wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2020 – 12:22 am BST

PDB ID	:	5OAL
Title	:	Crystal structure of mutant AChBP in complex with strychnine (T53F, Q74R, Y110A, I135S, G162E)
Authors	:	Dawson, A.; Hunter, W.N.; de Souza, J.O.; Trumper, P.
Deposited on	:	2017-06-22
Resolution	:	3.20 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 following versions of software and data (see references (1)) were used in the production of this report:

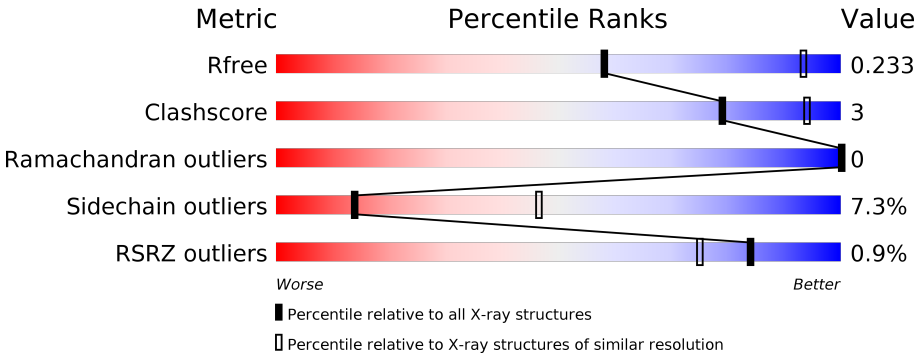
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.20 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))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	249	69% 10% • 17%
1	B	249	3% 69% 9% • • 17%
1	C	249	71% 10% • 17%
1	D	249	% 71% 9% • • 17%
1	E	249	70% 9% • 18%
1	F	249	71% 11% 17%

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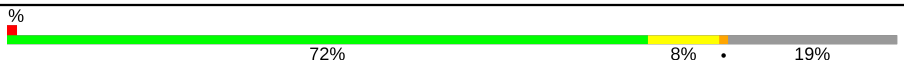
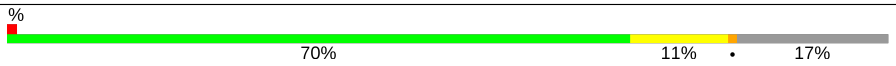
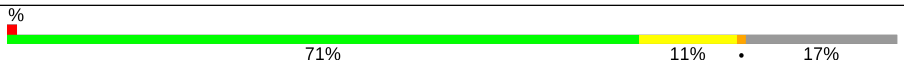
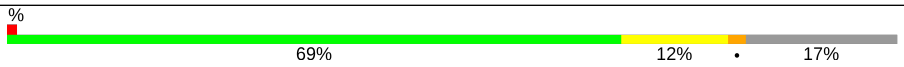
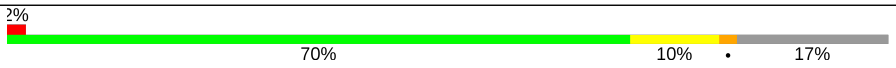
Mol	Chain	Length	Quality of chain
1	G	249	
1	H	249	
1	I	249	
1	J	249	
1	K	249	
1	L	249	
1	M	249	
1	N	249	
1	O	249	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25009 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 Soluble acetylcholine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	B	207	Total	C	N	O	S	0	0	0
			1654	1045	273	327	9			
1	C	207	Total	C	N	O	S	0	0	0
			1654	1045	273	327	9			
1	D	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	E	204	Total	C	N	O	S	0	0	0
			1627	1030	264	324	9			
1	F	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	G	202	Total	C	N	O	S	0	0	0
			1619	1024	268	320	7			
1	H	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	I	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	J	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	K	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	L	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	M	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			
1	N	198	Total	C	N	O	S	0	0	0
			1579	998	257	316	8			
1	O	206	Total	C	N	O	S	0	0	0
			1649	1042	272	326	9			

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	PHE	THR	engineered mutation	UNP Q8WSF8
A	60	VAL	ALA	conflict	UNP Q8WSF8
A	74	ARG	GLN	engineered mutation	UNP Q8WSF8
A	110	ALA	TYR	engineered mutation	UNP Q8WSF8
A	135	SER	ILE	engineered mutation	UNP Q8WSF8
A	155	VAL	ALA	conflict	UNP Q8WSF8
A	162	GLU	GLY	engineered mutation	UNP Q8WSF8
A	237	GLU	-	expression tag	UNP Q8WSF8
A	238	ASN	-	expression tag	UNP Q8WSF8
A	239	LEU	-	expression tag	UNP Q8WSF8
A	240	TYR	-	expression tag	UNP Q8WSF8
A	241	PHE	-	expression tag	UNP Q8WSF8
A	242	GLN	-	expression tag	UNP Q8WSF8
A	243	GLY	-	expression tag	UNP Q8WSF8
A	244	HIS	-	expression tag	UNP Q8WSF8
A	245	HIS	-	expression tag	UNP Q8WSF8
A	246	HIS	-	expression tag	UNP Q8WSF8
A	247	HIS	-	expression tag	UNP Q8WSF8
A	248	HIS	-	expression tag	UNP Q8WSF8
A	249	HIS	-	expression tag	UNP Q8WSF8
B	53	PHE	THR	engineered mutation	UNP Q8WSF8
B	60	VAL	ALA	conflict	UNP Q8WSF8
B	74	ARG	GLN	engineered mutation	UNP Q8WSF8
B	110	ALA	TYR	engineered mutation	UNP Q8WSF8
B	135	SER	ILE	engineered mutation	UNP Q8WSF8
B	155	VAL	ALA	conflict	UNP Q8WSF8
B	162	GLU	GLY	engineered mutation	UNP Q8WSF8
B	237	GLU	-	expression tag	UNP Q8WSF8
B	238	ASN	-	expression tag	UNP Q8WSF8
B	239	LEU	-	expression tag	UNP Q8WSF8
B	240	TYR	-	expression tag	UNP Q8WSF8
B	241	PHE	-	expression tag	UNP Q8WSF8
B	242	GLN	-	expression tag	UNP Q8WSF8
B	243	GLY	-	expression tag	UNP Q8WSF8
B	244	HIS	-	expression tag	UNP Q8WSF8
B	245	HIS	-	expression tag	UNP Q8WSF8
B	246	HIS	-	expression tag	UNP Q8WSF8
B	247	HIS	-	expression tag	UNP Q8WSF8
B	248	HIS	-	expression tag	UNP Q8WSF8
B	249	HIS	-	expression tag	UNP Q8WSF8
C	53	PHE	THR	engineered mutation	UNP Q8WSF8
C	60	VAL	ALA	conflict	UNP Q8WSF8
C	74	ARG	GLN	engineered mutation	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	110	ALA	TYR	engineered mutation	UNP Q8WSF8
C	135	SER	ILE	engineered mutation	UNP Q8WSF8
C	155	VAL	ALA	conflict	UNP Q8WSF8
C	162	GLU	GLY	engineered mutation	UNP Q8WSF8
C	237	GLU	-	expression tag	UNP Q8WSF8
C	238	ASN	-	expression tag	UNP Q8WSF8
C	239	LEU	-	expression tag	UNP Q8WSF8
C	240	TYR	-	expression tag	UNP Q8WSF8
C	241	PHE	-	expression tag	UNP Q8WSF8
C	242	GLN	-	expression tag	UNP Q8WSF8
C	243	GLY	-	expression tag	UNP Q8WSF8
C	244	HIS	-	expression tag	UNP Q8WSF8
C	245	HIS	-	expression tag	UNP Q8WSF8
C	246	HIS	-	expression tag	UNP Q8WSF8
C	247	HIS	-	expression tag	UNP Q8WSF8
C	248	HIS	-	expression tag	UNP Q8WSF8
C	249	HIS	-	expression tag	UNP Q8WSF8
D	53	PHE	THR	engineered mutation	UNP Q8WSF8
D	60	VAL	ALA	conflict	UNP Q8WSF8
D	74	ARG	GLN	engineered mutation	UNP Q8WSF8
D	110	ALA	TYR	engineered mutation	UNP Q8WSF8
D	135	SER	ILE	engineered mutation	UNP Q8WSF8
D	155	VAL	ALA	conflict	UNP Q8WSF8
D	162	GLU	GLY	engineered mutation	UNP Q8WSF8
D	237	GLU	-	expression tag	UNP Q8WSF8
D	238	ASN	-	expression tag	UNP Q8WSF8
D	239	LEU	-	expression tag	UNP Q8WSF8
D	240	TYR	-	expression tag	UNP Q8WSF8
D	241	PHE	-	expression tag	UNP Q8WSF8
D	242	GLN	-	expression tag	UNP Q8WSF8
D	243	GLY	-	expression tag	UNP Q8WSF8
D	244	HIS	-	expression tag	UNP Q8WSF8
D	245	HIS	-	expression tag	UNP Q8WSF8
D	246	HIS	-	expression tag	UNP Q8WSF8
D	247	HIS	-	expression tag	UNP Q8WSF8
D	248	HIS	-	expression tag	UNP Q8WSF8
D	249	HIS	-	expression tag	UNP Q8WSF8
E	53	PHE	THR	engineered mutation	UNP Q8WSF8
E	60	VAL	ALA	conflict	UNP Q8WSF8
E	74	ARG	GLN	engineered mutation	UNP Q8WSF8
E	110	ALA	TYR	engineered mutation	UNP Q8WSF8
E	135	SER	ILE	engineered mutation	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	155	VAL	ALA	conflict	UNP Q8WSF8
E	162	GLU	GLY	engineered mutation	UNP Q8WSF8
E	237	GLU	-	expression tag	UNP Q8WSF8
E	238	ASN	-	expression tag	UNP Q8WSF8
E	239	LEU	-	expression tag	UNP Q8WSF8
E	240	TYR	-	expression tag	UNP Q8WSF8
E	241	PHE	-	expression tag	UNP Q8WSF8
E	242	GLN	-	expression tag	UNP Q8WSF8
E	243	GLY	-	expression tag	UNP Q8WSF8
E	244	HIS	-	expression tag	UNP Q8WSF8
E	245	HIS	-	expression tag	UNP Q8WSF8
E	246	HIS	-	expression tag	UNP Q8WSF8
E	247	HIS	-	expression tag	UNP Q8WSF8
E	248	HIS	-	expression tag	UNP Q8WSF8
E	249	HIS	-	expression tag	UNP Q8WSF8
F	53	PHE	THR	engineered mutation	UNP Q8WSF8
F	60	VAL	ALA	conflict	UNP Q8WSF8
F	74	ARG	GLN	engineered mutation	UNP Q8WSF8
F	110	ALA	TYR	engineered mutation	UNP Q8WSF8
F	135	SER	ILE	engineered mutation	UNP Q8WSF8
F	155	VAL	ALA	conflict	UNP Q8WSF8
F	162	GLU	GLY	engineered mutation	UNP Q8WSF8
F	237	GLU	-	expression tag	UNP Q8WSF8
F	238	ASN	-	expression tag	UNP Q8WSF8
F	239	LEU	-	expression tag	UNP Q8WSF8
F	240	TYR	-	expression tag	UNP Q8WSF8
F	241	PHE	-	expression tag	UNP Q8WSF8
F	242	GLN	-	expression tag	UNP Q8WSF8
F	243	GLY	-	expression tag	UNP Q8WSF8
F	244	HIS	-	expression tag	UNP Q8WSF8
F	245	HIS	-	expression tag	UNP Q8WSF8
F	246	HIS	-	expression tag	UNP Q8WSF8
F	247	HIS	-	expression tag	UNP Q8WSF8
F	248	HIS	-	expression tag	UNP Q8WSF8
F	249	HIS	-	expression tag	UNP Q8WSF8
G	53	PHE	THR	engineered mutation	UNP Q8WSF8
G	60	VAL	ALA	conflict	UNP Q8WSF8
G	74	ARG	GLN	engineered mutation	UNP Q8WSF8
G	110	ALA	TYR	engineered mutation	UNP Q8WSF8
G	135	SER	ILE	engineered mutation	UNP Q8WSF8
G	155	VAL	ALA	conflict	UNP Q8WSF8
G	162	GLU	GLY	engineered mutation	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	237	GLU	-	expression tag	UNP Q8WSF8
G	238	ASN	-	expression tag	UNP Q8WSF8
G	239	LEU	-	expression tag	UNP Q8WSF8
G	240	TYR	-	expression tag	UNP Q8WSF8
G	241	PHE	-	expression tag	UNP Q8WSF8
G	242	GLN	-	expression tag	UNP Q8WSF8
G	243	GLY	-	expression tag	UNP Q8WSF8
G	244	HIS	-	expression tag	UNP Q8WSF8
G	245	HIS	-	expression tag	UNP Q8WSF8
G	246	HIS	-	expression tag	UNP Q8WSF8
G	247	HIS	-	expression tag	UNP Q8WSF8
G	248	HIS	-	expression tag	UNP Q8WSF8
G	249	HIS	-	expression tag	UNP Q8WSF8
H	53	PHE	THR	engineered mutation	UNP Q8WSF8
H	60	VAL	ALA	conflict	UNP Q8WSF8
H	74	ARG	GLN	engineered mutation	UNP Q8WSF8
H	110	ALA	TYR	engineered mutation	UNP Q8WSF8
H	135	SER	ILE	engineered mutation	UNP Q8WSF8
H	155	VAL	ALA	conflict	UNP Q8WSF8
H	162	GLU	GLY	engineered mutation	UNP Q8WSF8
H	237	GLU	-	expression tag	UNP Q8WSF8
H	238	ASN	-	expression tag	UNP Q8WSF8
H	239	LEU	-	expression tag	UNP Q8WSF8
H	240	TYR	-	expression tag	UNP Q8WSF8
H	241	PHE	-	expression tag	UNP Q8WSF8
H	242	GLN	-	expression tag	UNP Q8WSF8
H	243	GLY	-	expression tag	UNP Q8WSF8
H	244	HIS	-	expression tag	UNP Q8WSF8
H	245	HIS	-	expression tag	UNP Q8WSF8
H	246	HIS	-	expression tag	UNP Q8WSF8
H	247	HIS	-	expression tag	UNP Q8WSF8
H	248	HIS	-	expression tag	UNP Q8WSF8
H	249	HIS	-	expression tag	UNP Q8WSF8
I	53	PHE	THR	engineered mutation	UNP Q8WSF8
I	60	VAL	ALA	conflict	UNP Q8WSF8
I	74	ARG	GLN	engineered mutation	UNP Q8WSF8
I	110	ALA	TYR	engineered mutation	UNP Q8WSF8
I	135	SER	ILE	engineered mutation	UNP Q8WSF8
I	155	VAL	ALA	conflict	UNP Q8WSF8
I	162	GLU	GLY	engineered mutation	UNP Q8WSF8
I	237	GLU	-	expression tag	UNP Q8WSF8
I	238	ASN	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	239	LEU	-	expression tag	UNP Q8WSF8
I	240	TYR	-	expression tag	UNP Q8WSF8
I	241	PHE	-	expression tag	UNP Q8WSF8
I	242	GLN	-	expression tag	UNP Q8WSF8
I	243	GLY	-	expression tag	UNP Q8WSF8
I	244	HIS	-	expression tag	UNP Q8WSF8
I	245	HIS	-	expression tag	UNP Q8WSF8
I	246	HIS	-	expression tag	UNP Q8WSF8
I	247	HIS	-	expression tag	UNP Q8WSF8
I	248	HIS	-	expression tag	UNP Q8WSF8
I	249	HIS	-	expression tag	UNP Q8WSF8
J	53	PHE	THR	engineered mutation	UNP Q8WSF8
J	60	VAL	ALA	conflict	UNP Q8WSF8
J	74	ARG	GLN	engineered mutation	UNP Q8WSF8
J	110	ALA	TYR	engineered mutation	UNP Q8WSF8
J	135	SER	ILE	engineered mutation	UNP Q8WSF8
J	155	VAL	ALA	conflict	UNP Q8WSF8
J	162	GLU	GLY	engineered mutation	UNP Q8WSF8
J	237	GLU	-	expression tag	UNP Q8WSF8
J	238	ASN	-	expression tag	UNP Q8WSF8
J	239	LEU	-	expression tag	UNP Q8WSF8
J	240	TYR	-	expression tag	UNP Q8WSF8
J	241	PHE	-	expression tag	UNP Q8WSF8
J	242	GLN	-	expression tag	UNP Q8WSF8
J	243	GLY	-	expression tag	UNP Q8WSF8
J	244	HIS	-	expression tag	UNP Q8WSF8
J	245	HIS	-	expression tag	UNP Q8WSF8
J	246	HIS	-	expression tag	UNP Q8WSF8
J	247	HIS	-	expression tag	UNP Q8WSF8
J	248	HIS	-	expression tag	UNP Q8WSF8
J	249	HIS	-	expression tag	UNP Q8WSF8
K	53	PHE	THR	engineered mutation	UNP Q8WSF8
K	60	VAL	ALA	conflict	UNP Q8WSF8
K	74	ARG	GLN	engineered mutation	UNP Q8WSF8
K	110	ALA	TYR	engineered mutation	UNP Q8WSF8
K	135	SER	ILE	engineered mutation	UNP Q8WSF8
K	155	VAL	ALA	conflict	UNP Q8WSF8
K	162	GLU	GLY	engineered mutation	UNP Q8WSF8
K	237	GLU	-	expression tag	UNP Q8WSF8
K	238	ASN	-	expression tag	UNP Q8WSF8
K	239	LEU	-	expression tag	UNP Q8WSF8
K	240	TYR	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	241	PHE	-	expression tag	UNP Q8WSF8
K	242	GLN	-	expression tag	UNP Q8WSF8
K	243	GLY	-	expression tag	UNP Q8WSF8
K	244	HIS	-	expression tag	UNP Q8WSF8
K	245	HIS	-	expression tag	UNP Q8WSF8
K	246	HIS	-	expression tag	UNP Q8WSF8
K	247	HIS	-	expression tag	UNP Q8WSF8
K	248	HIS	-	expression tag	UNP Q8WSF8
K	249	HIS	-	expression tag	UNP Q8WSF8
L	53	PHE	THR	engineered mutation	UNP Q8WSF8
L	60	VAL	ALA	conflict	UNP Q8WSF8
L	74	ARG	GLN	engineered mutation	UNP Q8WSF8
L	110	ALA	TYR	engineered mutation	UNP Q8WSF8
L	135	SER	ILE	engineered mutation	UNP Q8WSF8
L	155	VAL	ALA	conflict	UNP Q8WSF8
L	162	GLU	GLY	engineered mutation	UNP Q8WSF8
L	237	GLU	-	expression tag	UNP Q8WSF8
L	238	ASN	-	expression tag	UNP Q8WSF8
L	239	LEU	-	expression tag	UNP Q8WSF8
L	240	TYR	-	expression tag	UNP Q8WSF8
L	241	PHE	-	expression tag	UNP Q8WSF8
L	242	GLN	-	expression tag	UNP Q8WSF8
L	243	GLY	-	expression tag	UNP Q8WSF8
L	244	HIS	-	expression tag	UNP Q8WSF8
L	245	HIS	-	expression tag	UNP Q8WSF8
L	246	HIS	-	expression tag	UNP Q8WSF8
L	247	HIS	-	expression tag	UNP Q8WSF8
L	248	HIS	-	expression tag	UNP Q8WSF8
L	249	HIS	-	expression tag	UNP Q8WSF8
M	53	PHE	THR	engineered mutation	UNP Q8WSF8
M	60	VAL	ALA	conflict	UNP Q8WSF8
M	74	ARG	GLN	engineered mutation	UNP Q8WSF8
M	110	ALA	TYR	engineered mutation	UNP Q8WSF8
M	135	SER	ILE	engineered mutation	UNP Q8WSF8
M	155	VAL	ALA	conflict	UNP Q8WSF8
M	162	GLU	GLY	engineered mutation	UNP Q8WSF8
M	237	GLU	-	expression tag	UNP Q8WSF8
M	238	ASN	-	expression tag	UNP Q8WSF8
M	239	LEU	-	expression tag	UNP Q8WSF8
M	240	TYR	-	expression tag	UNP Q8WSF8
M	241	PHE	-	expression tag	UNP Q8WSF8
M	242	GLN	-	expression tag	UNP Q8WSF8

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Chain	Residue	Modelled	Actual	Comment	Reference
M	243	GLY	-	expression tag	UNP Q8WSF8
M	244	HIS	-	expression tag	UNP Q8WSF8
M	245	HIS	-	expression tag	UNP Q8WSF8
M	246	HIS	-	expression tag	UNP Q8WSF8
M	247	HIS	-	expression tag	UNP Q8WSF8
M	248	HIS	-	expression tag	UNP Q8WSF8
M	249	HIS	-	expression tag	UNP Q8WSF8
N	53	PHE	THR	engineered mutation	UNP Q8WSF8
N	60	VAL	ALA	conflict	UNP Q8WSF8
N	74	ARG	GLN	engineered mutation	UNP Q8WSF8
N	110	ALA	TYR	engineered mutation	UNP Q8WSF8
N	135	SER	ILE	engineered mutation	UNP Q8WSF8
N	155	VAL	ALA	conflict	UNP Q8WSF8
N	162	GLU	GLY	engineered mutation	UNP Q8WSF8
N	237	GLU	-	expression tag	UNP Q8WSF8
N	238	ASN	-	expression tag	UNP Q8WSF8
N	239	LEU	-	expression tag	UNP Q8WSF8
N	240	TYR	-	expression tag	UNP Q8WSF8
N	241	PHE	-	expression tag	UNP Q8WSF8
N	242	GLN	-	expression tag	UNP Q8WSF8
N	243	GLY	-	expression tag	UNP Q8WSF8
N	244	HIS	-	expression tag	UNP Q8WSF8
N	245	HIS	-	expression tag	UNP Q8WSF8
N	246	HIS	-	expression tag	UNP Q8WSF8
N	247	HIS	-	expression tag	UNP Q8WSF8
N	248	HIS	-	expression tag	UNP Q8WSF8
N	249	HIS	-	expression tag	UNP Q8WSF8
O	53	PHE	THR	engineered mutation	UNP Q8WSF8
O	60	VAL	ALA	conflict	UNP Q8WSF8
O	74	ARG	GLN	engineered mutation	UNP Q8WSF8
O	110	ALA	TYR	engineered mutation	UNP Q8WSF8
O	135	SER	ILE	engineered mutation	UNP Q8WSF8
O	155	VAL	ALA	conflict	UNP Q8WSF8
O	162	GLU	GLY	engineered mutation	UNP Q8WSF8
O	237	GLU	-	expression tag	UNP Q8WSF8
O	238	ASN	-	expression tag	UNP Q8WSF8
O	239	LEU	-	expression tag	UNP Q8WSF8
O	240	TYR	-	expression tag	UNP Q8WSF8
O	241	PHE	-	expression tag	UNP Q8WSF8
O	242	GLN	-	expression tag	UNP Q8WSF8
O	243	GLY	-	expression tag	UNP Q8WSF8
O	244	HIS	-	expression tag	UNP Q8WSF8

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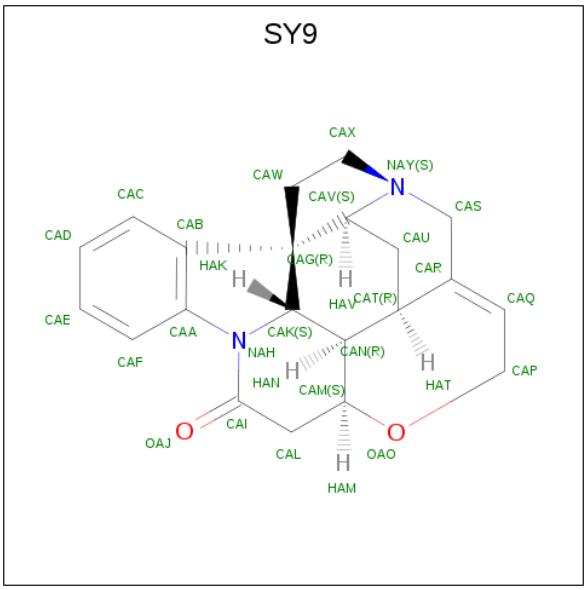
Chain	Residue	Modelled	Actual	Comment	Reference
O	245	HIS	-	expression tag	UNP Q8WSF8
O	246	HIS	-	expression tag	UNP Q8WSF8
O	247	HIS	-	expression tag	UNP Q8WSF8
O	248	HIS	-	expression tag	UNP Q8WSF8
O	249	HIS	-	expression tag	UNP Q8WSF8

- Molecule 2 is STRYCHNINE (three-letter code: SY9) (formula: $C_{21}H_{22}N_2O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 25 21 2 2	0	0
2	C	1	Total C N O 25 21 2 2	0	0
2	C	1	Total C N O 25 21 2 2	0	0
2	D	1	Total C N O 25 21 2 2	0	0
2	E	1	Total C N O 25 21 2 2	0	0
2	G	1	Total C N O 25 21 2 2	0	0
2	H	1	Total C N O 25 21 2 2	0	0
2	H	1	Total C N O 25 21 2 2	0	0

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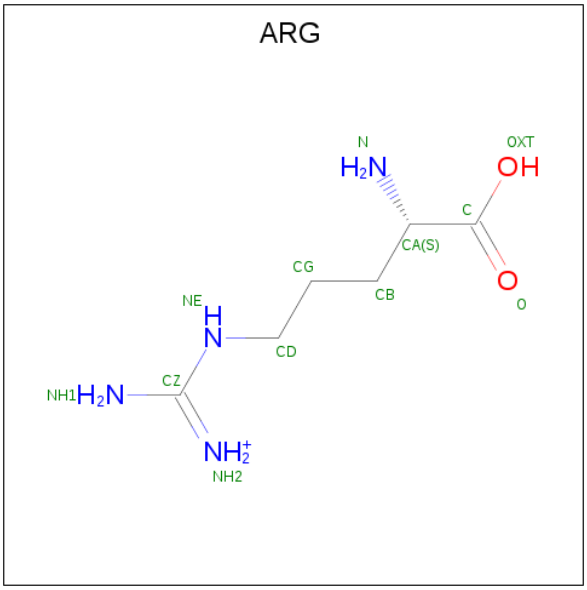
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total	C	N	O	0	0
			25	21	2	2		
2	J	1	Total	C	N	O	0	0
			25	21	2	2		
2	K	1	Total	C	N	O	0	0
			25	21	2	2		
2	K	1	Total	C	N	O	0	0
			25	21	2	2		
2	L	1	Total	C	N	O	0	0
			25	21	2	2		
2	M	1	Total	C	N	O	0	0
			25	21	2	2		
2	N	1	Total	C	N	O	0	0
			25	21	2	2		

- Molecule 3 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



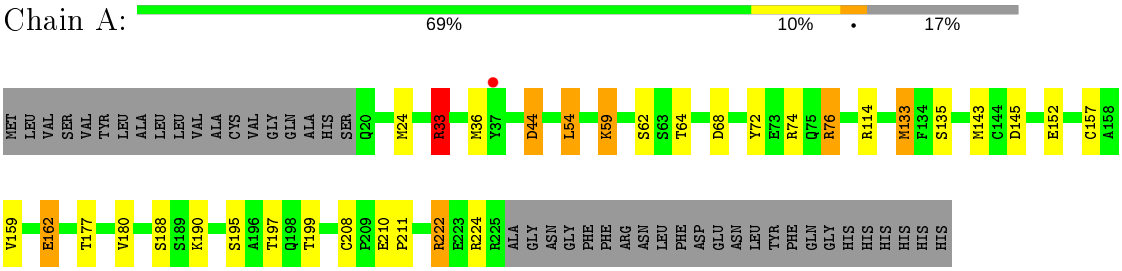
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	N	1	Total	C	N	O	0	0
			11	6	4	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

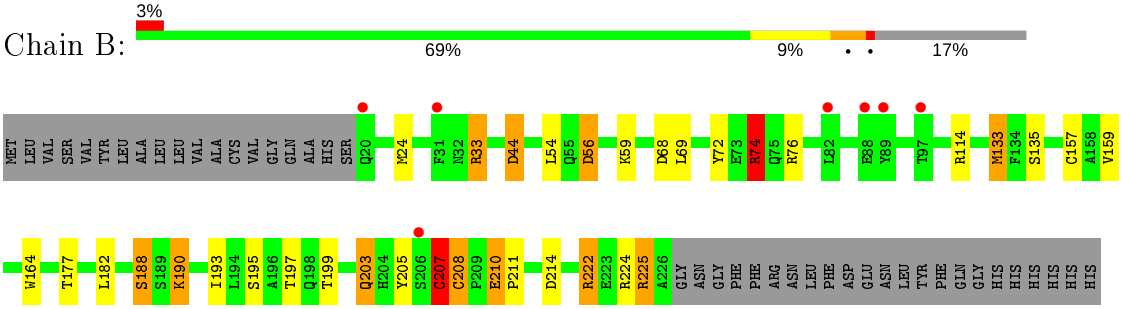
- Molecule 1: Soluble acetylcholine receptor

Chain A:



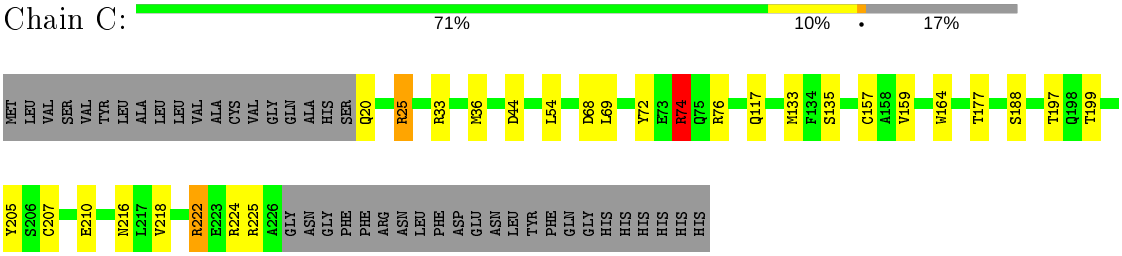
- Molecule 1: Soluble acetylcholine receptor

Chain B:



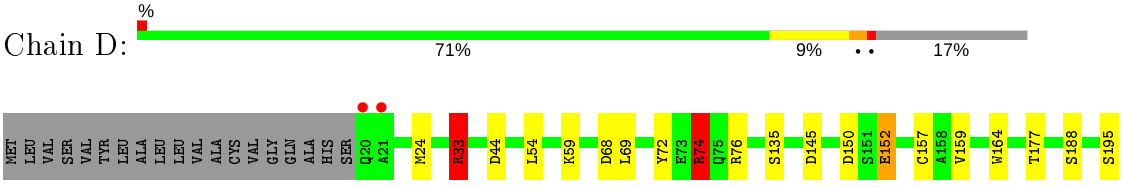
- Molecule 1: Soluble acetylcholine receptor

Chain C:



- Molecule 1: Soluble acetylcholine receptor

Chain D:

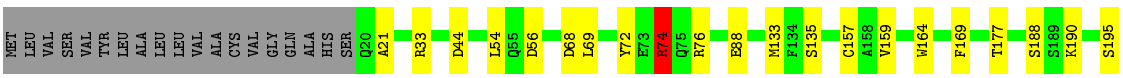


• Molecule 1: Soluble acetylcholine receptor

Chain E:

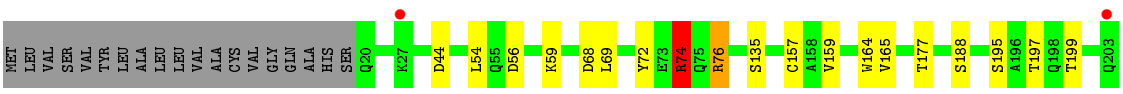
• Molecule 1: Soluble acetylcholine receptor

Chain F:



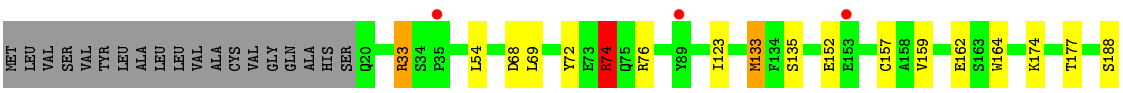
• Molecule 1: Soluble acetylcholine receptor

Chain G:



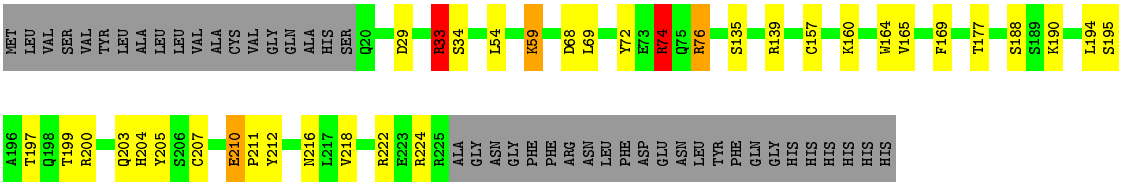
• Molecule 1: Soluble acetylcholine receptor

Chain H:



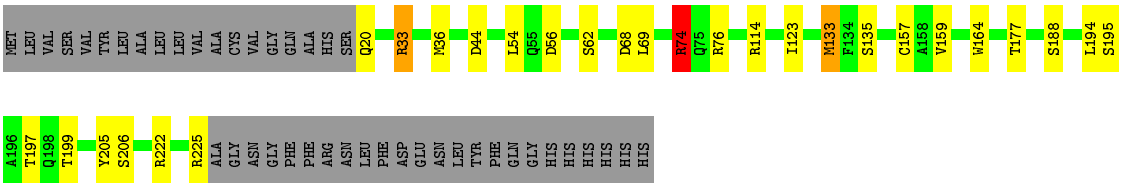
• Molecule 1: Soluble acetylcholine receptor

Chain I:



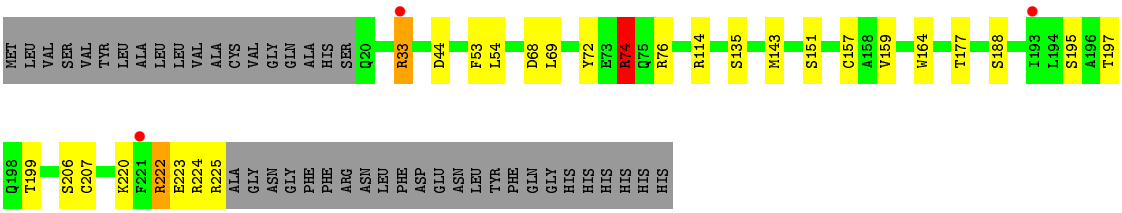
• Molecule 1: Soluble acetylcholine receptor

Chain J:



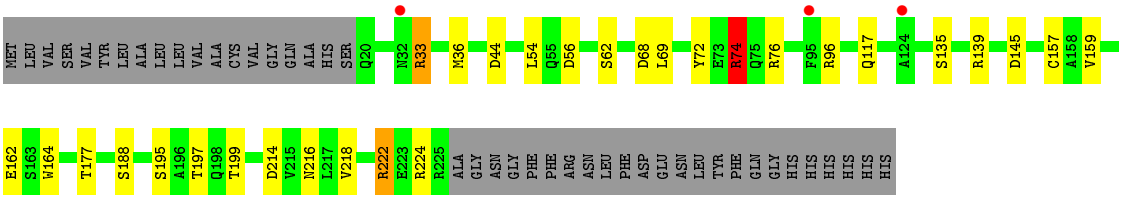
• Molecule 1: Soluble acetylcholine receptor

Chain K:



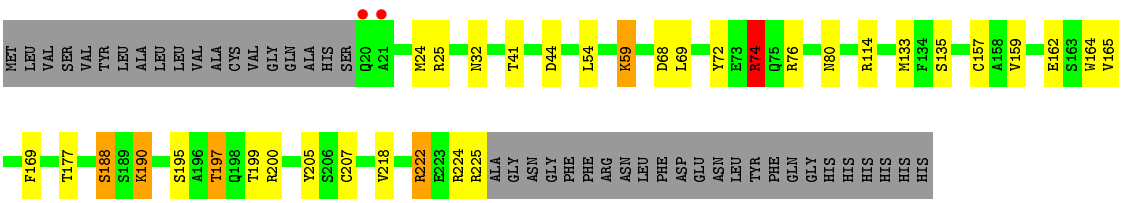
• Molecule 1: Soluble acetylcholine receptor

Chain L:



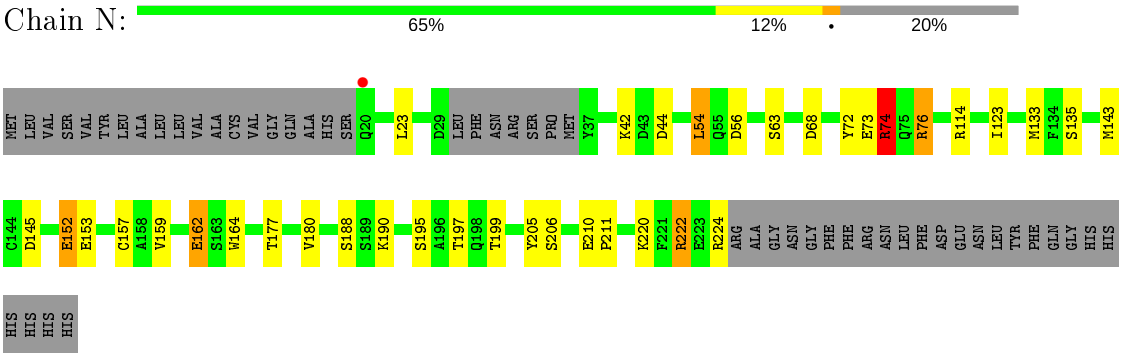
• Molecule 1: Soluble acetylcholine receptor

Chain M:



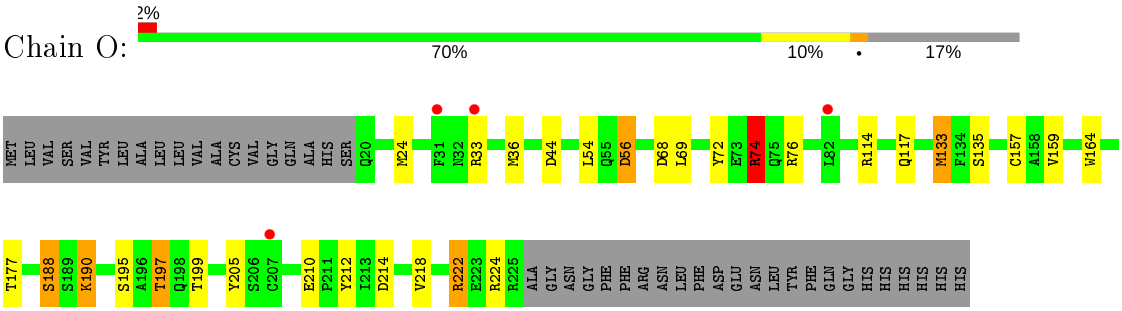
• Molecule 1: Soluble acetylcholine receptor

Chain N:



• Molecule 1: Soluble acetylcholine receptor

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	130.90Å 130.90Å 190.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.85 – 3.20 72.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (72.85-3.20) 98.7 (72.84-3.20)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.188 , 0.231 0.191 , 0.233	Depositor DCC
R_{free} test set	2910 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	62.9	Xtriage
Anisotropy	0.696	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 37.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l 0.054 for h,-h-k,-l 0.049 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25009	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: SY9

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	0.85	0/1689	1.09	12/2302 (0.5%)
1	B	0.86	2/1694 (0.1%)	1.12	13/2309 (0.6%)
1	C	0.82	1/1694 (0.1%)	1.06	7/2309 (0.3%)
1	D	0.91	3/1689 (0.2%)	1.11	10/2302 (0.4%)
1	E	0.89	2/1667 (0.1%)	1.06	9/2274 (0.4%)
1	F	0.85	2/1689 (0.1%)	1.08	8/2302 (0.3%)
1	G	0.79	0/1657	1.03	6/2256 (0.3%)
1	H	0.79	1/1689 (0.1%)	1.04	9/2302 (0.4%)
1	I	0.97	3/1689 (0.2%)	1.13	10/2302 (0.4%)
1	J	0.82	0/1689	1.04	9/2302 (0.4%)
1	K	0.79	1/1689 (0.1%)	1.04	7/2302 (0.3%)
1	L	0.80	0/1689	1.08	13/2302 (0.6%)
1	M	0.87	3/1689 (0.2%)	1.10	10/2302 (0.4%)
1	N	0.91	2/1616 (0.1%)	1.12	11/2203 (0.5%)
1	O	0.82	2/1689 (0.1%)	1.10	13/2302 (0.6%)
All	All	0.85	22/25218 (0.1%)	1.08	147/34371 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
1	E	0	2
1	F	0	2
1	H	0	1
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	2
1	L	0	1
1	M	0	2
1	O	0	1
All	All	0	19

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	208	CYS	CB-SG	8.92	1.97	1.82
1	N	152	GLU	CG-CD	8.26	1.64	1.51
1	E	210	GLU	CD-OE1	7.73	1.34	1.25
1	B	208	CYS	CB-SG	7.44	1.94	1.82
1	I	212	TYR	CE1-CZ	-7.12	1.29	1.38

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	74	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	N	222	ARG	NE-CZ-NH2	-10.53	115.04	120.30
1	I	74	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	L	36	MET	CG-SD-CE	9.91	116.05	100.20
1	G	74	ARG	NE-CZ-NH1	9.68	125.14	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	ARG	Peptide
1	B	207	CYS	Peptide
1	B	33	ARG	Peptide
1	C	207	CYS	Peptide
1	C	33	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1649	0	1582	14	0
1	B	1654	0	1587	19	0
1	C	1654	0	1587	14	1
1	D	1649	0	1582	10	0
1	E	1627	0	1556	9	0
1	F	1649	0	1582	8	0
1	G	1619	0	1560	6	0
1	H	1649	0	1582	11	1
1	I	1649	0	1582	14	1
1	J	1649	0	1582	12	1
1	K	1649	0	1582	11	1
1	L	1649	0	1582	12	0
1	M	1649	0	1582	12	2
1	N	1579	0	1508	13	1
1	O	1649	0	1582	12	0
2	A	25	0	22	7	0
2	C	50	0	44	1	0
2	D	25	0	22	0	0
2	E	25	0	22	0	0
2	G	25	0	22	0	0
2	H	50	0	44	4	0
2	I	25	0	22	3	0
2	J	25	0	22	3	0
2	K	50	0	44	5	0
2	L	25	0	22	1	0
2	M	25	0	22	1	0
2	N	25	0	22	2	0
3	N	11	0	12	0	0
All	All	25009	0	23960	137	4

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 3.

The worst 5 of 137 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:J:54:LEU:HD11	1:J:69:LEU:HD11	1.33	1.10
1:I:29:ASP:O	1:I:33:ARG:HD3	1.58	1.02
1:B:44:ASP:CG	1:C:20:GLN:HE22	1.73	0.92
1:H:205:TYR:CE2	2:H:302:SY9:HAP2	2.09	0.87
1:J:205:TYR:CE2	2:J:401:SY9:HAP2	2.11	0.86

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:204:HIS:CB	1:M:80:ASN:OD1[1_445]	1.74	0.46
1:C:25:ARG:CD	1:M:32:ASN:O[1_445]	1.98	0.22
1:K:206:SER:OG	1:N:206:SER:OG[3_555]	2.07	0.13
1:H:206:SER:OG	1:J:206:SER:OG[2_444]	2.17	0.03

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	204/249 (82%)	193 (95%)	11 (5%)	0	100	100
1	B	205/249 (82%)	192 (94%)	13 (6%)	0	100	100
1	C	205/249 (82%)	191 (93%)	14 (7%)	0	100	100
1	D	204/249 (82%)	192 (94%)	12 (6%)	0	100	100
1	E	202/249 (81%)	190 (94%)	12 (6%)	0	100	100
1	F	204/249 (82%)	192 (94%)	12 (6%)	0	100	100
1	G	198/249 (80%)	186 (94%)	12 (6%)	0	100	100
1	H	204/249 (82%)	192 (94%)	12 (6%)	0	100	100
1	I	204/249 (82%)	192 (94%)	12 (6%)	0	100	100
1	J	204/249 (82%)	192 (94%)	12 (6%)	0	100	100
1	K	204/249 (82%)	192 (94%)	12 (6%)	0	100	100
1	L	204/249 (82%)	191 (94%)	13 (6%)	0	100	100
1	M	204/249 (82%)	191 (94%)	13 (6%)	0	100	100
1	N	194/249 (78%)	182 (94%)	12 (6%)	0	100	100
1	O	204/249 (82%)	191 (94%)	13 (6%)	0	100	100
All	All	3044/3735 (82%)	2859 (94%)	185 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	189/224 (84%)	174 (92%)	15 (8%)	12 43
1	B	189/224 (84%)	171 (90%)	18 (10%)	8 32
1	C	189/224 (84%)	178 (94%)	11 (6%)	20 55
1	D	189/224 (84%)	172 (91%)	17 (9%)	9 34
1	E	187/224 (84%)	174 (93%)	13 (7%)	15 48
1	F	189/224 (84%)	176 (93%)	13 (7%)	15 49
1	G	185/224 (83%)	172 (93%)	13 (7%)	15 48
1	H	189/224 (84%)	175 (93%)	14 (7%)	13 46
1	I	189/224 (84%)	176 (93%)	13 (7%)	15 49
1	J	189/224 (84%)	177 (94%)	12 (6%)	18 52
1	K	189/224 (84%)	178 (94%)	11 (6%)	20 55
1	L	189/224 (84%)	177 (94%)	12 (6%)	18 52
1	M	189/224 (84%)	175 (93%)	14 (7%)	13 46
1	N	181/224 (81%)	164 (91%)	17 (9%)	8 33
1	O	189/224 (84%)	175 (93%)	14 (7%)	13 46
All	All	2821/3360 (84%)	2614 (93%)	207 (7%)	14 46

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	159	VAL
1	I	59	LYS
1	N	222	ARG
1	G	195	SER
1	H	177	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such

sidechains are listed below:

Mol	Chain	Res	Type
1	E	80	ASN
1	F	80	ASN
1	L	80	ASN
1	D	80	ASN
1	E	32	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

16 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	SY9	H	302	-	31,31,31	0.63	0	51,51,51	0.80	3 (5%)
2	SY9	N	302	-	31,31,31	0.49	0	51,51,51	0.80	2 (3%)
2	SY9	C	401	-	31,31,31	0.29	0	51,51,51	0.45	0
2	SY9	I	301	-	31,31,31	0.55	0	51,51,51	0.74	1 (1%)
2	SY9	A	401	-	31,31,31	0.47	0	51,51,51	0.82	3 (5%)
2	SY9	D	401	-	31,31,31	0.38	0	51,51,51	0.73	0
2	SY9	G	401	-	31,31,31	0.46	0	51,51,51	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SY9	E	401	-	31,31,31	0.51	0	51,51,51	0.71	2 (3%)
2	SY9	C	402	-	31,31,31	0.39	0	51,51,51	0.70	0
2	SY9	K	401	-	31,31,31	0.29	0	51,51,51	0.53	0
2	SY9	L	401	-	31,31,31	0.42	0	51,51,51	0.53	0
2	SY9	H	301	-	31,31,31	0.44	0	51,51,51	0.62	1 (1%)
2	SY9	J	401	-	31,31,31	0.45	0	51,51,51	0.83	3 (5%)
2	SY9	M	401	-	31,31,31	0.44	0	51,51,51	0.56	1 (1%)
2	SY9	K	402	-	31,31,31	0.39	0	51,51,51	0.44	0

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	302	SY9	CAW-CAG-CAB	2.60	117.09	112.35
2	A	401	SY9	CAP-CAQ-CAR	2.55	127.58	122.31
2	E	401	SY9	CAR-CAS-NAY	2.44	117.65	112.91
2	J	401	SY9	CAW-CAG-CAB	2.32	116.58	112.35
2	J	401	SY9	CAP-CAQ-CAR	2.26	126.98	122.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

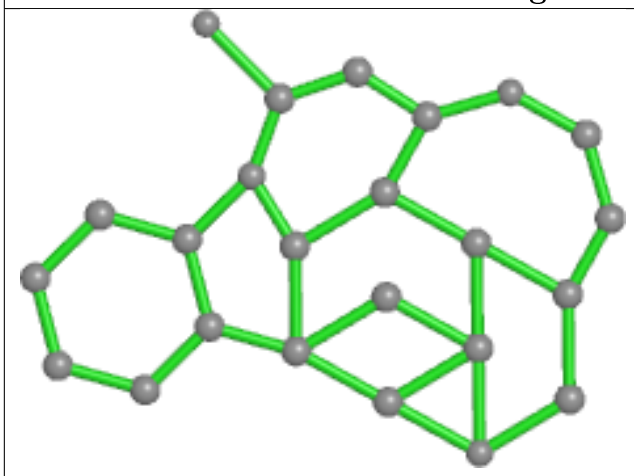
10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	302	SY9	4	0
2	N	302	SY9	2	0
2	I	301	SY9	3	0
2	A	401	SY9	7	0
2	C	402	SY9	1	0
2	K	401	SY9	2	0
2	L	401	SY9	1	0
2	J	401	SY9	3	0
2	M	401	SY9	1	0
2	K	402	SY9	3	0

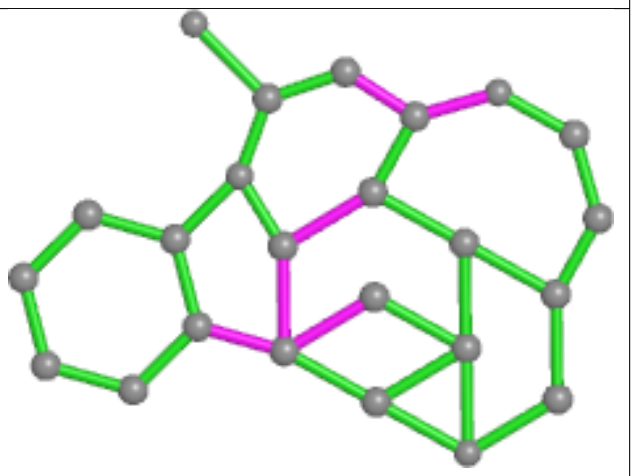
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

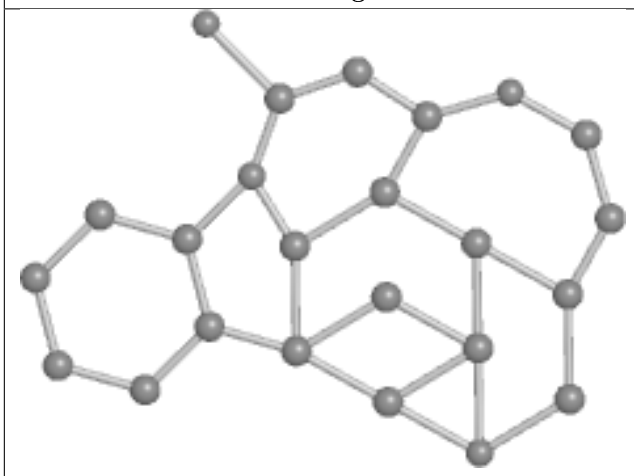
Ligand SY9 H 302



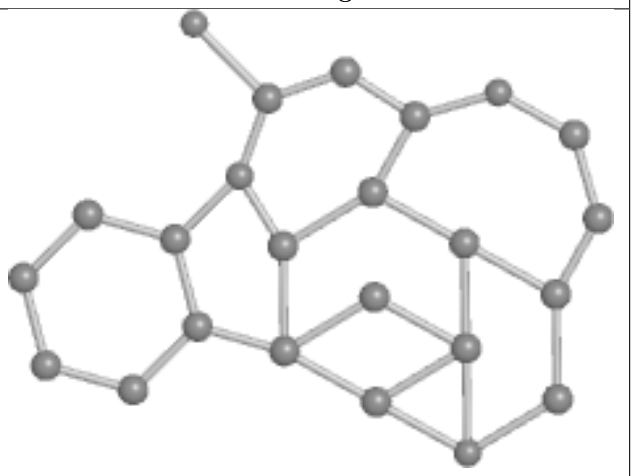
Bond lengths



Bond angles

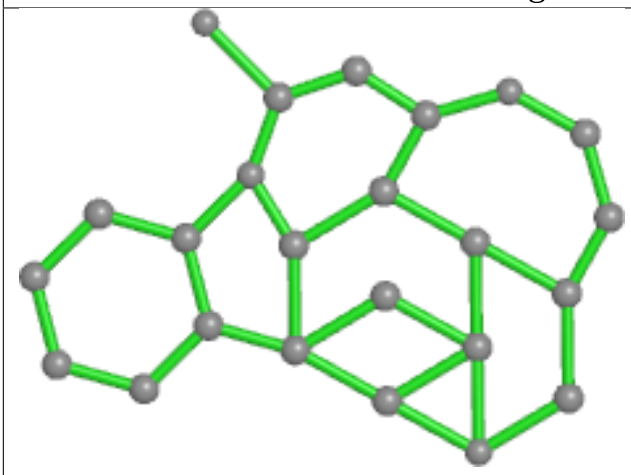


Torsions



Rings

Ligand SY9 N 302



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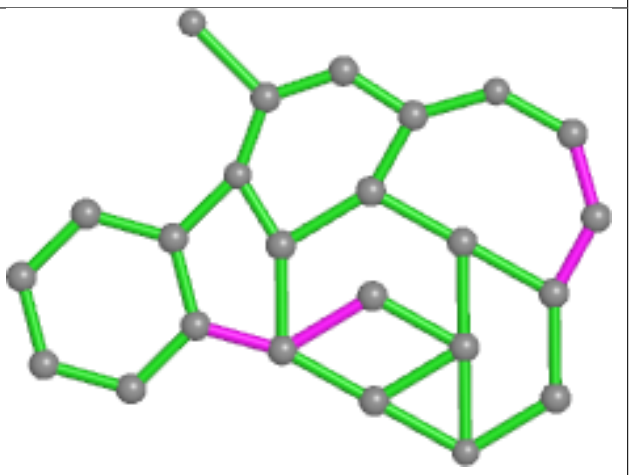

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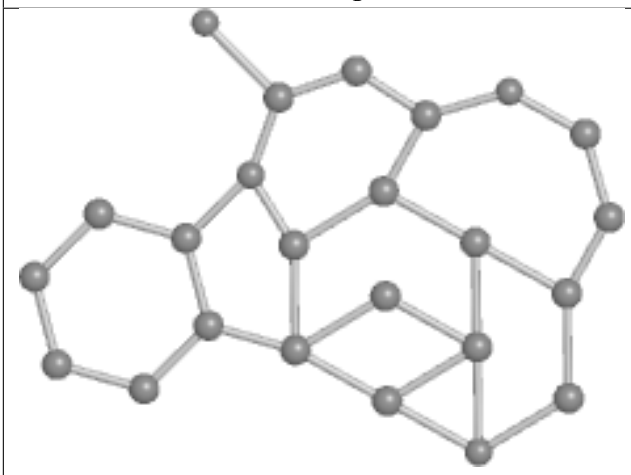

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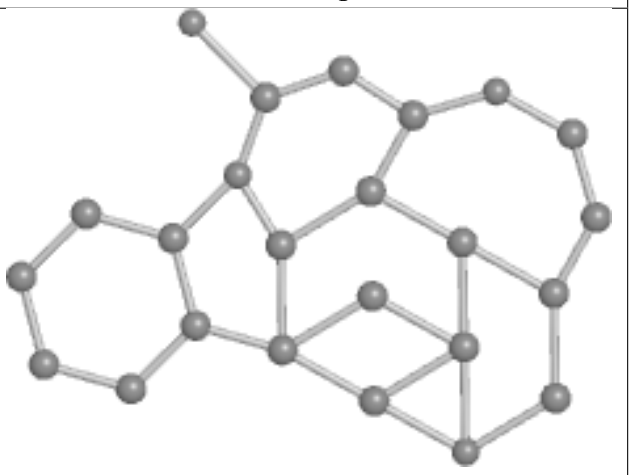
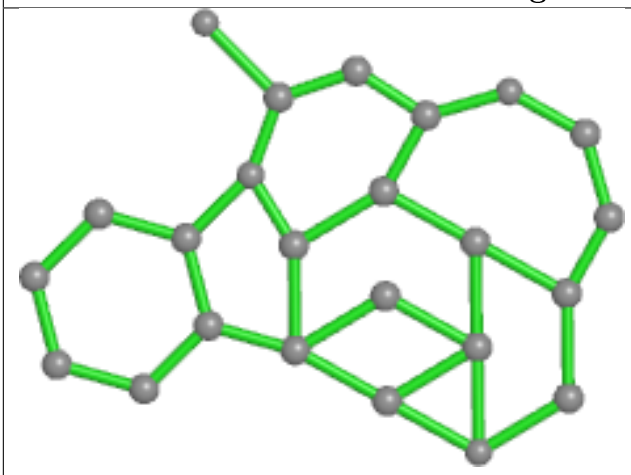


Rings

Ligand SY9 C 401



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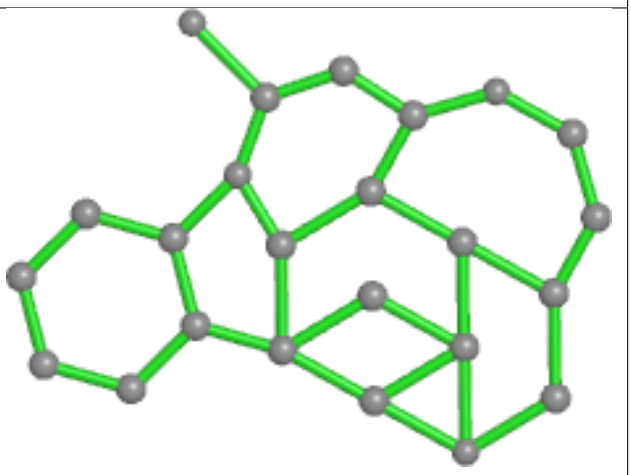

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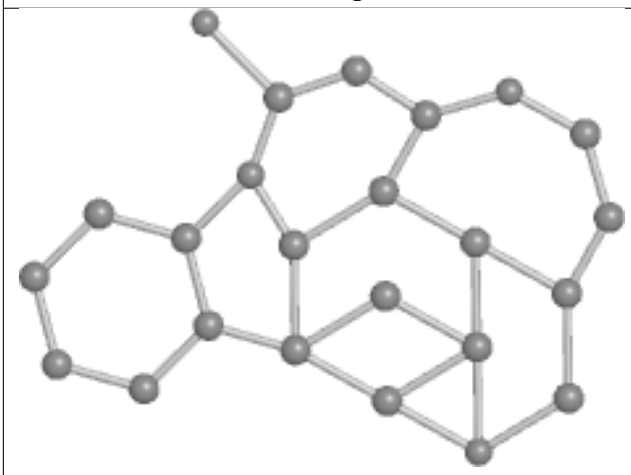

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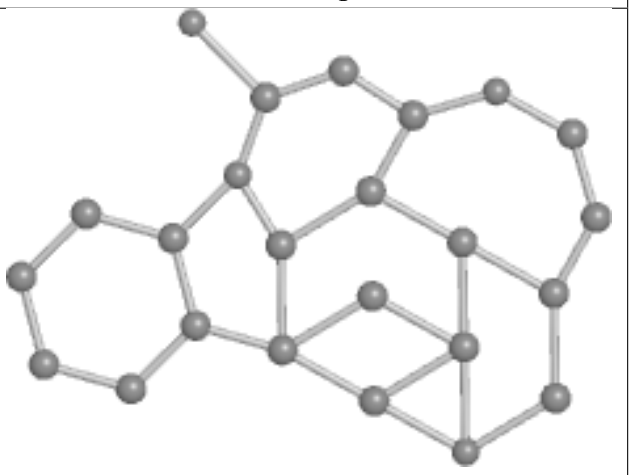

Rings

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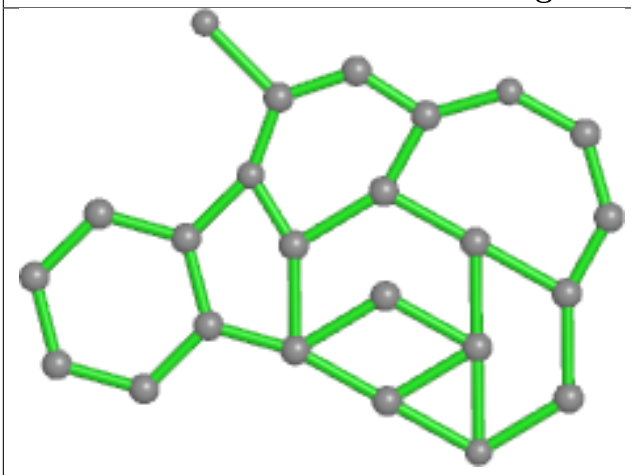

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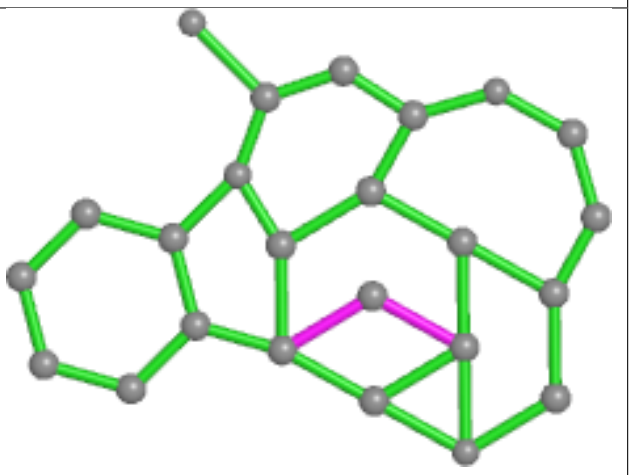

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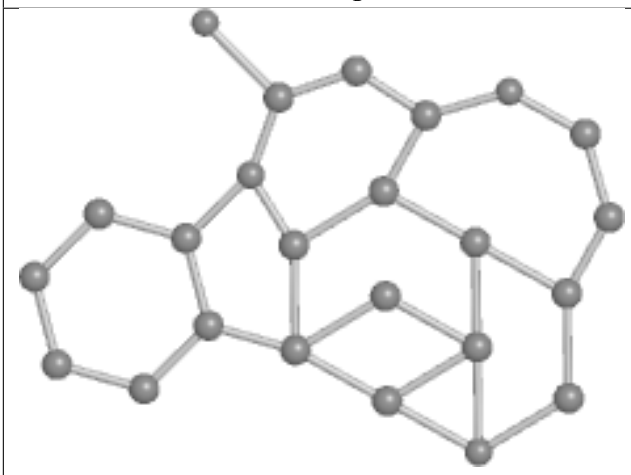

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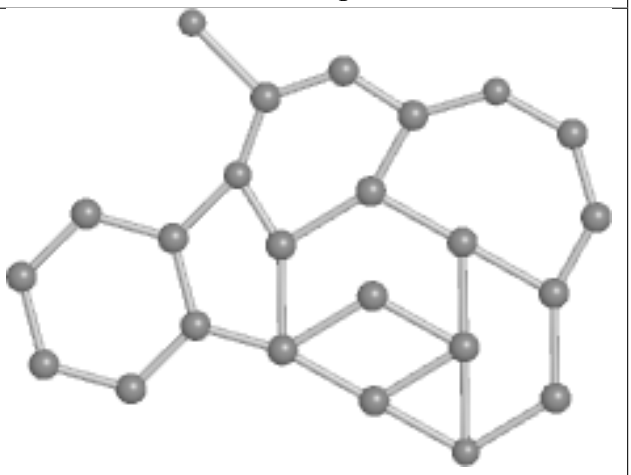

Rings

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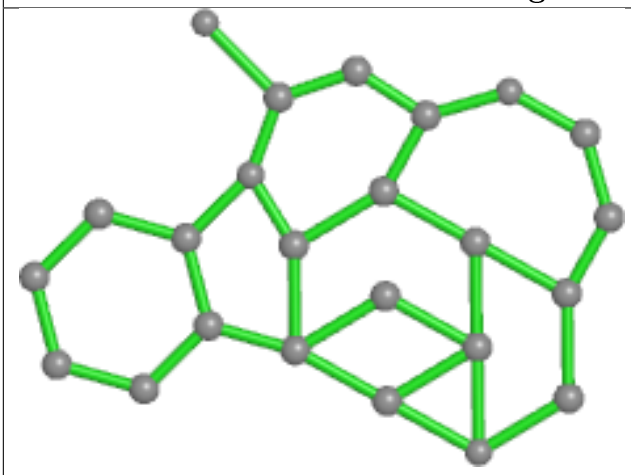

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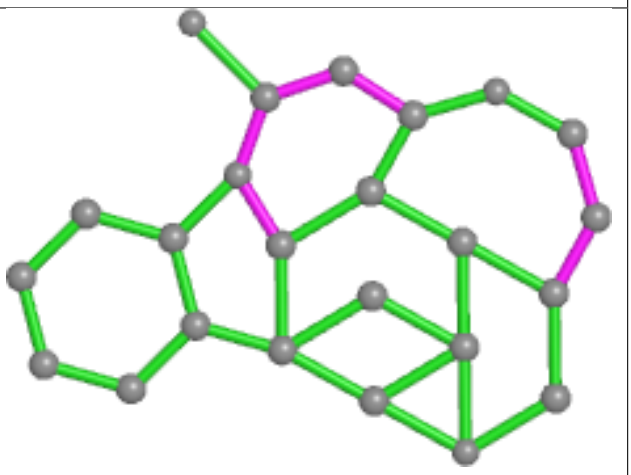

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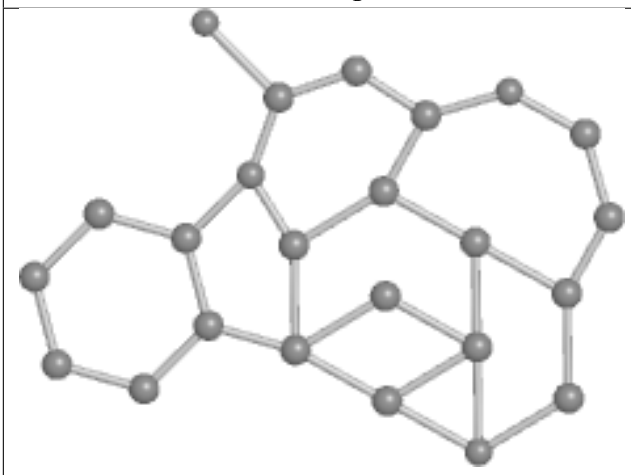

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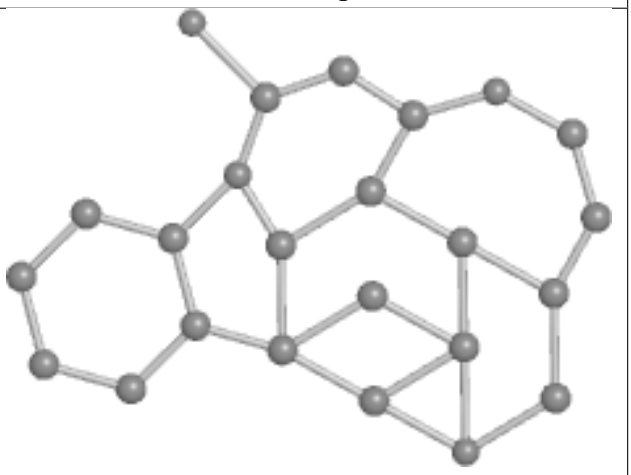
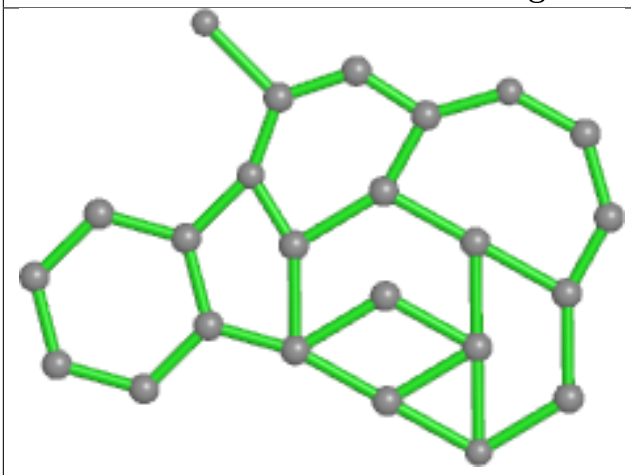


Rings

Ligand SY9 D 401



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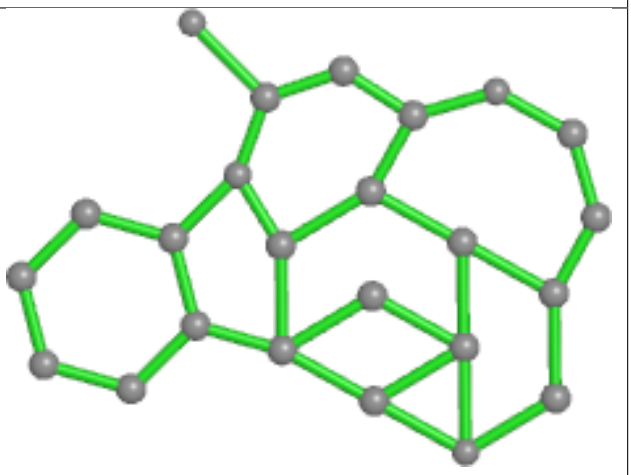

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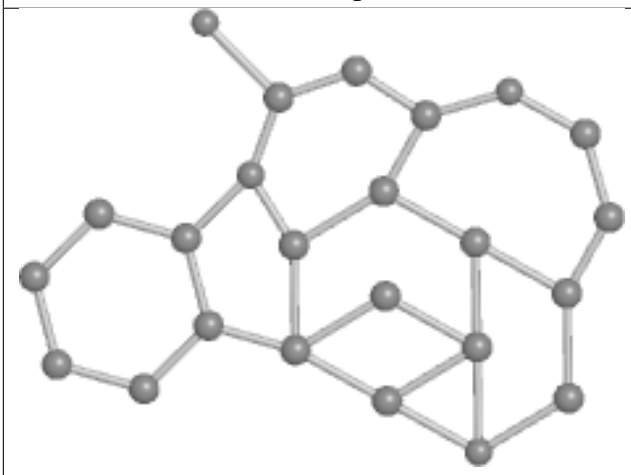

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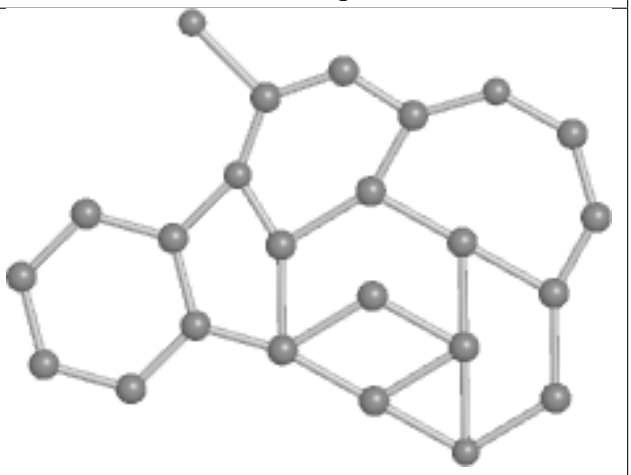
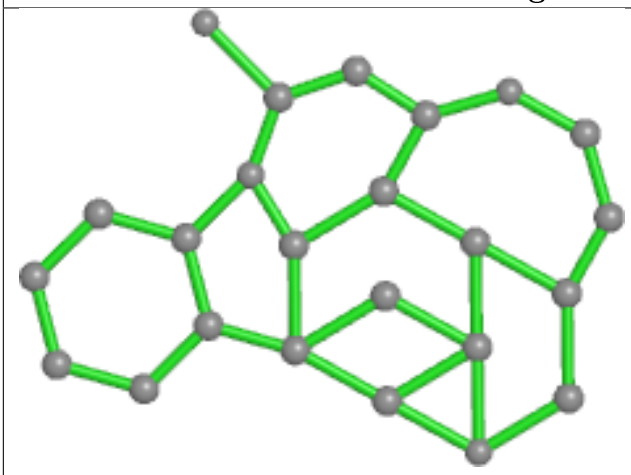


Rings

Ligand SY9 G 401



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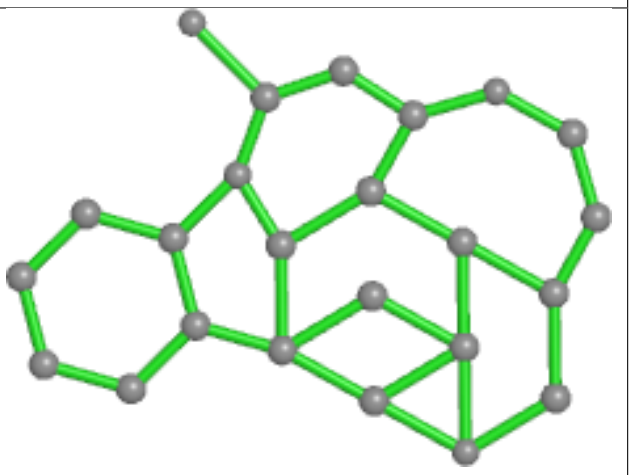

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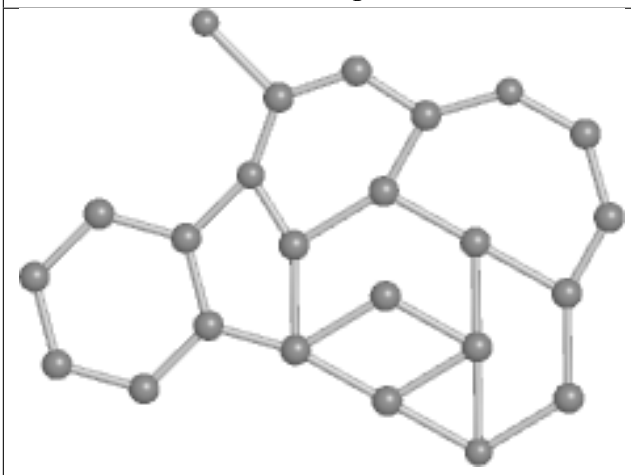

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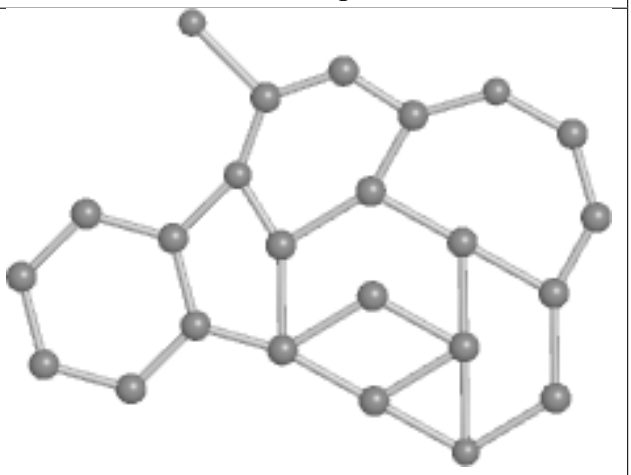

Rings

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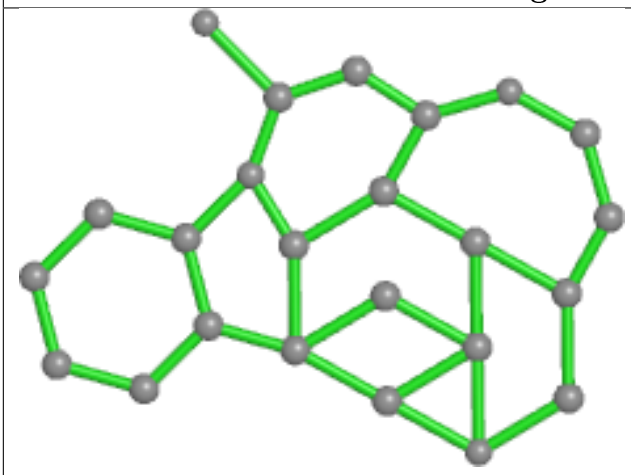

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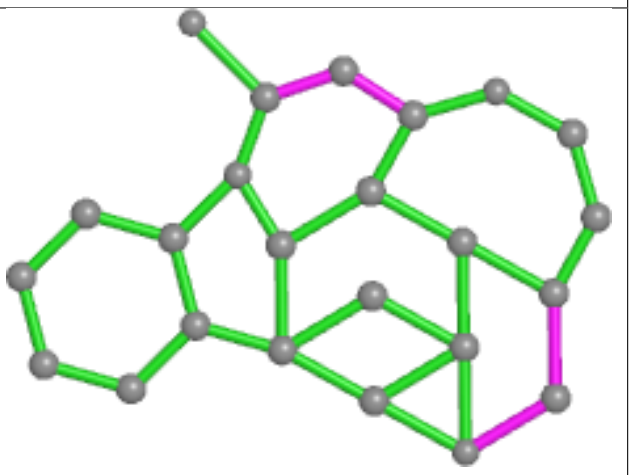
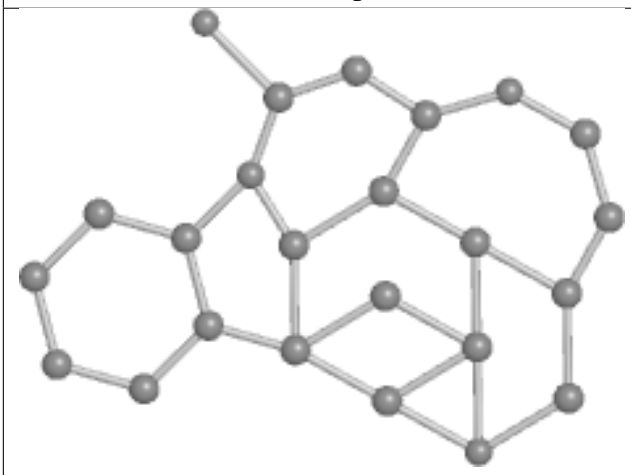


Bond angles



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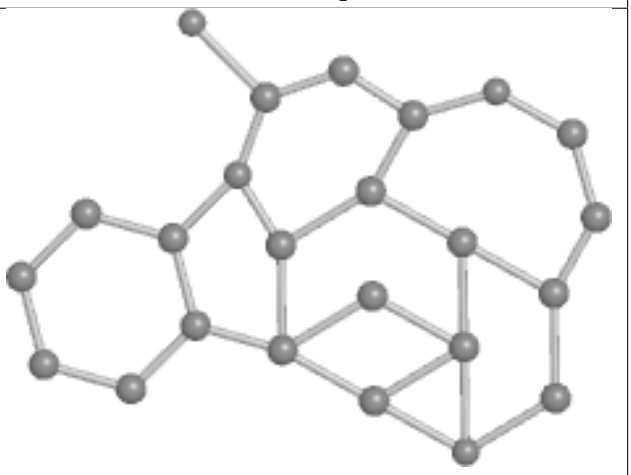
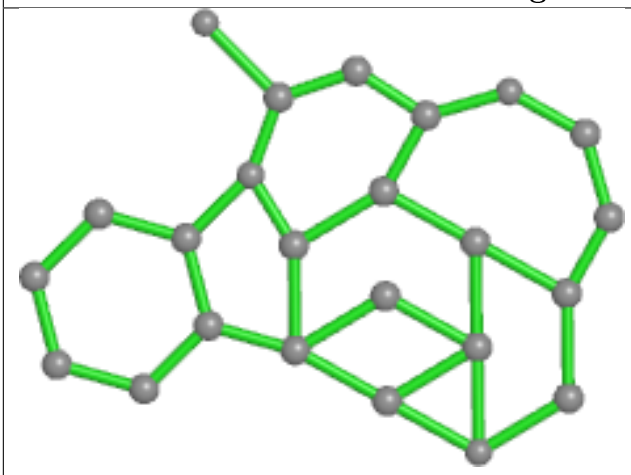


Rings

Ligand SY9 C 402



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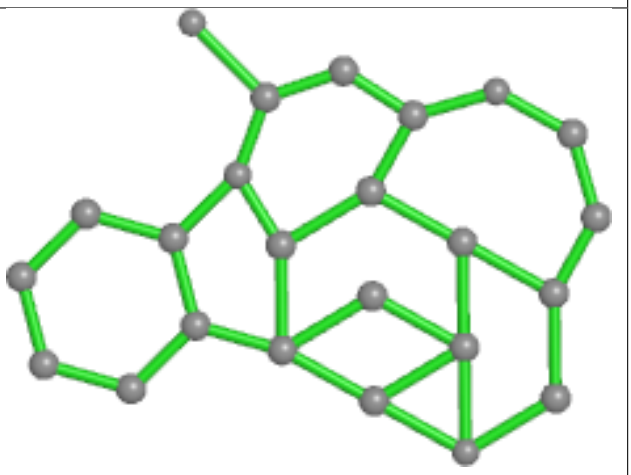

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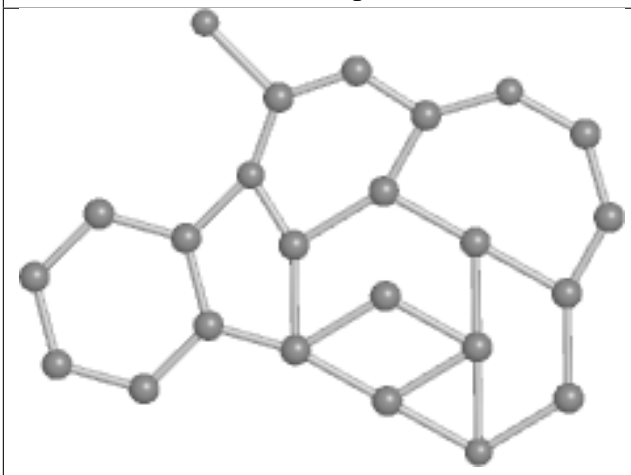

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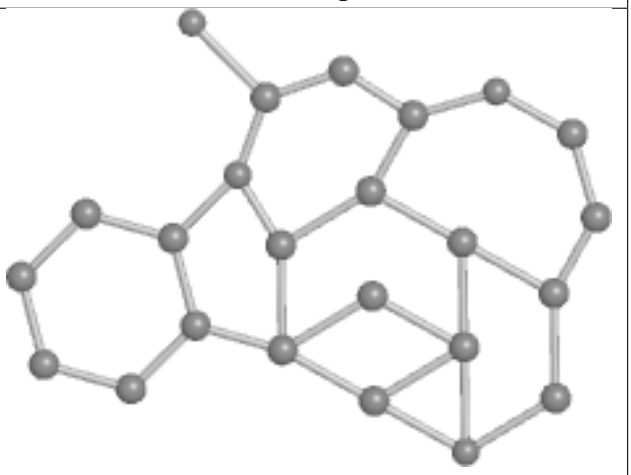
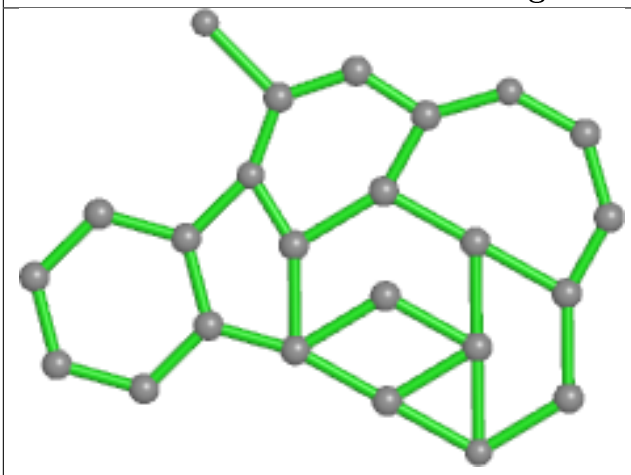


Rings

Ligand SY9 K 401



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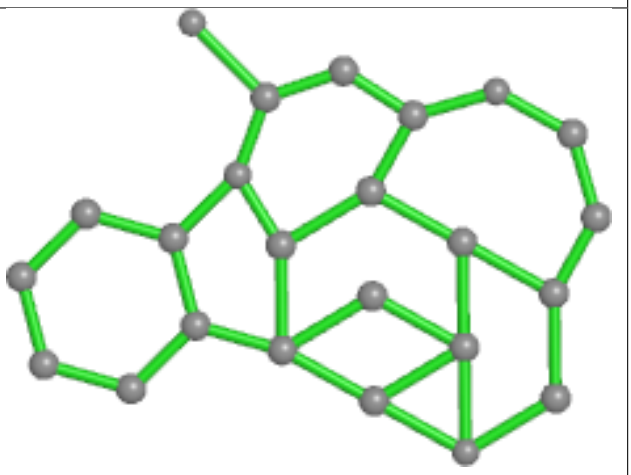
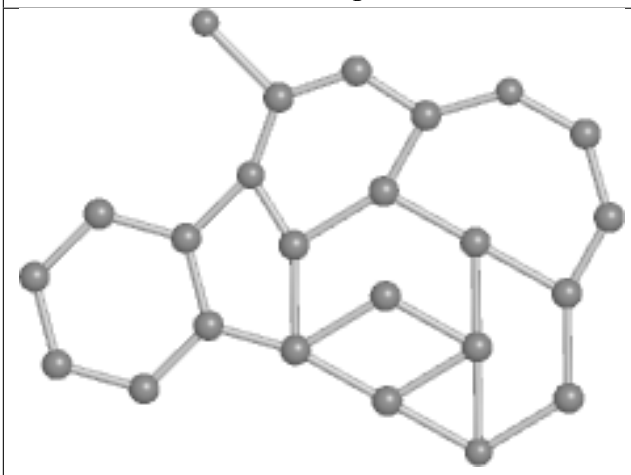
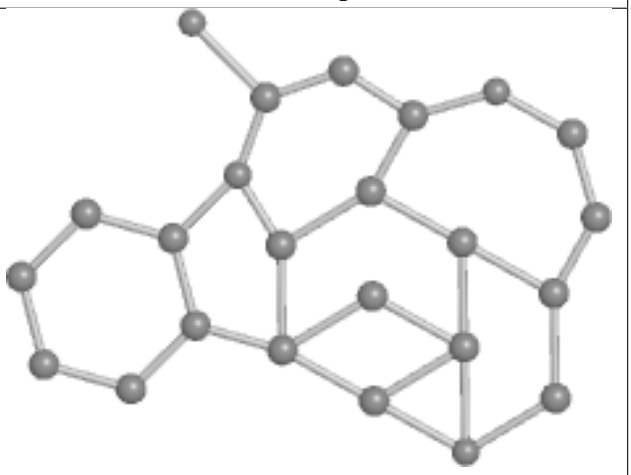


Bond angles

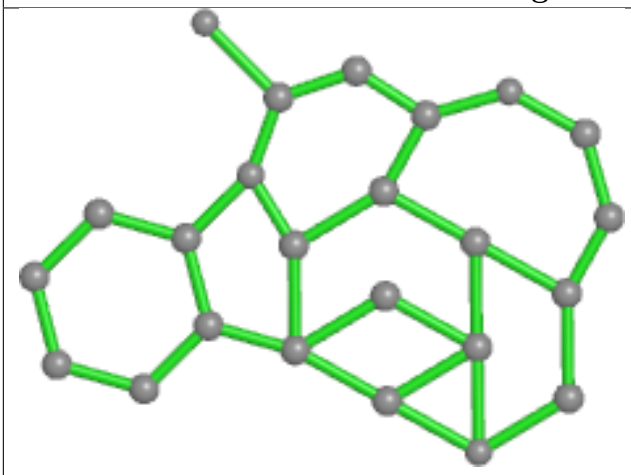


Torsions

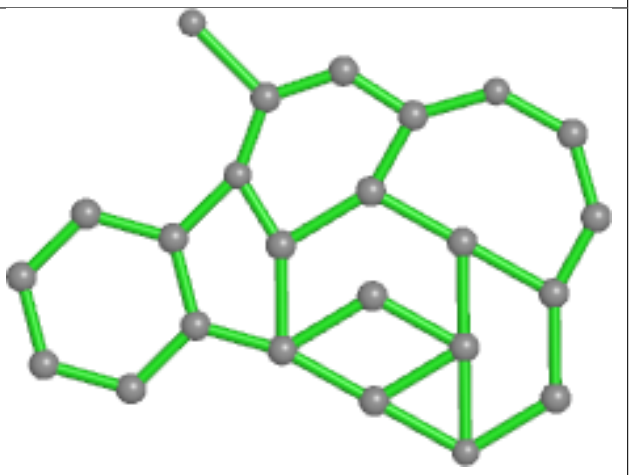


Rings

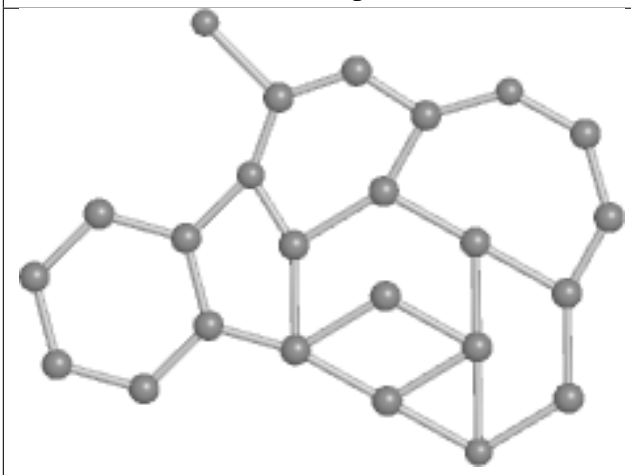
Ligand SY9 L 401



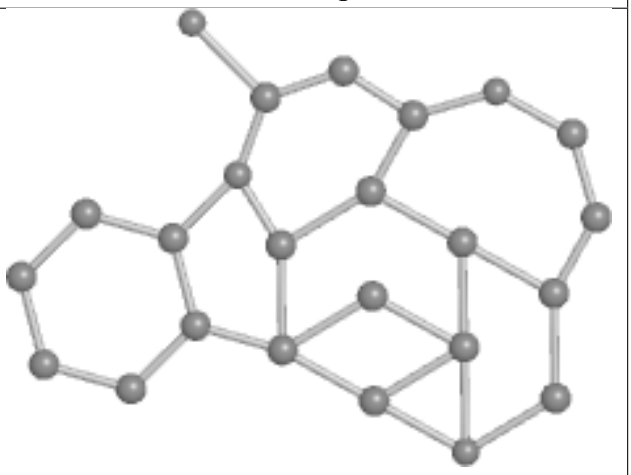
Bond lengths



Bond angles

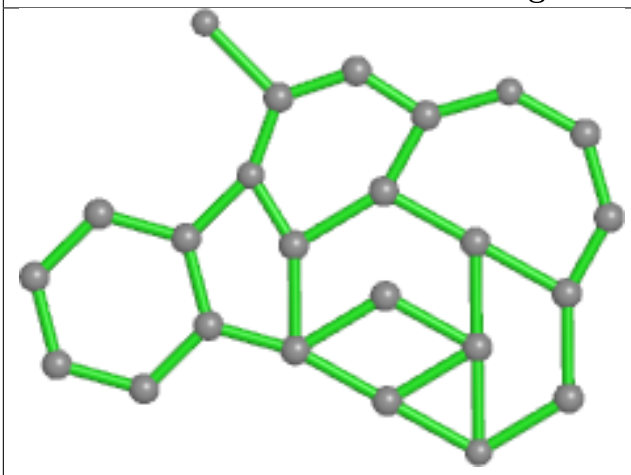


Torsions

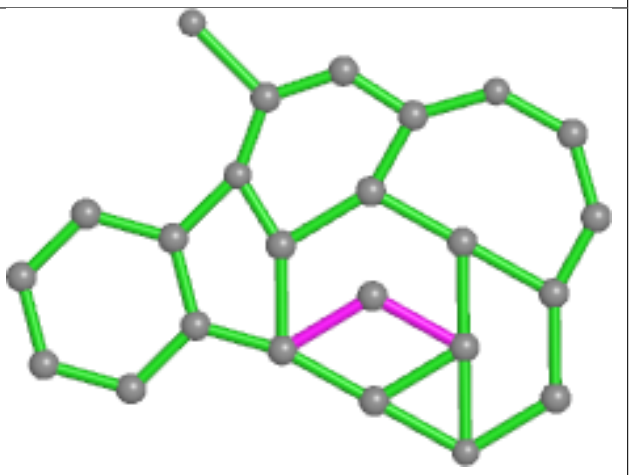


Rings

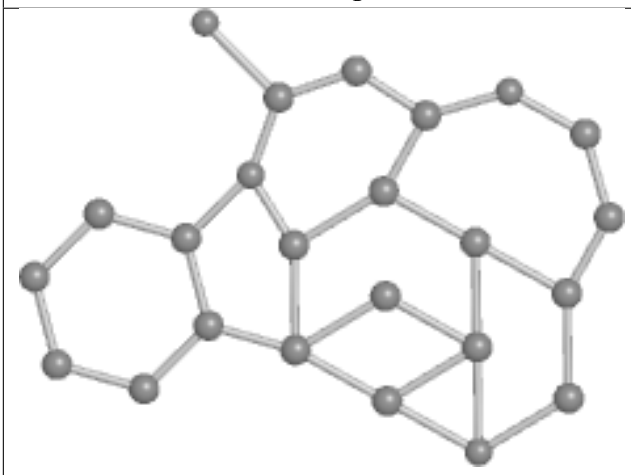
Ligand SY9 H 301



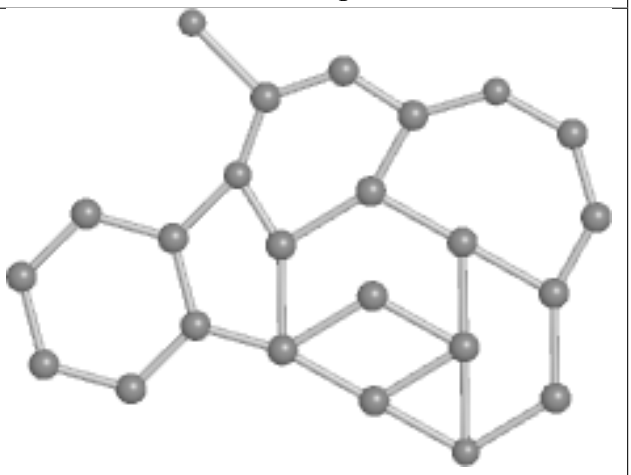
Bond lengths



Bond angles

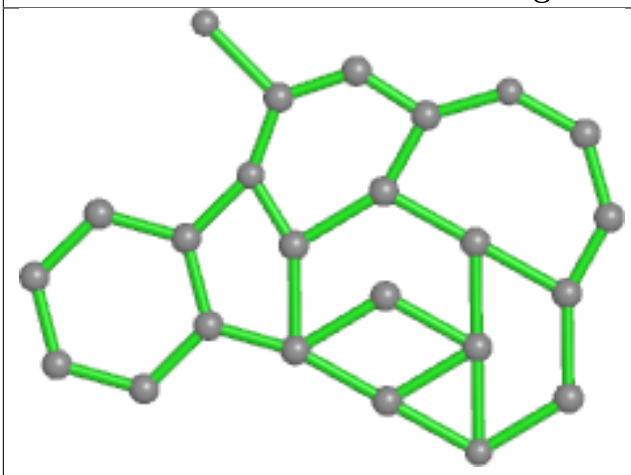


Torsions

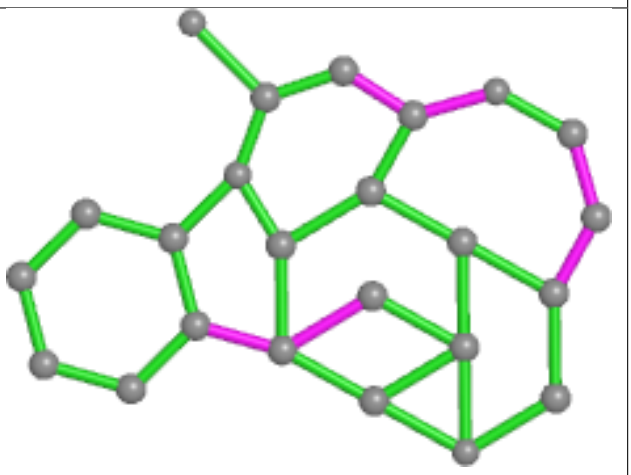


Rings

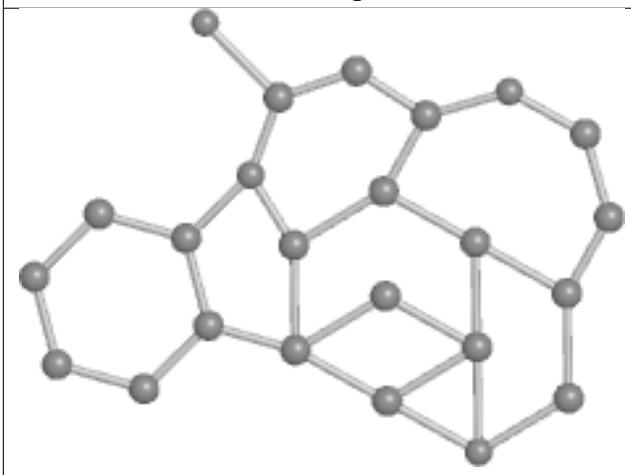
Ligand SY9 J 401



Bond lengths



Bond angles



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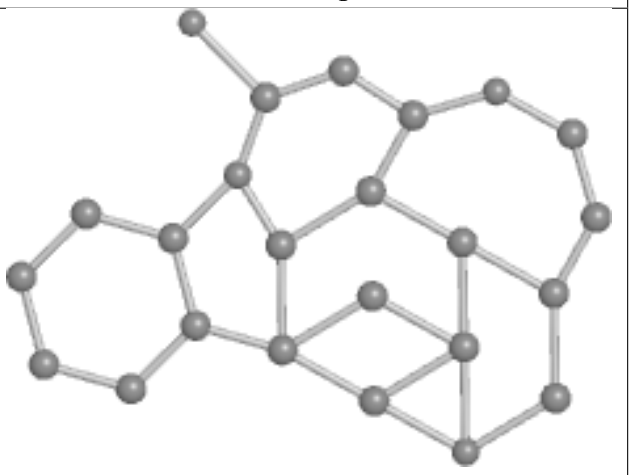
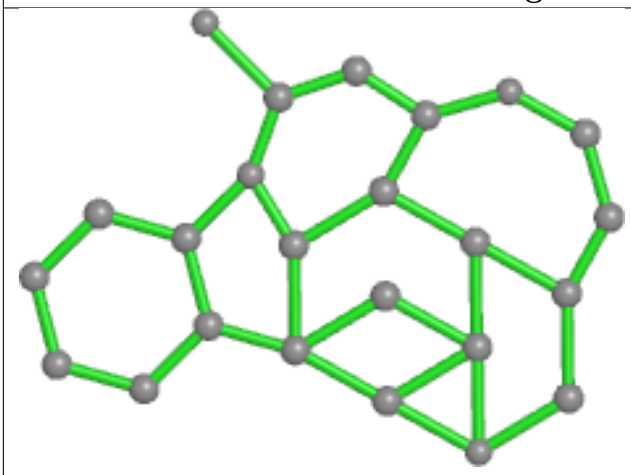


Rings

Ligand SY9 M 401



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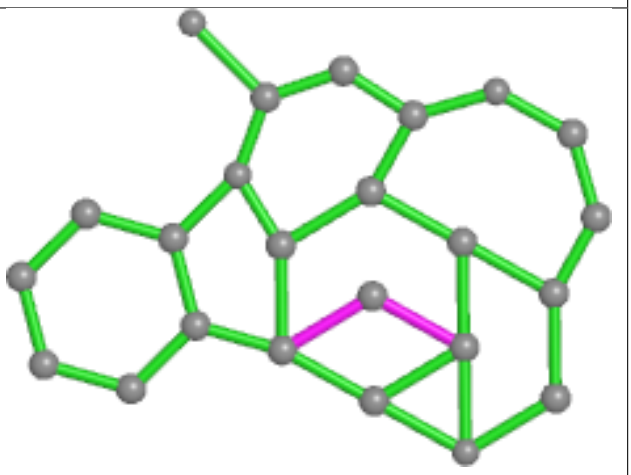
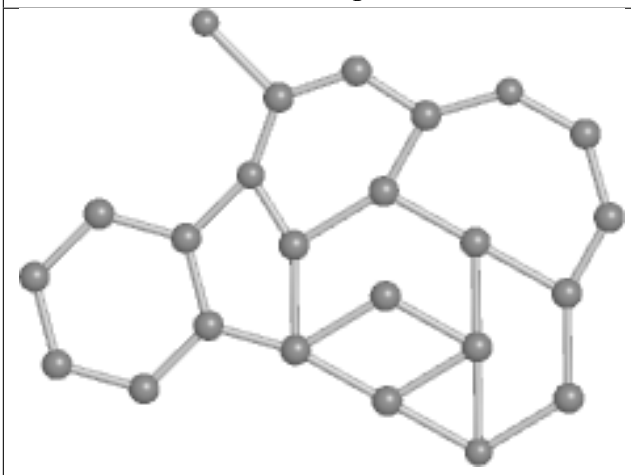
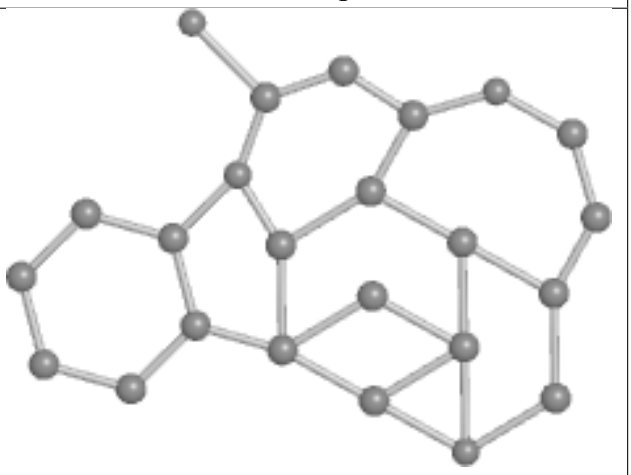


Bond angles

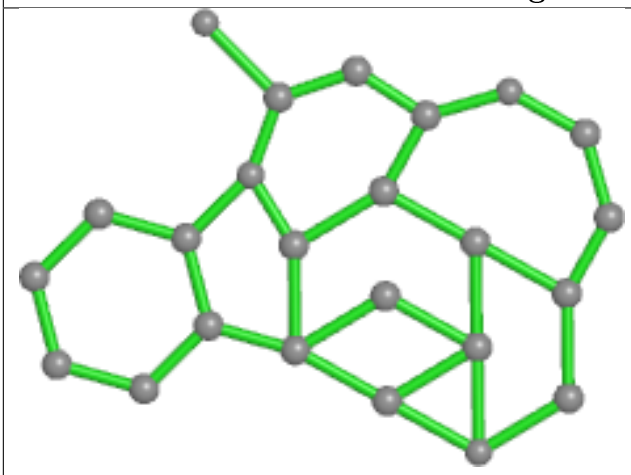


Torsions

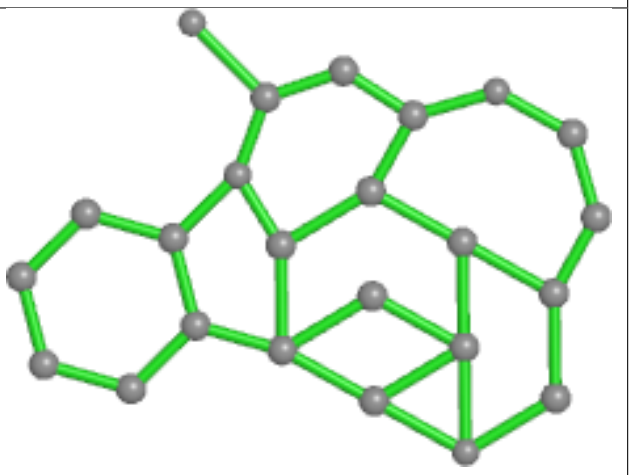


Rings

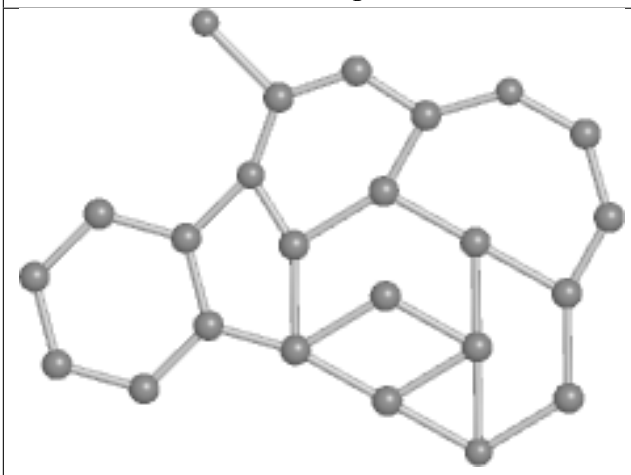
Ligand SY9 K 402



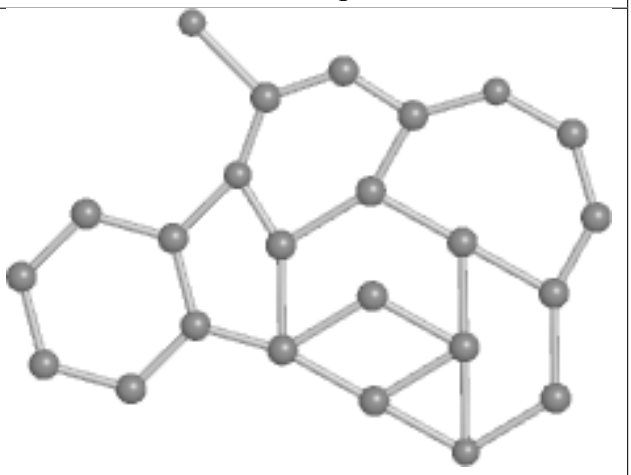
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	206/249 (82%)	-0.17	1 (0%) 91 86	32, 62, 96, 146	0
1	B	207/249 (83%)	-0.09	7 (3%) 45 29	35, 75, 137, 169	0
1	C	207/249 (83%)	-0.13	0 100 100	37, 73, 121, 166	0
1	D	206/249 (82%)	-0.21	2 (0%) 82 72	34, 69, 120, 177	0
1	E	204/249 (81%)	-0.50	0 100 100	39, 67, 100, 143	0
1	F	206/249 (82%)	-0.28	0 100 100	37, 66, 117, 163	0
1	G	202/249 (81%)	-0.23	3 (1%) 73 61	42, 79, 134, 157	0
1	H	206/249 (82%)	-0.01	3 (1%) 73 61	36, 67, 115, 141	0
1	I	206/249 (82%)	-0.34	0 100 100	36, 65, 104, 152	0
1	J	206/249 (82%)	-0.26	0 100 100	35, 63, 100, 135	0
1	K	206/249 (82%)	0.02	3 (1%) 73 61	55, 97, 136, 174	0
1	L	206/249 (82%)	-0.09	3 (1%) 73 61	49, 87, 133, 148	0
1	M	206/249 (82%)	-0.23	2 (0%) 82 72	45, 78, 126, 179	0
1	N	198/249 (79%)	-0.21	1 (0%) 91 86	39, 69, 120, 170	0
1	O	206/249 (82%)	-0.00	4 (1%) 66 53	49, 97, 145, 187	0
All	All	3078/3735 (82%)	-0.18	29 (0%) 84 75	32, 74, 130, 187	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	89	TYR	4.7
1	D	20	GLN	4.1
1	K	193	ILE	3.7
1	G	203	GLN	3.5
1	N	20	GLN	3.4

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

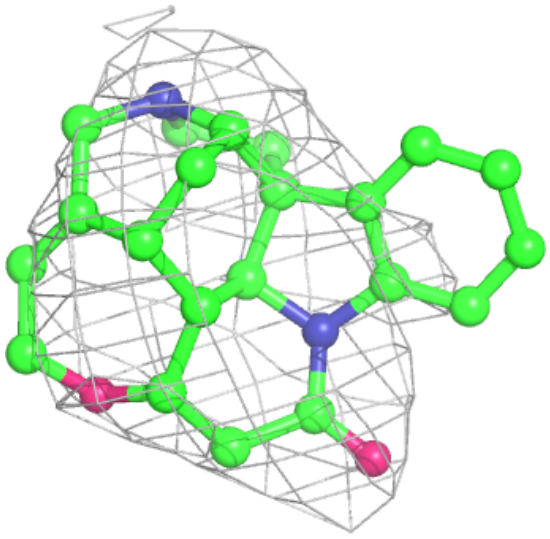
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

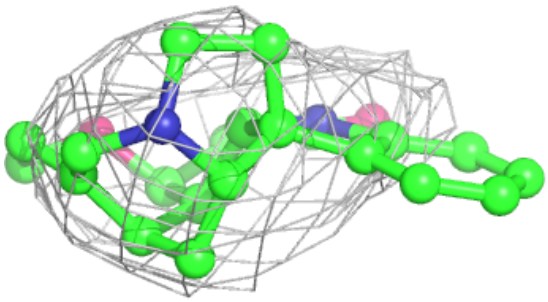
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ARG	N	301	11/12	0.81	0.24	68,83,96,98	0
2	SY9	K	402	25/25	0.89	0.34	107,153,175,185	0
2	SY9	I	301	25/25	0.93	0.25	63,84,115,117	0
2	SY9	E	401	25/25	0.94	0.28	64,71,84,84	0
2	SY9	H	301	25/25	0.94	0.41	100,133,141,146	0
2	SY9	A	401	25/25	0.94	0.28	84,99,147,158	0
2	SY9	D	401	25/25	0.95	0.21	92,103,121,122	0
2	SY9	N	302	25/25	0.95	0.29	93,101,118,122	0
2	SY9	L	401	25/25	0.96	0.34	94,106,116,126	0
2	SY9	C	401	25/25	0.96	0.27	94,123,132,134	0
2	SY9	K	401	25/25	0.96	0.22	91,102,110,125	0
2	SY9	G	401	25/25	0.97	0.25	75,92,105,115	0
2	SY9	J	401	25/25	0.97	0.20	63,75,81,90	0
2	SY9	M	401	25/25	0.97	0.22	68,76,97,107	0
2	SY9	C	402	25/25	0.97	0.15	61,68,78,83	0
2	SY9	H	302	25/25	0.98	0.25	57,72,83,89	0

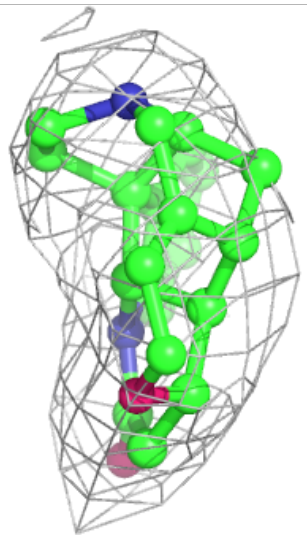
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SY9 K 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

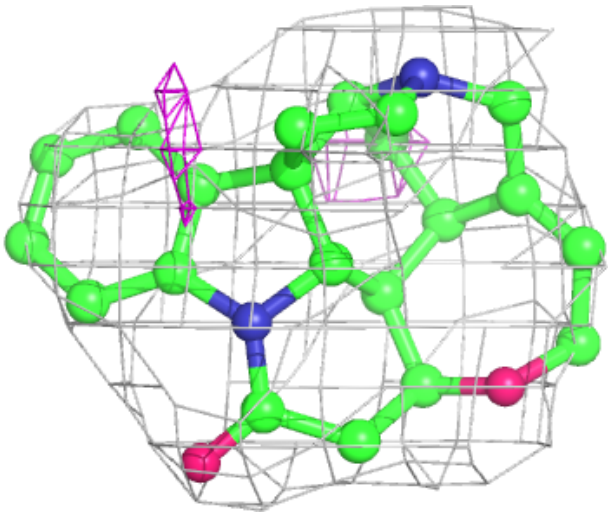


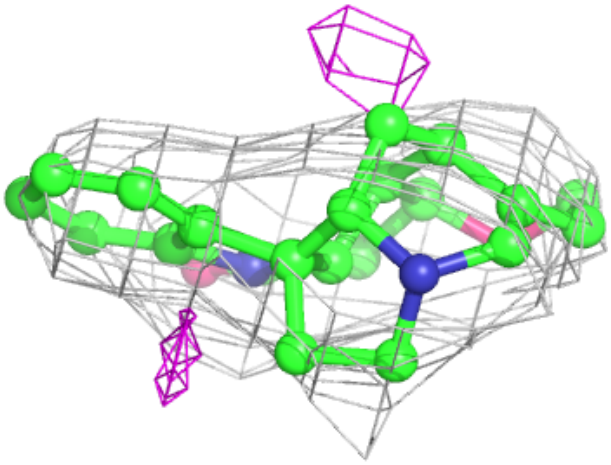


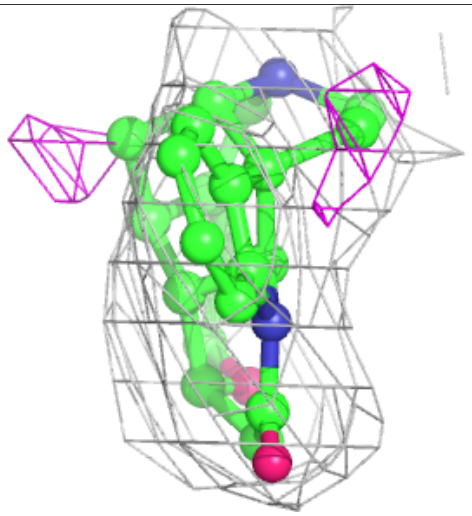


Electron density around SY9 I 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around SY9 E 401:

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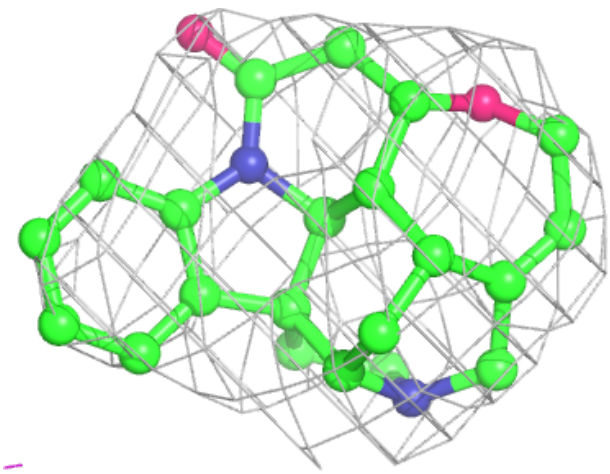
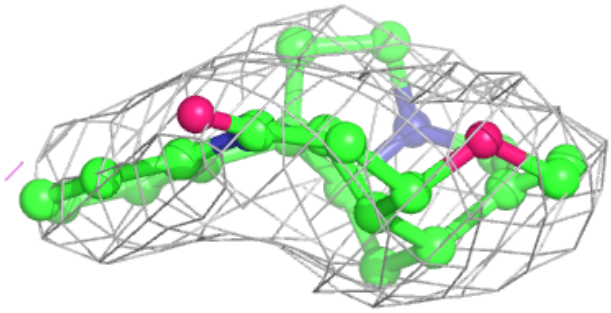
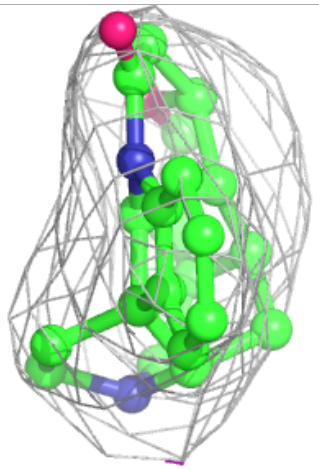
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

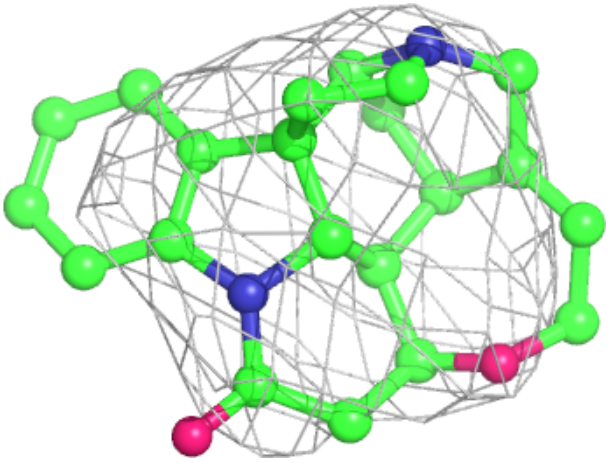


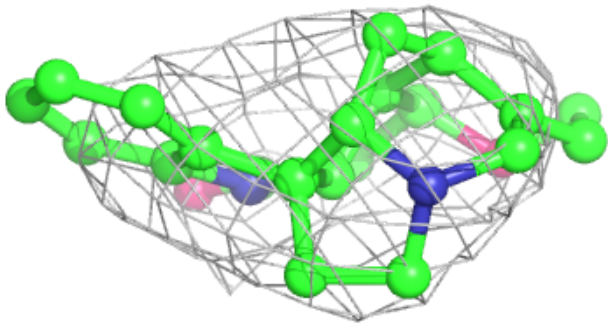


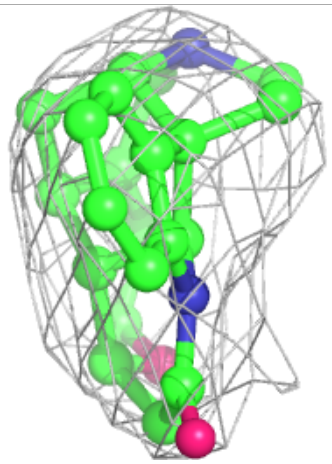


Electron density around SY9 H 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around SY9 A 401:

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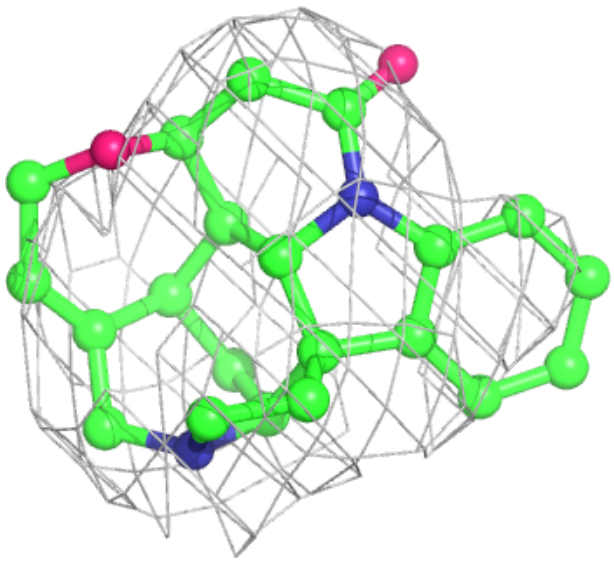
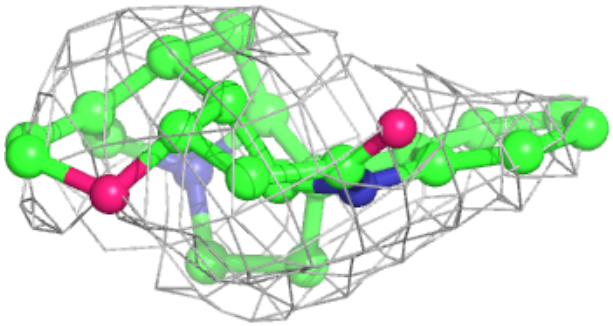
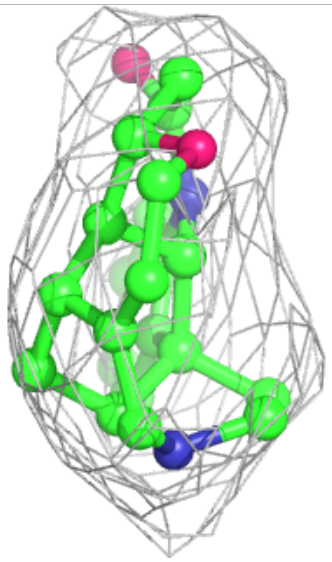
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

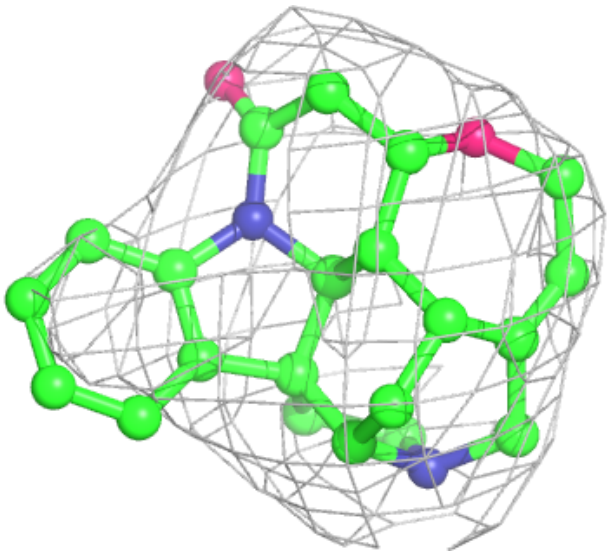


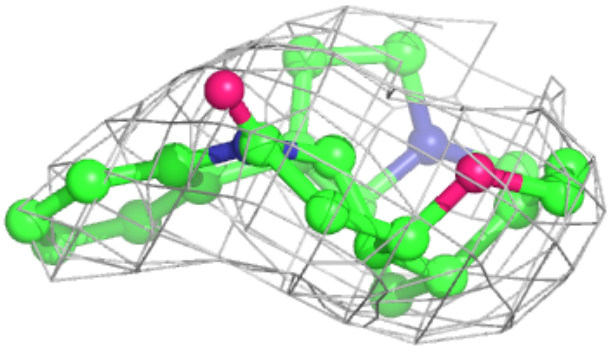


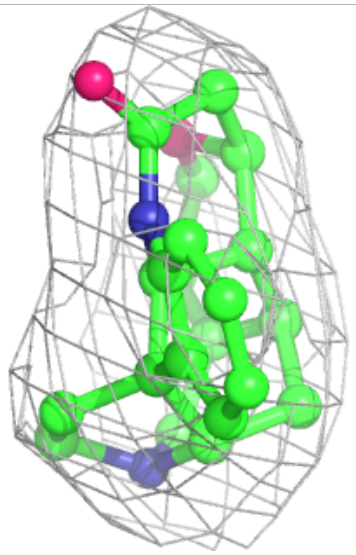


Electron density around SY9 D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around SY9 N 302:

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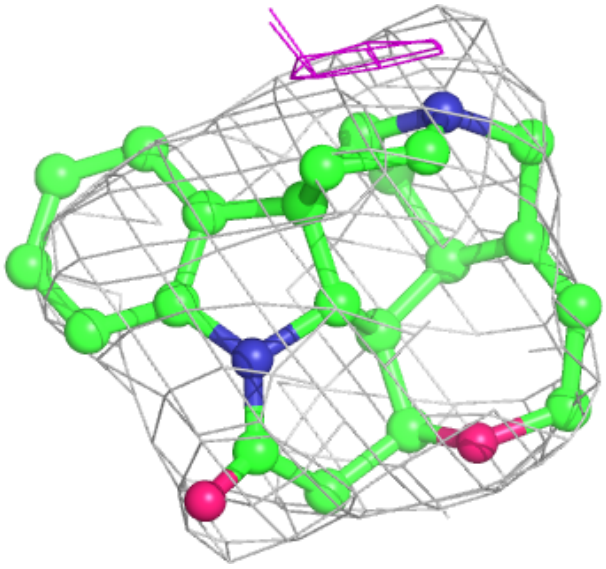
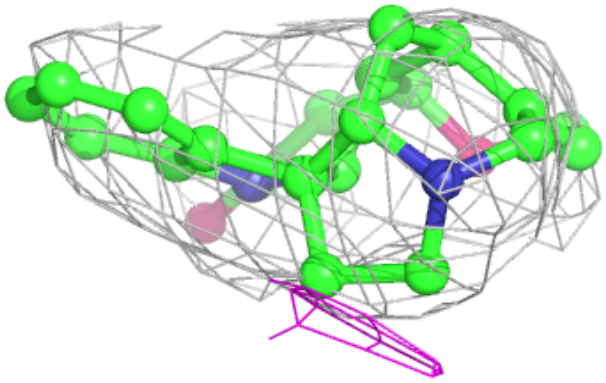
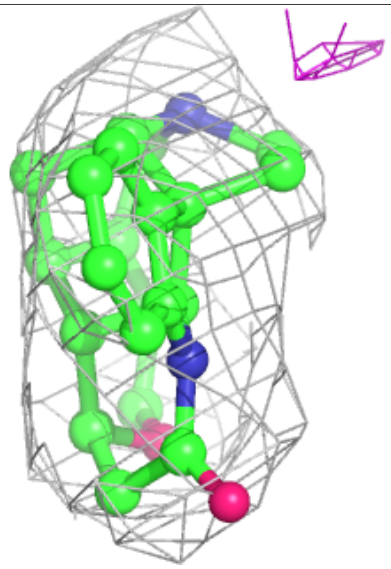
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

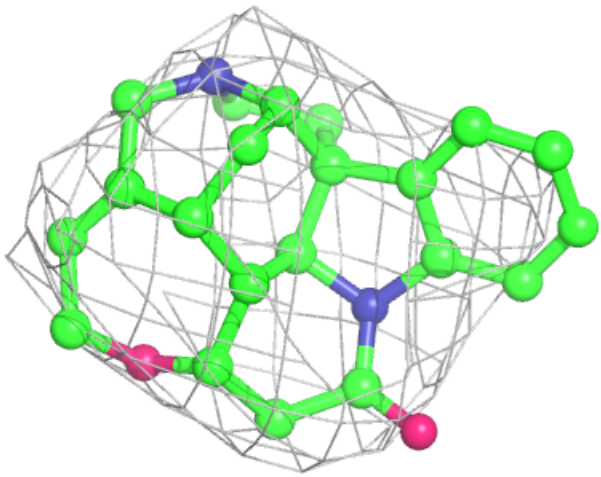


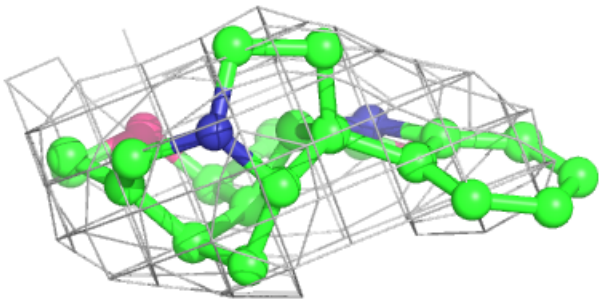


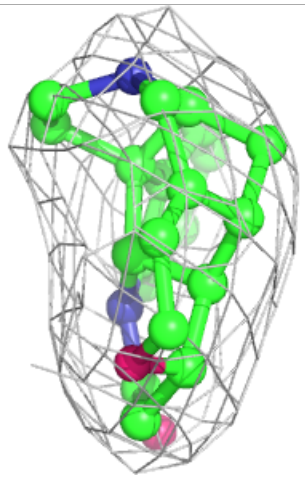


Electron density around SY9 L 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

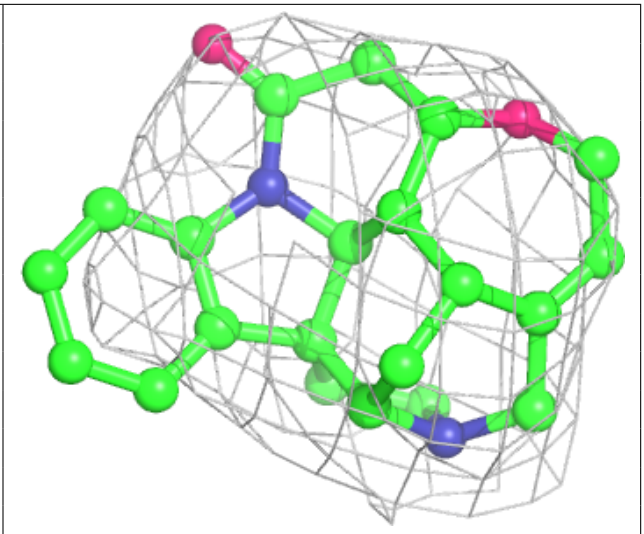


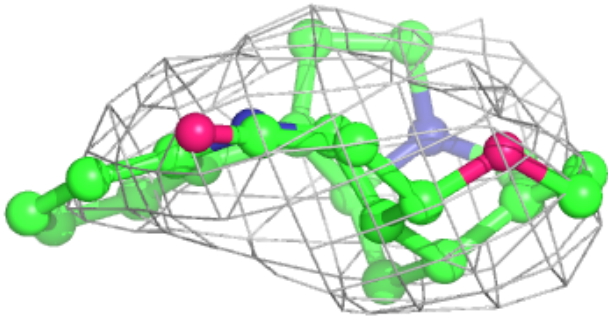


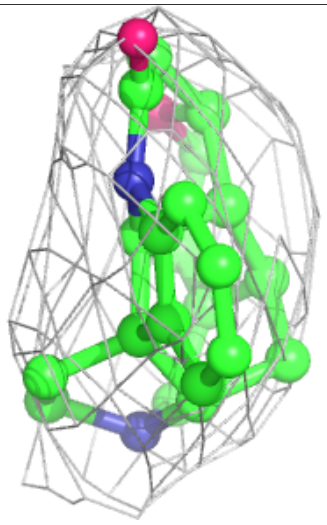


Electron density around SY9 C 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

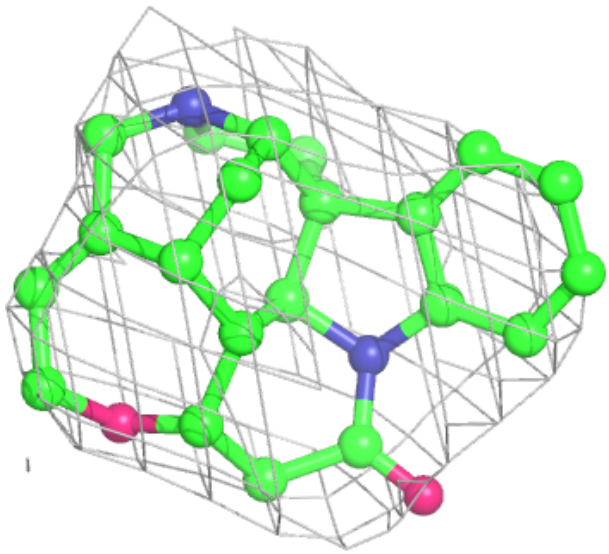


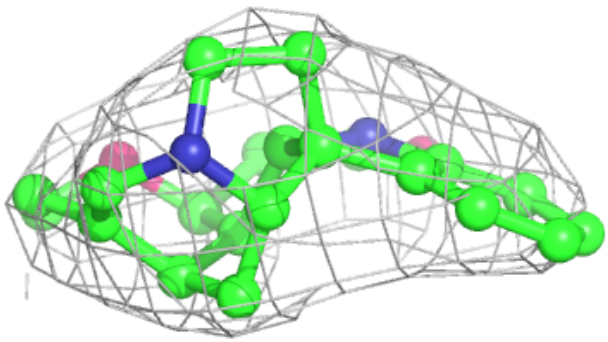


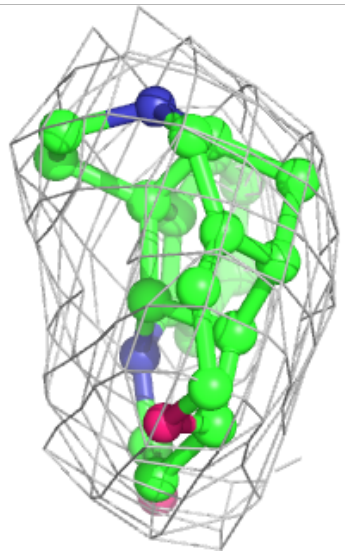


Electron density around SY9 K 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

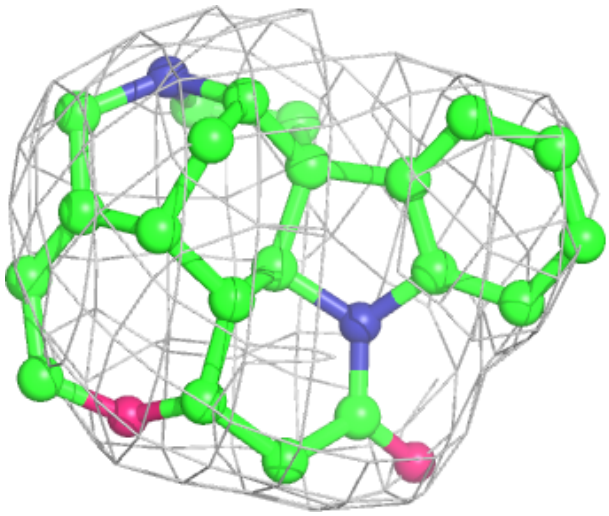


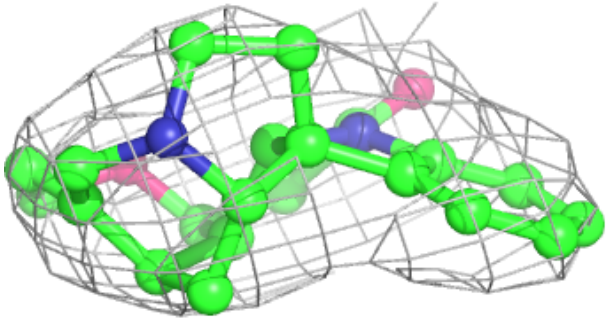


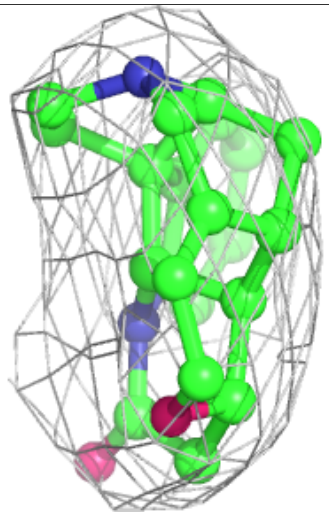


Electron density around SY9 G 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

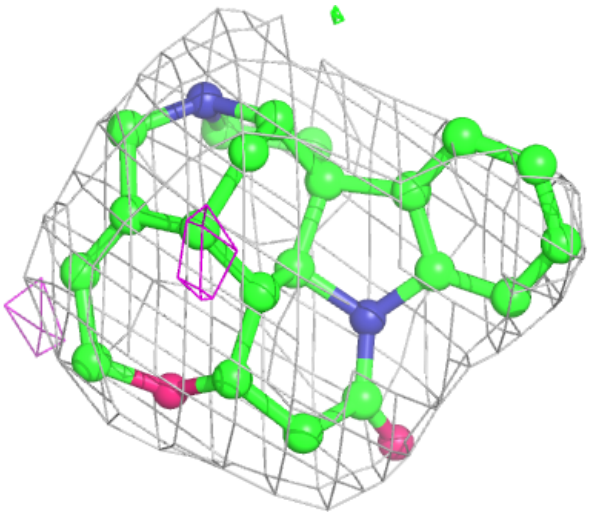


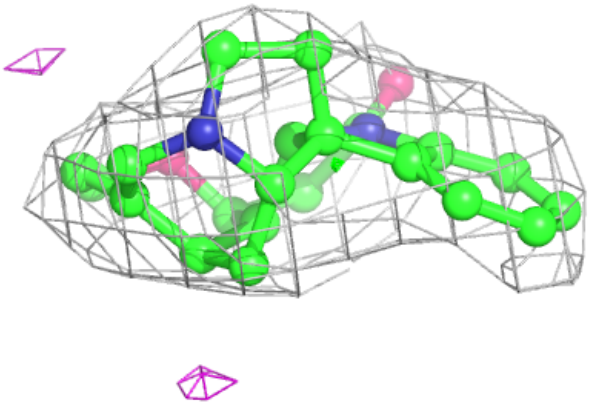


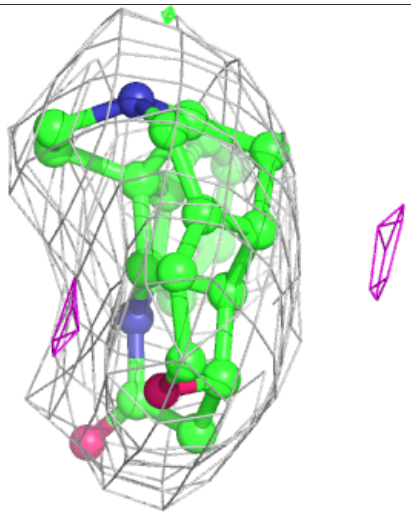


Electron density around SY9 J 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

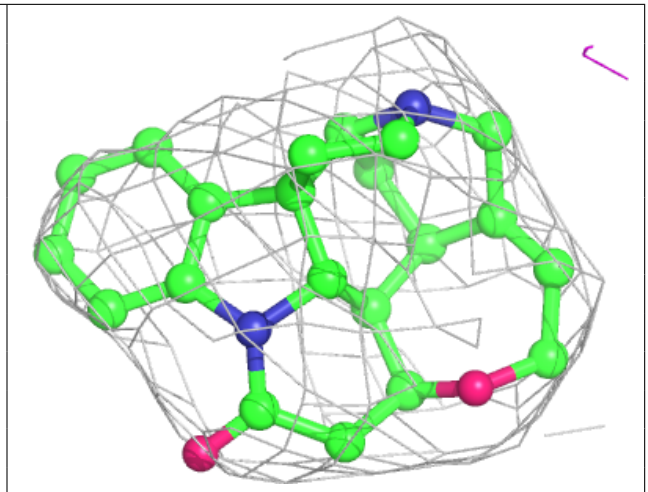


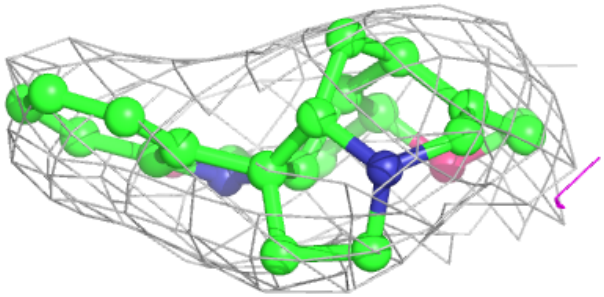


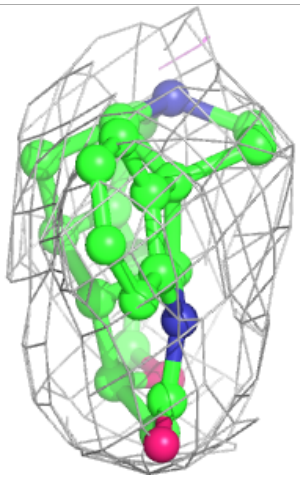


Electron density around SY9 M 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

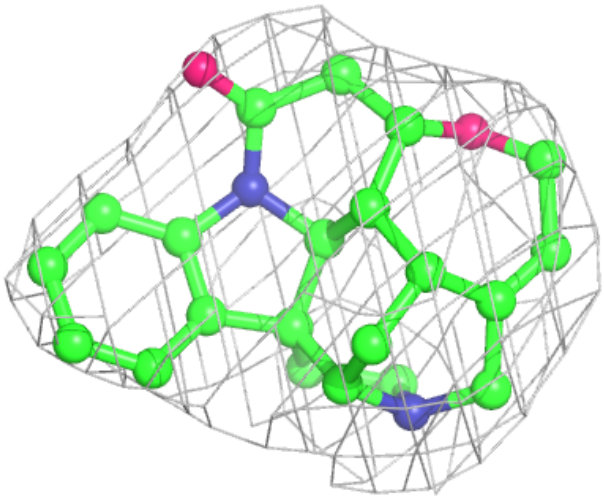


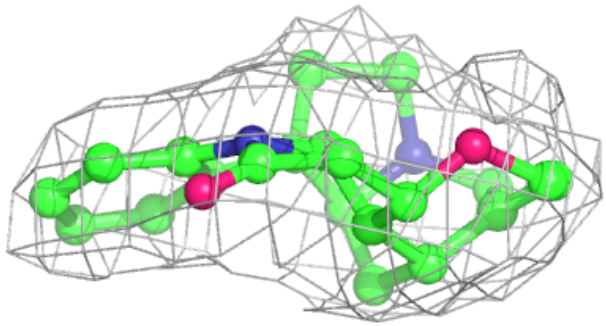


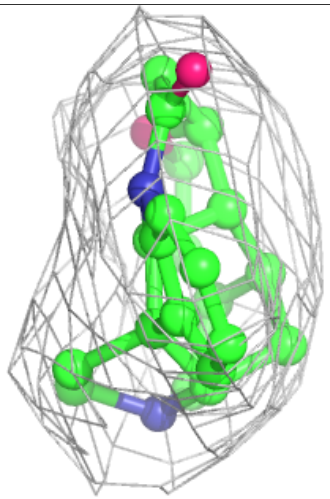


Electron density around SY9 C 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

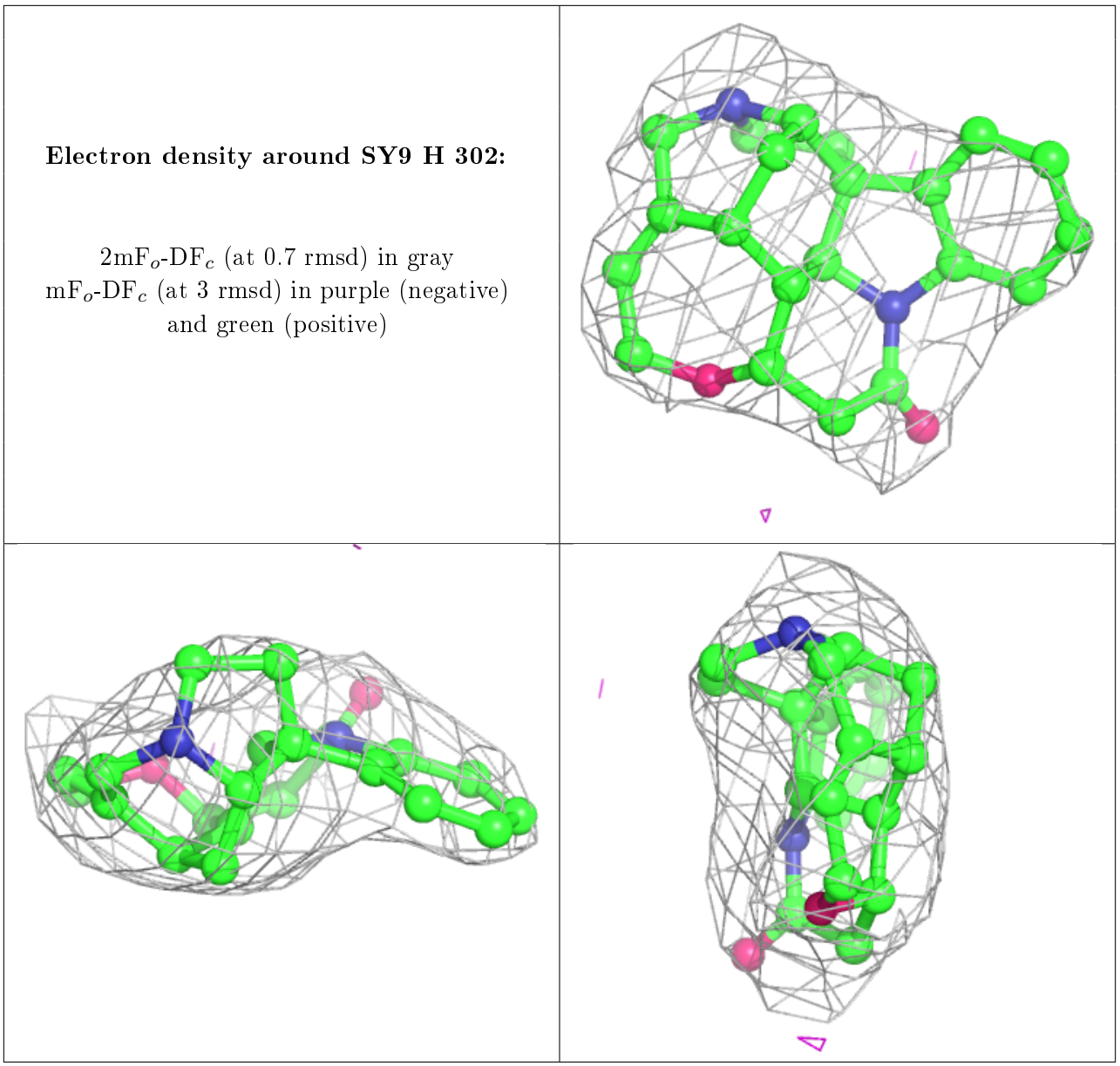






Electron density around SY9 H 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.