Ls-AChBP with alpha4-alpha4 binding pocket in complex with NS3920
Authors	:	Shahsavar, A.; Kastrup, J.S.; Balle, T.; Gajhede, M.
Deposited on	:	2014-05-14
Resolution	:	2.70 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:

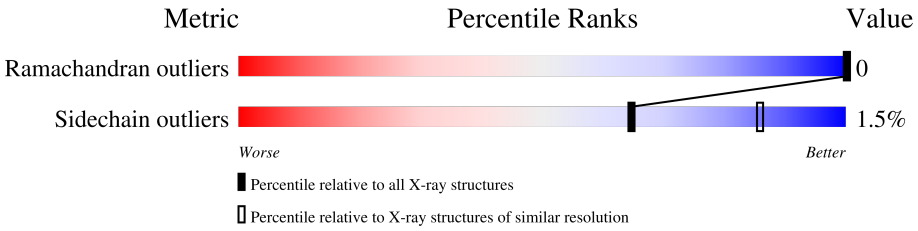
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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))
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	229	86% · 12%
1	B	229	86% 14%
1	C	229	87% · 12%
1	D	229	86% · 12%
1	E	229	85% 15%
1	F	229	84% · 14%
1	G	229	86% · 13%
1	H	229	85% · 14%
1	I	229	85% · 13%

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Mol	Chain	Length	Quality of chain
1	J	229	86% 13%
1	K	229	85% 14%
1	L	229	84% 15%
1	M	229	86% 14%
1	N	229	85% 14%
1	O	229	84% 14%
1	Q	229	85% 14%
1	R	229	86% 14%
1	T	229	84% 15%
1	U	229	84% 14%
1	V	229	85% 13%
1	W	229	85% 14%
1	X	229	86% 12%
1	Y	229	85% 14%
1	Z	229	85% 14%
1	a	229	86% 14%
1	b	229	84% 14%
1	c	229	86% 13%
1	d	229	85% 14%
1	e	229	84% 14%
1	f	229	84% 15%
1	g	229	86% 14%
1	h	229	86% 13%
1	i	229	86% 14%
1	j	229	85% 14%

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Mol	Chain	Length	Quality of chain
1	k	229	85% 14%
1	l	229	85% 13%
1	m	229	86% 12%
1	n	229	83% 14%
2	P	228	86% 12%
3	S	229	86% 12%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 64774 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
1	A	201	Total	C	N	O	S	0	2	0
			1619	1015	280	320	4			
1	B	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	C	201	Total	C	N	O	S	0	0	0
			1608	1007	278	319	4			
1	D	201	Total	C	N	O	S	0	0	0
			1605	1005	275	321	4			
1	E	195	Total	C	N	O	S	0	1	0
			1560	983	265	308	4			
1	F	196	Total	C	N	O	S	0	1	0
			1572	989	270	309	4			
1	G	200	Total	C	N	O	S	0	0	0
			1597	1001	274	318	4			
1	H	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	I	200	Total	C	N	O	S	0	1	0
			1603	1005	274	320	4			
1	J	200	Total	C	N	O	S	0	1	0
			1605	1006	277	318	4			
1	K	197	Total	C	N	O	S	0	1	0
			1575	990	268	313	4			
1	L	195	Total	C	N	O	S	0	1	0
			1565	985	268	308	4			
1	M	198	Total	C	N	O	S	0	1	0
			1590	998	272	316	4			
1	N	196	Total	C	N	O	S	0	1	0
			1564	984	264	312	4			
1	O	196	Total	C	N	O	S	0	0	0
			1563	983	264	312	4			
1	Q	196	Total	C	N	O	S	0	2	0
			1574	991	269	310	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	T	194	Total	C	N	O	S	0	0	0
			1552	978	265	305	4			
1	U	197	Total	C	N	O	S	0	0	0
			1575	990	271	310	4			
1	V	199	Total	C	N	O	S	0	0	0
			1589	997	273	315	4			
1	W	197	Total	C	N	O	S	0	0	0
			1570	987	268	311	4			
1	X	202	Total	C	N	O	S	0	0	0
			1611	1008	276	323	4			
1	Y	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	Z	196	Total	C	N	O	S	0	0	0
			1564	984	267	309	4			
1	a	197	Total	C	N	O	S	0	1	0
			1575	990	268	313	4			
1	b	198	Total	C	N	O	S	0	1	0
			1590	999	274	313	4			
1	c	200	Total	C	N	O	S	0	2	0
			1604	1005	273	322	4			
1	d	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	e	198	Total	C	N	O	S	0	0	0
			1583	994	272	313	4			
1	f	195	Total	C	N	O	S	0	0	0
			1560	982	266	308	4			
1	g	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	h	199	Total	C	N	O	S	0	1	0
			1596	1001	273	318	4			
1	i	197	Total	C	N	O	S	0	0	0
			1567	985	265	313	4			
1	j	198	Total	C	N	O	S	0	0	0
			1585	995	272	314	4			
1	k	198	Total	C	N	O	S	0	0	0
			1578	991	269	314	4			
1	l	200	Total	C	N	O	S	0	0	0
			1597	1001	274	318	4			
1	m	201	Total	C	N	O	S	0	0	0
			1605	1005	275	321	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	n	196	Total	C	N	O	S	0	0	0
			1559	981	264	310	4			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	HIS	ARG	engineered mutation	UNP P58154
A	112	GLN	LEU	engineered mutation	UNP P58154
A	114	THR	MET	engineered mutation	UNP P58154
B	104	HIS	ARG	engineered mutation	UNP P58154
B	112	GLN	LEU	engineered mutation	UNP P58154
B	114	THR	MET	engineered mutation	UNP P58154
C	104	HIS	ARG	engineered mutation	UNP P58154
C	112	GLN	LEU	engineered mutation	UNP P58154
C	114	THR	MET	engineered mutation	UNP P58154
D	104	HIS	ARG	engineered mutation	UNP P58154
D	112	GLN	LEU	engineered mutation	UNP P58154
D	114	THR	MET	engineered mutation	UNP P58154
E	104	HIS	ARG	engineered mutation	UNP P58154
E	112	GLN	LEU	engineered mutation	UNP P58154
E	114	THR	MET	engineered mutation	UNP P58154
F	104	HIS	ARG	engineered mutation	UNP P58154
F	112	GLN	LEU	engineered mutation	UNP P58154
F	114	THR	MET	engineered mutation	UNP P58154
G	104	HIS	ARG	engineered mutation	UNP P58154
G	112	GLN	LEU	engineered mutation	UNP P58154
G	114	THR	MET	engineered mutation	UNP P58154
H	104	HIS	ARG	engineered mutation	UNP P58154
H	112	GLN	LEU	engineered mutation	UNP P58154
H	114	THR	MET	engineered mutation	UNP P58154
I	104	HIS	ARG	engineered mutation	UNP P58154
I	112	GLN	LEU	engineered mutation	UNP P58154
I	114	THR	MET	engineered mutation	UNP P58154
J	104	HIS	ARG	engineered mutation	UNP P58154
J	112	GLN	LEU	engineered mutation	UNP P58154
J	114	THR	MET	engineered mutation	UNP P58154
K	104	HIS	ARG	engineered mutation	UNP P58154
K	112	GLN	LEU	engineered mutation	UNP P58154
K	114	THR	MET	engineered mutation	UNP P58154
L	104	HIS	ARG	engineered mutation	UNP P58154
L	112	GLN	LEU	engineered mutation	UNP P58154
L	114	THR	MET	engineered mutation	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
M	104	HIS	ARG	engineered mutation	UNP P58154
M	112	GLN	LEU	engineered mutation	UNP P58154
M	114	THR	MET	engineered mutation	UNP P58154
N	104	HIS	ARG	engineered mutation	UNP P58154
N	112	GLN	LEU	engineered mutation	UNP P58154
N	114	THR	MET	engineered mutation	UNP P58154
O	104	HIS	ARG	engineered mutation	UNP P58154
O	112	GLN	LEU	engineered mutation	UNP P58154
O	114	THR	MET	engineered mutation	UNP P58154
Q	104	HIS	ARG	engineered mutation	UNP P58154
Q	112	GLN	LEU	engineered mutation	UNP P58154
Q	114	THR	MET	engineered mutation	UNP P58154
R	104	HIS	ARG	engineered mutation	UNP P58154
R	112	GLN	LEU	engineered mutation	UNP P58154
R	114	THR	MET	engineered mutation	UNP P58154
T	104	HIS	ARG	engineered mutation	UNP P58154
T	112	GLN	LEU	engineered mutation	UNP P58154
T	114	THR	MET	engineered mutation	UNP P58154
U	104	HIS	ARG	engineered mutation	UNP P58154
U	112	GLN	LEU	engineered mutation	UNP P58154
U	114	THR	MET	engineered mutation	UNP P58154
V	104	HIS	ARG	engineered mutation	UNP P58154
V	112	GLN	LEU	engineered mutation	UNP P58154
V	114	THR	MET	engineered mutation	UNP P58154
W	104	HIS	ARG	engineered mutation	UNP P58154
W	112	GLN	LEU	engineered mutation	UNP P58154
W	114	THR	MET	engineered mutation	UNP P58154
X	104	HIS	ARG	engineered mutation	UNP P58154
X	112	GLN	LEU	engineered mutation	UNP P58154
X	114	THR	MET	engineered mutation	UNP P58154
Y	104	HIS	ARG	engineered mutation	UNP P58154
Y	112	GLN	LEU	engineered mutation	UNP P58154
Y	114	THR	MET	engineered mutation	UNP P58154
Z	104	HIS	ARG	engineered mutation	UNP P58154
Z	112	GLN	LEU	engineered mutation	UNP P58154
Z	114	THR	MET	engineered mutation	UNP P58154
a	104	HIS	ARG	engineered mutation	UNP P58154
a	112	GLN	LEU	engineered mutation	UNP P58154
a	114	THR	MET	engineered mutation	UNP P58154
b	104	HIS	ARG	engineered mutation	UNP P58154
b	112	GLN	LEU	engineered mutation	UNP P58154
b	114	THR	MET	engineered mutation	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
c	104	HIS	ARG	engineered mutation	UNP P58154
c	112	GLN	LEU	engineered mutation	UNP P58154
c	114	THR	MET	engineered mutation	UNP P58154
d	104	HIS	ARG	engineered mutation	UNP P58154
d	112	GLN	LEU	engineered mutation	UNP P58154
d	114	THR	MET	engineered mutation	UNP P58154
e	104	HIS	ARG	engineered mutation	UNP P58154
e	112	GLN	LEU	engineered mutation	UNP P58154
e	114	THR	MET	engineered mutation	UNP P58154
f	104	HIS	ARG	engineered mutation	UNP P58154
f	112	GLN	LEU	engineered mutation	UNP P58154
f	114	THR	MET	engineered mutation	UNP P58154
g	104	HIS	ARG	engineered mutation	UNP P58154
g	112	GLN	LEU	engineered mutation	UNP P58154
g	114	THR	MET	engineered mutation	UNP P58154
h	104	HIS	ARG	engineered mutation	UNP P58154
h	112	GLN	LEU	engineered mutation	UNP P58154
h	114	THR	MET	engineered mutation	UNP P58154
i	104	HIS	ARG	engineered mutation	UNP P58154
i	112	GLN	LEU	engineered mutation	UNP P58154
i	114	THR	MET	engineered mutation	UNP P58154
j	104	HIS	ARG	engineered mutation	UNP P58154
j	112	GLN	LEU	engineered mutation	UNP P58154
j	114	THR	MET	engineered mutation	UNP P58154
k	104	HIS	ARG	engineered mutation	UNP P58154
k	112	GLN	LEU	engineered mutation	UNP P58154
k	114	THR	MET	engineered mutation	UNP P58154
l	104	HIS	ARG	engineered mutation	UNP P58154
l	112	GLN	LEU	engineered mutation	UNP P58154
l	114	THR	MET	engineered mutation	UNP P58154
m	104	HIS	ARG	engineered mutation	UNP P58154
m	112	GLN	LEU	engineered mutation	UNP P58154
m	114	THR	MET	engineered mutation	UNP P58154
n	104	HIS	ARG	engineered mutation	UNP P58154
n	112	GLN	LEU	engineered mutation	UNP P58154
n	114	THR	MET	engineered mutation	UNP P58154

- Molecule 2 is a protein called ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	201	Total	C	N	O	S	0	0	0
			1608	1007	278	319	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	104	HIS	ARG	engineered mutation	UNP P58154
P	112	GLN	LEU	engineered mutation	UNP P58154
P	114	THR	MET	engineered mutation	UNP P58154
P	?	-	ASP	deletion	UNP P58154

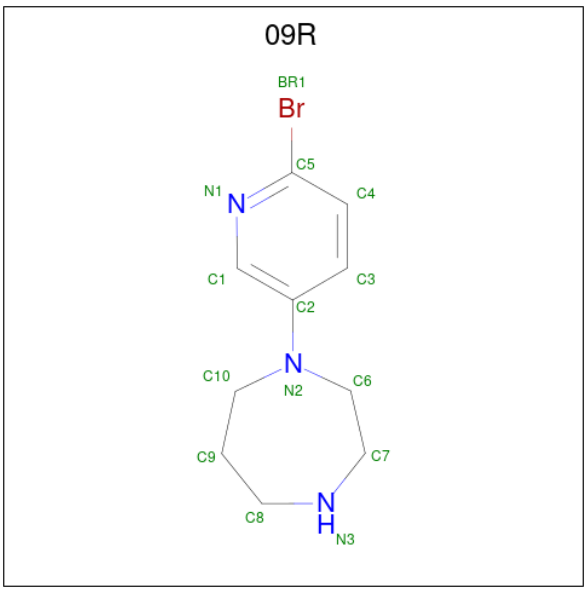
- Molecule 3 is a protein called ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	201	Total	C	N	O	S	0	0	0
			1603	1004	276	319	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	104	HIS	ARG	engineered mutation	UNP P58154
S	112	GLN	LEU	engineered mutation	UNP P58154
S	114	THR	MET	engineered mutation	UNP P58154
S	131	GLN	GLU	conflict	UNP P58154

- Molecule 4 is 1-(6-bromopyridin-3-yl)-1,4-diazepane (three-letter code: 09R) (formula: $C_{10}H_{14}BrN_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	N	0	0
			14	1	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	Br	C	N	0	0
			14	1	10	3		
4	C	1	Total	Br	C	N	0	0
			14	1	10	3		
4	D	1	Total	Br	C	N	0	0
			14	1	10	3		
4	E	1	Total	Br	C	N	0	0
			14	1	10	3		
4	F	1	Total	Br	C	N	0	0
			14	1	10	3		
4	G	1	Total	Br	C	N	0	0
			14	1	10	3		
4	H	1	Total	Br	C	N	0	0
			14	1	10	3		
4	I	1	Total	Br	C	N	0	0
			14	1	10	3		
4	J	1	Total	Br	C	N	0	0
			14	1	10	3		
4	K	1	Total	Br	C	N	0	0
			14	1	10	3		
4	L	1	Total	Br	C	N	0	0
			14	1	10	3		
4	M	1	Total	Br	C	N	0	0
			14	1	10	3		
4	N	1	Total	Br	C	N	0	0
			14	1	10	3		
4	O	1	Total	Br	C	N	0	0
			14	1	10	3		
4	P	1	Total	Br	C	N	0	0
			14	1	10	3		
4	Q	1	Total	Br	C	N	0	0
			14	1	10	3		
4	R	1	Total	Br	C	N	0	0
			14	1	10	3		
4	S	1	Total	Br	C	N	0	0
			14	1	10	3		
4	T	1	Total	Br	C	N	0	0
			14	1	10	3		
4	U	1	Total	Br	C	N	0	0
			14	1	10	3		
4	V	1	Total	Br	C	N	0	0
			14	1	10	3		

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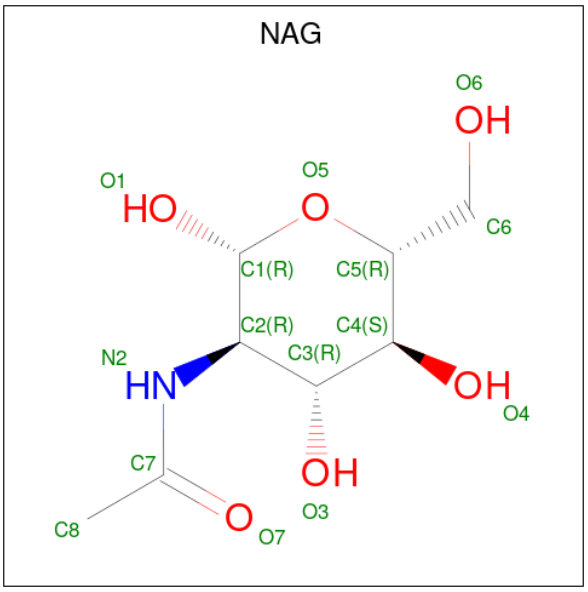
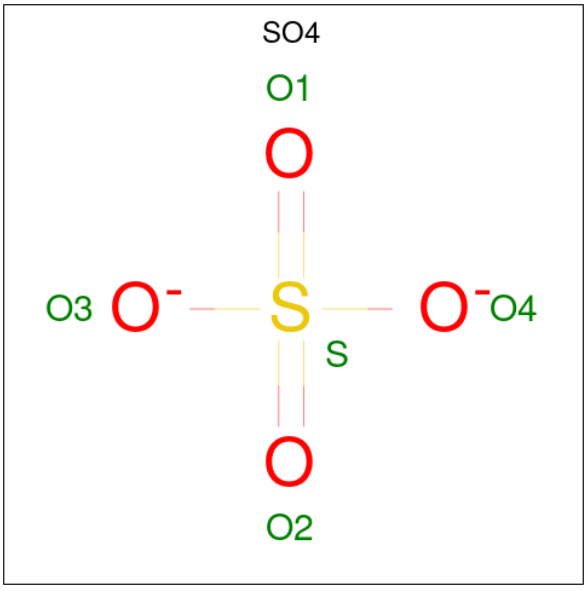
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	W	1	Total	Br	C	N	0	0
			14	1	10	3		
4	X	1	Total	Br	C	N	0	0
			14	1	10	3		
4	Y	1	Total	Br	C	N	0	0
			14	1	10	3		
4	Z	1	Total	Br	C	N	0	0
			14	1	10	3		
4	a	1	Total	Br	C	N	0	0
			14	1	10	3		
4	b	1	Total	Br	C	N	0	0
			14	1	10	3		
4	c	1	Total	Br	C	N	0	0
			14	1	10	3		
4	d	1	Total	Br	C	N	0	0
			14	1	10	3		
4	f	1	Total	Br	C	N	0	0
			14	1	10	3		
4	f	1	Total	Br	C	N	0	0
			14	1	10	3		
4	g	1	Total	Br	C	N	0	0
			14	1	10	3		
4	h	1	Total	Br	C	N	0	0
			14	1	10	3		
4	i	1	Total	Br	C	N	0	0
			14	1	10	3		
4	j	1	Total	Br	C	N	0	0
			14	1	10	3		
4	k	1	Total	Br	C	N	0	0
			14	1	10	3		
4	l	1	Total	Br	C	N	0	0
			14	1	10	3		
4	m	1	Total	Br	C	N	0	0
			14	1	10	3		
4	n	1	Total	Br	C	N	0	0
			14	1	10	3		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	d	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	V	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	41	Total O 41 41	0	0
7	B	31	Total O 31 31	0	0
7	C	25	Total O 25 25	0	0
7	D	26	Total O 26 26	0	0
7	E	25	Total O 25 25	0	0
7	F	29	Total O 29 29	0	0
7	G	29	Total O 29 29	0	0
7	H	22	Total O 22 22	0	0
7	I	28	Total O 28 28	0	0
7	J	37	Total O 37 37	0	0
7	K	29	Total O 29 29	0	0
7	L	23	Total O 23 23	0	0
7	M	19	Total O 19 19	0	0
7	N	21	Total O 21 21	0	0
7	O	30	Total O 30 30	0	0
7	P	40	Total O 40 40	0	0
7	Q	37	Total O 37 37	0	0
7	R	27	Total O 27 27	0	0
7	S	28	Total O 28 28	0	0
7	T	31	Total O 31 31	0	0
7	U	30	Total O 30 30	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	V	44	Total O 44 44	0	0
7	W	28	Total O 28 28	0	0
7	X	28	Total O 28 28	0	0
7	Y	16	Total O 16 16	0	0
7	Z	23	Total O 23 23	0	0
7	a	16	Total O 16 16	0	0
7	b	9	Total O 9 9	0	0
7	c	3	Total O 3 3	0	0
7	d	19	Total O 19 19	0	0
7	e	3	Total O 3 3	0	0
7	f	2	Total O 2 2	0	0
7	g	1	Total O 1 1	0	0
7	h	7	Total O 7 7	0	0
7	i	5	Total O 5 5	0	0
7	j	2	Total O 2 2	0	0
7	k	7	Total O 7 7	0	0
7	l	6	Total O 6 6	0	0
7	m	2	Total O 2 2	0	0
7	n	7	Total O 7 7	0	0

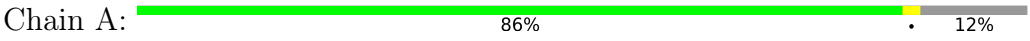
3 Residue-property plots (i)

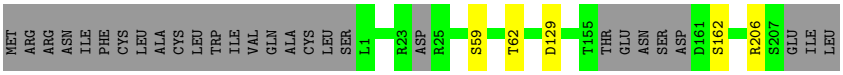
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

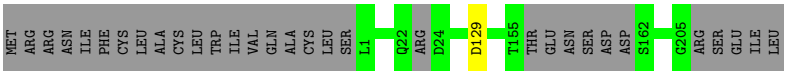
Chain A:





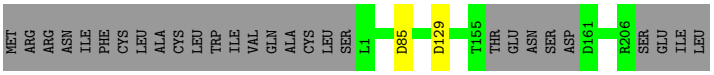
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain B:



- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain C:

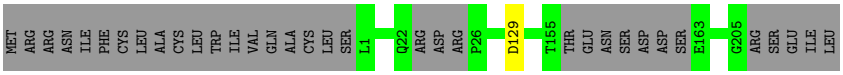


- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain D:

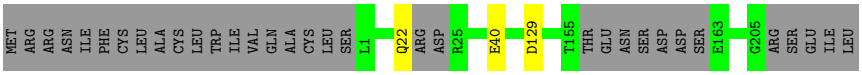
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain E:



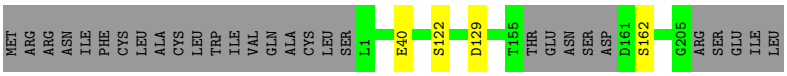
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain F:



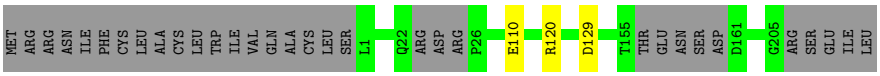
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain G:



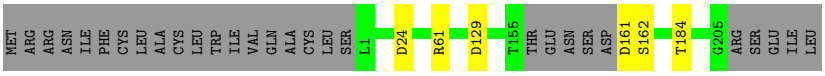
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain H:



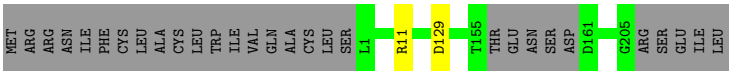
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain I:



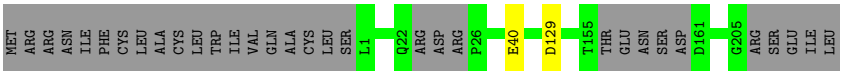
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain J:



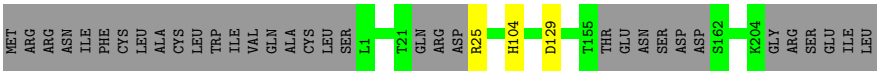
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain K:



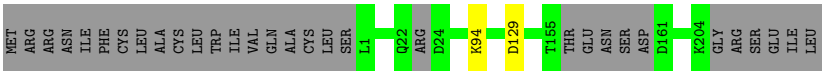
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain L:



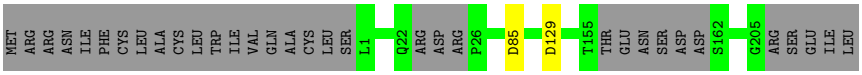
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain M:



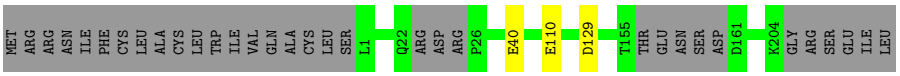
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain N:



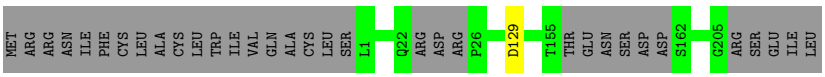
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain O:



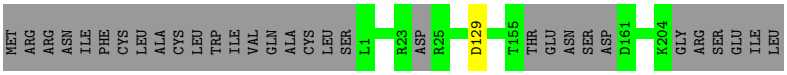
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain Q:



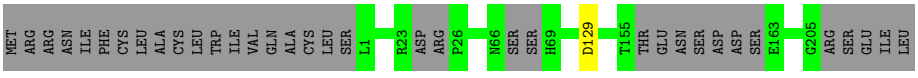
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain R:



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain T:

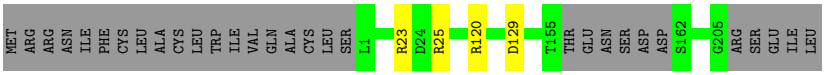


• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain U:

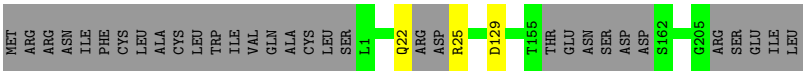
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain V:



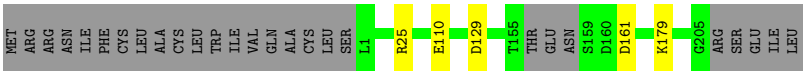
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain W:



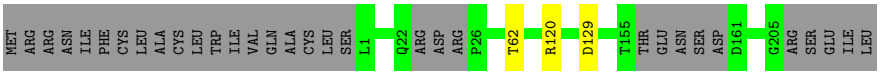
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain X:



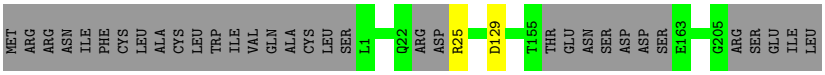
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain Y:



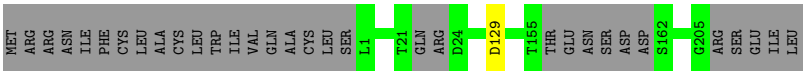
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain Z:



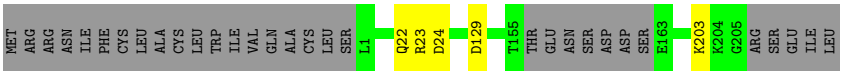
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain a:



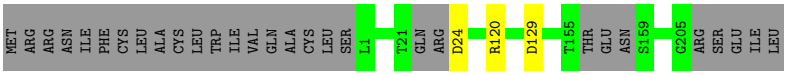
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain b:



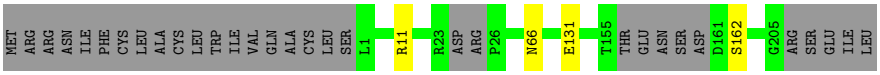
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain c:



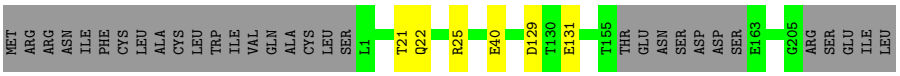
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain d:



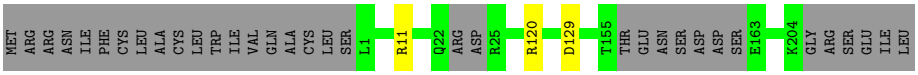
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain e:



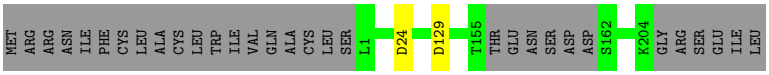
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain f:



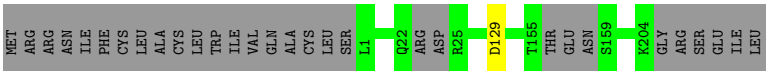
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain g:



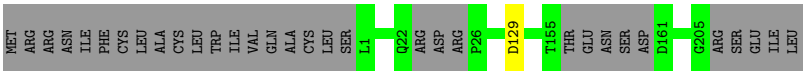
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain h:



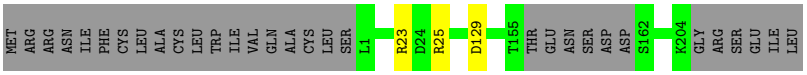
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain i:



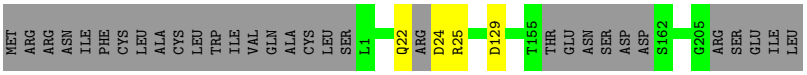
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain j:



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain k:



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

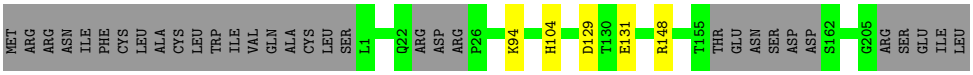
Chain l:

• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain m:

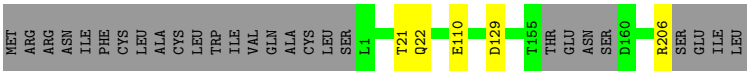
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain n:



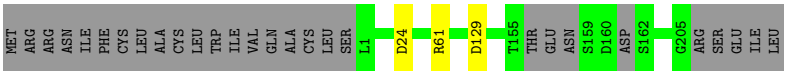
• Molecule 2: ACETYLCHOLINE BINDING PROTEIN

Chain P:



• Molecule 3: ACETYLCHOLINE BINDING PROTEIN

Chain S:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.49Å 145.42Å 234.91Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	30.07 – 2.70	Depositor
% Data completeness (in resolution range)	99.5 (30.07-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.72Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.244	Depositor
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.622	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	64774	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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, NAG, 09R

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	0.68	0/1661	0.64	0/2264
1	B	0.55	0/1613	0.58	0/2201
1	C	0.56	0/1644	0.67	2/2243 (0.1%)
1	D	0.60	0/1640	0.61	0/2237
1	E	0.59	0/1599	0.60	0/2182
1	F	0.63	0/1610	0.62	0/2196
1	G	0.56	0/1633	0.59	0/2229
1	H	0.53	0/1602	0.57	0/2186
1	I	0.61	0/1642	0.62	0/2241
1	J	0.55	0/1644	0.61	0/2243
1	K	0.47	0/1613	0.55	0/2200
1	L	0.50	0/1603	0.58	1/2187 (0.0%)
1	M	0.47	0/1628	0.54	0/2221
1	N	0.53	0/1602	0.59	1/2187 (0.0%)
1	O	0.58	0/1598	0.58	0/2181
1	Q	0.51	0/1616	0.57	0/2204
1	R	0.57	0/1620	0.62	0/2210
1	T	0.59	0/1586	0.60	0/2162
1	U	0.65	0/1610	0.61	0/2196
1	V	0.61	0/1625	0.61	0/2218
1	W	0.54	0/1605	0.59	0/2190
1	X	0.56	0/1647	0.57	0/2248
1	Y	0.51	0/1602	0.58	0/2186
1	Z	0.52	0/1599	0.56	0/2182
1	a	0.53	0/1613	0.56	0/2201
1	b	0.55	0/1630	0.59	0/2225
1	c	0.50	0/1645	0.56	0/2245
1	d	0.52	0/1613	0.58	0/2200
1	e	0.49	0/1619	0.56	0/2210
1	f	0.46	0/1595	0.57	0/2177
1	g	0.50	0/1621	0.54	0/2213
1	h	0.47	0/1634	0.55	0/2229

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	i	0.51	0/1602	0.57	0/2186
1	j	0.46	0/1621	0.53	0/2213
1	k	0.45	0/1613	0.54	0/2201
1	l	0.47	0/1633	0.57	0/2229
1	m	0.43	0/1640	0.53	0/2237
1	n	0.45	0/1594	0.54	0/2175
2	P	0.63	0/1644	0.63	0/2243
3	S	0.60	0/1638	0.57	0/2234
All	All	0.54	0/64797	0.58	4/88412 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	85	ASP	CB-CG-OD2	-9.30	109.93	118.30
1	C	85	ASP	CB-CG-OD1	7.45	125.00	118.30
1	L	25	ARG	C-N-CD	5.93	140.85	128.40
1	N	85	ASP	CB-CG-OD2	5.29	123.06	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	197/229 (86%)	194 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	192/229 (84%)	192 (100%)	0	0	100	100
1	C	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
1	D	195/229 (85%)	195 (100%)	0	0	100	100
1	E	190/229 (83%)	190 (100%)	0	0	100	100
1	F	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	G	196/229 (86%)	194 (99%)	2 (1%)	0	100	100
1	H	191/229 (83%)	188 (98%)	3 (2%)	0	100	100
1	I	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
1	J	197/229 (86%)	194 (98%)	3 (2%)	0	100	100
1	K	192/229 (84%)	189 (98%)	3 (2%)	0	100	100
1	L	190/229 (83%)	189 (100%)	1 (0%)	0	100	100
1	M	193/229 (84%)	190 (98%)	3 (2%)	0	100	100
1	N	191/229 (83%)	189 (99%)	2 (1%)	0	100	100
1	O	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
1	Q	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	R	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	T	186/229 (81%)	186 (100%)	0	0	100	100
1	U	191/229 (83%)	191 (100%)	0	0	100	100
1	V	195/229 (85%)	195 (100%)	0	0	100	100
1	W	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	X	198/229 (86%)	197 (100%)	1 (0%)	0	100	100
1	Y	191/229 (83%)	189 (99%)	2 (1%)	0	100	100
1	Z	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
1	a	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	b	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
1	c	196/229 (86%)	193 (98%)	3 (2%)	0	100	100
1	d	192/229 (84%)	190 (99%)	2 (1%)	0	100	100
1	e	194/229 (85%)	193 (100%)	1 (0%)	0	100	100
1	f	189/229 (82%)	187 (99%)	2 (1%)	0	100	100
1	g	194/229 (85%)	193 (100%)	1 (0%)	0	100	100
1	h	194/229 (85%)	190 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	i	191/229 (83%)	190 (100%)	1 (0%)	0	100	100
1	j	194/229 (85%)	192 (99%)	2 (1%)	0	100	100
1	k	192/229 (84%)	191 (100%)	1 (0%)	0	100	100
1	l	196/229 (86%)	195 (100%)	1 (0%)	0	100	100
1	m	195/229 (85%)	192 (98%)	3 (2%)	0	100	100
1	n	190/229 (83%)	188 (99%)	2 (1%)	0	100	100
2	P	197/228 (86%)	194 (98%)	3 (2%)	0	100	100
3	S	195/229 (85%)	194 (100%)	1 (0%)	0	100	100
All	All	7721/9159 (84%)	7657 (99%)	64 (1%)	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 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	189/213 (89%)	184 (97%)	5 (3%)	46	75
1	B	184/213 (86%)	183 (100%)	1 (0%)	88	96
1	C	187/213 (88%)	186 (100%)	1 (0%)	88	96
1	D	187/213 (88%)	184 (98%)	3 (2%)	62	85
1	E	182/213 (85%)	181 (100%)	1 (0%)	88	96
1	F	183/213 (86%)	180 (98%)	3 (2%)	62	85
1	G	186/213 (87%)	182 (98%)	4 (2%)	52	79
1	H	183/213 (86%)	180 (98%)	3 (2%)	62	85
1	I	187/213 (88%)	182 (97%)	5 (3%)	44	74
1	J	187/213 (88%)	185 (99%)	2 (1%)	73	90
1	K	184/213 (86%)	182 (99%)	2 (1%)	73	90
1	L	183/213 (86%)	181 (99%)	2 (1%)	73	90
1	M	186/213 (87%)	184 (99%)	2 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	183/213 (86%)	182 (100%)	1 (0%)	88 96
1	O	183/213 (86%)	180 (98%)	3 (2%)	62 85
1	Q	184/213 (86%)	183 (100%)	1 (0%)	88 96
1	R	185/213 (87%)	184 (100%)	1 (0%)	88 96
1	T	180/213 (84%)	179 (99%)	1 (1%)	86 95
1	U	183/213 (86%)	179 (98%)	4 (2%)	52 79
1	V	185/213 (87%)	182 (98%)	3 (2%)	62 85
1	W	183/213 (86%)	180 (98%)	3 (2%)	62 85
1	X	188/213 (88%)	183 (97%)	5 (3%)	44 74
1	Y	183/213 (86%)	180 (98%)	3 (2%)	62 85
1	Z	182/213 (85%)	180 (99%)	2 (1%)	73 90
1	a	184/213 (86%)	183 (100%)	1 (0%)	88 96
1	b	185/213 (87%)	180 (97%)	5 (3%)	44 74
1	c	188/213 (88%)	184 (98%)	4 (2%)	53 80
1	d	184/213 (86%)	181 (98%)	3 (2%)	62 85
1	e	184/213 (86%)	178 (97%)	6 (3%)	38 67
1	f	182/213 (85%)	179 (98%)	3 (2%)	62 85
1	g	185/213 (87%)	183 (99%)	2 (1%)	73 90
1	h	187/213 (88%)	186 (100%)	1 (0%)	88 96
1	i	183/213 (86%)	182 (100%)	1 (0%)	88 96
1	j	185/213 (87%)	182 (98%)	3 (2%)	62 85
1	k	184/213 (86%)	181 (98%)	3 (2%)	62 85
1	l	186/213 (87%)	181 (97%)	5 (3%)	44 74
1	m	187/213 (88%)	183 (98%)	4 (2%)	53 80
1	n	182/213 (85%)	177 (97%)	5 (3%)	44 74
2	P	187/212 (88%)	182 (97%)	5 (3%)	44 74
3	S	187/213 (88%)	184 (98%)	3 (2%)	62 85
All	All	7387/8519 (87%)	7272 (98%)	115 (2%)	65 85

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	25	ARG

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Mol	Chain	Res	Type
1	n	94	LYS
1	b	23	ARG
1	m	129	ASP
1	k	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	12	GLN
1	W	104	HIS
1	n	104	HIS
1	j	12	GLN
1	T	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)

44 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	09R	E	301	-	13,15,15	3.45	3 (23%)	15,19,19	1.95	5 (33%)
4	09R	V	302	-	13,15,15	3.54	3 (23%)	15,19,19	1.79	5 (33%)
4	09R	B	301	-	13,15,15	3.39	3 (23%)	15,19,19	1.77	5 (33%)
4	09R	Z	301	-	13,15,15	3.35	3 (23%)	15,19,19	1.75	4 (26%)
4	09R	F	301	-	13,15,15	3.48	3 (23%)	15,19,19	1.67	4 (26%)
4	09R	g	301	-	13,15,15	3.39	3 (23%)	15,19,19	1.87	5 (33%)
4	09R	h	301	-	13,15,15	3.33	3 (23%)	15,19,19	2.30	6 (40%)
4	09R	i	301	-	13,15,15	3.59	3 (23%)	15,19,19	1.70	4 (26%)
4	09R	m	301	-	13,15,15	3.80	3 (23%)	15,19,19	2.15	6 (40%)
6	SO4	V	301	-	4,4,4	0.11	0	6,6,6	0.28	0
4	09R	D	301	-	13,15,15	3.10	3 (23%)	15,19,19	2.22	4 (26%)
4	09R	J	301	-	13,15,15	3.47	3 (23%)	15,19,19	1.78	4 (26%)
4	09R	G	301	-	13,15,15	2.93	3 (23%)	15,19,19	2.59	5 (33%)
4	09R	N	301	-	13,15,15	3.67	3 (23%)	15,19,19	1.82	4 (26%)
4	09R	X	301	-	13,15,15	3.34	3 (23%)	15,19,19	2.52	4 (26%)
5	NAG	d	302	1	14,14,15	0.71	0	17,19,21	3.48	11 (64%)
4	09R	C	301	-	13,15,15	3.42	5 (38%)	15,19,19	1.31	2 (13%)
4	09R	S	301	-	13,15,15	3.37	3 (23%)	15,19,19	1.83	4 (26%)
4	09R	f	301	-	13,15,15	3.19	3 (23%)	15,19,19	3.21	8 (53%)
4	09R	j	301	-	13,15,15	3.50	3 (23%)	15,19,19	2.17	6 (40%)
4	09R	b	301	-	13,15,15	3.23	3 (23%)	15,19,19	2.54	6 (40%)
4	09R	K	301	-	13,15,15	3.45	3 (23%)	15,19,19	1.63	3 (20%)
4	09R	c	301	-	13,15,15	3.41	3 (23%)	15,19,19	1.80	5 (33%)
4	09R	l	301	-	13,15,15	3.40	3 (23%)	15,19,19	2.27	5 (33%)
4	09R	T	301	-	13,15,15	3.51	4 (30%)	15,19,19	1.52	2 (13%)
4	09R	R	301	-	13,15,15	3.40	3 (23%)	15,19,19	1.28	2 (13%)
4	09R	d	301	-	13,15,15	3.64	3 (23%)	15,19,19	2.14	5 (33%)
4	09R	f	302	-	13,15,15	3.55	3 (23%)	15,19,19	2.02	5 (33%)
4	09R	Y	301	-	13,15,15	3.29	4 (30%)	15,19,19	2.43	6 (40%)
4	09R	A	301	-	13,15,15	3.12	3 (23%)	15,19,19	2.24	5 (33%)
5	NAG	O	302	1	14,14,15	1.51	2 (14%)	17,19,21	3.55	10 (58%)
4	09R	a	301	-	13,15,15	3.30	3 (23%)	15,19,19	2.53	7 (46%)
4	09R	L	301	-	13,15,15	3.26	3 (23%)	15,19,19	2.76	6 (40%)
4	09R	n	301	-	13,15,15	3.55	3 (23%)	15,19,19	2.21	6 (40%)
5	NAG	A	302	1	14,14,15	0.71	0	17,19,21	3.48	11 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	09R	U	301	-	13,15,15	3.37	4 (30%)	15,19,19	1.86	5 (33%)
4	09R	W	301	-	13,15,15	3.32	3 (23%)	15,19,19	2.42	6 (40%)
4	09R	Q	301	-	13,15,15	3.53	4 (30%)	15,19,19	1.09	2 (13%)
4	09R	O	301	-	13,15,15	3.23	2 (15%)	15,19,19	1.67	5 (33%)
4	09R	k	301	-	13,15,15	3.41	3 (23%)	15,19,19	2.33	6 (40%)
4	09R	M	301	-	13,15,15	3.39	3 (23%)	15,19,19	1.81	6 (40%)
4	09R	I	301	-	13,15,15	3.90	3 (23%)	15,19,19	2.72	7 (46%)
4	09R	P	301	-	13,15,15	3.36	3 (23%)	15,19,19	1.98	5 (33%)
4	09R	H	301	-	13,15,15	3.25	3 (23%)	15,19,19	2.48	7 (46%)

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	09R	E	301	-	-	0/4/13/13	0/2/2/2
4	09R	V	302	-	-	0/4/13/13	0/2/2/2
4	09R	B	301	-	-	0/4/13/13	0/2/2/2
4	09R	Z	301	-	-	0/4/13/13	0/2/2/2
4	09R	F	301	-	-	0/4/13/13	0/2/2/2
4	09R	g	301	-	-	1/4/13/13	0/2/2/2
4	09R	h	301	-	-	0/4/13/13	0/2/2/2
4	09R	i	301	-	-	0/4/13/13	0/2/2/2
4	09R	m	301	-	-	0/4/13/13	0/2/2/2
4	09R	D	301	-	-	0/4/13/13	0/2/2/2
4	09R	J	301	-	-	0/4/13/13	0/2/2/2
4	09R	G	301	-	-	0/4/13/13	0/2/2/2
4	09R	N	301	-	-	0/4/13/13	0/2/2/2
4	09R	X	301	-	-	0/4/13/13	0/2/2/2
5	NAG	d	302	1	-	4/6/23/26	0/1/1/1
4	09R	C	301	-	-	0/4/13/13	0/2/2/2
4	09R	S	301	-	-	0/4/13/13	0/2/2/2
4	09R	f	301	-	-	0/4/13/13	0/2/2/2
4	09R	j	301	-	-	0/4/13/13	0/2/2/2
4	09R	b	301	-	-	0/4/13/13	0/2/2/2
4	09R	K	301	-	-	0/4/13/13	0/2/2/2
4	09R	c	301	-	-	0/4/13/13	0/2/2/2
4	09R	l	301	-	-	0/4/13/13	0/2/2/2
4	09R	T	301	-	-	0/4/13/13	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	09R	R	301	-	-	0/4/13/13	0/2/2/2
4	09R	d	301	-	-	0/4/13/13	0/2/2/2
4	09R	f	302	-	-	0/4/13/13	0/2/2/2
4	09R	Y	301	-	-	0/4/13/13	0/2/2/2
4	09R	A	301	-	-	0/4/13/13	0/2/2/2
5	NAG	O	302	1	-	2/6/23/26	0/1/1/1
4	09R	a	301	-	-	1/4/13/13	0/2/2/2
4	09R	L	301	-	-	0/4/13/13	0/2/2/2
4	09R	n	301	-	-	4/4/13/13	0/2/2/2
5	NAG	A	302	1	-	4/6/23/26	0/1/1/1
4	09R	U	301	-	-	0/4/13/13	0/2/2/2
4	09R	W	301	-	-	0/4/13/13	0/2/2/2
4	09R	Q	301	-	-	0/4/13/13	0/2/2/2
4	09R	O	301	-	-	0/4/13/13	0/2/2/2
4	09R	k	301	-	-	2/4/13/13	0/2/2/2
4	09R	M	301	-	-	0/4/13/13	0/2/2/2
4	09R	I	301	-	-	0/4/13/13	0/2/2/2
4	09R	P	301	-	-	0/4/13/13	0/2/2/2
4	09R	H	301	-	-	0/4/13/13	0/2/2/2

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	301	09R	BR1-C5	-13.19	1.71	1.90
4	m	301	09R	BR1-C5	-12.64	1.71	1.90
4	N	301	09R	BR1-C5	-12.04	1.72	1.90
4	d	301	09R	BR1-C5	-11.92	1.72	1.90
4	i	301	09R	BR1-C5	-11.85	1.73	1.90

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	302	NAG	C1-O5-C5	7.90	122.89	112.19
5	d	302	NAG	C1-O5-C5	7.89	122.88	112.19
5	A	302	NAG	C2-N2-C7	7.28	133.27	122.90
5	d	302	NAG	C2-N2-C7	7.28	133.26	122.90
5	O	302	NAG	C1-O5-C5	6.84	121.46	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

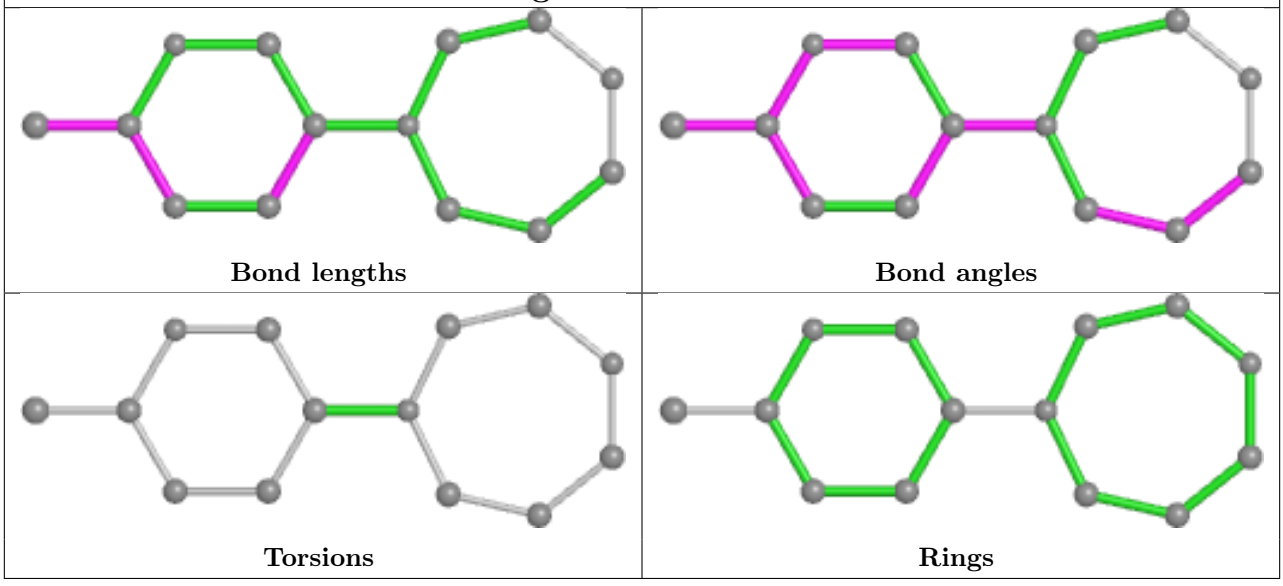
Mol	Chain	Res	Type	Atoms
5	O	302	NAG	O5-C5-C6-O6
5	O	302	NAG	C4-C5-C6-O6
5	A	302	NAG	C8-C7-N2-C2
5	A	302	NAG	O7-C7-N2-C2
5	d	302	NAG	C8-C7-N2-C2

There are no ring outliers.

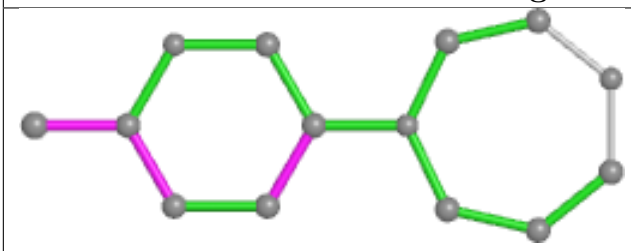
No monomer is involved in short contacts.

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.

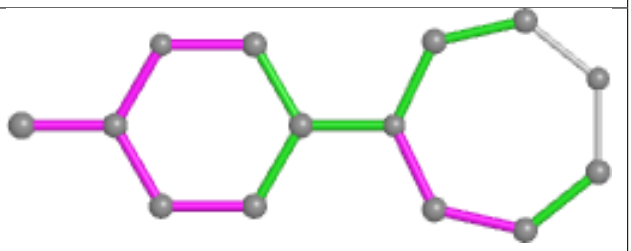
Ligand 09R E 301



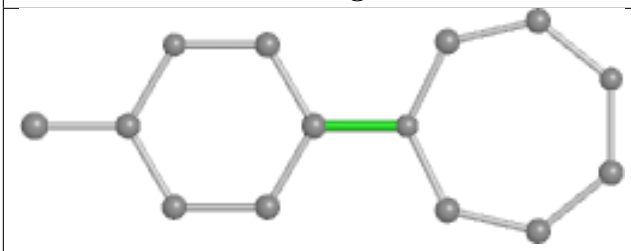
Ligand 09R V 302



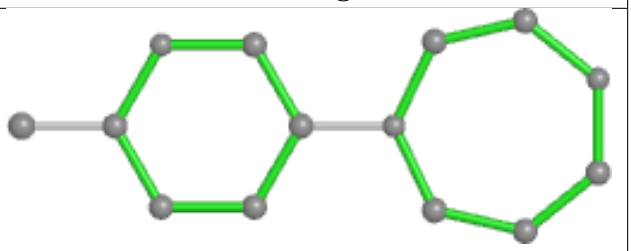
Bond lengths



Bond angles

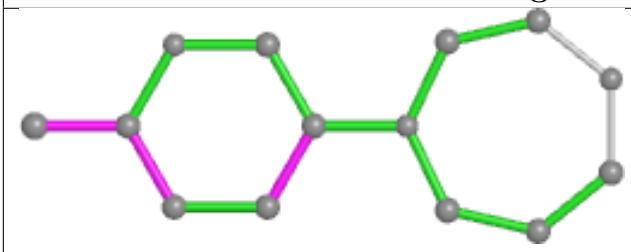


Torsions



Rings

Ligand 09R B 301



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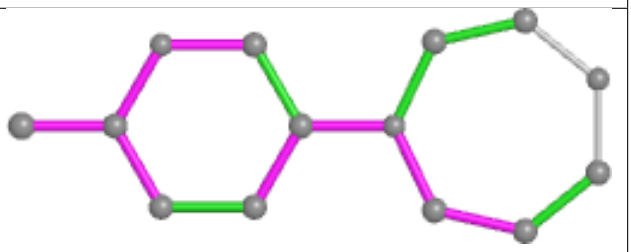

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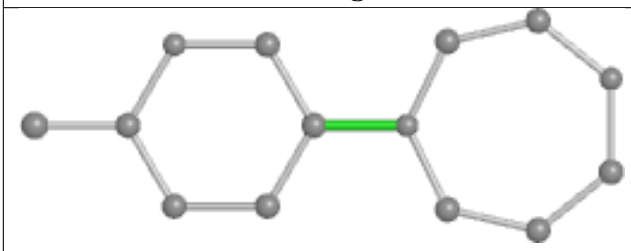

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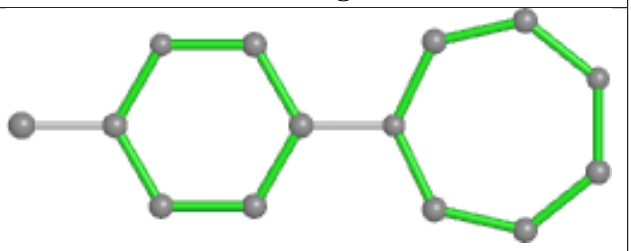

Rings

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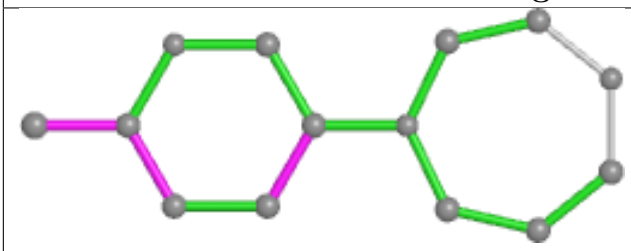

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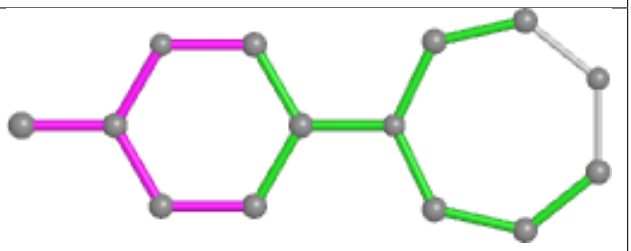

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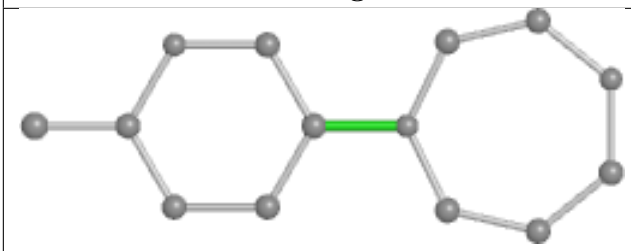

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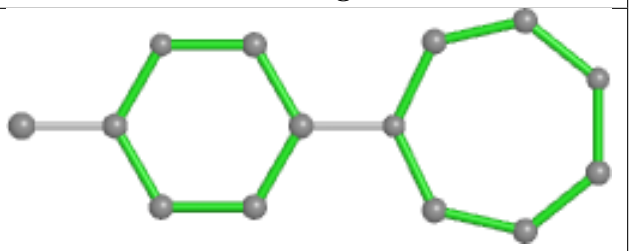

Rings

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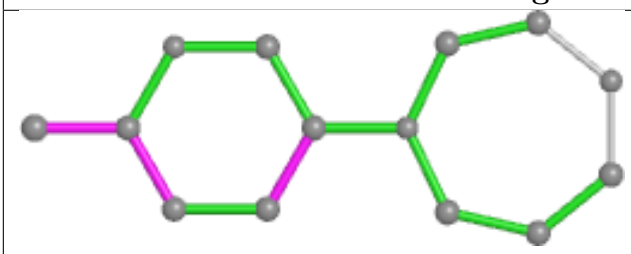

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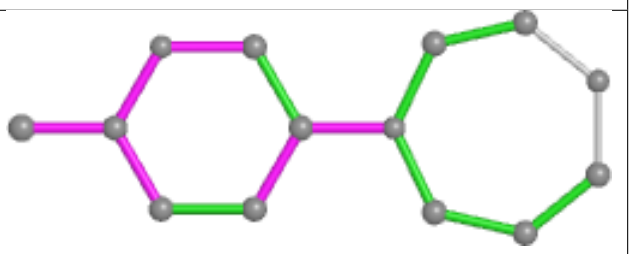

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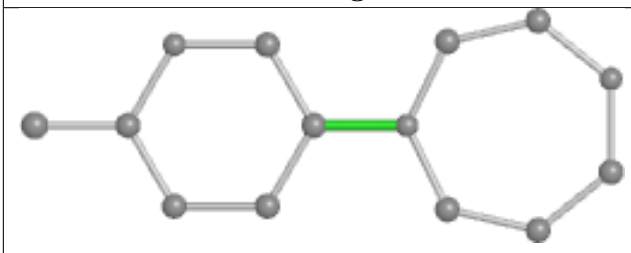

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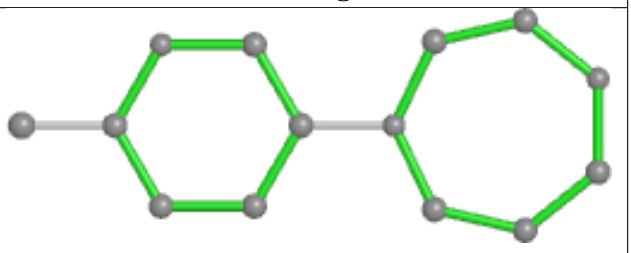

Rings

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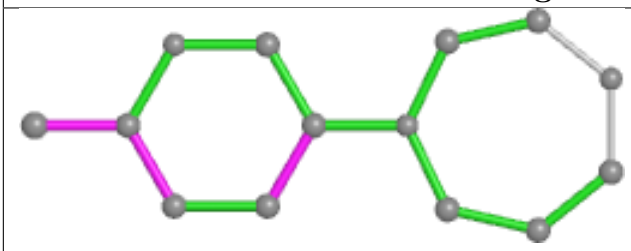

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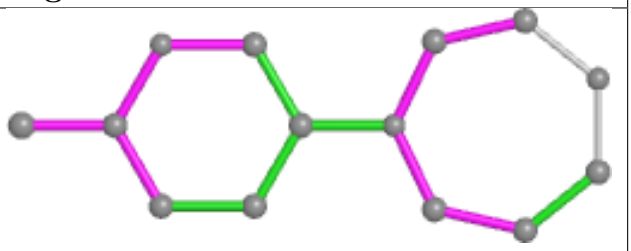

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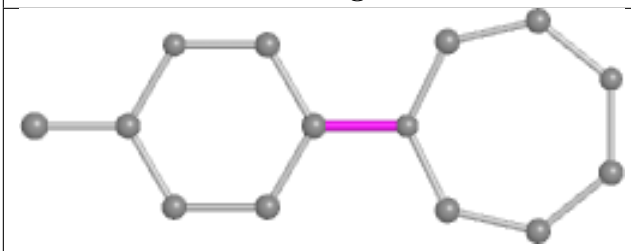

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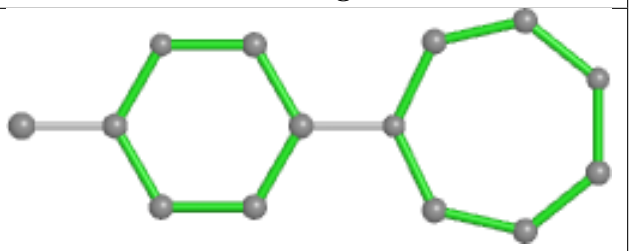

Rings

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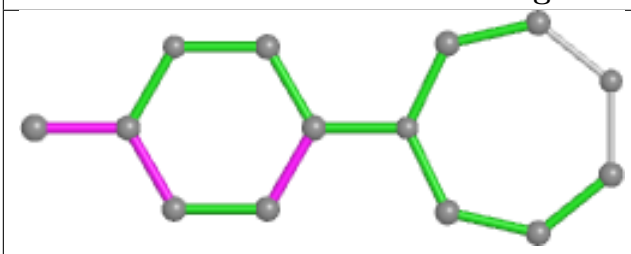

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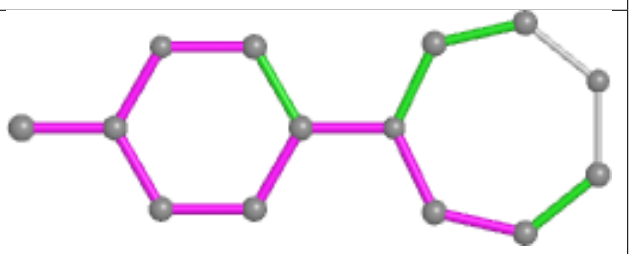

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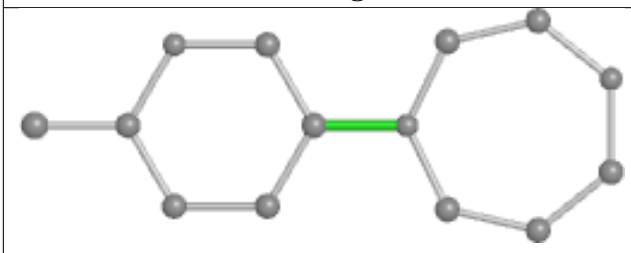

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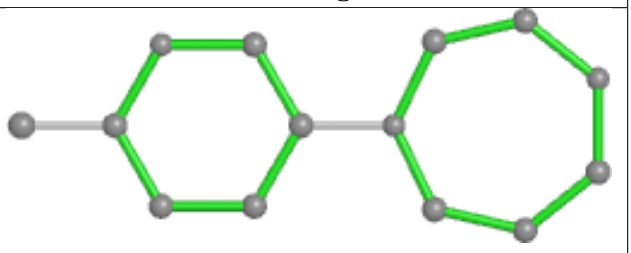

Rings

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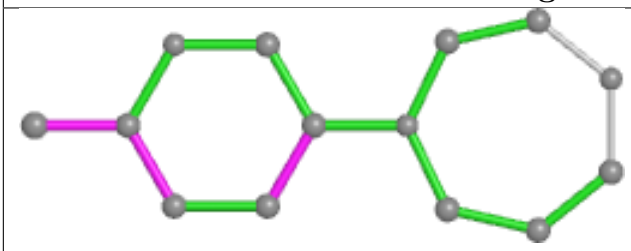

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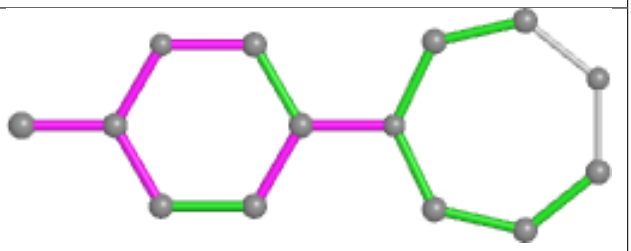

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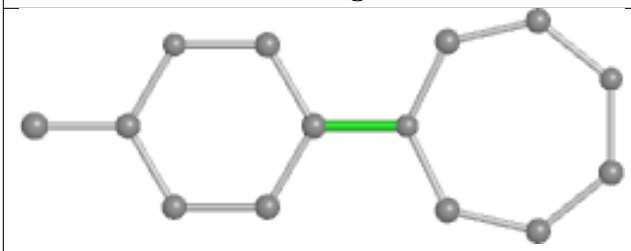

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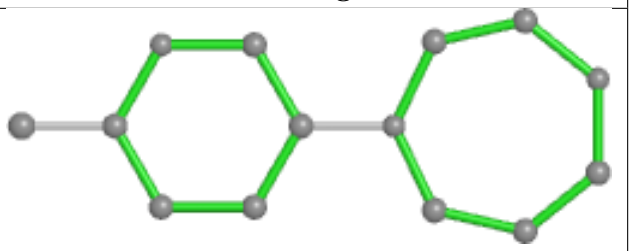

Rings

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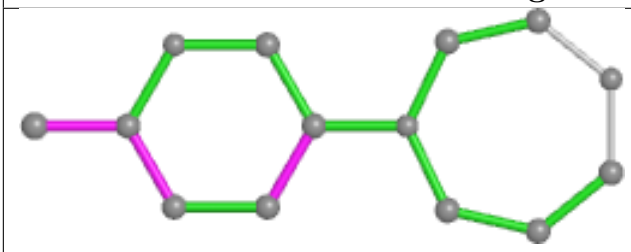

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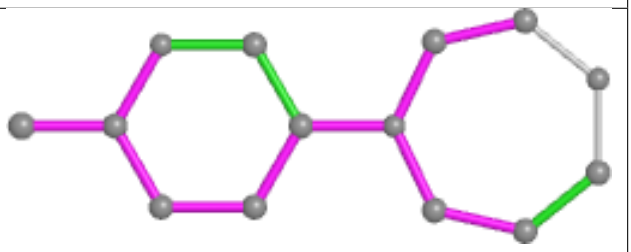

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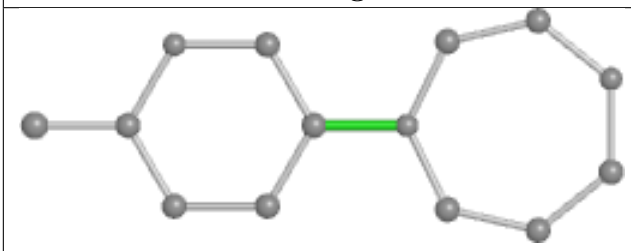

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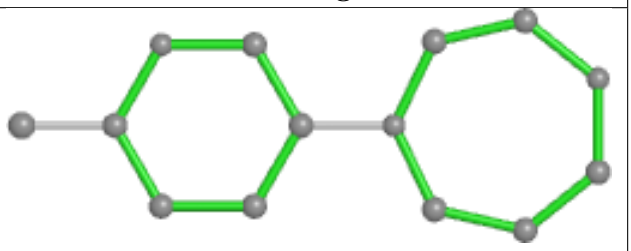

Rings

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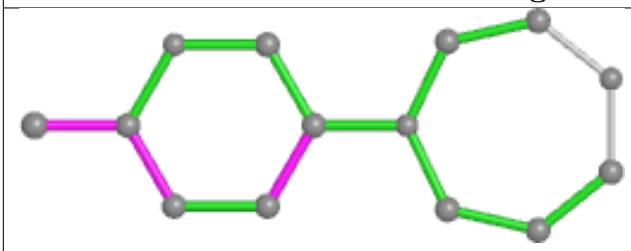

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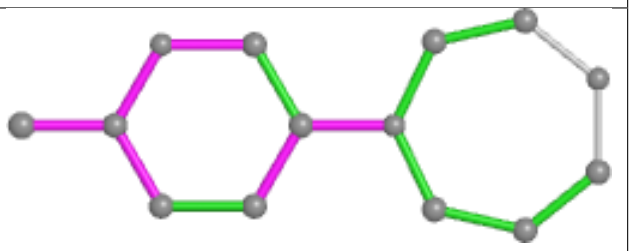

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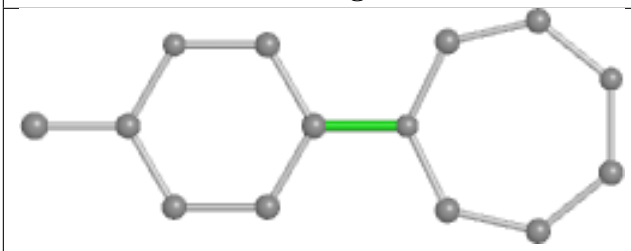

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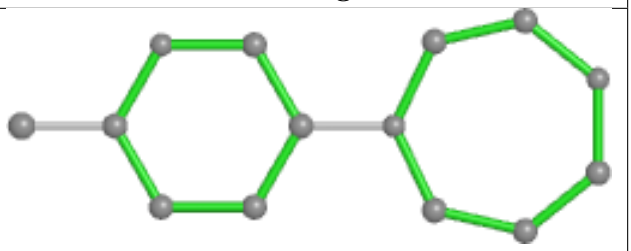

Rings

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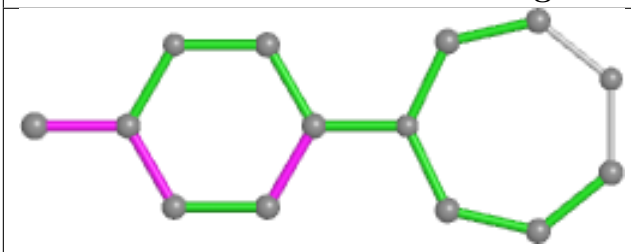

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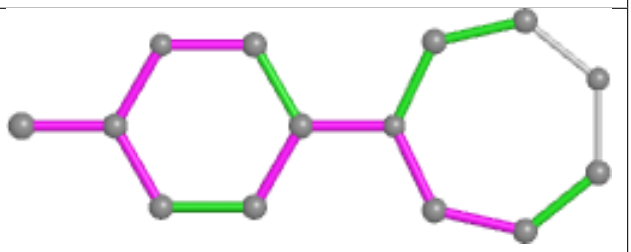

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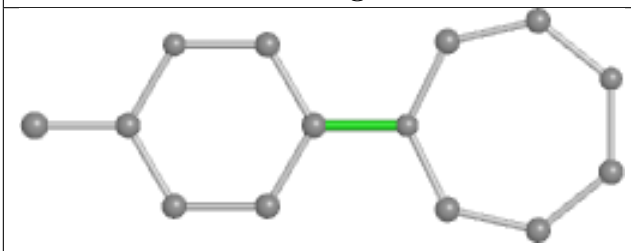

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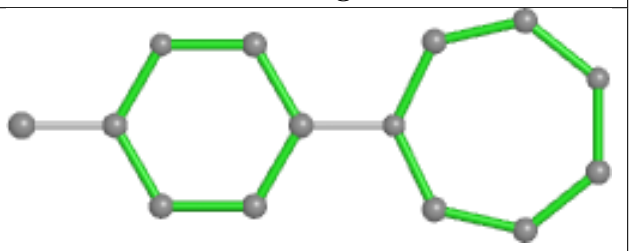

Rings

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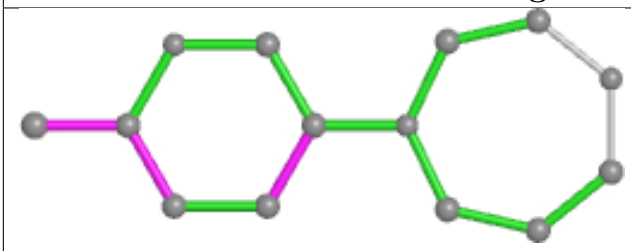

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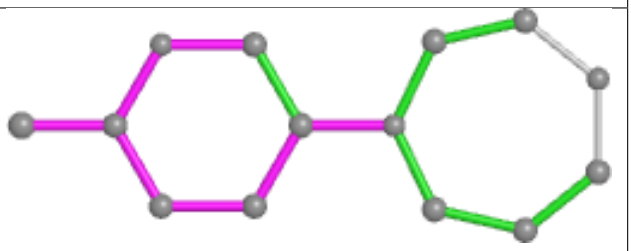

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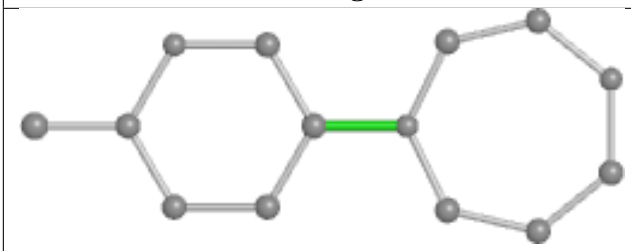

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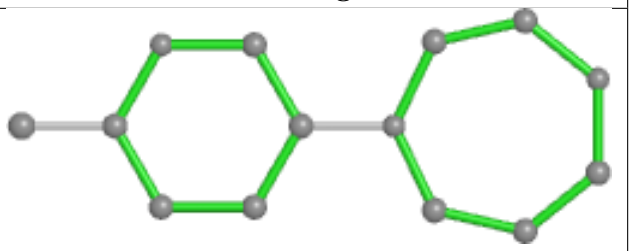

Rings

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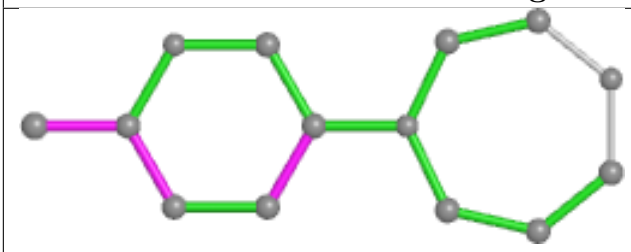

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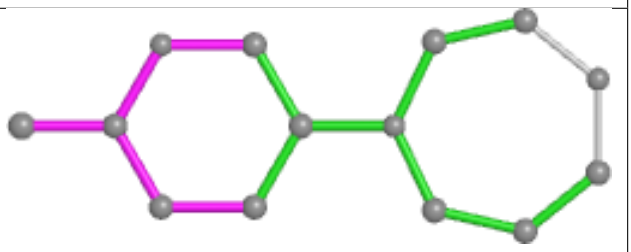

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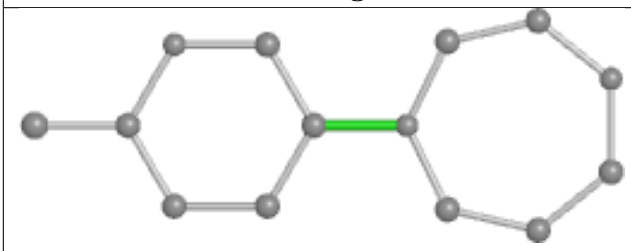

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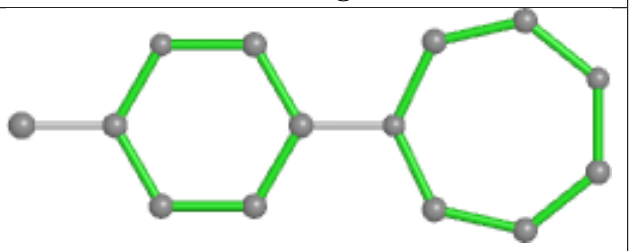

Rings

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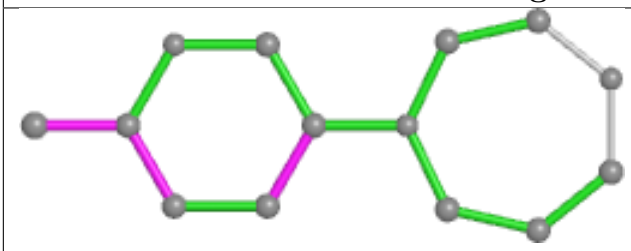

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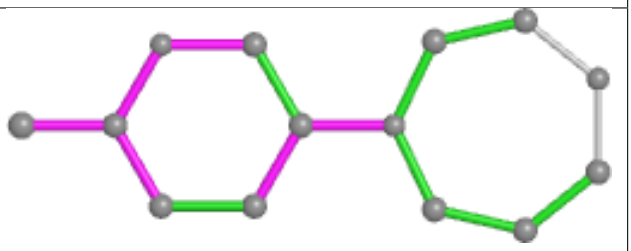

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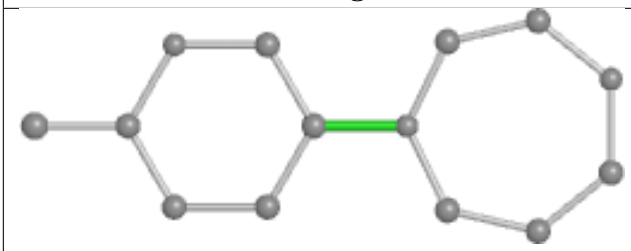

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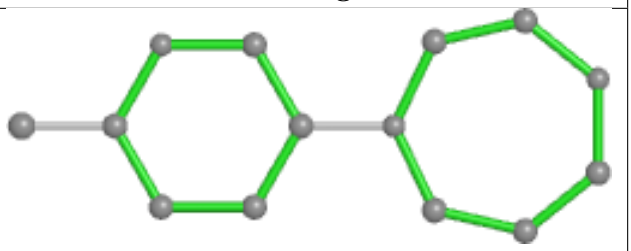
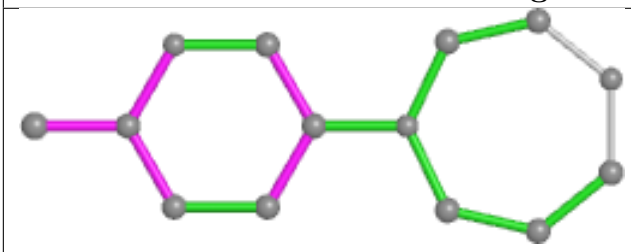


Rings

Ligand 09R C 301



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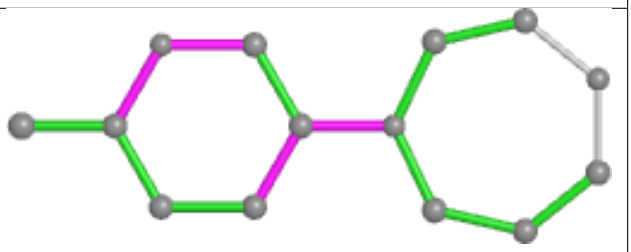

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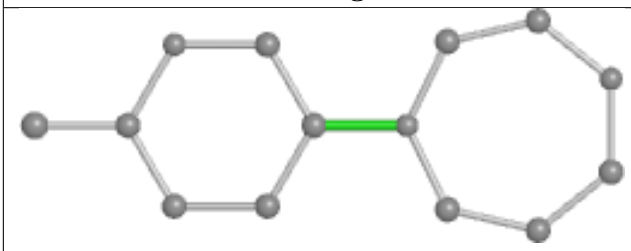
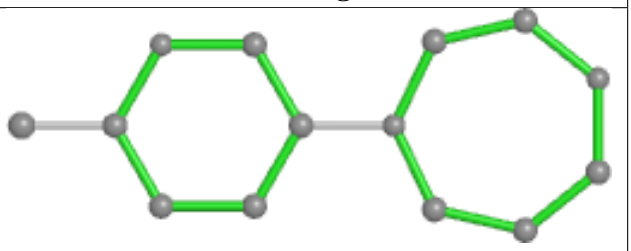
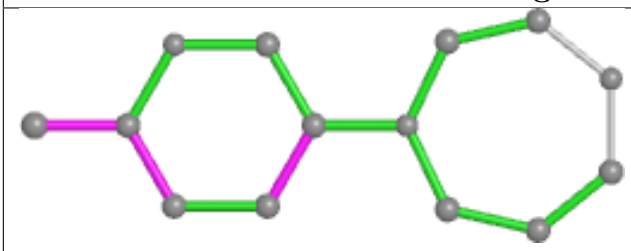


Torsions



Rings

Ligand 09R S 301



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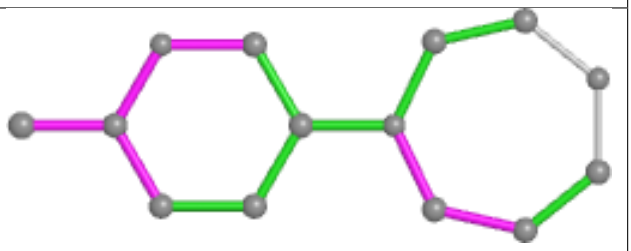
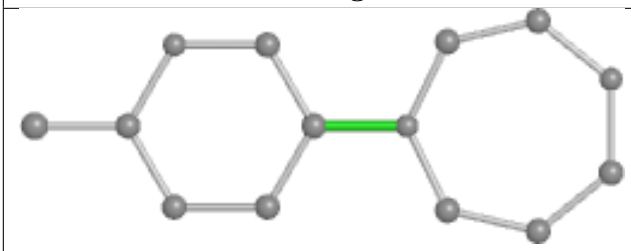


Bond angles



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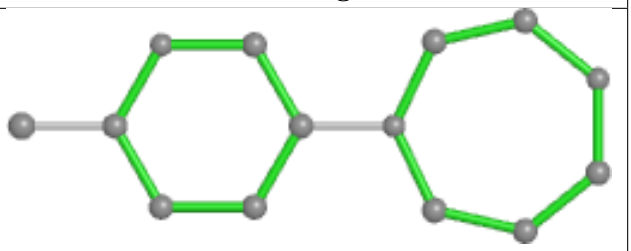

Rings

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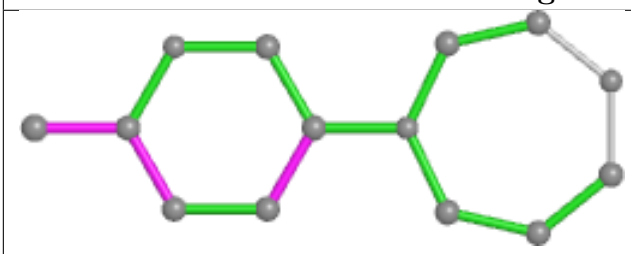

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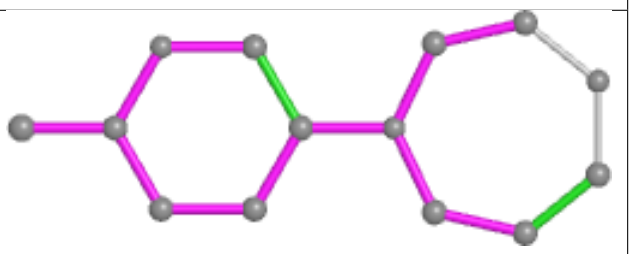

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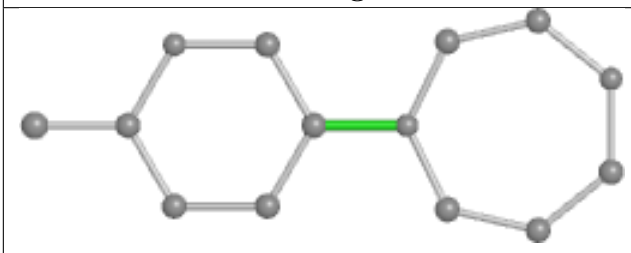

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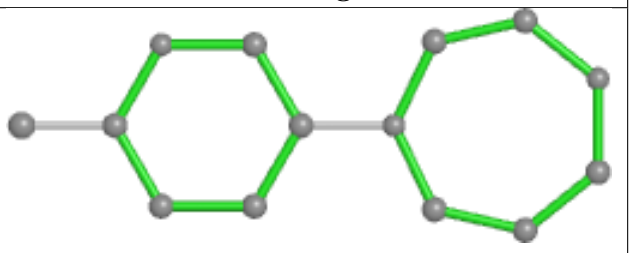

Rings

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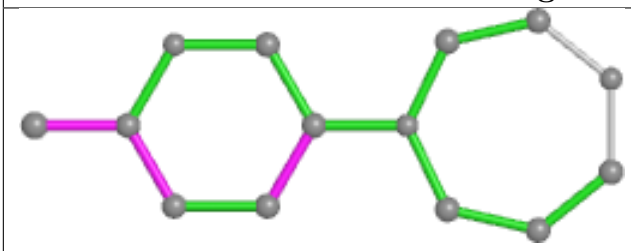

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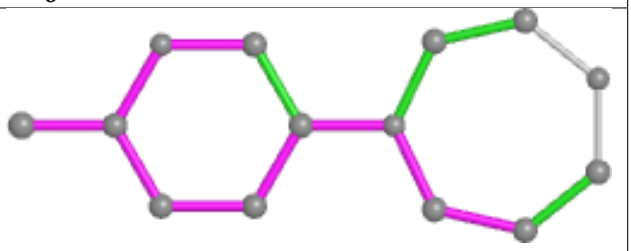

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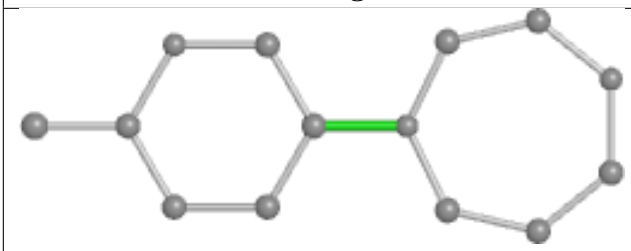

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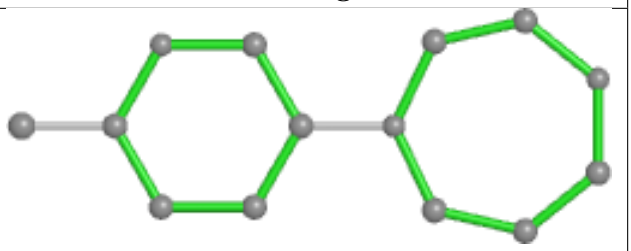

Rings

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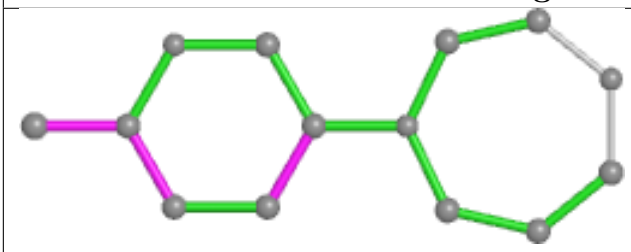

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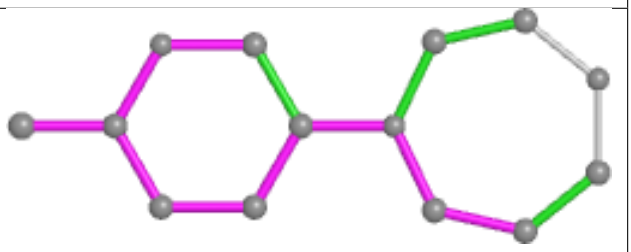

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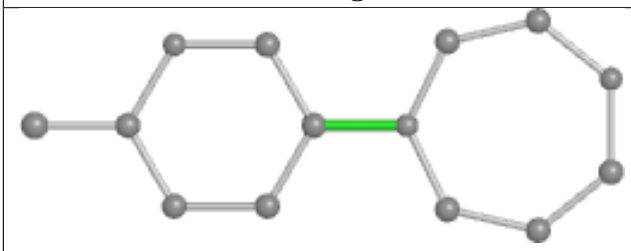

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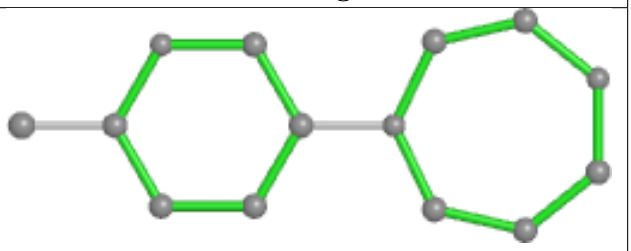

Rings

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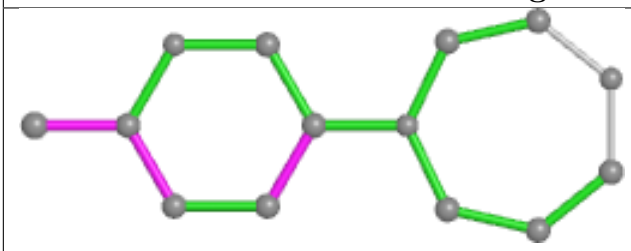

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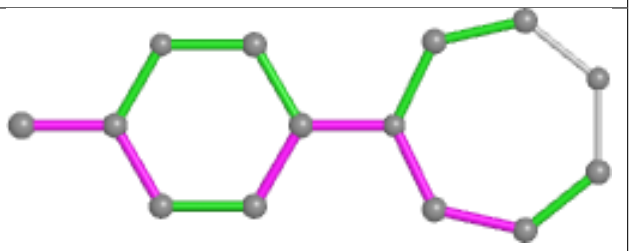

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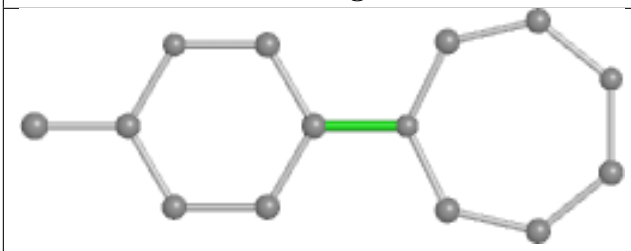

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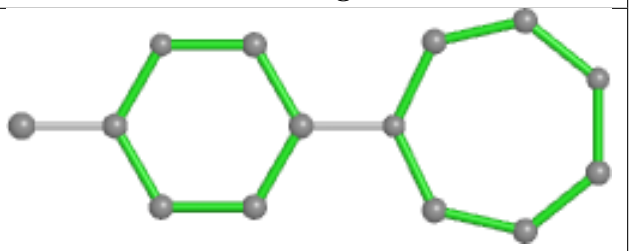

Rings

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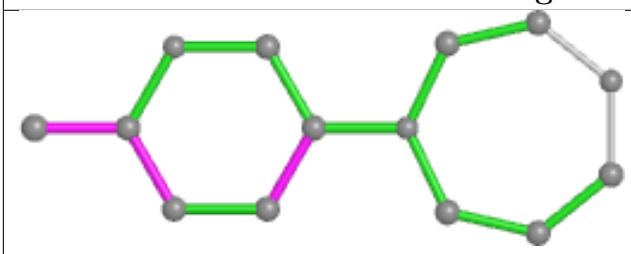

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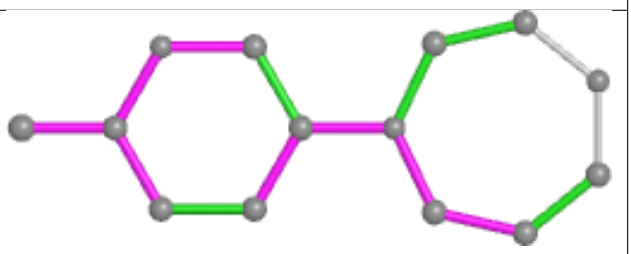

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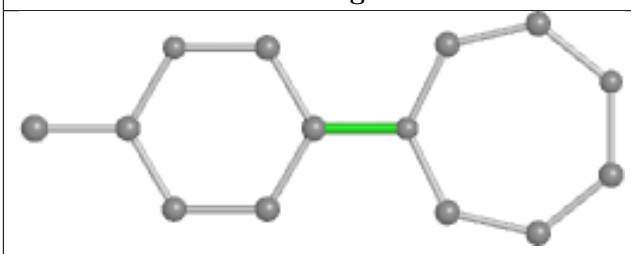

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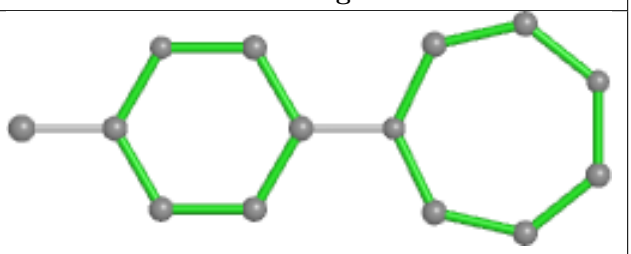

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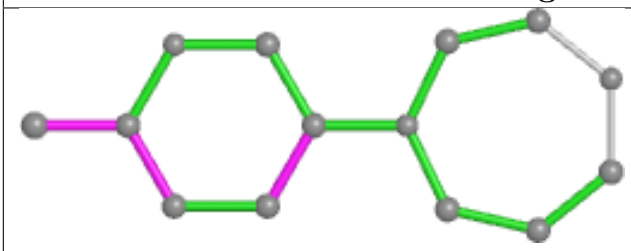

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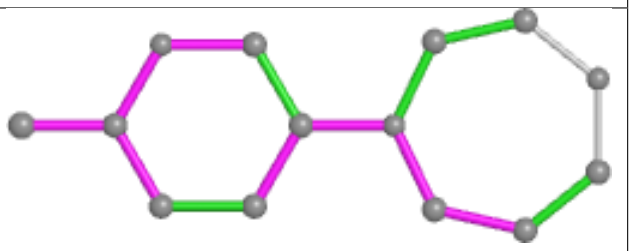

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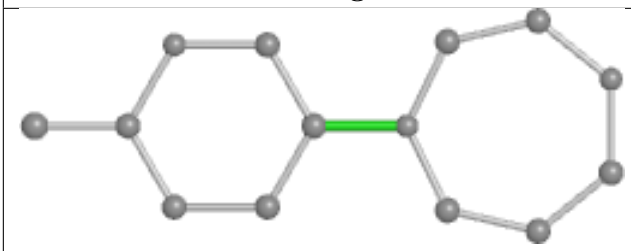

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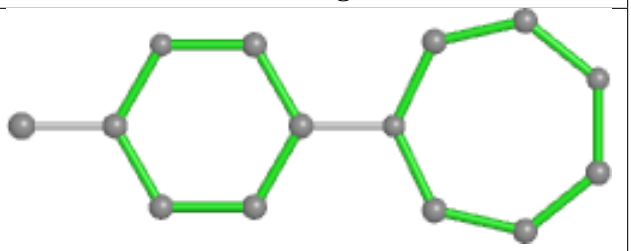

Rings

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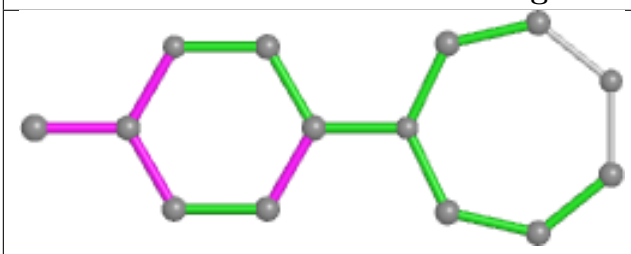

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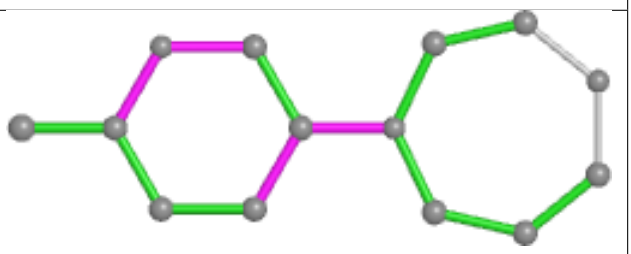

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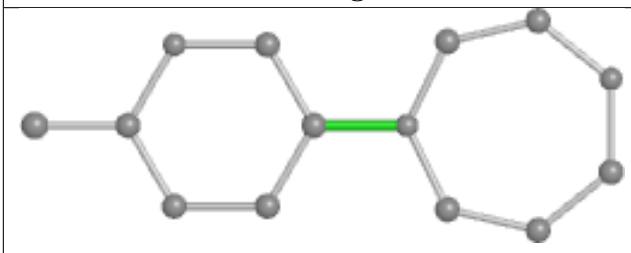

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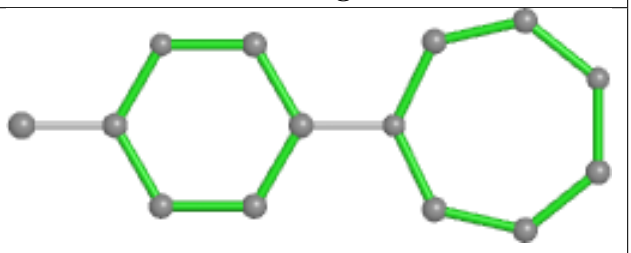

Rings

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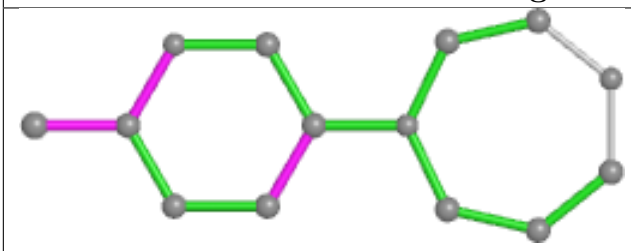

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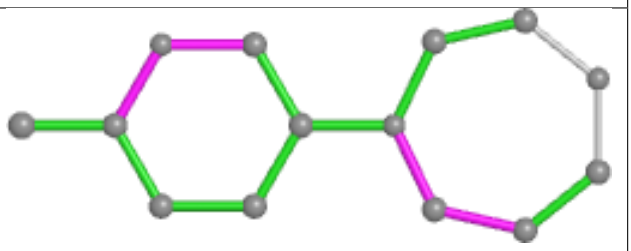

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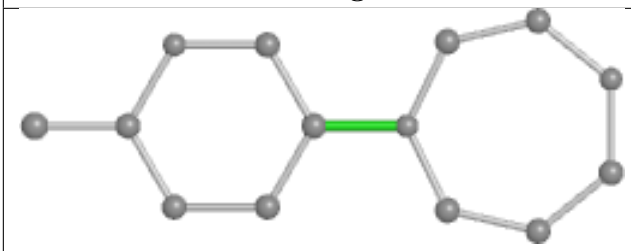

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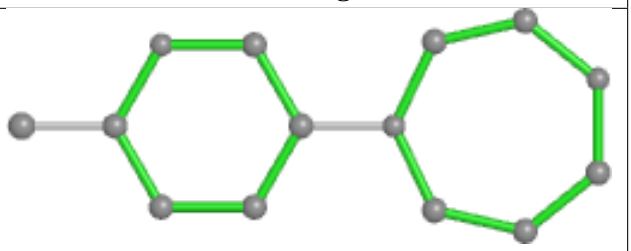

Rings

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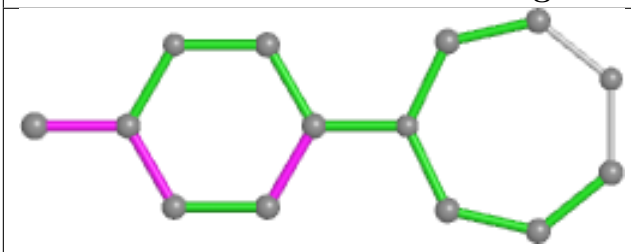

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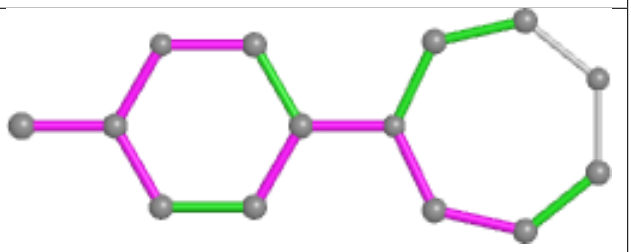

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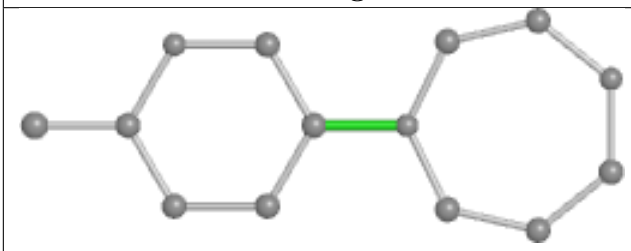

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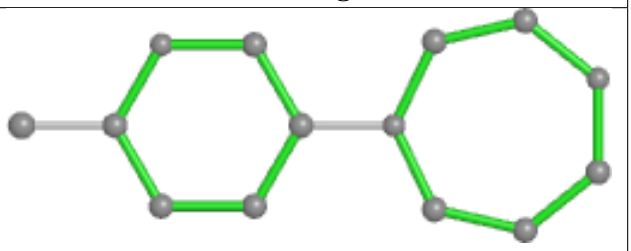

Rings

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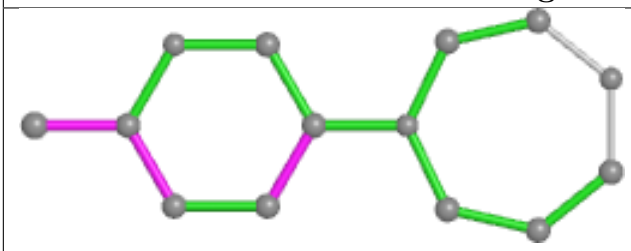

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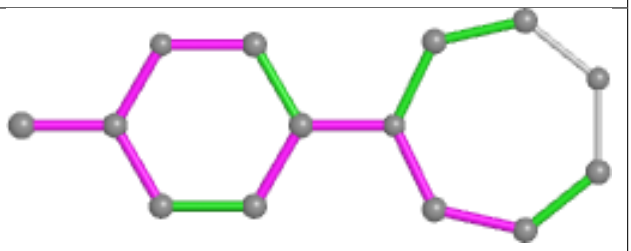

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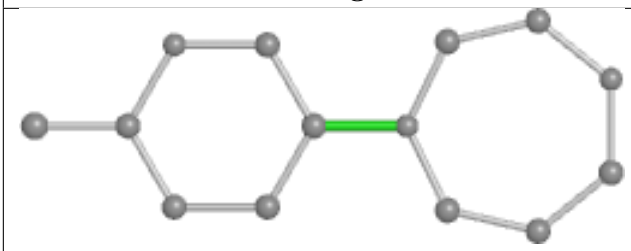

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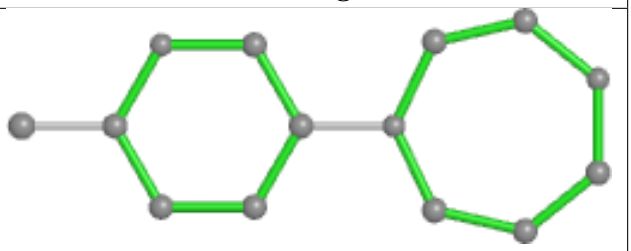

Rings

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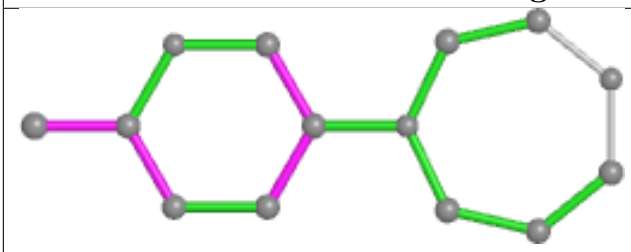

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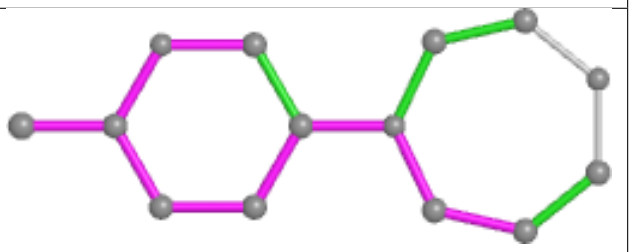

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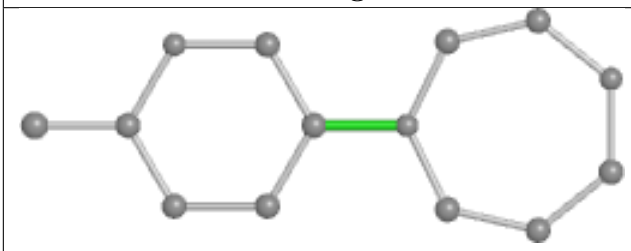

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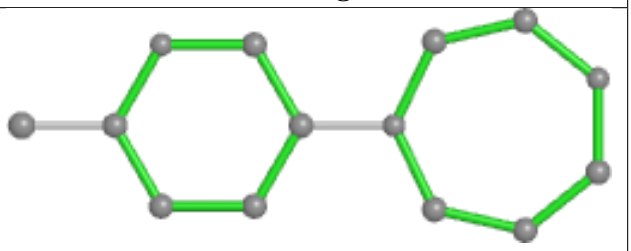

Rings

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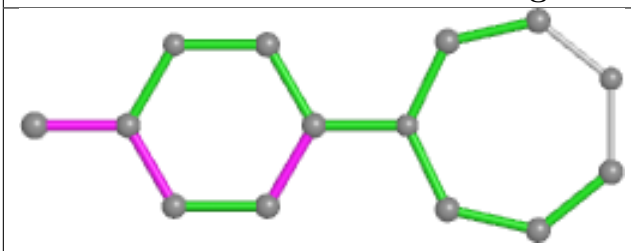

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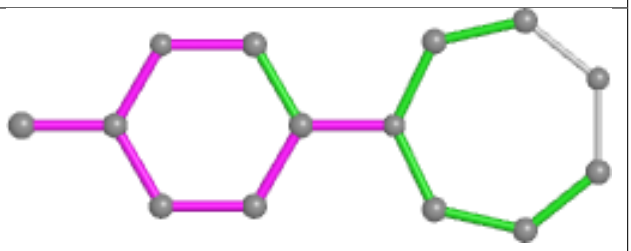

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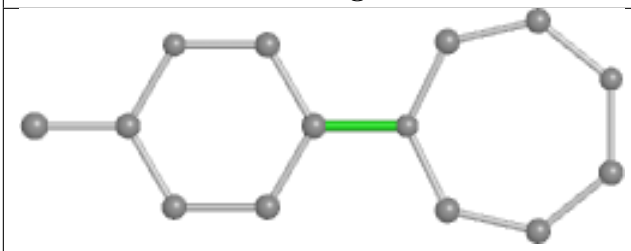

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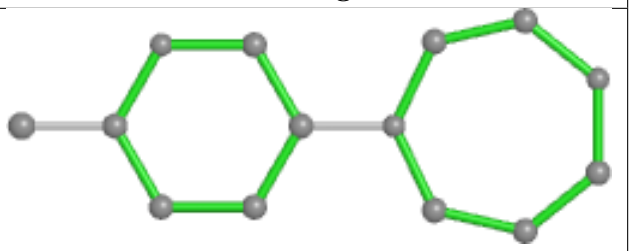
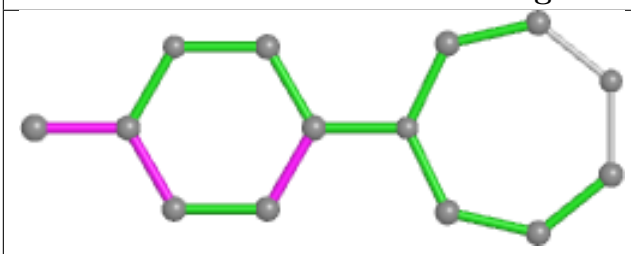
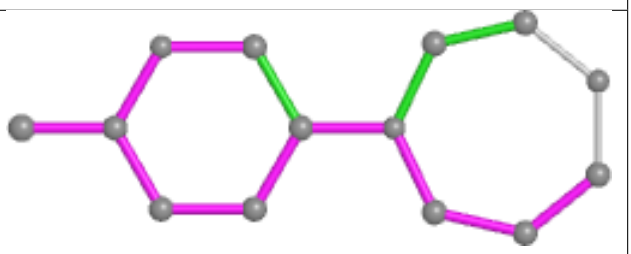


Rings

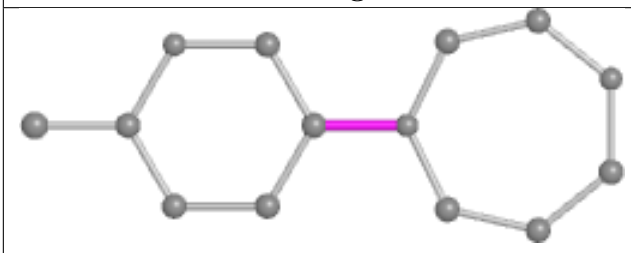
Ligand 09R a 301



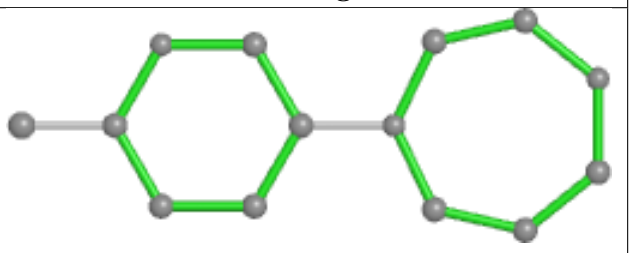
Bond lengths



Bond angles

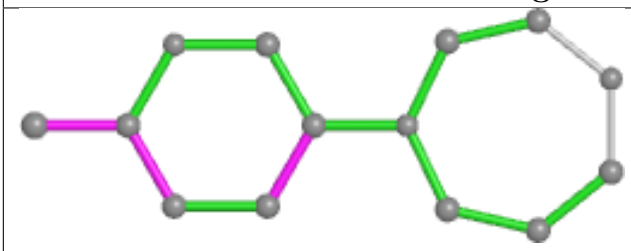


Torsions



Rings

Ligand 09R L 301



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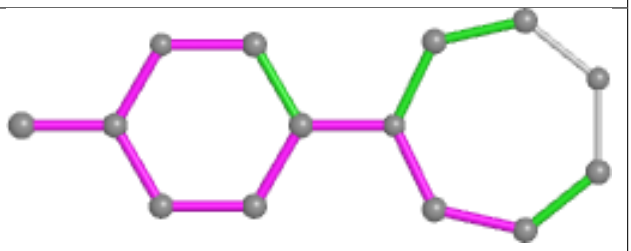

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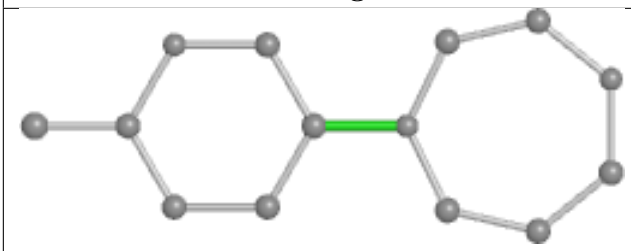

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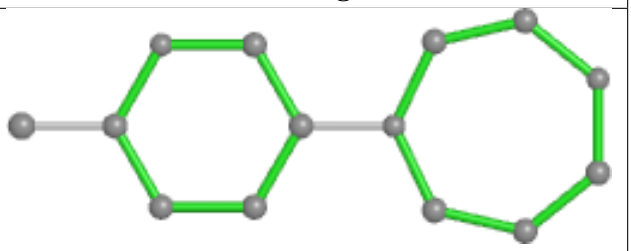
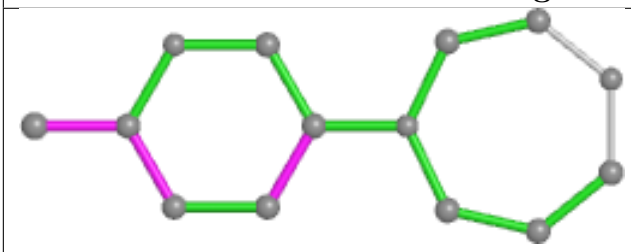


Rings

Ligand 09R n 301



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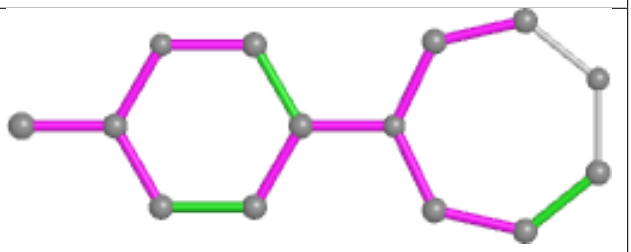

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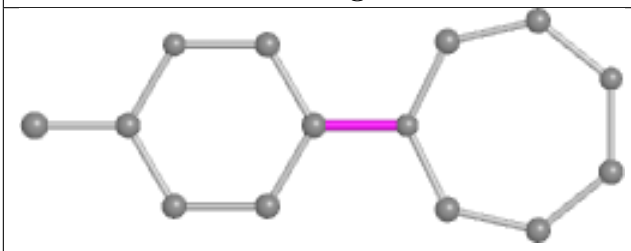

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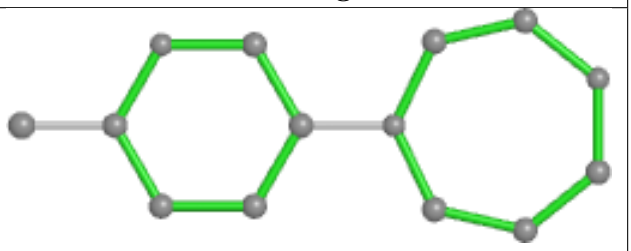
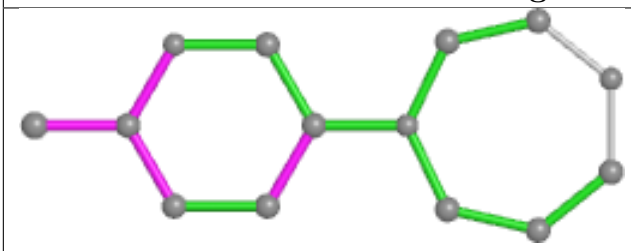


Rings

Ligand 09R U 301



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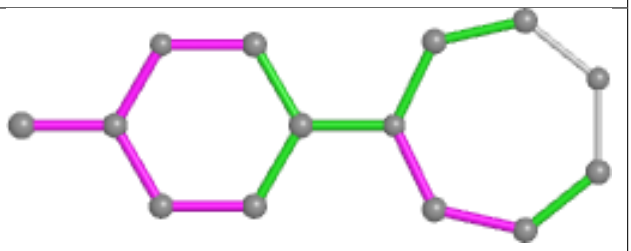

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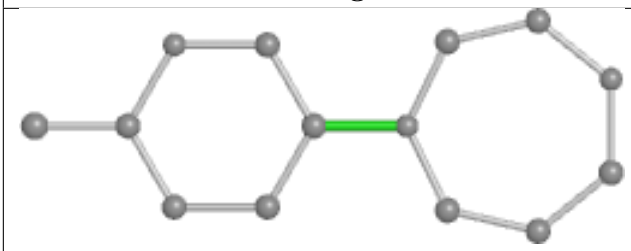

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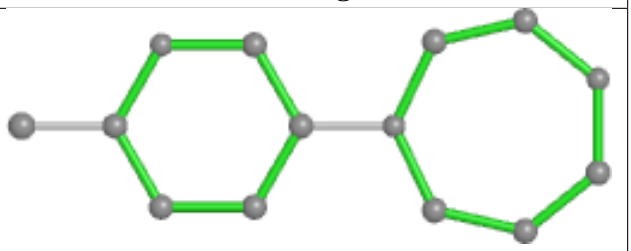
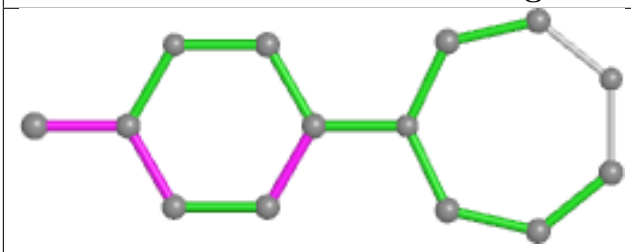


Rings

Ligand 09R W 301



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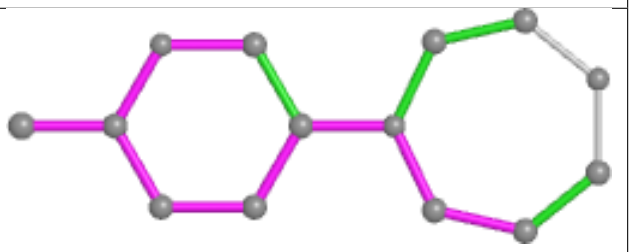

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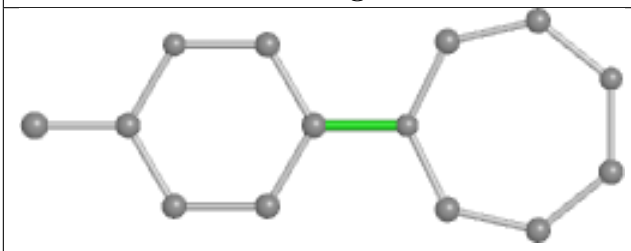

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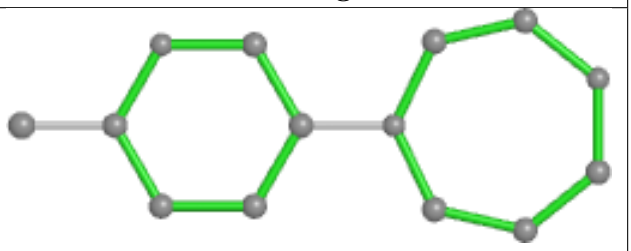

Rings

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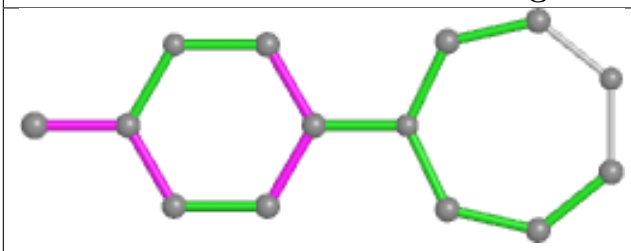

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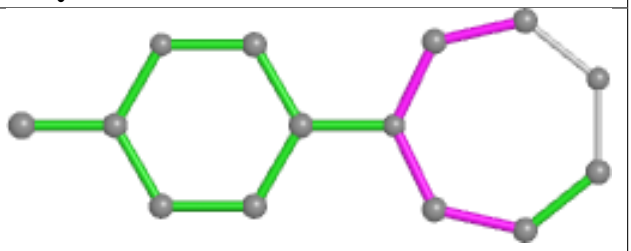

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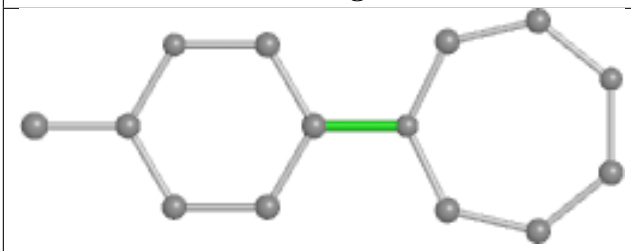

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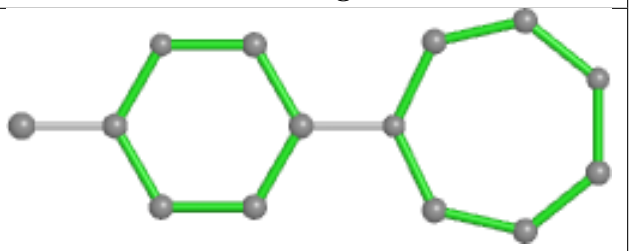

Rings

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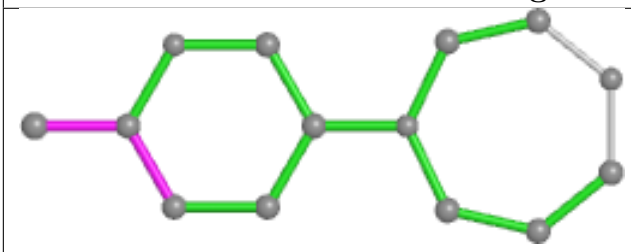

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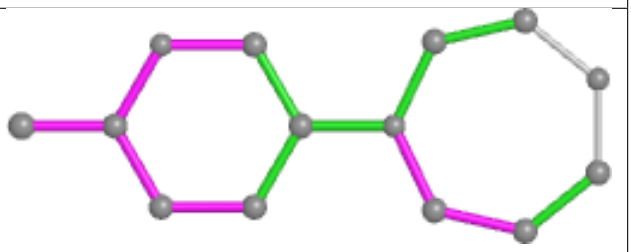

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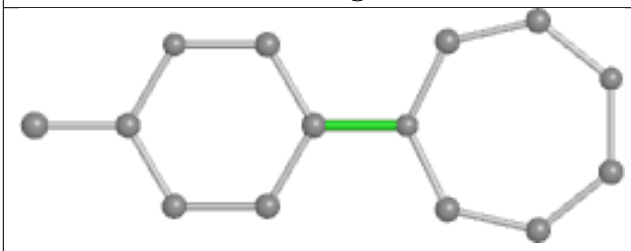

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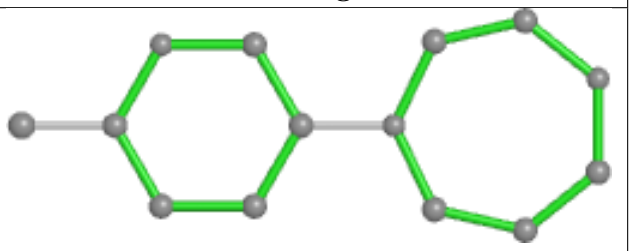
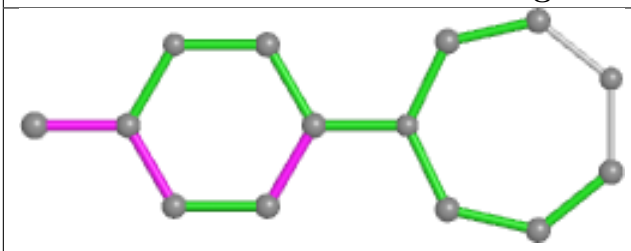


Rings

Ligand 09R k 301



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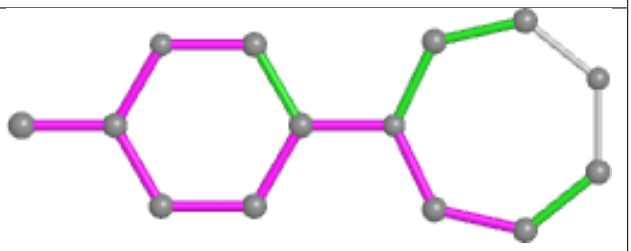

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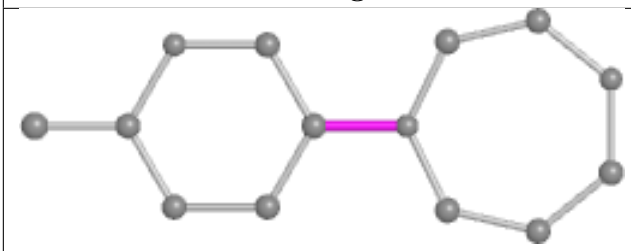

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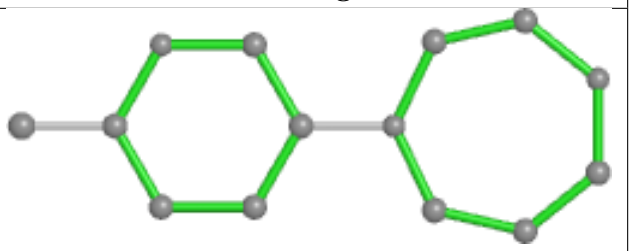
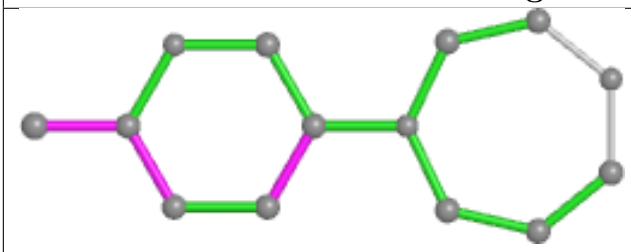


Rings

Ligand 09R M 301



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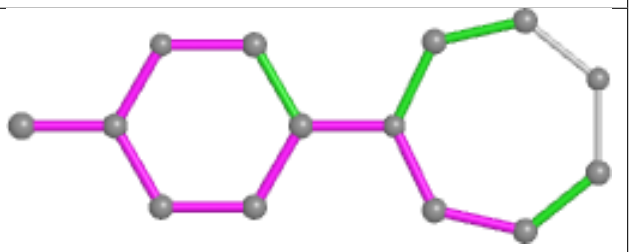

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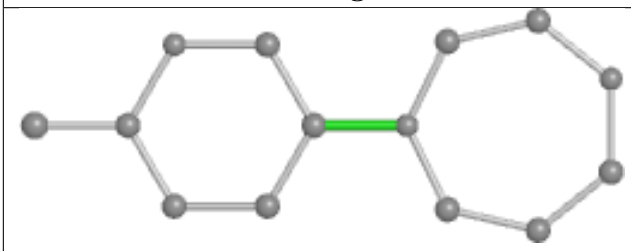

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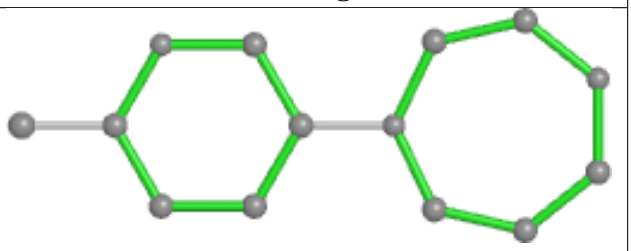
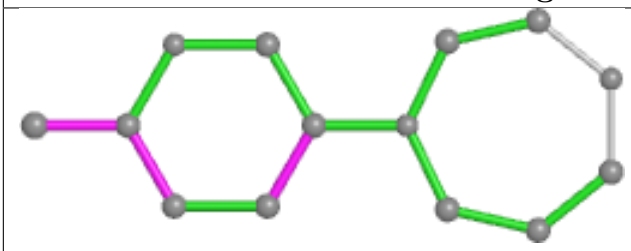


Rings

Ligand 09R I 301



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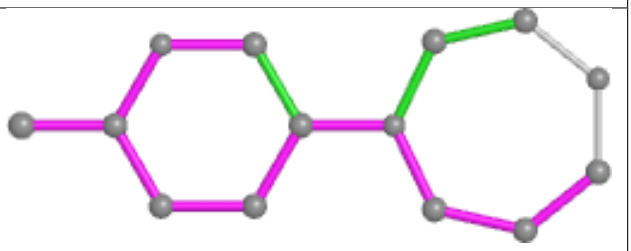

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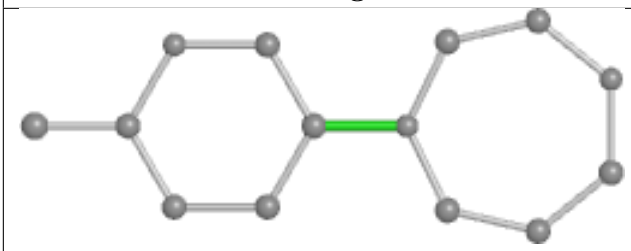

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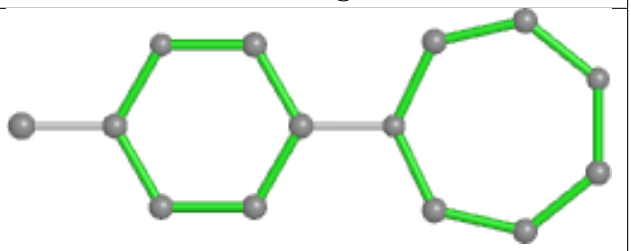
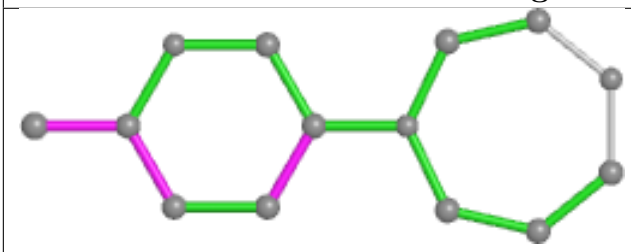


Rings

Ligand 09R P 301



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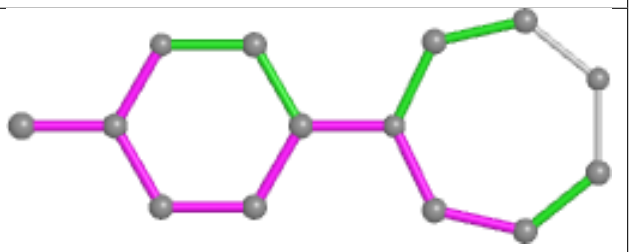

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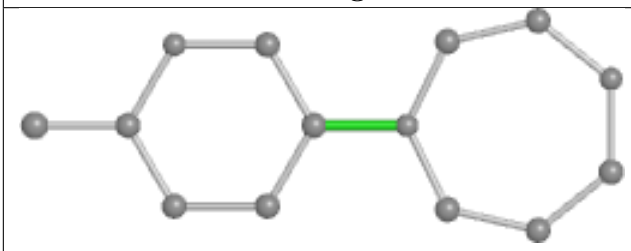

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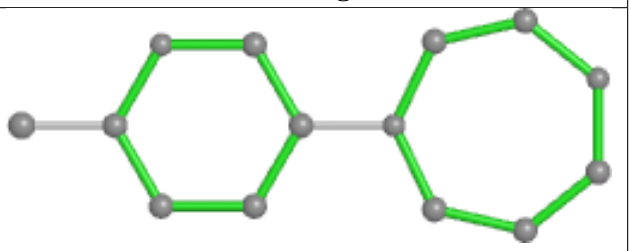
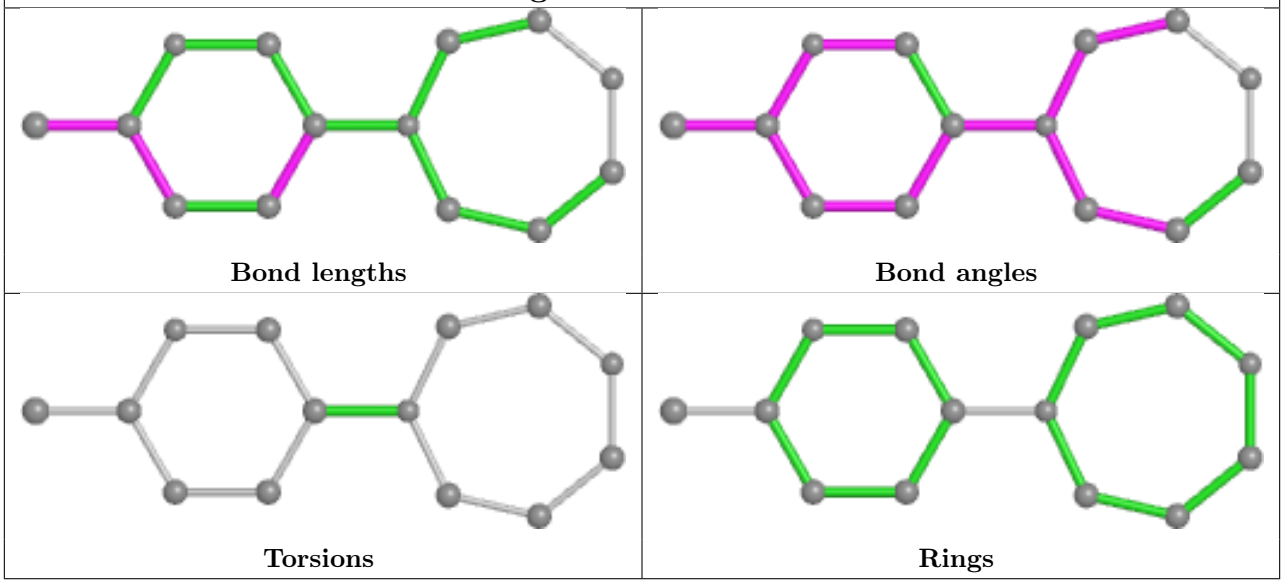


Rings

Ligand 09R H 301



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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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