wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2023 – 09:50 AM EDT

PDB ID	:	3U8M
Title	:	Crystal structure of the acetylcholine binding protein (AChBP) from Lymnaea stagnalis in complex with NS3920 (1-(6-bromopyridin-3-yl)-1,4-diazepane)
Authors	:	Rohde, L.A.H.; Ahring, P.K.; Jensen, M.L.; Nielsen, E.O.; Peters, D.; Helgstrand, C.; Krintel, C.; Harpsoe, K.; Gajhede, M.; Kastrup, J.S.; Balle, T.
Deposited on	:	2011-10-17
Resolution	:	2.70 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:

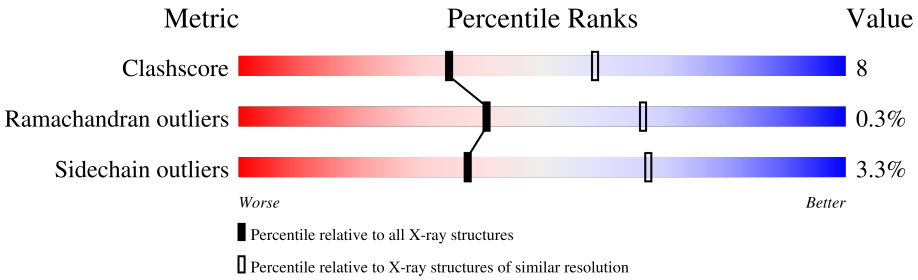
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

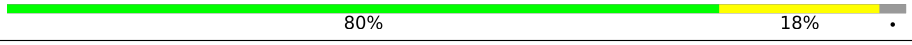
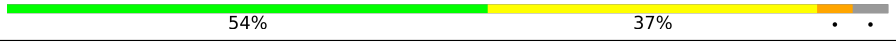
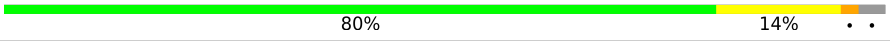
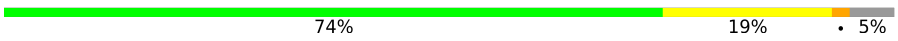
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	210	84% 11% • •
1	B	210	80% 14% • 5%
1	C	210	83% 12% •
1	D	210	77% 18% • •
1	E	210	81% 12% 7%
1	F	210	82% 16% •
1	G	210	78% 16% 5%
1	H	210	81% 13% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	210	
1	J	210	
1	K	210	
1	L	210	
1	M	210	
1	N	210	
1	O	210	
1	P	210	
1	Q	210	
1	R	210	
1	S	210	
1	T	210	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32783 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.

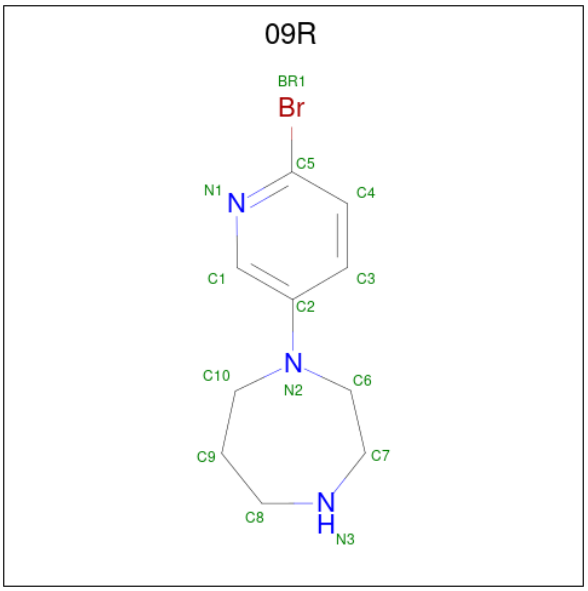
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	1	0
			1623	1017	279	322	5			
1	B	199	Total	C	N	O	S	0	0	0
			1590	999	273	313	5			
1	C	201	Total	C	N	O	S	0	0	0
			1609	1009	278	317	5			
1	D	202	Total	C	N	O	S	0	1	0
			1617	1013	276	323	5			
1	E	196	Total	C	N	O	S	0	1	0
			1575	992	270	308	5			
1	F	205	Total	C	N	O	S	0	0	0
			1639	1025	282	327	5			
1	G	199	Total	C	N	O	S	0	0	0
			1590	999	273	313	5			
1	H	198	Total	C	N	O	S	0	0	0
			1584	996	272	311	5			
1	I	204	Total	C	N	O	S	0	0	0
			1629	1019	281	324	5			
1	J	201	Total	C	N	O	S	0	0	0
			1608	1008	275	320	5			
1	K	204	Total	C	N	O	S	0	0	0
			1632	1021	281	325	5			
1	L	203	Total	C	N	O	S	0	0	0
			1623	1016	280	322	5			
1	M	200	Total	C	N	O	S	0	1	0
			1604	1007	274	318	5			
1	N	201	Total	C	N	O	S	0	1	0
			1611	1010	275	320	6			
1	O	197	Total	C	N	O	S	0	0	0
			1580	994	271	310	5			
1	P	200	Total	C	N	O	S	0	0	0
			1597	1003	274	315	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	199	Total	C	N	O	S	0	0	0
			1590	999	273	313	5			
1	R	199	Total	C	N	O	S	0	1	0
			1593	1001	273	314	5			
1	S	200	Total	C	N	O	S	0	0	0
			1598	1003	274	316	5			
1	T	200	Total	C	N	O	S	0	0	0
			1598	1003	274	316	5			

- Molecule 2 is 1-(6-bromopyridin-3-yl)-1,4-diazepane (three-letter code: 09R) (formula: $C_{10}H_{14}BrN_3$).



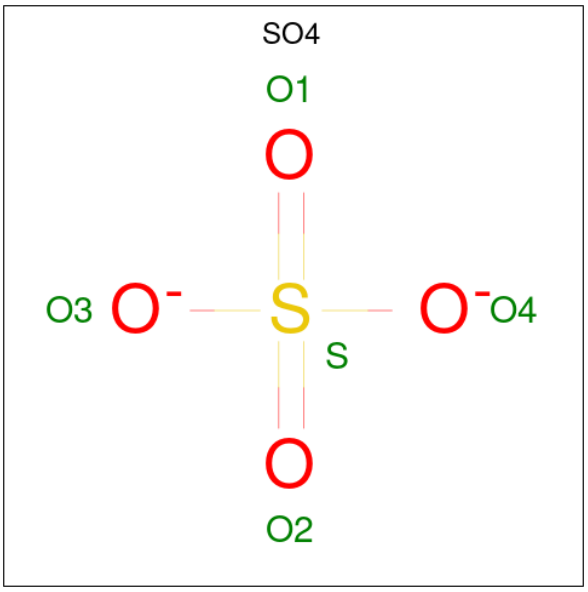
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Br	C	N	0	0
			14	1	10	3		
2	B	1	Total	Br	C	N	0	0
			14	1	10	3		
2	C	1	Total	Br	C	N	0	0
			14	1	10	3		
2	D	1	Total	Br	C	N	0	0
			14	1	10	3		
2	E	1	Total	Br	C	N	0	0
			14	1	10	3		
2	F	1	Total	Br	C	N	0	0
			14	1	10	3		
2	G	1	Total	Br	C	N	0	0
			14	1	10	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	Br	C	N	0	0
			14	1	10	3		
2	I	1	Total	Br	C	N	0	0
			14	1	10	3		
2	J	1	Total	Br	C	N	0	0
			14	1	10	3		
2	K	1	Total	Br	C	N	0	0
			14	1	10	3		
2	L	1	Total	Br	C	N	0	0
			14	1	10	3		
2	M	1	Total	Br	C	N	0	0
			14	1	10	3		
2	N	1	Total	Br	C	N	0	0
			14	1	10	3		
2	O	1	Total	Br	C	N	0	0
			14	1	10	3		
2	P	1	Total	Br	C	N	0	0
			14	1	10	3		
2	Q	1	Total	Br	C	N	0	0
			14	1	10	3		
2	R	1	Total	Br	C	N	0	0
			14	1	10	3		
2	S	1	Total	Br	C	N	0	0
			14	1	10	3		
2	T	1	Total	Br	C	N	0	0
			14	1	10	3		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	N	1	Total O S 5 4 1	0	0
3	R	1	Total O S 5 4 1	0	0
3	T	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	23	Total O 23 23	0	0
4	B	16	Total O 16 16	0	0
4	C	20	Total O 20 20	0	0
4	D	21	Total O 21 21	0	0
4	E	15	Total O 15 15	0	0
4	F	19	Total O 19 19	0	0
4	G	14	Total O 14 14	0	0
4	H	18	Total O 18 18	0	0
4	I	15	Total O 15 15	0	0
4	J	9	Total O 9 9	0	0
4	K	19	Total O 19 19	0	0
4	L	20	Total O 20 20	0	0
4	M	11	Total O 11 11	0	0
4	N	18	Total O 18 18	0	0
4	O	12	Total O 12 12	0	0
4	P	13	Total O 13 13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Q	19	Total O 19 19	0	0
4	R	13	Total O 13 13	0	0
4	S	14	Total O 14 14	0	0
4	T	19	Total O 19 19	0	0

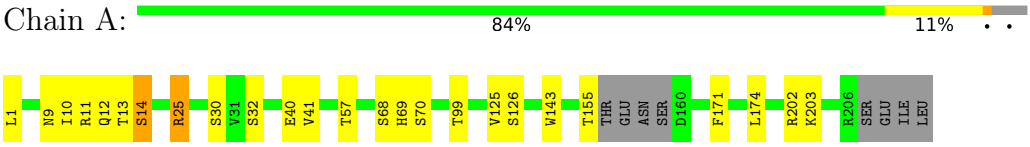
3 Residue-property plots (i)

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.

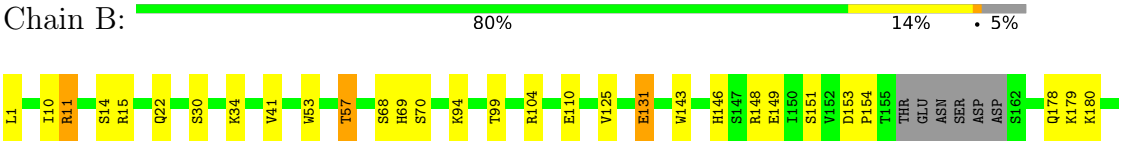
• Molecule 1: Acetylcholine-binding protein

Chain A:



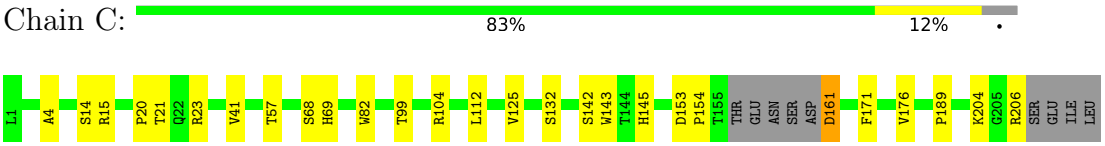
• Molecule 1: Acetylcholine-binding protein

Chain B:



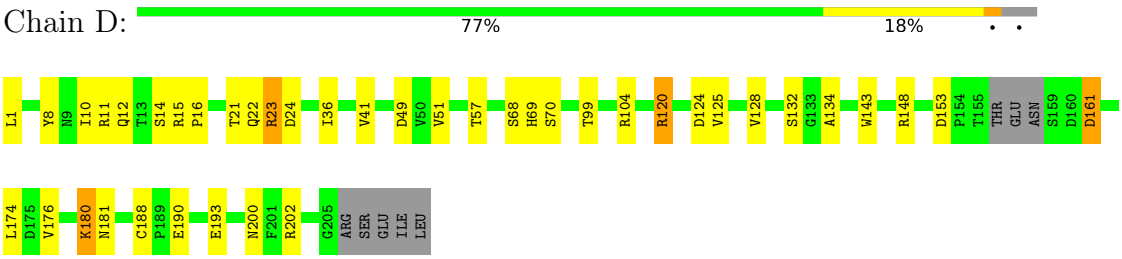
• Molecule 1: Acetylcholine-binding protein

Chain C:



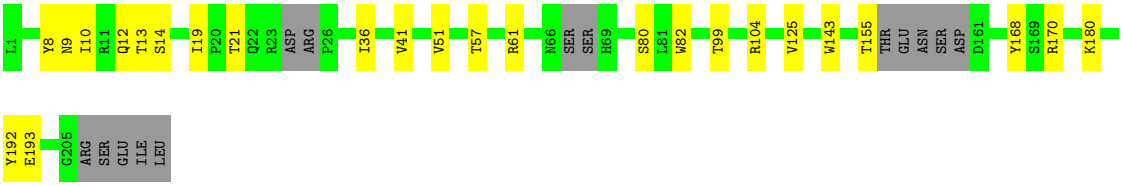
• Molecule 1: Acetylcholine-binding protein

Chain D:



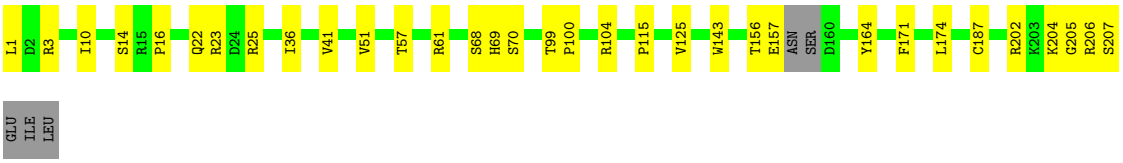
• Molecule 1: Acetylcholine-binding protein

Chain E:



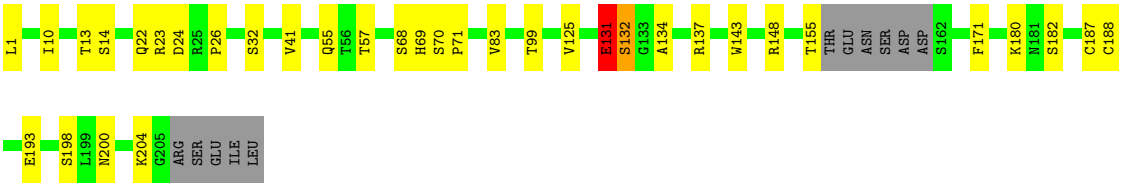
• Molecule 1: Acetylcholine-binding protein

Chain F:



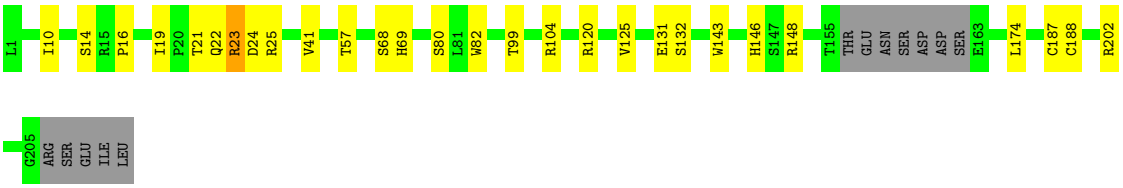
• Molecule 1: Acetylcholine-binding protein

Chain G:



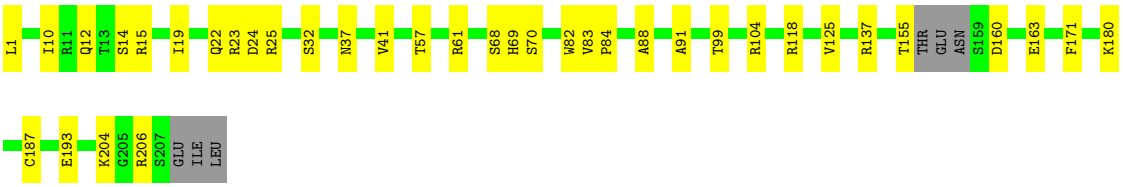
• Molecule 1: Acetylcholine-binding protein

Chain H:



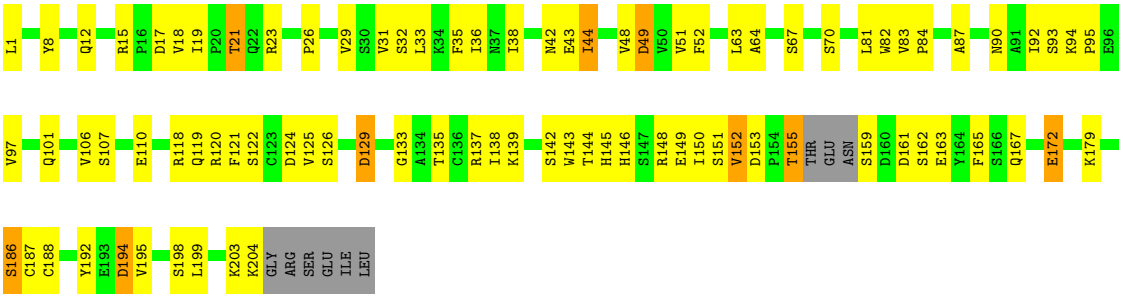
• Molecule 1: Acetylcholine-binding protein

Chain I:



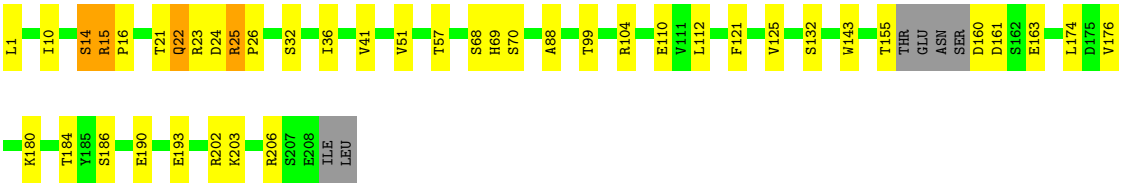
• Molecule 1: Acetylcholine-binding protein

Chain J:



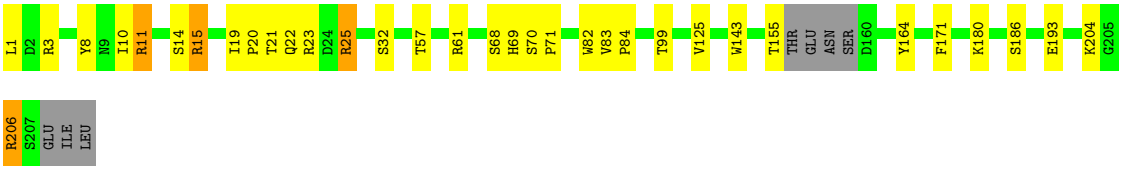
• Molecule 1: Acetylcholine-binding protein

Chain K:



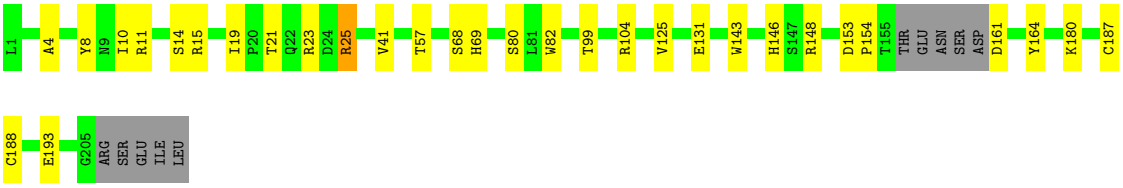
• Molecule 1: Acetylcholine-binding protein

Chain L:



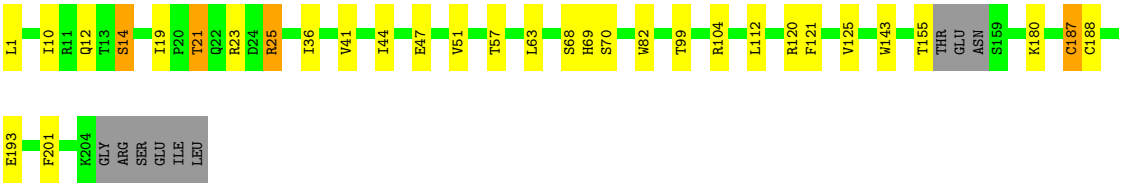
• Molecule 1: Acetylcholine-binding protein

Chain M:



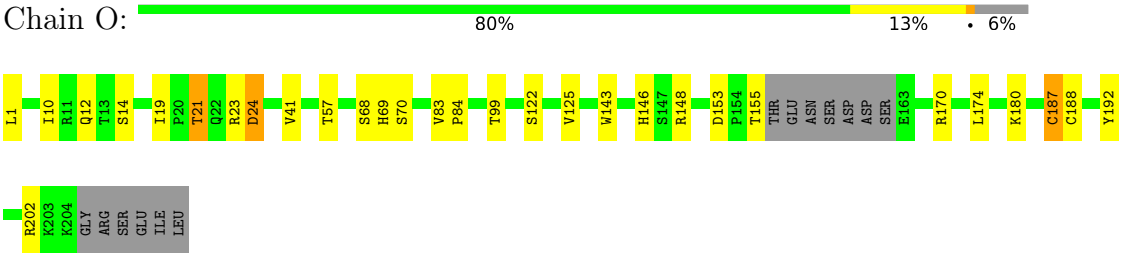
• Molecule 1: Acetylcholine-binding protein

Chain N:



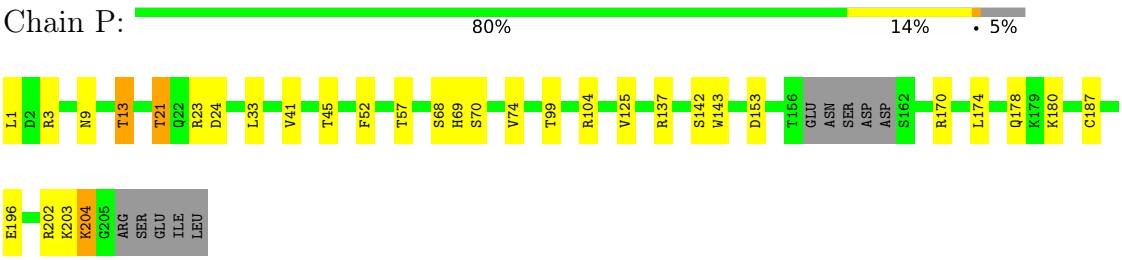
• Molecule 1: Acetylcholine-binding protein

Chain O:



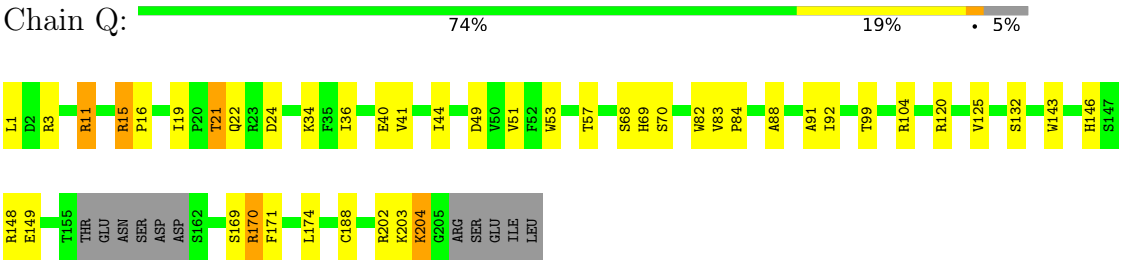
• Molecule 1: Acetylcholine-binding protein

Chain P:



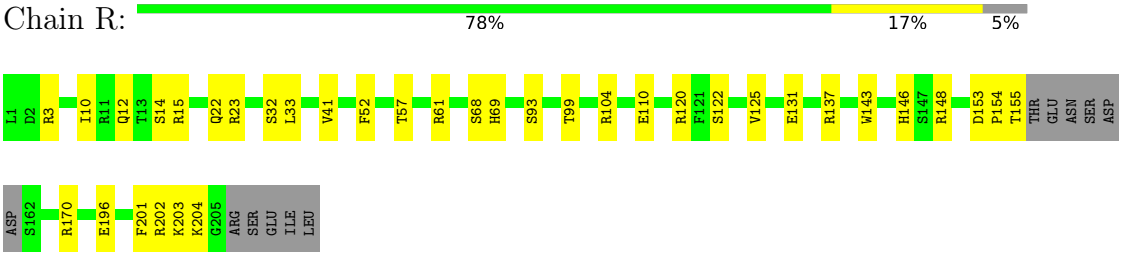
• Molecule 1: Acetylcholine-binding protein

Chain Q:



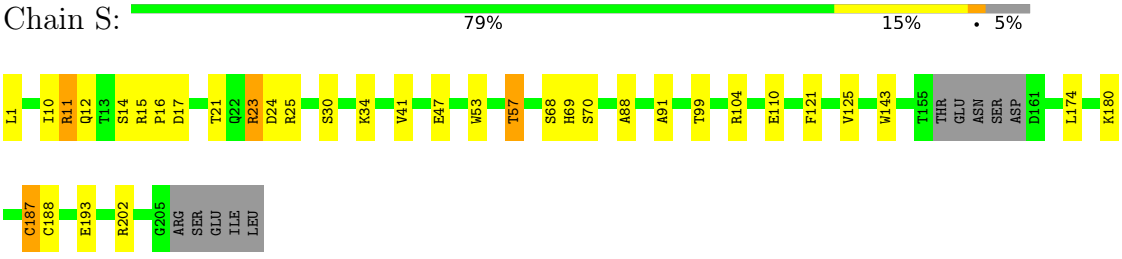
• Molecule 1: Acetylcholine-binding protein

Chain R:



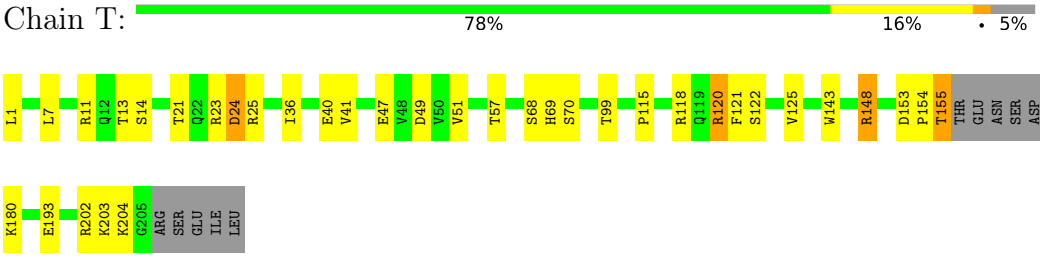
• Molecule 1: Acetylcholine-binding protein

Chain S:



• Molecule 1: Acetylcholine-binding protein

Chain T:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	233.06Å 268.45Å 73.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.01 – 2.70	Depositor
% Data completeness (in resolution range)	97.8 (30.01-2.70)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	4.00 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.219 , 0.275	Depositor
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.870	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32783	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 09R, SO4

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	0.43	0/1661	0.56	0/2264
1	B	0.43	0/1625	0.55	0/2216
1	C	0.44	0/1644	0.54	0/2241
1	D	0.43	0/1655	0.56	0/2258
1	E	0.43	0/1611	0.55	0/2193
1	F	0.43	0/1674	0.56	0/2282
1	G	0.43	0/1625	0.56	0/2216
1	H	0.44	0/1619	0.55	0/2208
1	I	0.42	0/1664	0.55	0/2268
1	J	0.47	0/1643	0.66	0/2241
1	K	0.42	0/1667	0.57	1/2272 (0.0%)
1	L	0.44	0/1658	0.57	0/2260
1	M	0.42	0/1642	0.55	0/2239
1	N	0.41	0/1649	0.58	0/2249
1	O	0.43	0/1615	0.57	0/2203
1	P	0.43	0/1632	0.55	0/2226
1	Q	0.46	0/1625	0.86	3/2216 (0.1%)
1	R	0.43	0/1631	0.55	0/2224
1	S	0.41	0/1633	0.55	0/2227
1	T	0.42	0/1633	0.56	0/2227
All	All	0.43	0/32806	0.58	4/44730 (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	Q	170	ARG	NE-CZ-NH1	-21.23	109.69	120.30
1	Q	170	ARG	NE-CZ-NH2	19.18	129.89	120.30
1	Q	170	ARG	CD-NE-CZ	8.79	135.90	123.60
1	K	112	LEU	CB-CG-CD2	5.22	119.87	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1623	0	1575	20	0
1	B	1590	0	1548	32	0
1	C	1609	0	1565	23	0
1	D	1617	0	1565	34	0
1	E	1575	0	1537	24	0
1	F	1639	0	1587	26	0
1	G	1590	0	1548	39	0
1	H	1584	0	1543	20	0
1	I	1629	0	1579	26	0
1	J	1608	0	1558	66	0
1	K	1632	0	1580	35	0
1	L	1623	0	1574	36	0
1	M	1604	0	1558	24	0
1	N	1611	0	1563	29	0
1	O	1580	0	1540	22	0
1	P	1597	0	1555	28	0
1	Q	1590	0	1548	33	0
1	R	1593	0	1553	35	0
1	S	1598	0	1552	27	0
1	T	1598	0	1552	36	0
2	A	14	0	14	1	0
2	B	14	0	14	2	0
2	C	14	0	14	1	0
2	D	14	0	14	1	0
2	E	14	0	14	1	0
2	F	14	0	14	2	0
2	G	14	0	14	3	0
2	H	14	0	14	1	0
2	I	14	0	14	0	0
2	J	14	0	14	2	0
2	K	14	0	14	0	0
2	L	14	0	14	3	0
2	M	14	0	14	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	14	0	14	2	0
2	O	14	0	14	3	0
2	P	14	0	14	2	0
2	Q	14	0	14	1	0
2	R	14	0	14	1	0
2	S	14	0	14	2	0
2	T	14	0	14	4	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	D	15	0	0	0	0
3	F	10	0	0	1	0
3	H	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	10	0	0	0	0
3	N	5	0	0	0	0
3	R	5	0	0	0	0
3	T	5	0	0	0	0
4	A	23	0	0	1	0
4	B	16	0	0	1	0
4	C	20	0	0	2	0
4	D	21	0	0	2	0
4	E	15	0	0	1	0
4	F	19	0	0	2	0
4	G	14	0	0	2	0
4	H	18	0	0	0	0
4	I	15	0	0	1	0
4	J	9	0	0	0	0
4	K	19	0	0	0	0
4	L	20	0	0	0	0
4	M	11	0	0	0	0
4	N	18	0	0	0	0
4	O	12	0	0	0	0
4	P	13	0	0	2	0
4	Q	19	0	0	1	0
4	R	13	0	0	0	0
4	S	14	0	0	0	0
4	T	19	0	0	1	0
All	All	32783	0	31460	529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 529 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170[B]:ARG:HG2	1:E:170[B]:ARG:HH11	1.00	1.10
1:L:15:ARG:HG2	1:L:15:ARG:HH11	1.15	1.07
1:A:25:ARG:HG3	1:A:25:ARG:HH11	1.19	1.07
1:P:9:ASN:O	1:P:13:THR:HG22	1.58	1.04
1:G:131:GLU:HG2	1:G:132:SER:H	1.23	1.03

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/210 (95%)	196 (98%)	3 (2%)	0	100	100
1	B	195/210 (93%)	193 (99%)	2 (1%)	0	100	100
1	C	197/210 (94%)	195 (99%)	2 (1%)	0	100	100
1	D	199/210 (95%)	195 (98%)	3 (2%)	1 (0%)	29	54
1	E	189/210 (90%)	188 (100%)	1 (0%)	0	100	100
1	F	201/210 (96%)	194 (96%)	6 (3%)	1 (0%)	29	54
1	G	195/210 (93%)	192 (98%)	2 (1%)	1 (0%)	29	54
1	H	194/210 (92%)	192 (99%)	2 (1%)	0	100	100
1	I	200/210 (95%)	198 (99%)	2 (1%)	0	100	100
1	J	197/210 (94%)	182 (92%)	12 (6%)	3 (2%)	10	26
1	K	200/210 (95%)	194 (97%)	4 (2%)	2 (1%)	15	37
1	L	199/210 (95%)	197 (99%)	2 (1%)	0	100	100
1	M	197/210 (94%)	192 (98%)	5 (2%)	0	100	100
1	N	198/210 (94%)	194 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	193/210 (92%)	188 (97%)	5 (3%)	0	100	100
1	P	196/210 (93%)	192 (98%)	3 (2%)	1 (0%)	29	54
1	Q	195/210 (93%)	189 (97%)	6 (3%)	0	100	100
1	R	196/210 (93%)	190 (97%)	6 (3%)	0	100	100
1	S	196/210 (93%)	191 (97%)	5 (3%)	0	100	100
1	T	196/210 (93%)	191 (97%)	4 (2%)	1 (0%)	29	54
All	All	3932/4200 (94%)	3843 (98%)	79 (2%)	10 (0%)	41	66

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	23	ARG
1	T	24	ASP
1	D	23	ARG
1	F	206	ARG
1	G	131	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/196 (96%)	184 (97%)	5 (3%)	46	75
1	B	185/196 (94%)	180 (97%)	5 (3%)	44	74
1	C	187/196 (95%)	181 (97%)	6 (3%)	39	68
1	D	189/196 (96%)	181 (96%)	8 (4%)	30	58
1	E	183/196 (93%)	180 (98%)	3 (2%)	62	85
1	F	191/196 (97%)	187 (98%)	4 (2%)	53	80
1	G	185/196 (94%)	181 (98%)	4 (2%)	52	79
1	H	184/196 (94%)	178 (97%)	6 (3%)	38	67
1	I	190/196 (97%)	187 (98%)	3 (2%)	62	85
1	J	188/196 (96%)	173 (92%)	15 (8%)	12	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	190/196 (97%)	182 (96%)	8 (4%)	30	58
1	L	189/196 (96%)	183 (97%)	6 (3%)	39	68
1	M	187/196 (95%)	182 (97%)	5 (3%)	44	74
1	N	189/196 (96%)	181 (96%)	8 (4%)	30	58
1	O	184/196 (94%)	177 (96%)	7 (4%)	33	62
1	P	186/196 (95%)	179 (96%)	7 (4%)	33	62
1	Q	185/196 (94%)	178 (96%)	7 (4%)	33	62
1	R	186/196 (95%)	183 (98%)	3 (2%)	62	85
1	S	186/196 (95%)	180 (97%)	6 (3%)	39	68
1	T	186/196 (95%)	179 (96%)	7 (4%)	33	62
All	All	3739/3920 (95%)	3616 (97%)	123 (3%)	38	67

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	179	LYS
1	S	11	ARG
1	L	57	THR
1	R	122	SER
1	T	120	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	9	ASN
1	T	69	HIS
1	M	55	GLN
1	R	69	HIS
1	L	69	HIS

5.3.3 RNA

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)

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	09R	D	211	-	13,15,15	3.45	2 (15%)	15,19,19	1.57	3 (20%)
2	09R	S	211	-	13,15,15	3.34	2 (15%)	15,19,19	1.55	3 (20%)
2	09R	T	211	-	13,15,15	3.39	1 (7%)	15,19,19	1.67	4 (26%)
2	09R	J	211	-	13,15,15	3.15	2 (15%)	15,19,19	1.98	4 (26%)
3	SO4	B	212	-	4,4,4	0.19	0	6,6,6	0.17	0
3	SO4	B	213	-	4,4,4	0.16	0	6,6,6	0.16	0
2	09R	G	211	-	13,15,15	3.53	2 (15%)	15,19,19	1.40	2 (13%)
3	SO4	D	213	-	4,4,4	0.19	0	6,6,6	0.12	0
2	09R	A	211	-	13,15,15	3.57	3 (23%)	15,19,19	2.77	7 (46%)
3	SO4	F	212	-	4,4,4	0.14	0	6,6,6	0.17	0
3	SO4	K	212	-	4,4,4	0.13	0	6,6,6	0.22	0
3	SO4	D	212	-	4,4,4	0.15	0	6,6,6	0.19	0
2	09R	F	211	-	13,15,15	3.32	2 (15%)	15,19,19	2.04	4 (26%)
2	09R	E	211	-	13,15,15	3.84	1 (7%)	15,19,19	1.02	1 (6%)
2	09R	K	211	-	13,15,15	3.41	2 (15%)	15,19,19	1.53	3 (20%)
2	09R	P	211	-	13,15,15	3.42	2 (15%)	15,19,19	1.70	2 (13%)
3	SO4	F	213	-	4,4,4	0.16	0	6,6,6	0.16	0
2	09R	I	211	-	13,15,15	3.46	3 (23%)	15,19,19	1.24	1 (6%)
3	SO4	J	212	-	4,4,4	0.11	0	6,6,6	0.20	0
3	SO4	N	212	-	4,4,4	0.16	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	09R	N	211	-	13,15,15	3.39	2 (15%)	15,19,19	2.03	5 (33%)
2	09R	R	211	-	13,15,15	3.40	2 (15%)	15,19,19	1.53	4 (26%)
3	SO4	D	214	-	4,4,4	0.16	0	6,6,6	0.37	0
2	09R	C	211	-	13,15,15	3.55	2 (15%)	15,19,19	1.11	0
2	09R	O	211	-	13,15,15	3.36	1 (7%)	15,19,19	1.56	3 (20%)
2	09R	H	211	-	13,15,15	3.40	3 (23%)	15,19,19	1.85	4 (26%)
2	09R	B	211	-	13,15,15	3.53	1 (7%)	15,19,19	1.22	2 (13%)
2	09R	L	211	-	13,15,15	3.51	2 (15%)	15,19,19	1.68	4 (26%)
3	SO4	L	213	-	4,4,4	0.22	0	6,6,6	0.18	0
3	SO4	I	212	-	4,4,4	0.17	0	6,6,6	0.09	0
2	09R	Q	211	-	13,15,15	3.32	4 (30%)	15,19,19	1.59	4 (26%)
3	SO4	A	212	-	4,4,4	0.11	0	6,6,6	0.15	0
2	09R	M	211	-	13,15,15	3.36	1 (7%)	15,19,19	1.46	3 (20%)
3	SO4	R	212	-	4,4,4	0.24	0	6,6,6	0.42	0
3	SO4	H	212	-	4,4,4	0.17	0	6,6,6	0.30	0
3	SO4	L	212	-	4,4,4	0.24	0	6,6,6	0.33	0
3	SO4	T	212	-	4,4,4	0.19	0	6,6,6	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	09R	D	211	-	-	0/4/13/13	0/2/2/2
2	09R	S	211	-	-	0/4/13/13	0/2/2/2
2	09R	T	211	-	-	0/4/13/13	0/2/2/2
2	09R	J	211	-	-	0/4/13/13	0/2/2/2
2	09R	G	211	-	-	0/4/13/13	0/2/2/2
2	09R	A	211	-	-	0/4/13/13	0/2/2/2
2	09R	F	211	-	-	0/4/13/13	0/2/2/2
2	09R	E	211	-	-	0/4/13/13	0/2/2/2
2	09R	K	211	-	-	0/4/13/13	0/2/2/2
2	09R	P	211	-	-	2/4/13/13	0/2/2/2
2	09R	I	211	-	-	0/4/13/13	0/2/2/2
2	09R	N	211	-	-	0/4/13/13	0/2/2/2
2	09R	R	211	-	-	0/4/13/13	0/2/2/2
2	09R	C	211	-	-	0/4/13/13	0/2/2/2
2	09R	O	211	-	-	2/4/13/13	0/2/2/2
2	09R	H	211	-	-	0/4/13/13	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	09R	B	211	-	-	0/4/13/13	0/2/2/2
2	09R	L	211	-	-	0/4/13/13	0/2/2/2
2	09R	Q	211	-	-	0/4/13/13	0/2/2/2
2	09R	M	211	-	-	0/4/13/13	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	211	09R	BR1-C5	-13.32	1.70	1.90
2	B	211	09R	BR1-C5	-12.17	1.72	1.90
2	C	211	09R	BR1-C5	-12.14	1.72	1.90
2	L	211	09R	BR1-C5	-12.10	1.72	1.90
2	G	211	09R	BR1-C5	-11.92	1.72	1.90

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	211	09R	BR1-C5-C4	5.99	124.77	118.64
2	F	211	09R	C3-C4-C5	4.62	120.47	117.38
2	P	211	09R	C3-C4-C5	4.51	120.40	117.38
2	A	211	09R	C3-C2-N2	4.14	127.09	121.38
2	A	211	09R	C9-C10-N2	4.02	121.20	113.46

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	211	09R	C1-C2-N2-C6
2	P	211	09R	C1-C2-N2-C6
2	O	211	09R	C3-C2-N2-C6
2	P	211	09R	C3-C2-N2-C6

There are no ring outliers.

19 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	211	09R	1	0
2	S	211	09R	2	0
2	T	211	09R	4	0
2	J	211	09R	2	0
2	G	211	09R	3	0

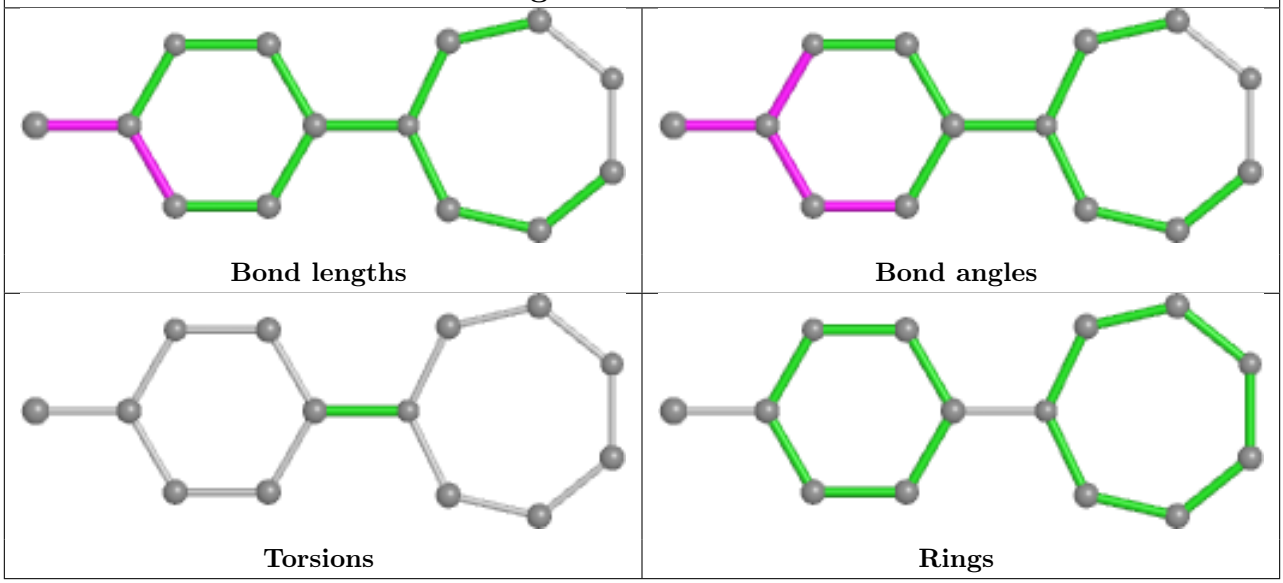
Continued on next page...

Continued from previous page...

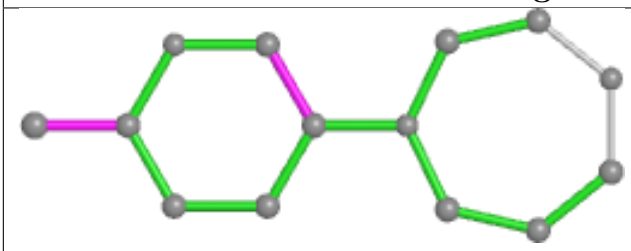
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	211	09R	1	0
2	F	211	09R	2	0
2	E	211	09R	1	0
2	P	211	09R	2	0
3	F	213	SO4	1	0
2	N	211	09R	2	0
2	R	211	09R	1	0
2	C	211	09R	1	0
2	O	211	09R	3	0
2	H	211	09R	1	0
2	B	211	09R	2	0
2	L	211	09R	3	0
2	Q	211	09R	1	0
2	M	211	09R	2	0

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

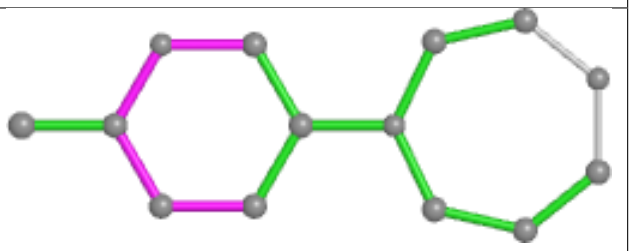
Ligand 09R D 211



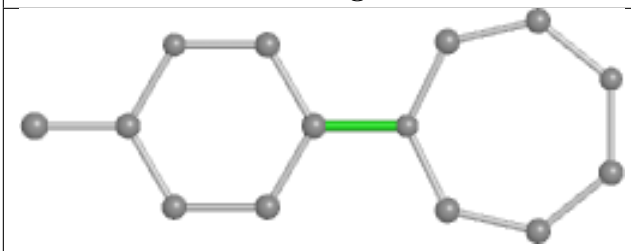
Ligand 09R S 211



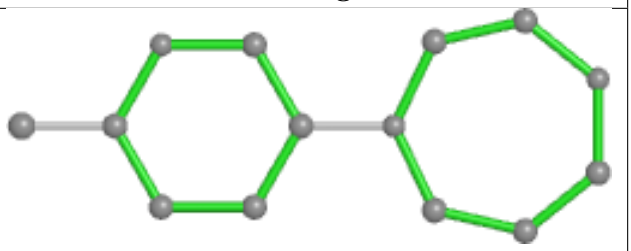
Bond lengths



Bond angles

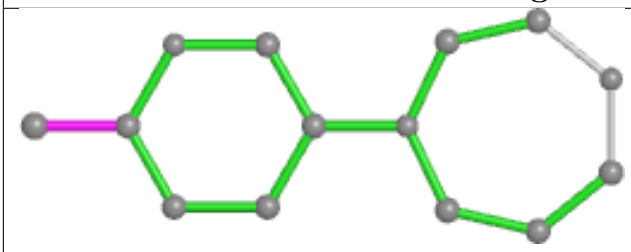


Torsions

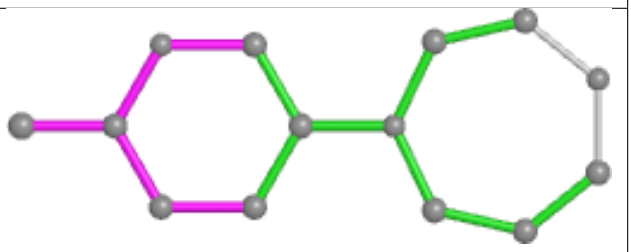


Rings

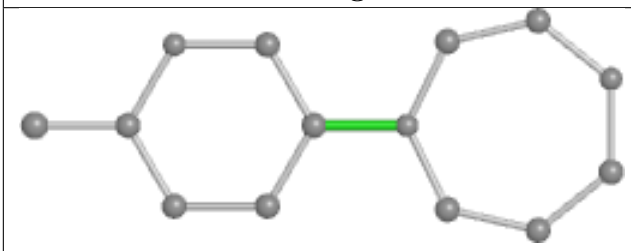
Ligand 09R T 211



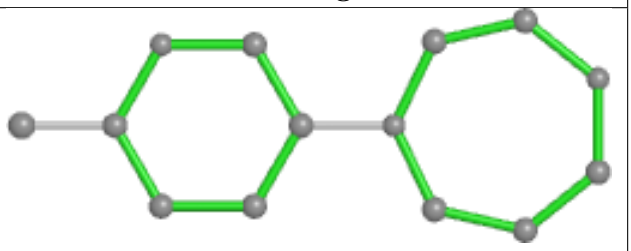
Bond lengths



Bond angles

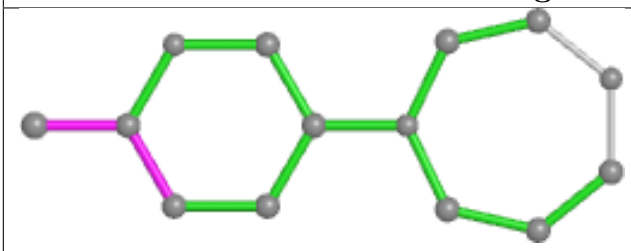


Torsions

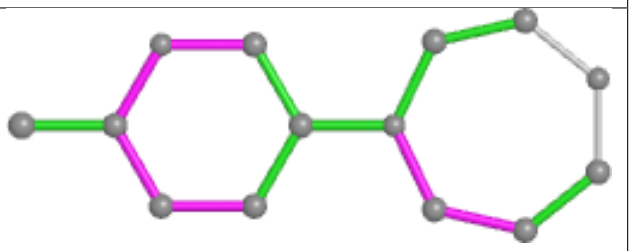


Rings

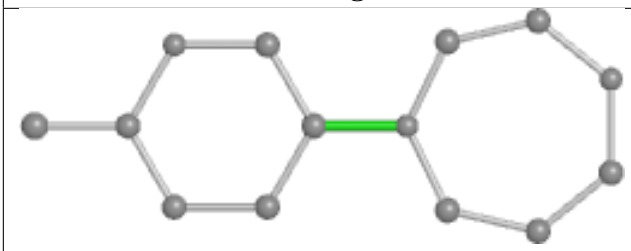
Ligand 09R J 211



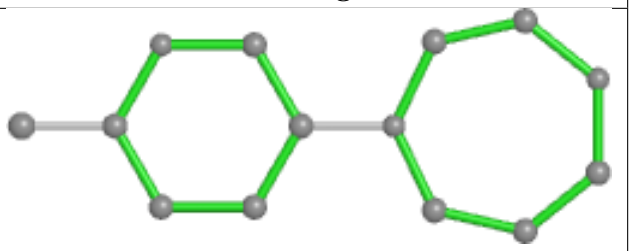
Bond lengths



Bond angles

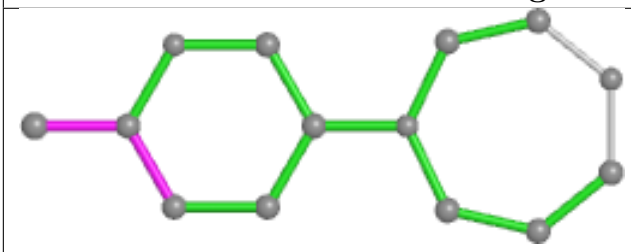


Torsions

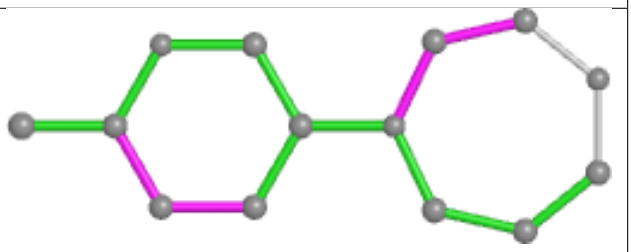


Rings

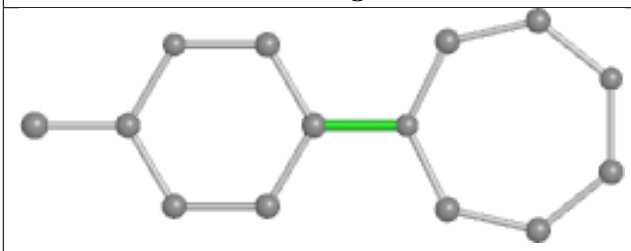
Ligand 09R G 211



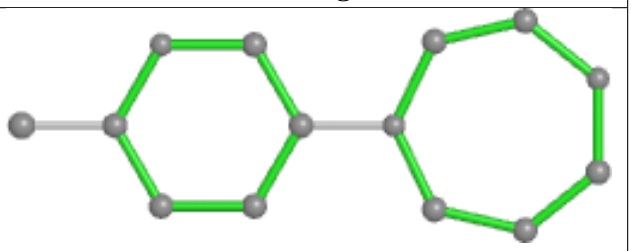
Bond lengths



Bond angles

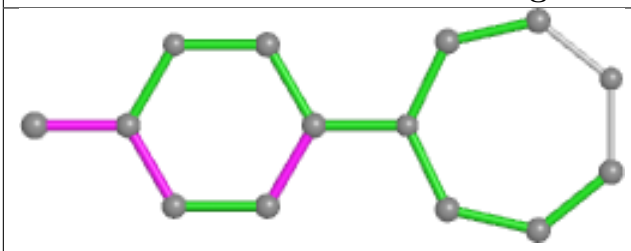


Torsions

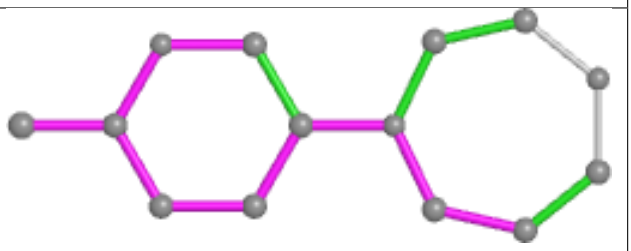


Rings

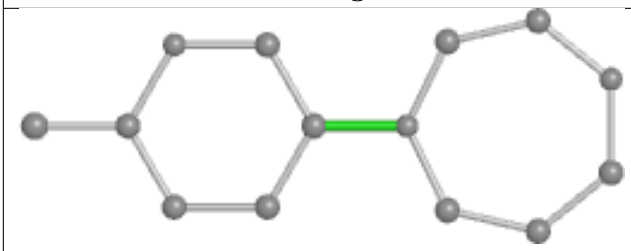
Ligand 09R A 211



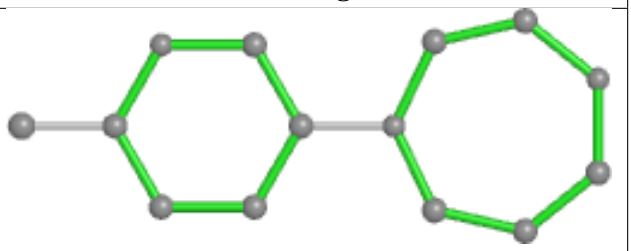
Bond lengths



Bond angles

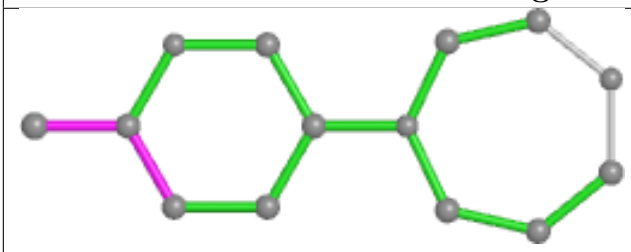


Torsions

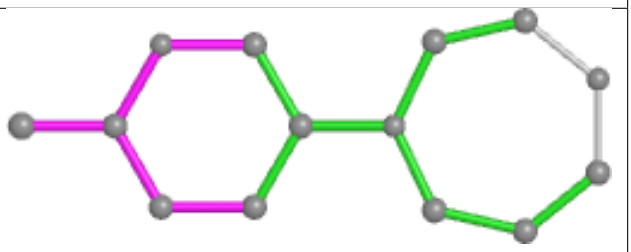


Rings

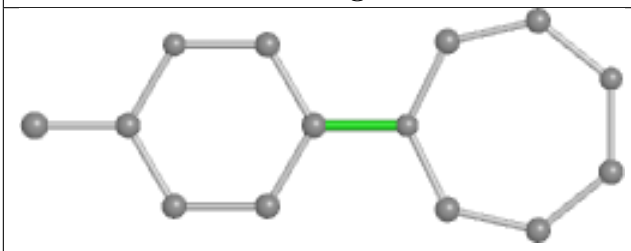
Ligand 09R F 211



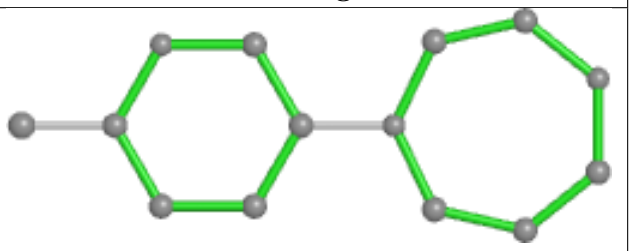
Bond lengths



Bond angles

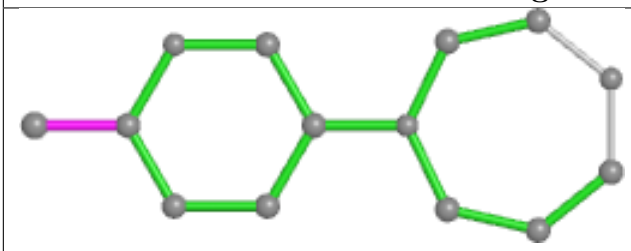


Torsions

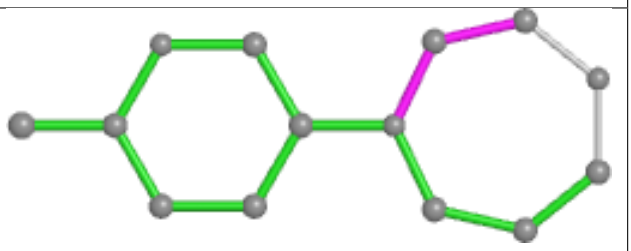


Rings

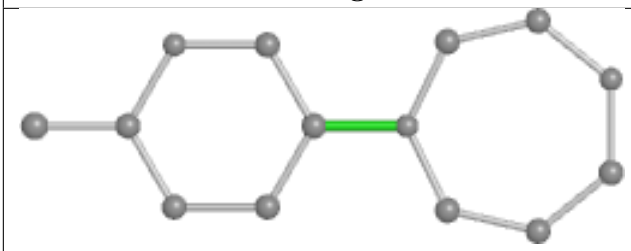
Ligand 09R E 211



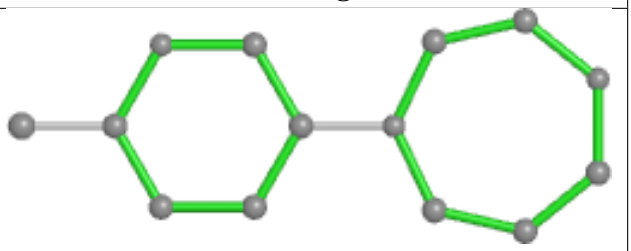
Bond lengths



Bond angles

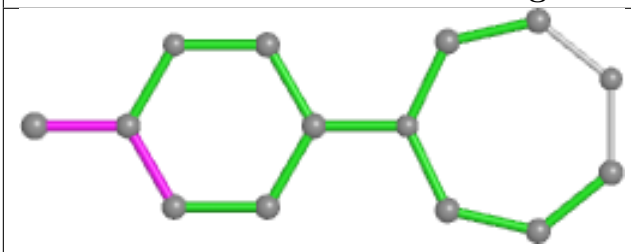


Torsions

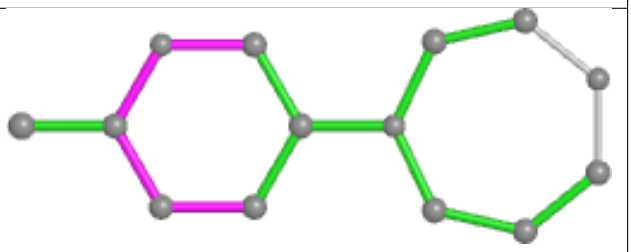


Rings

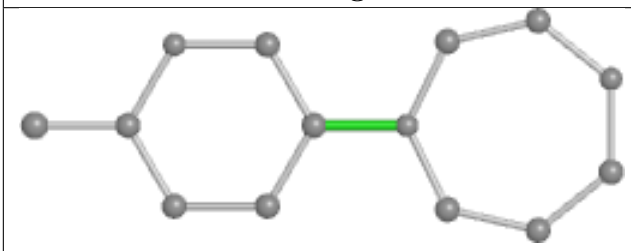
Ligand 09R K 211



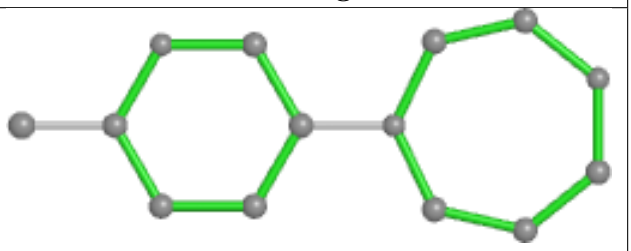
Bond lengths



Bond angles

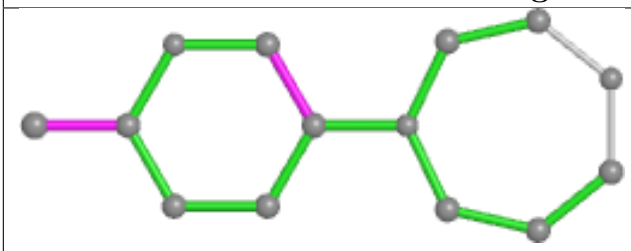


Torsions

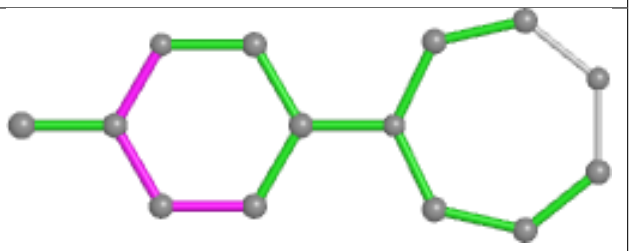


Rings

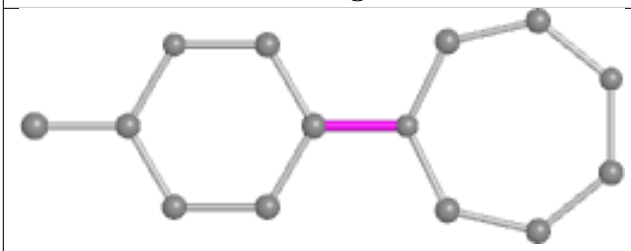
Ligand 09R P 211



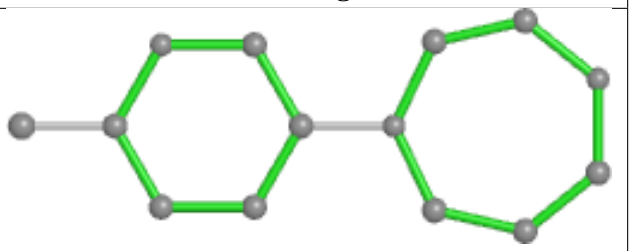
Bond lengths



Bond angles

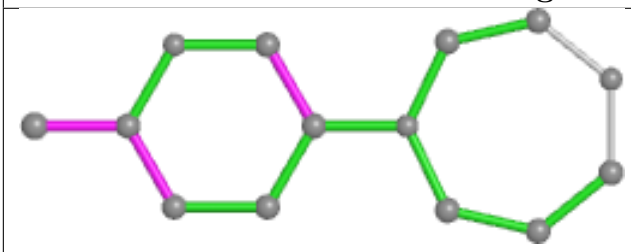


Torsions

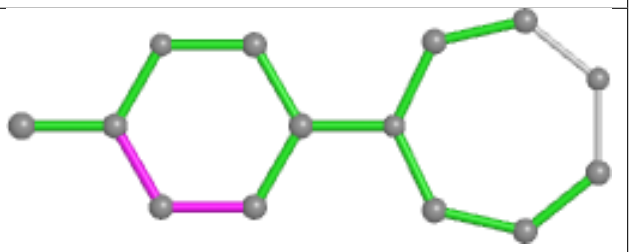


Rings

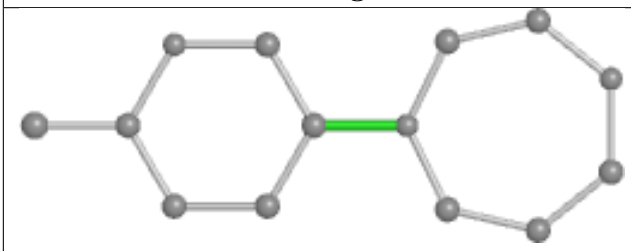
Ligand 09R I 211



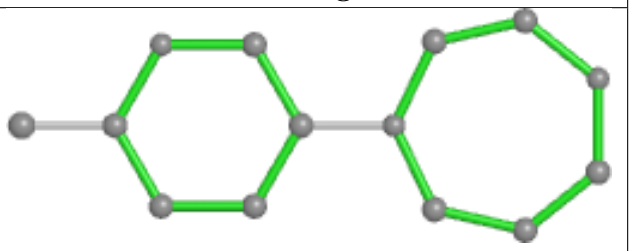
Bond lengths



Bond angles

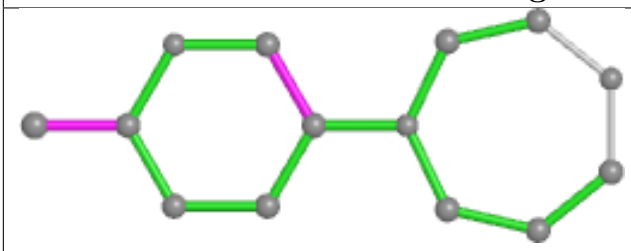


Torsions

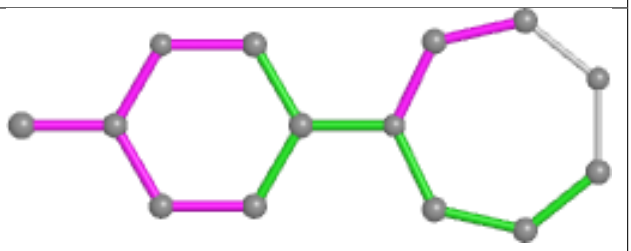


Rings

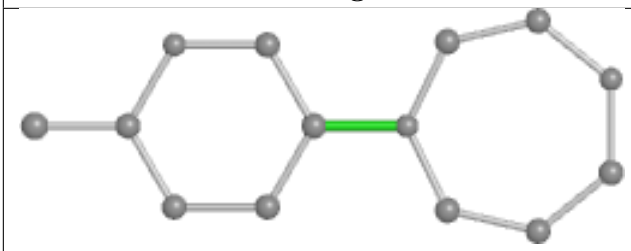
Ligand 09R N 211



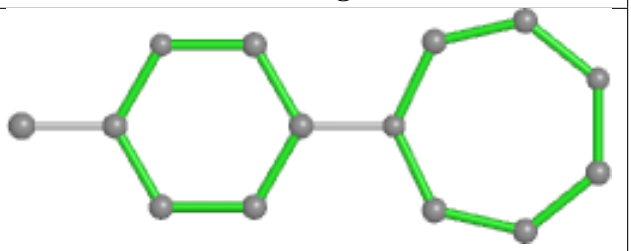
Bond lengths



Bond angles

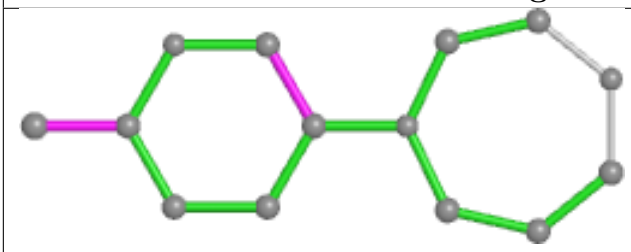


Torsions

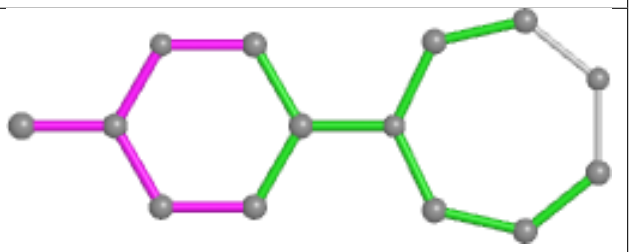


Rings

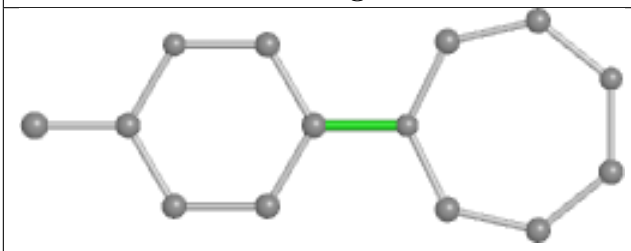
Ligand 09R R 211



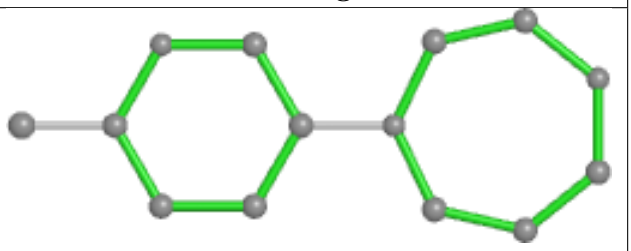
Bond lengths



Bond angles

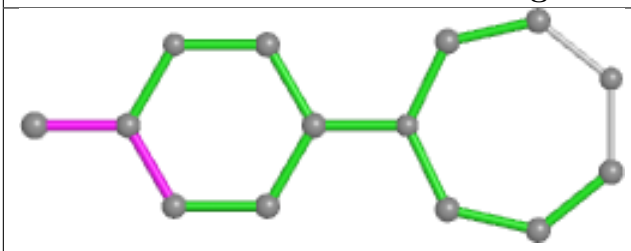


Torsions

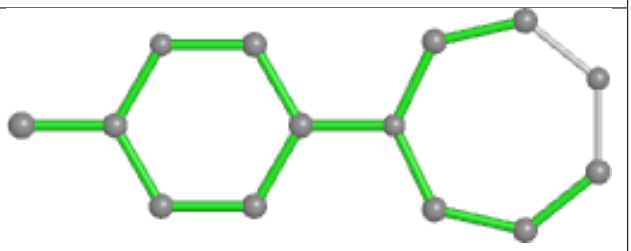


Rings

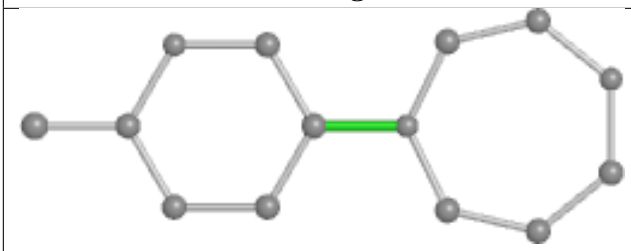
Ligand 09R C 211



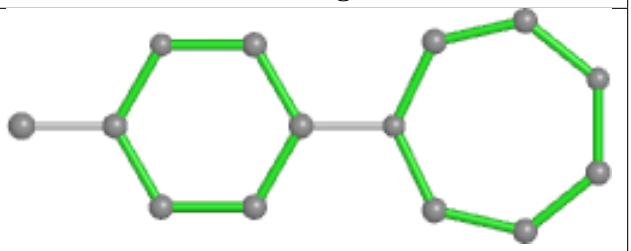
Bond lengths



Bond angles

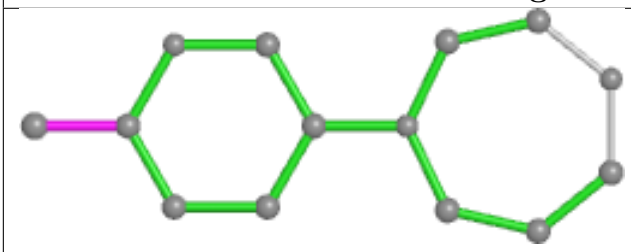


Torsions

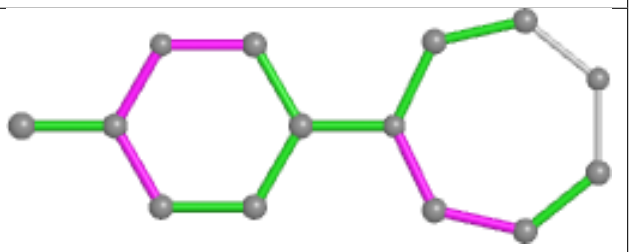


Rings

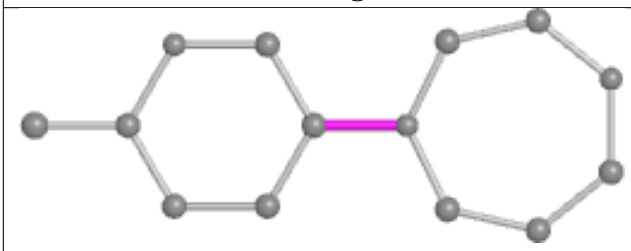
Ligand 09R O 211



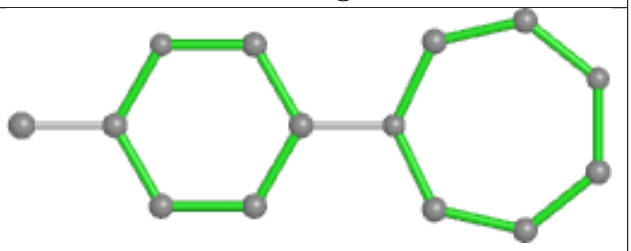
Bond lengths



Bond angles

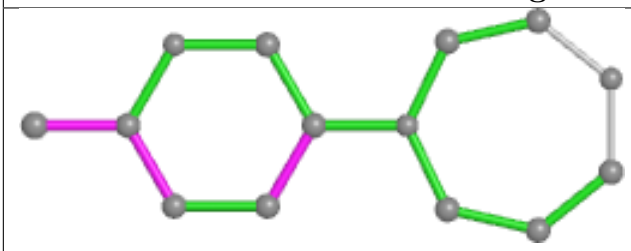


Torsions

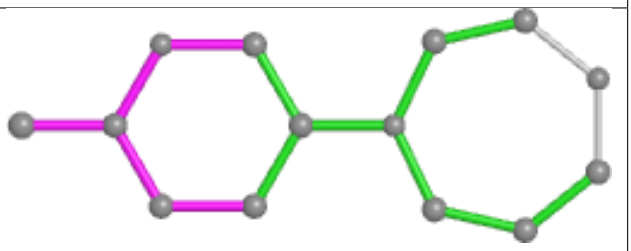


Rings

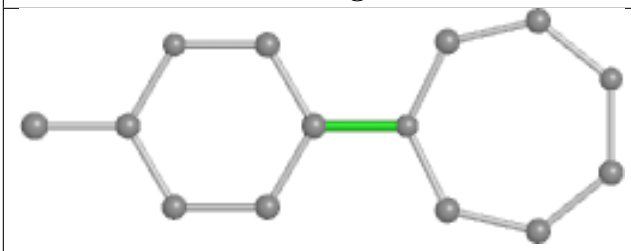
Ligand 09R H 211



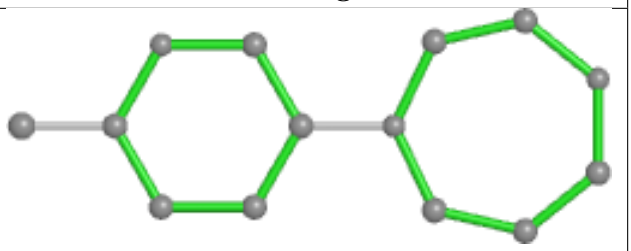
Bond lengths



Bond angles

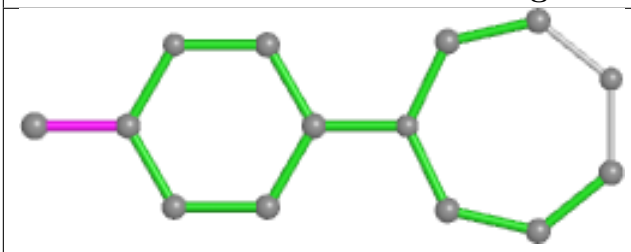


Torsions

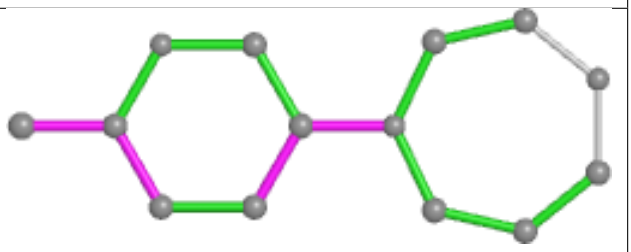


Rings

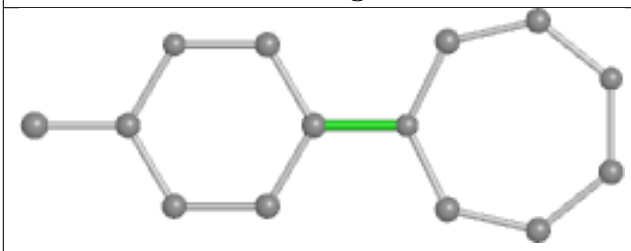
Ligand 09R B 211



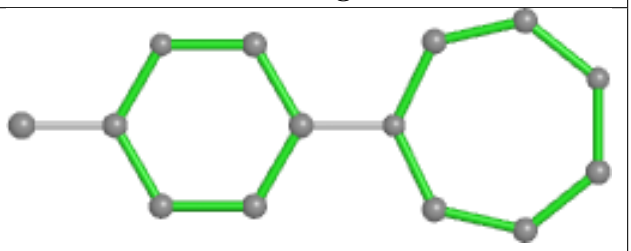
Bond lengths



Bond angles

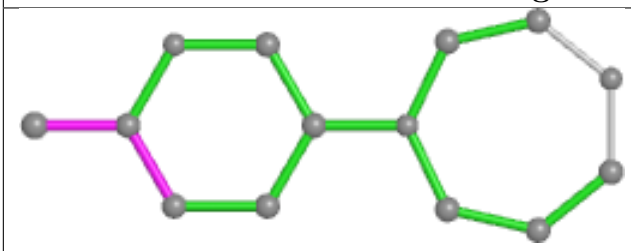


Torsions

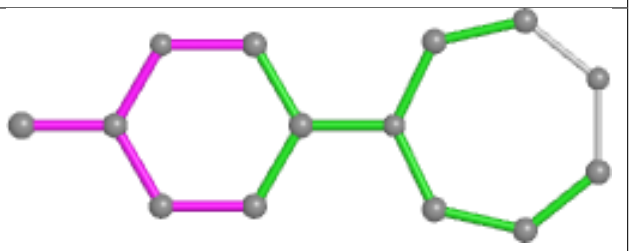


Rings

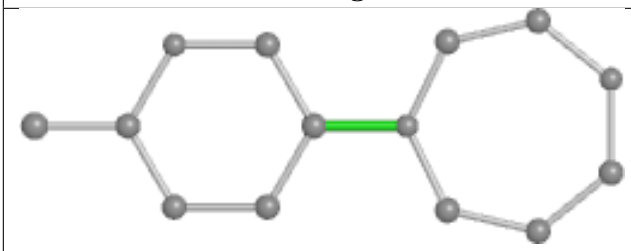
Ligand 09R L 211



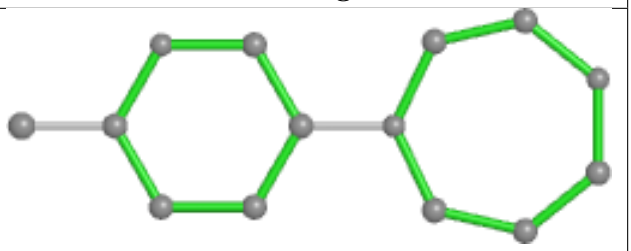
Bond lengths



Bond angles

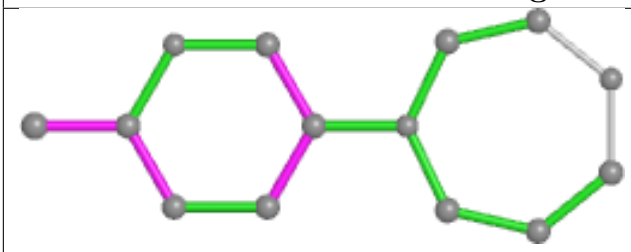


Torsions

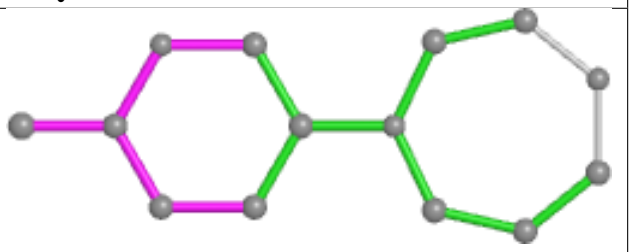


Rings

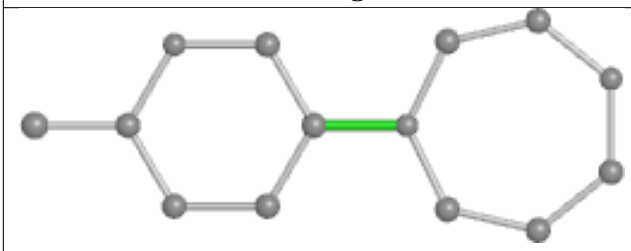
Ligand 09R Q 211



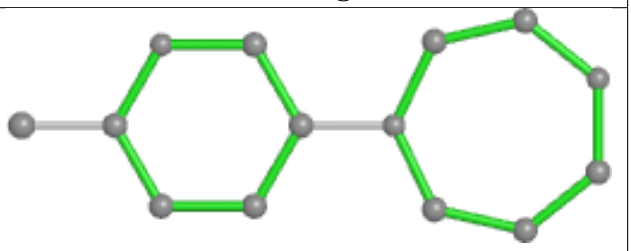
Bond lengths



Bond angles

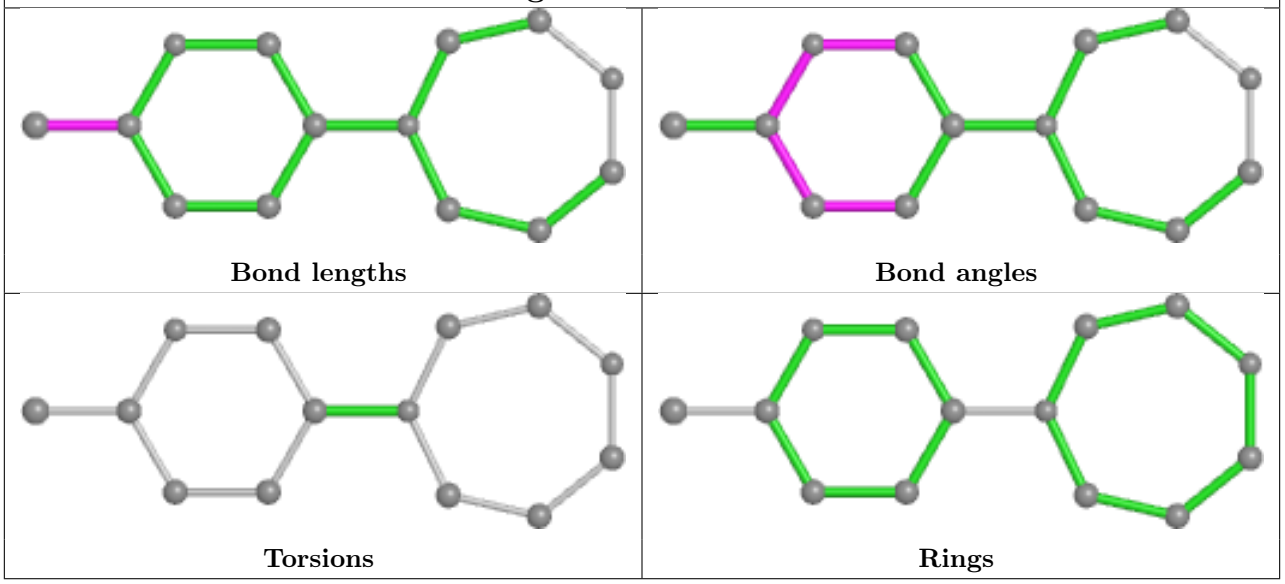


Torsions



Rings

Ligand 09R M 211



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.