wwPDB X-ray Structure Validation Summary Report (i)

Mar 30, 2025 – 04:00 am BST

PDB ID	:	9ETB / pdb_00009etb
Title	:	CDK2-cyclin A in complex with FragLite 2
Authors	:	Hope, I.; Martin, M.P.; Waring, M.J.; Noble, M.E.M.; Endicott, J.A.; Tatum, N.J.
Deposited on	:	2024-03-26
Resolution	:	2.76 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 (i)) were used in the production of this report:

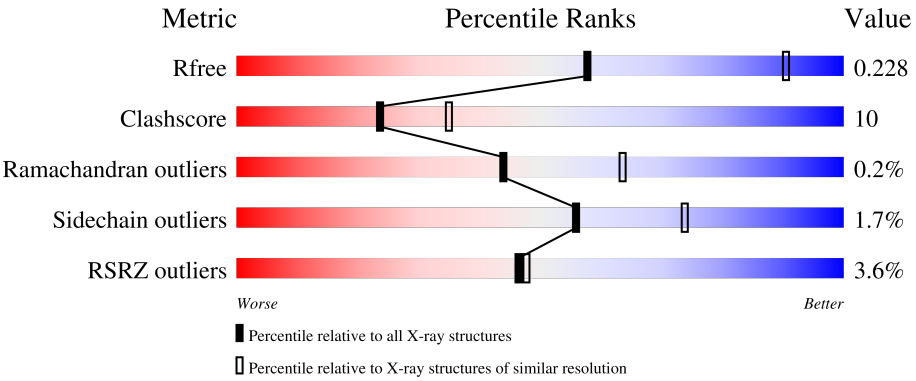
MolProbity	:	4.02b-467
Mogul	:	?.? (???), CSD ??CSD?? (????)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.76 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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% 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	B	268	84% 15%
1	D	268	3% 81% 16%
2	A	302	4% 73% 25%
2	C	302	6% 74% 21% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PYZ	A	604[A]	-	-	X	-
3	PYZ	A	604[B]	-	-	X	-
3	PYZ	B	503	-	-	X	-
3	PYZ	B	504[A]	-	-	X	-
3	PYZ	B	504[B]	-	-	X	-
4	EPE	C	505	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9347 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 Cyclin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	262	Total	C	N	O	S	0	0	0
			2110	1366	344	390	10			
1	B	268	Total	C	N	O	S	0	0	0
			2170	1402	362	396	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	171	GLY	-	expression tag	UNP P30274
D	433	HIS	-	expression tag	UNP P30274
D	434	HIS	-	expression tag	UNP P30274
D	435	HIS	-	expression tag	UNP P30274
D	436	HIS	-	expression tag	UNP P30274
D	437	HIS	-	expression tag	UNP P30274
D	438	HIS	-	expression tag	UNP P30274
B	171	GLY	-	expression tag	UNP P30274
B	433	HIS	-	expression tag	UNP P30274
B	434	HIS	-	expression tag	UNP P30274
B	435	HIS	-	expression tag	UNP P30274
B	436	HIS	-	expression tag	UNP P30274
B	437	HIS	-	expression tag	UNP P30274
B	438	HIS	-	expression tag	UNP P30274

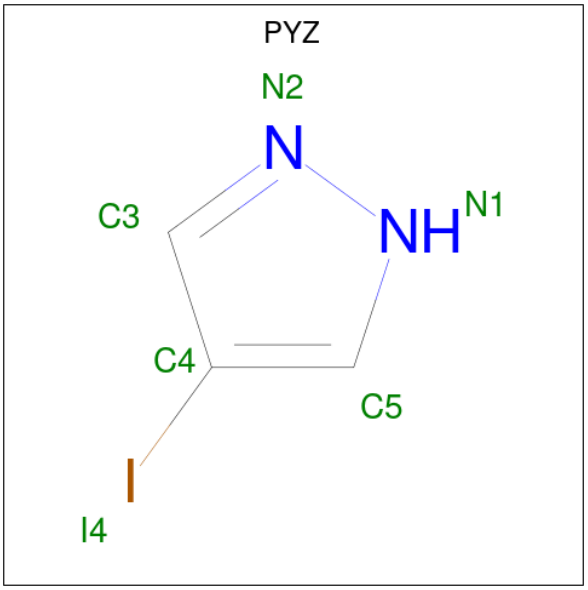
- Molecule 2 is a protein called Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	301	Total	C	N	O	P	S	0	1	0
			2427	1574	412	432	1	8			
2	C	285	Total	C	N	O	P	S	0	0	0
			2285	1482	385	409	1	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P24941
A	-2	PRO	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-3	GLY	-	expression tag	UNP P24941
C	-2	PRO	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

- Molecule 3 is 4-IODOPYRAZOLE (CCD ID: PYZ) (formula: $C_3H_3IN_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	I	N	0	0
			6	3	1	2		
3	A	1	Total	C	I	N	0	0
			6	3	1	2		
3	A	1	Total	C	I	N	0	1
			12	6	2	4		
3	A	1	Total	C	I	N	0	1
			12	6	2	4		
3	A	1	Total	C	I	N	0	0
			6	3	1	2		
3	B	1	Total	C	I	N	0	0
			6	3	1	2		
3	B	1	Total	C	I	N	0	0
			6	3	1	2		

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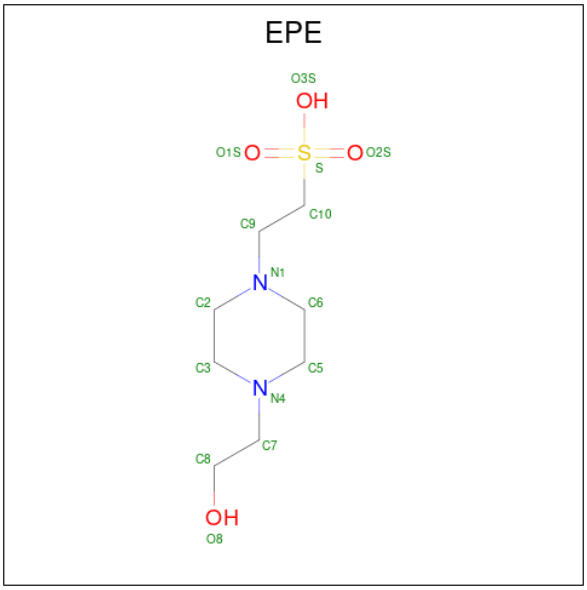
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C I N 6 3 1 2	0	0
3	B	1	Total C I N 12 6 2 4	0	1
3	C	1	Total C I N 12 6 2 4	0	1
3	C	1	Total C I N 6 3 1 2	0	0
3	C	1	Total C I N 6 3 1 2	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	47	Total O 47 47	0	0
5	A	85	Total O 85 85	0	0
5	B	74	Total O 74 74	0	0

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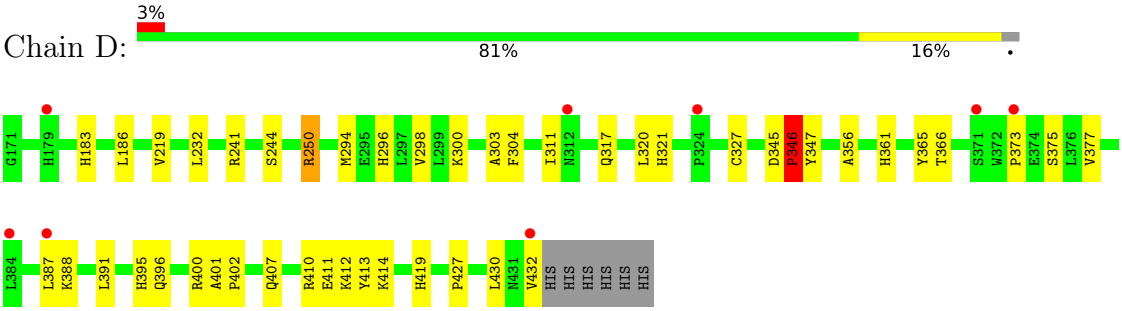
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	38	Total O 38 38	0	0

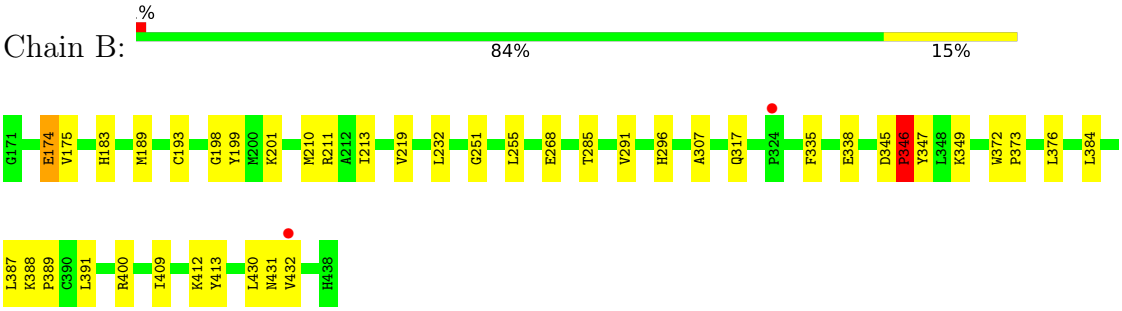
3 Residue-property plots

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 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.

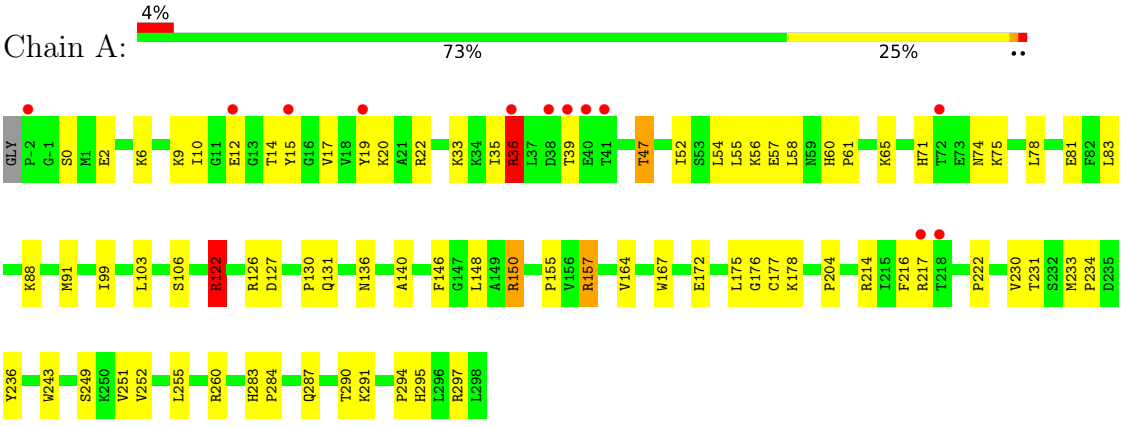
• Molecule 1: Cyclin-A2



• Molecule 1: Cyclin-A2

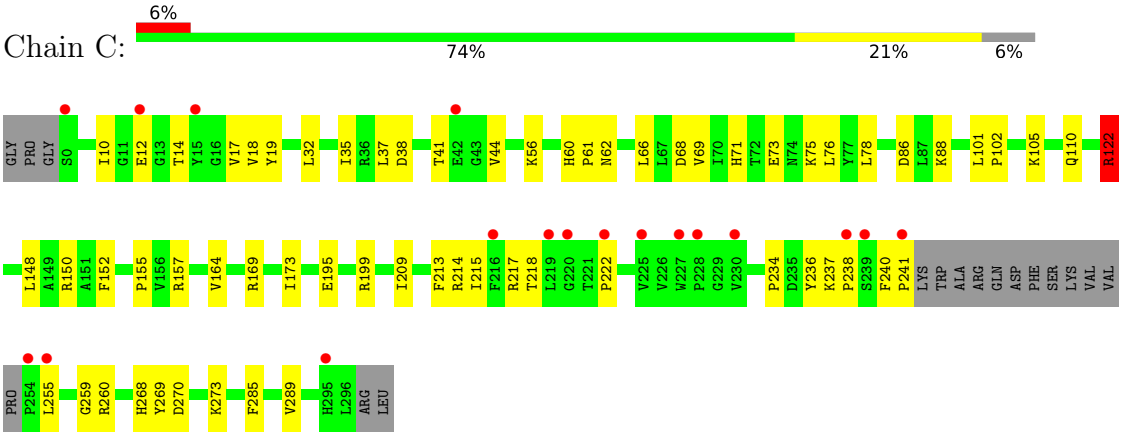


• Molecule 2: Cyclin-dependent kinase 2



• Molecule 2: Cyclin-dependent kinase 2

Chain C:


6%
74%
21%
6%
GLY PRO GLY S0 I10 G11 E12 G13 T14 Y15 G16 V17 V18 Y19 L32 I35 R36 L37 D38 T41 E42 G43 V44 K56 H60 P61 N62 L66 L67 D68 V69 I70 H71 T72 E73 N74 K75 L76 Y77 L78 D86 L87 K88 L101 P102 K105 Q110 R122
L148 A149 R150 A151 F152 P155 V156 R157 V164 R169 I173 E195 R199 I209 F213 R214 I215 F216 R217 T218 L219 G220 T221 P222 V225 V226 W227 P228 G229 V230 P234 D235 Y236 K237 P238 S239 F240 P241 LYS TRP ALA ARG GLN ASP PHE SER LYS VAL VAL
PRO P254 L255 G259 R260 H268 Y269 D270 K273 F285 V289 H295 L296 ARG LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.15Å 133.67Å 147.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.38 – 2.76 99.18 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.1 (99.38-2.76) 99.1 (99.18-2.76)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.212 , 0.228 0.209 , 0.228	Depositor DCC
R_{free} test set	1861 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9347	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: EPE, PYZ, TPO

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	B	0.47	1/2226 (0.0%)	0.85	1/3027 (0.0%)
1	D	0.44	0/2160	0.81	1/2937 (0.0%)
2	A	0.47	1/2478 (0.0%)	0.90	1/3361 (0.0%)
2	C	0.46	0/2330	0.83	0/3159
All	All	0.46	2/9194 (0.0%)	0.85	3/12484 (0.0%)

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	B	0	1
1	D	0	1
2	A	0	5
2	C	0	3
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	GLY	C-N	-5.38	1.21	1.34
2	A	36	ARG	C-N	-5.21	1.22	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	346	PRO	N-CA-CB	-11.71	89.24	103.30
1	B	346	PRO	N-CA-CB	-11.12	89.96	103.30
2	A	122	ARG	CA-CB-CG	5.65	125.83	113.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	122	ARG	Sidechain
2	A	150	ARG	Sidechain
2	A	217	ARG	Sidechain
2	A	36	ARG	Sidechain
1	D	250	ARG	Sidechain

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	B	2170	0	2169	32	0
1	D	2110	0	2128	35	0
2	A	2427	0	2468	66	0
2	C	2285	0	2325	58	0
3	A	36	0	18	8	0
3	B	30	0	15	12	0
3	C	24	0	12	2	0
3	D	6	0	3	0	0
4	C	15	0	17	13	0
5	A	85	0	0	4	0
5	B	74	0	0	2	0
5	C	38	0	0	0	0
5	D	47	0	0	0	0
All	All	9347	0	9155	182	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 10.

The worst 5 of 182 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:B:193:CYS:SG	3:B:504[B]:PYZ:I4	2.64	1.25
1:B:193:CYS:SG	3:B:504[A]:PYZ:I4	2.94	0.95
1:D:296:HIS:NE2	2:C:71:HIS:HD2	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:9:LYS:HG3	2:A:17:VAL:CG2	2.03	0.88
2:A:177:CYS:SG	2:A:233:MET:CE	2.64	0.86

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	B	266/268 (99%)	256 (96%)	10 (4%)	0	100	100
1	D	260/268 (97%)	250 (96%)	10 (4%)	0	100	100
2	A	299/302 (99%)	286 (96%)	12 (4%)	1 (0%)	37	55
2	C	280/302 (93%)	265 (95%)	14 (5%)	1 (0%)	30	47
All	All	1105/1140 (97%)	1057 (96%)	46 (4%)	2 (0%)	44	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	164	VAL
2	A	164	VAL

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	B	240/240 (100%)	235 (98%)	5 (2%)	48 69
1	D	234/240 (98%)	232 (99%)	2 (1%)	75 86
2	A	265/264 (100%)	258 (97%)	7 (3%)	41 63
2	C	250/264 (95%)	247 (99%)	3 (1%)	67 81
All	All	989/1008 (98%)	972 (98%)	17 (2%)	56 74

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	122	ARG
2	C	157	ARG
2	A	150	ARG
2	A	157	ARG
1	B	174	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	312	ASN
1	B	395	HIS
2	C	295	HIS
1	B	396	GLN
1	B	378	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

17 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

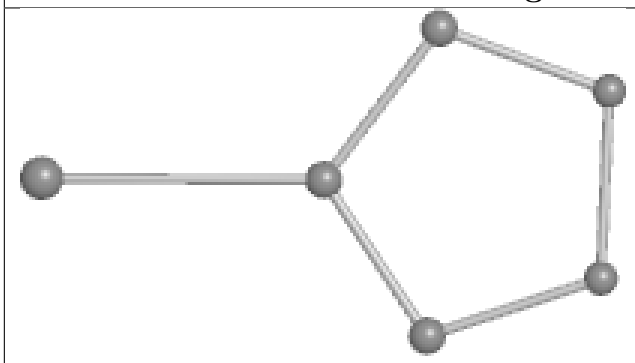
There are no torsion outliers.

There are no ring outliers.

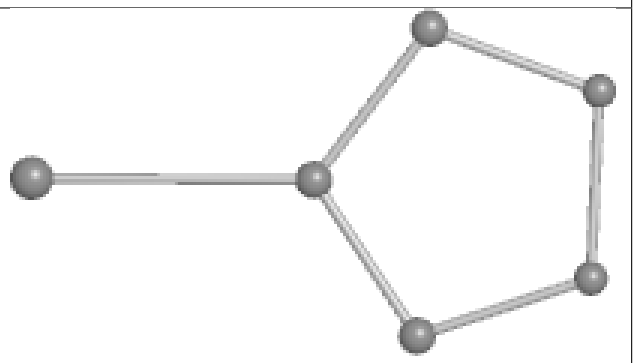
No monomer is involved in short contacts.

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

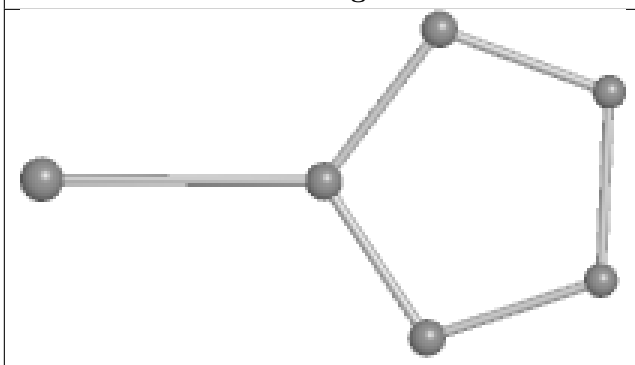
Ligand PYZ D 501



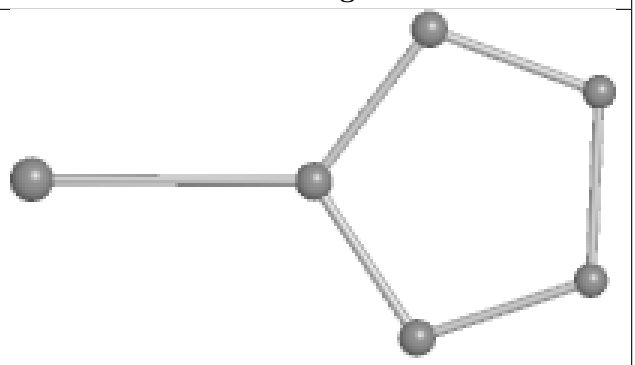
Bond lengths



Bond angles

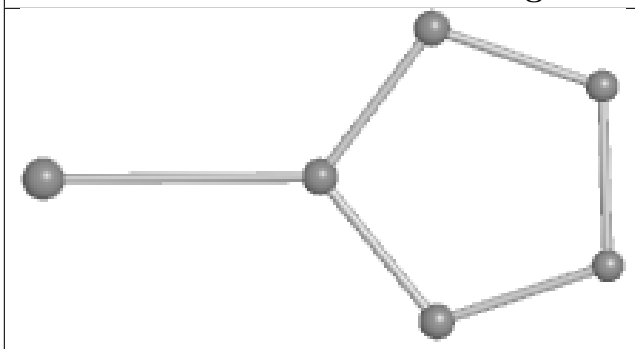


Torsions

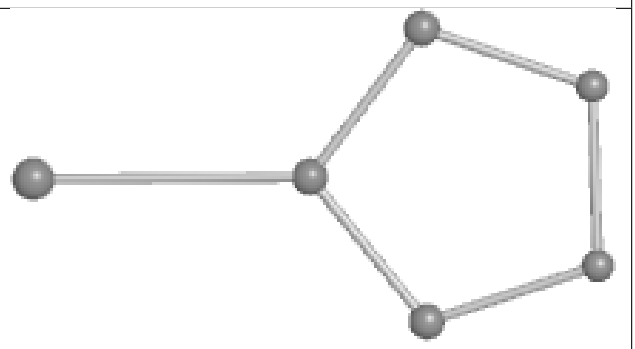


Rings

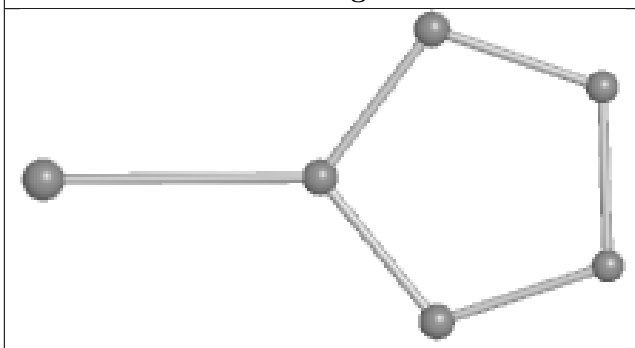
Ligand PYZ A 601



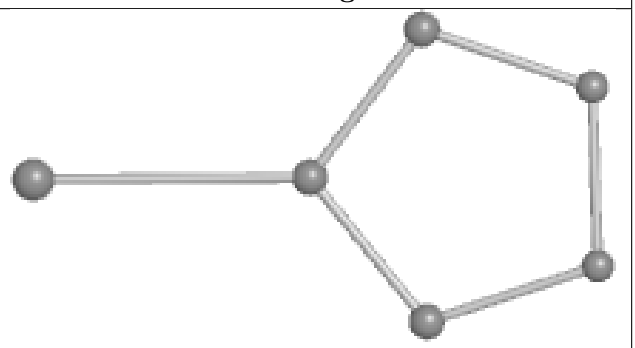
Bond lengths



Bond angles

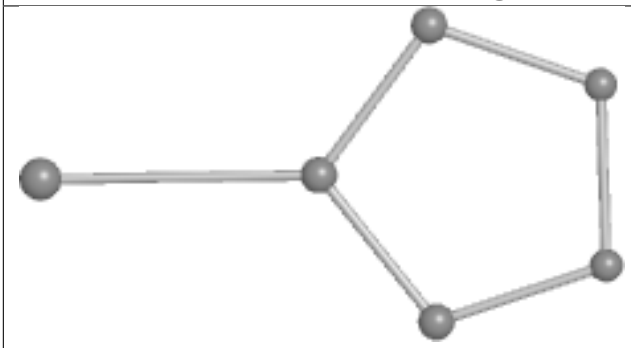


Torsions

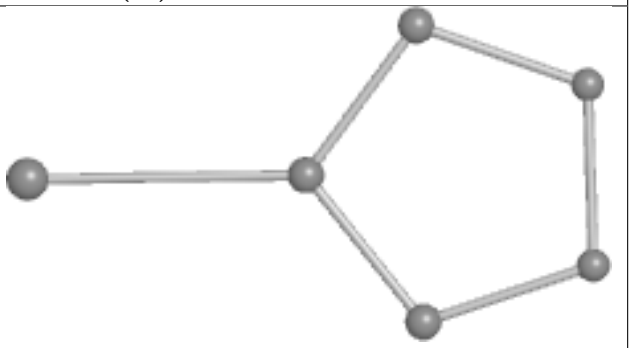


Rings

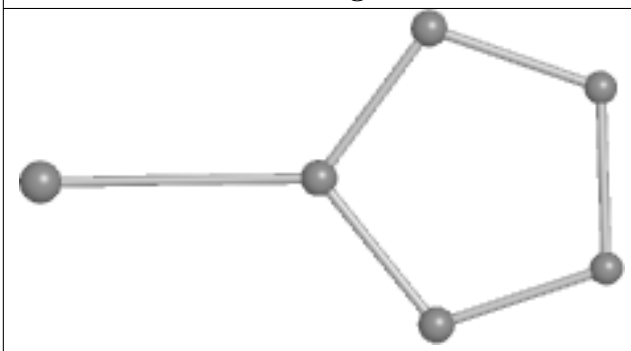
Ligand PYZ A 602 (A)



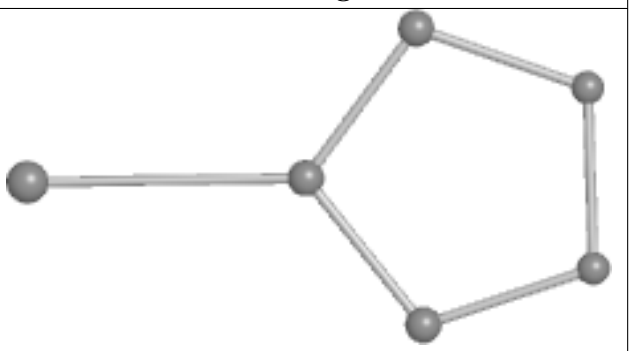
Bond lengths



Bond angles

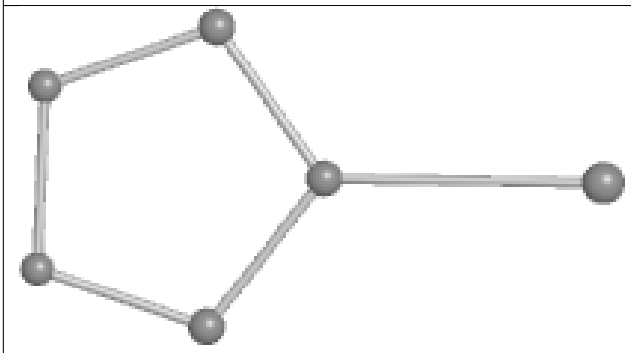


Torsions

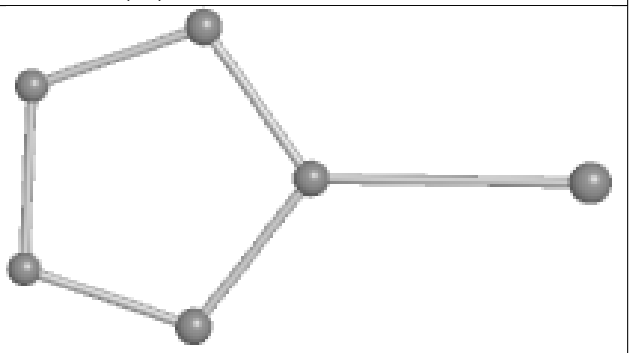


Rings

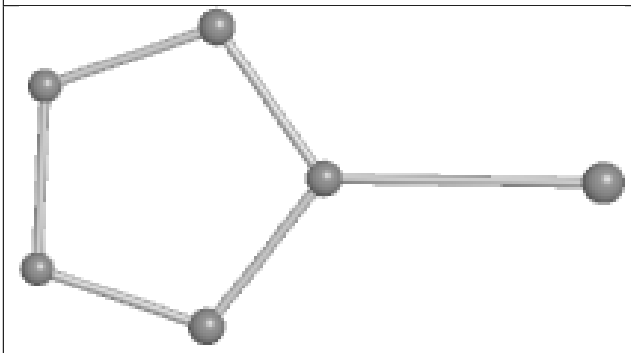
Ligand PYZ A 602 (B)



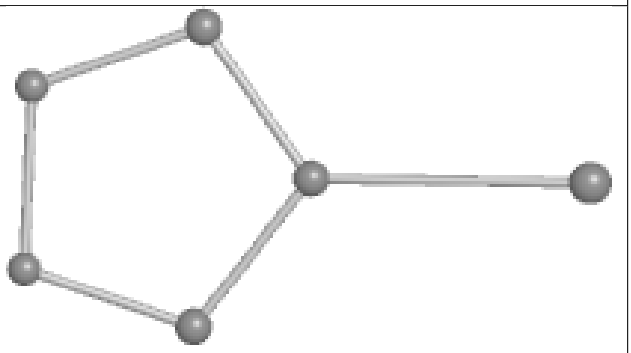
Bond lengths



Bond angles

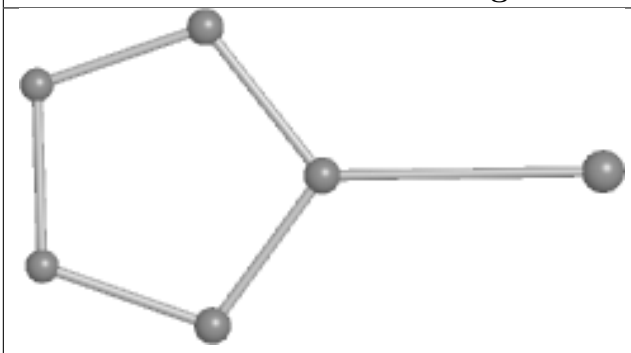


Torsions

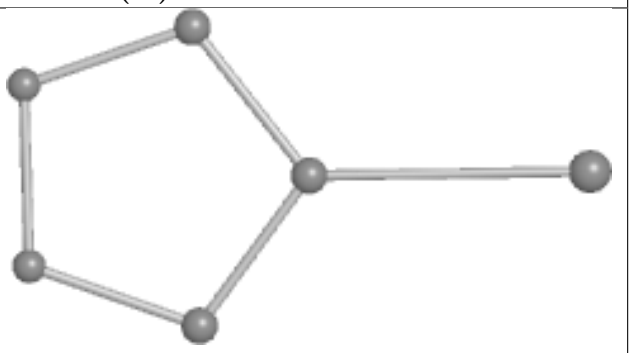


Rings

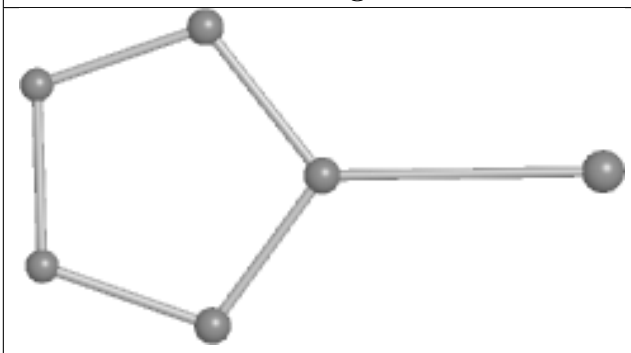
Ligand PYZ A 604 (A)



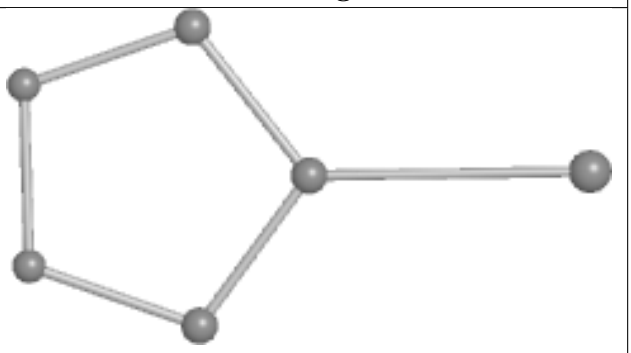
Bond lengths



Bond angles

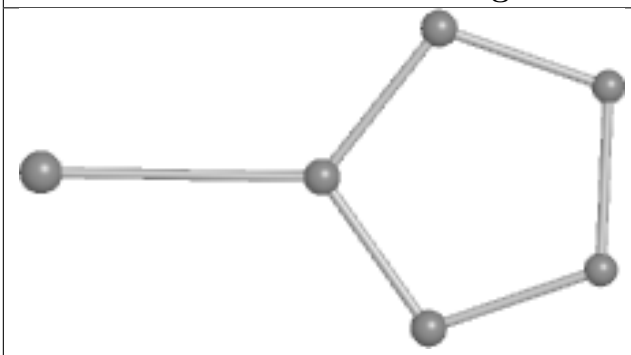


Torsions

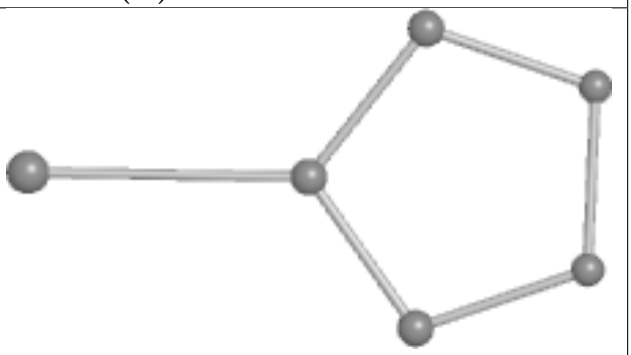


Rings

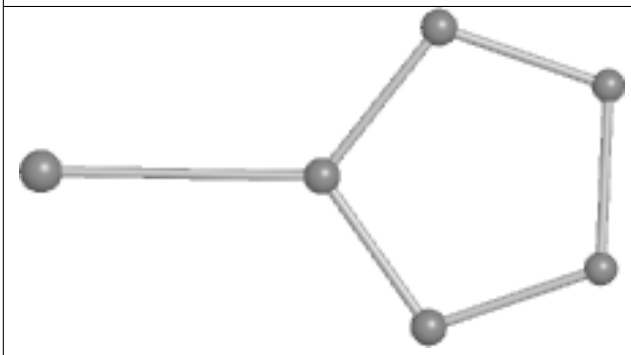
Ligand PYZ A 604 (B)



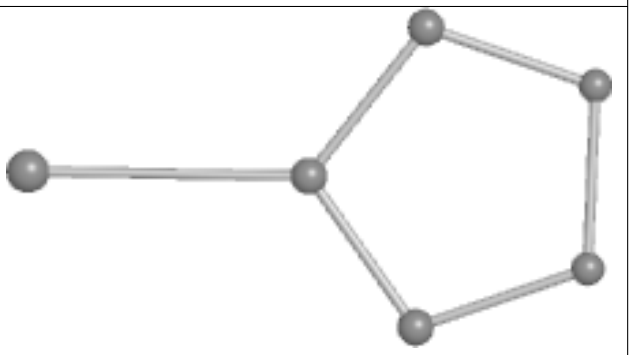
Bond lengths



Bond angles

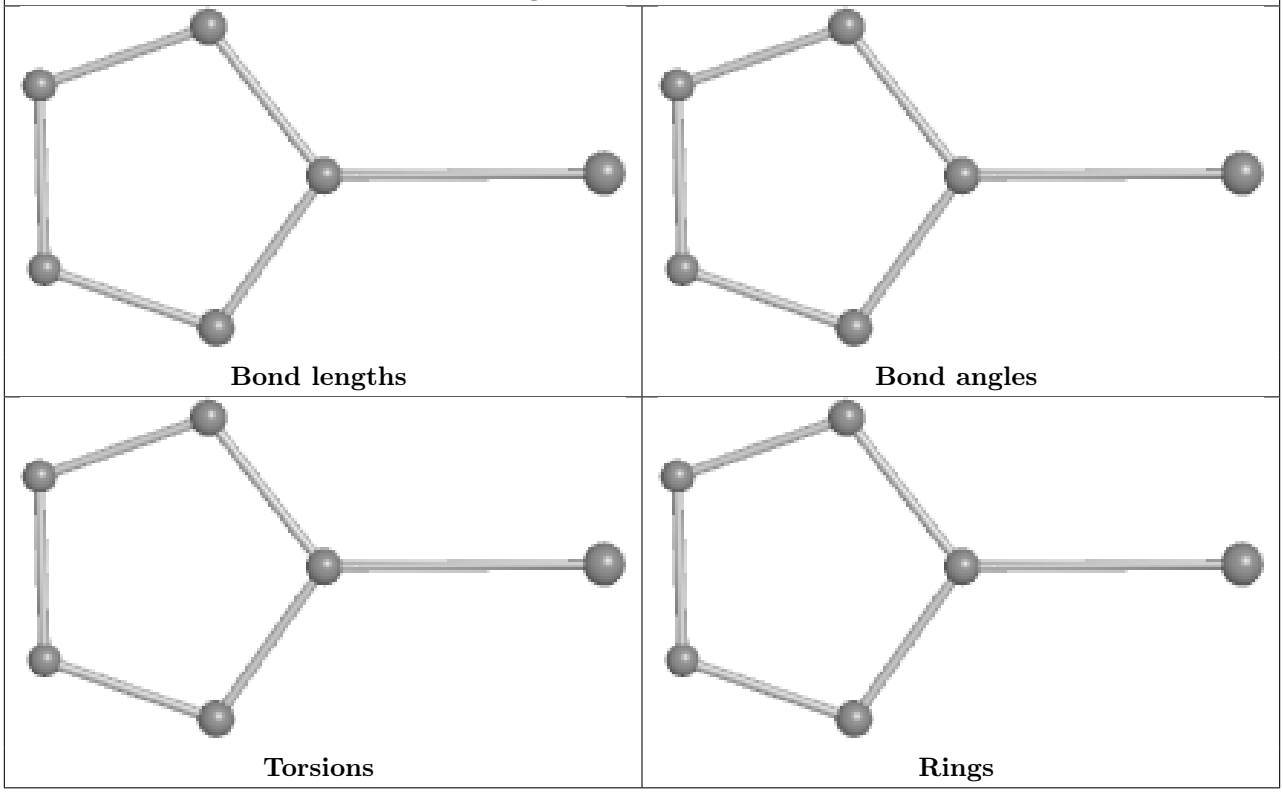


Torsions

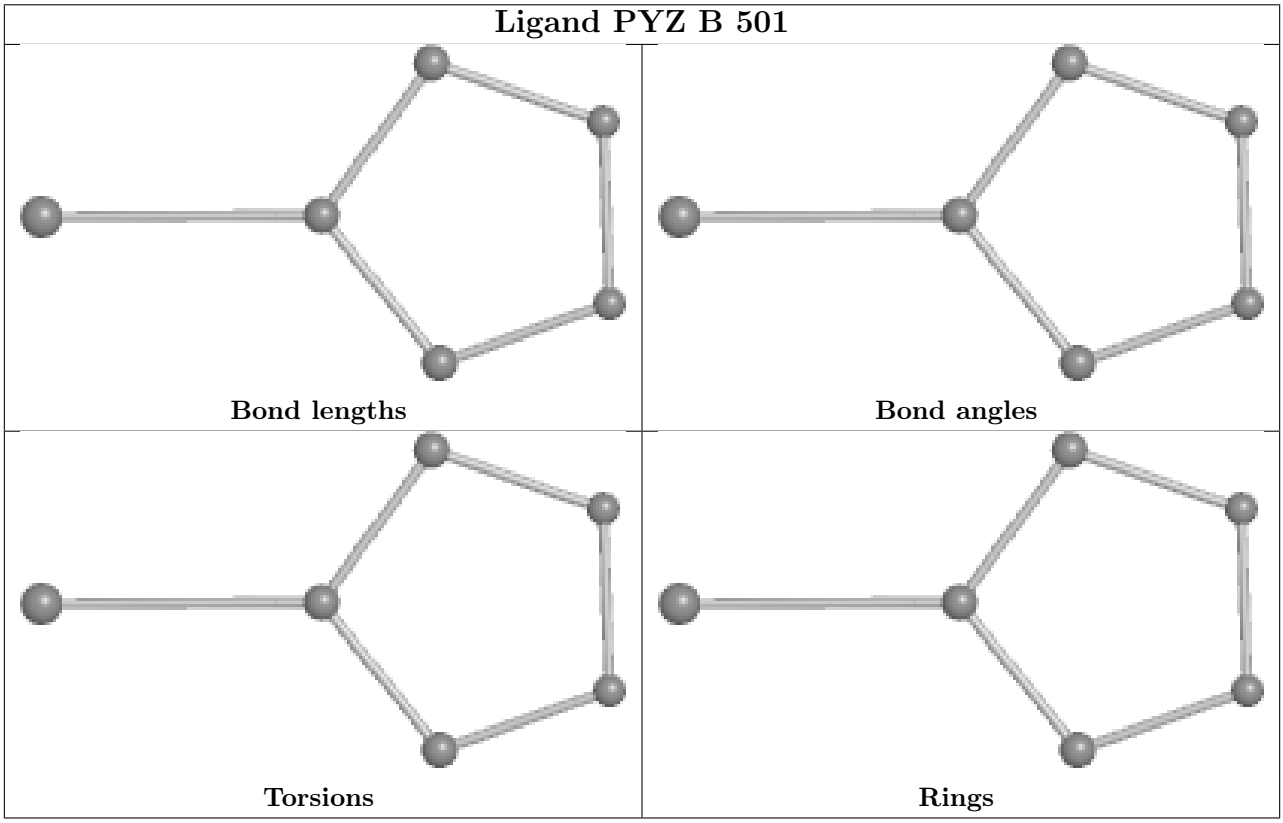


Rings

Ligand PYZ A 606



Ligand PYZ B 501



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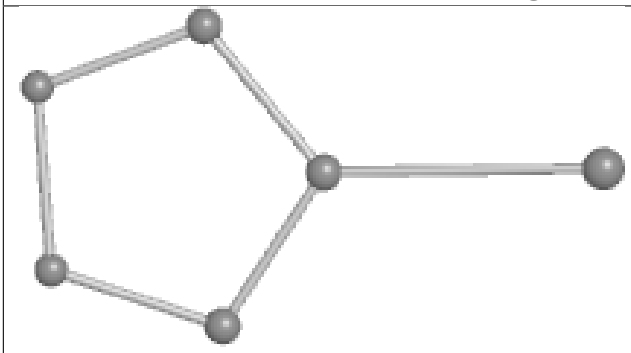
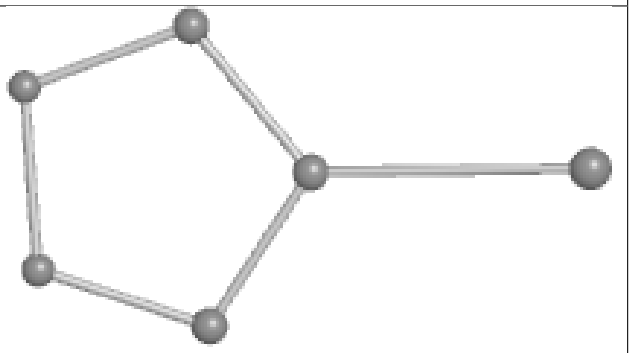
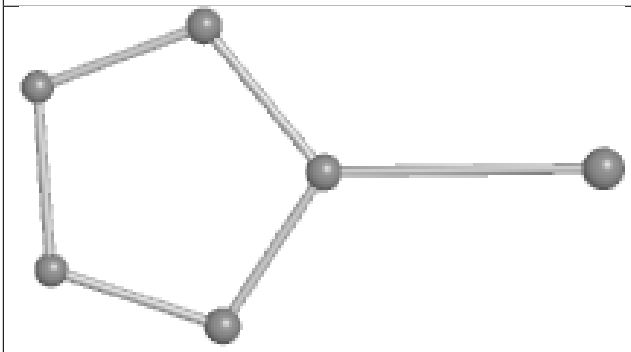


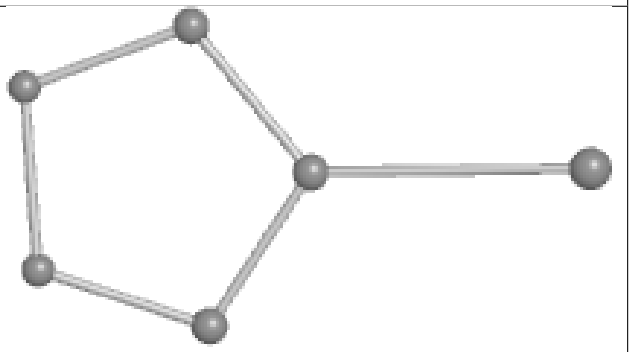
Bond lengths



Bond angles



Torsions



Rings

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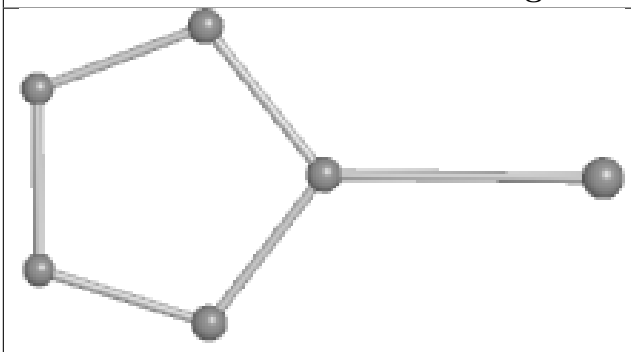
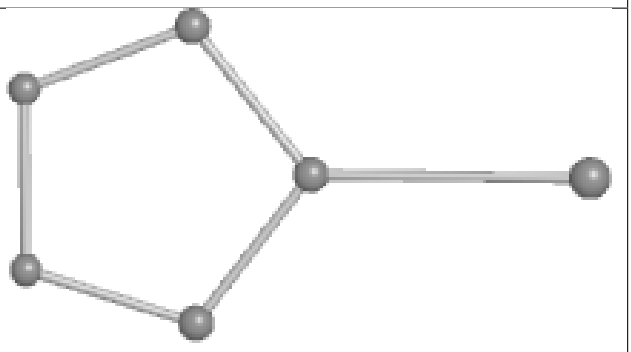
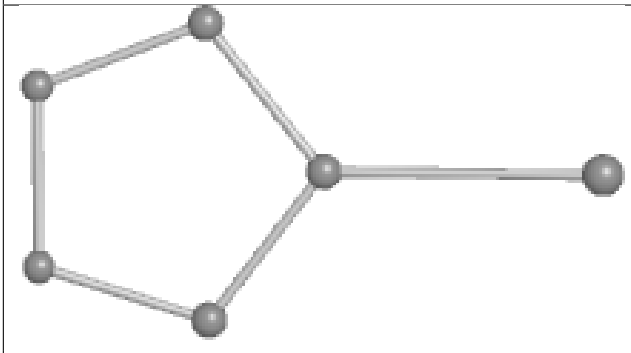


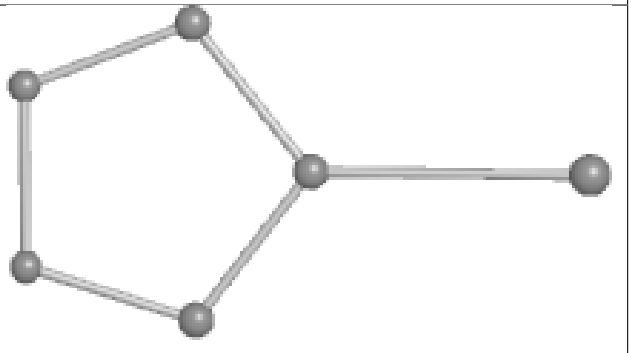
Bond lengths



Bond angles

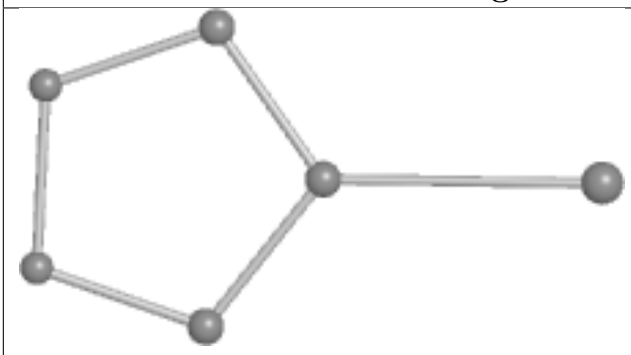


Torsions

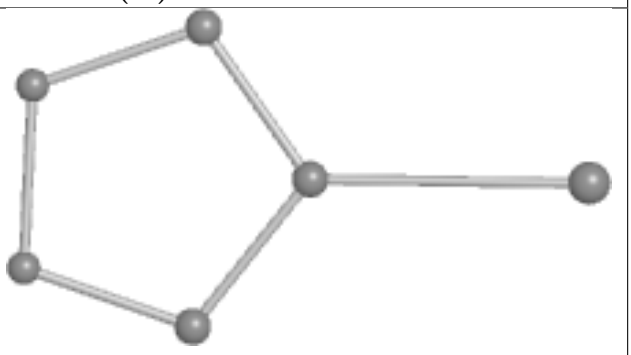


Rings

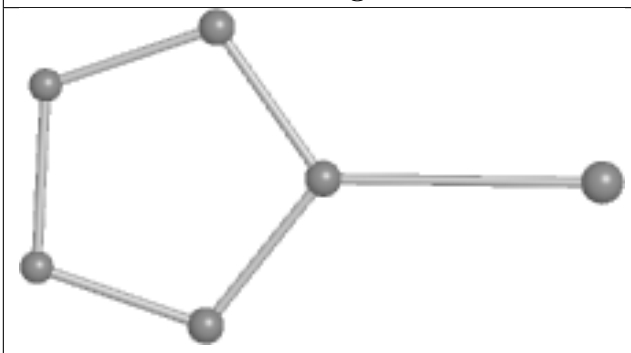
Ligand PYZ B 504 (A)



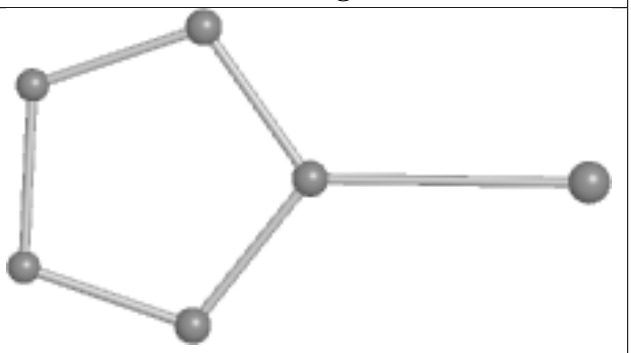
Bond lengths



Bond angles

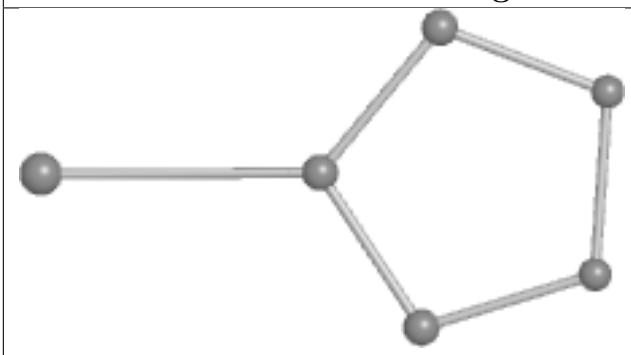


Torsions

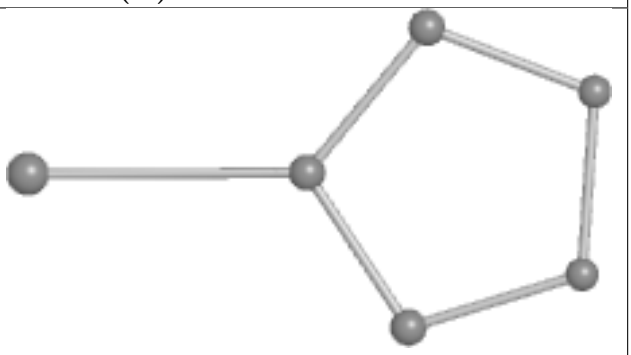


Rings

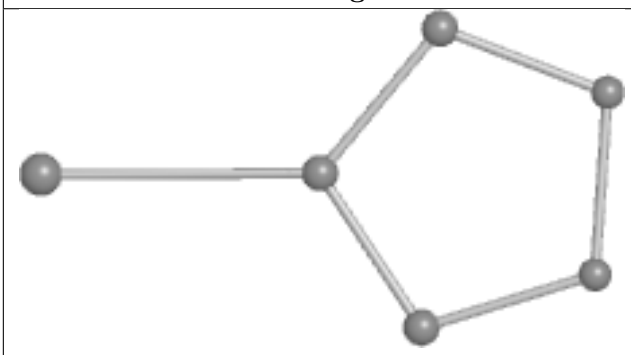
Ligand PYZ B 504 (B)



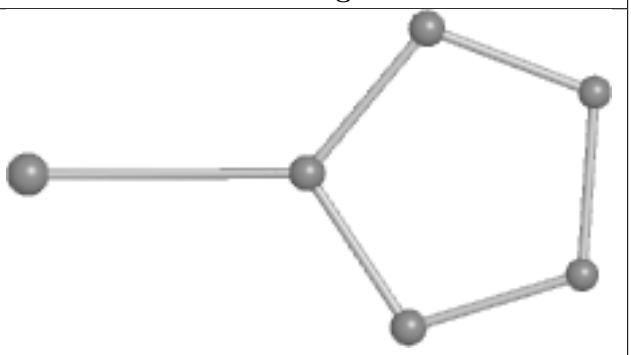
Bond lengths



Bond angles

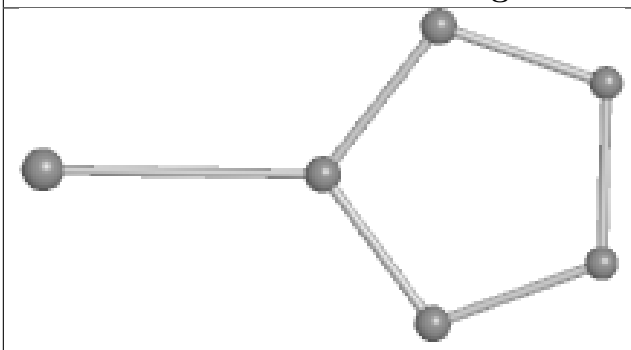


Torsions

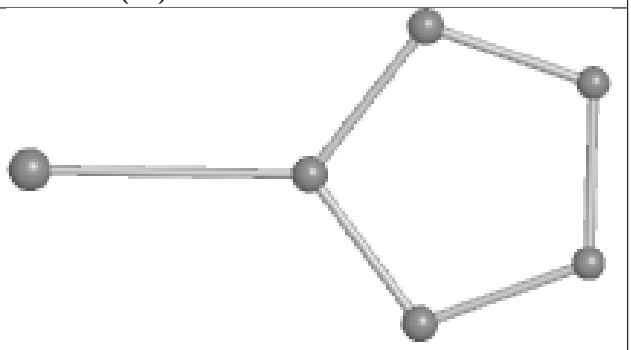


Rings

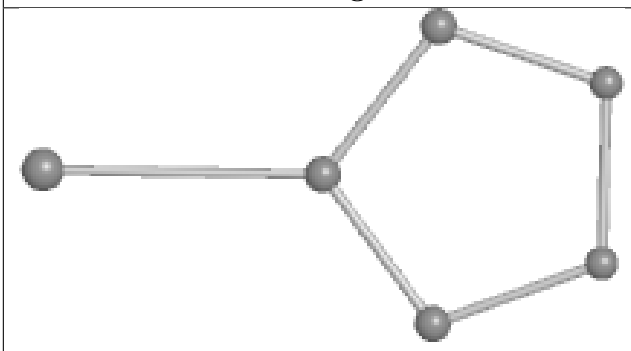
Ligand PYZ C 501 (A)



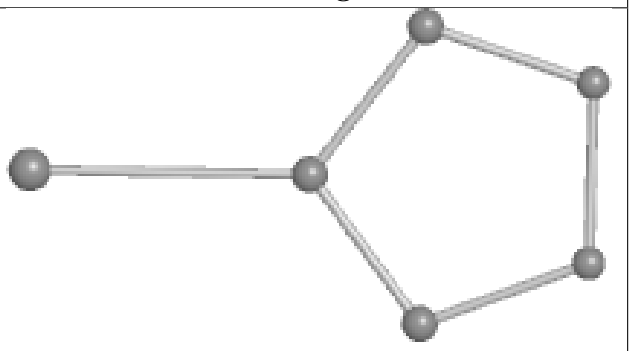
Bond lengths



Bond angles

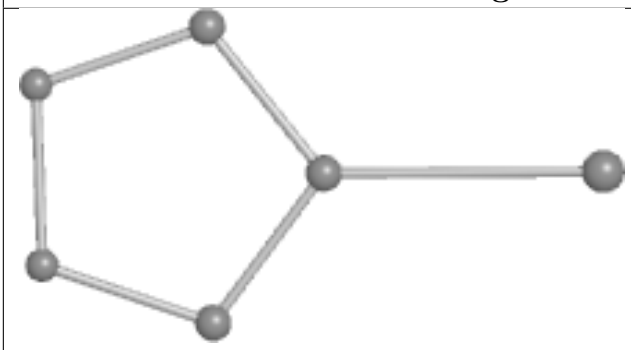


Torsions

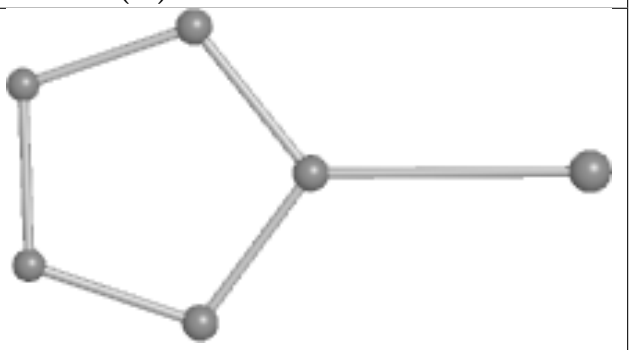


Rings

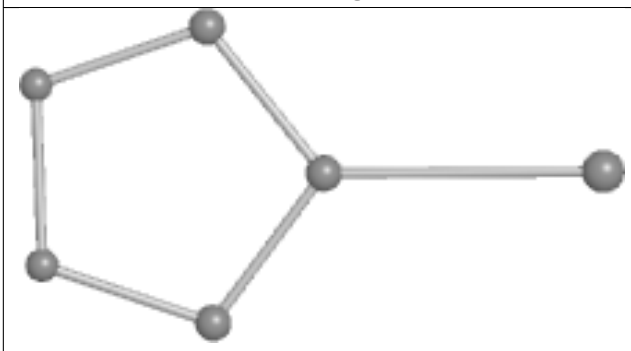
Ligand PYZ C 501 (B)



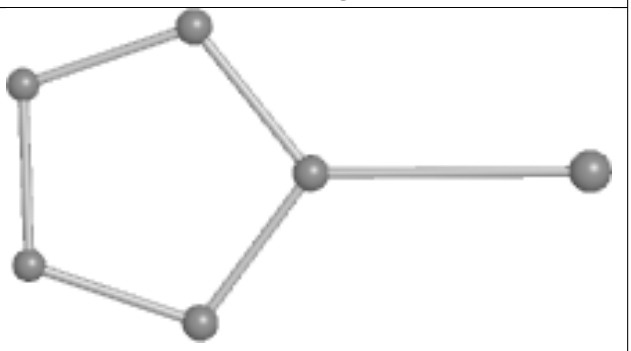
Bond lengths



Bond angles

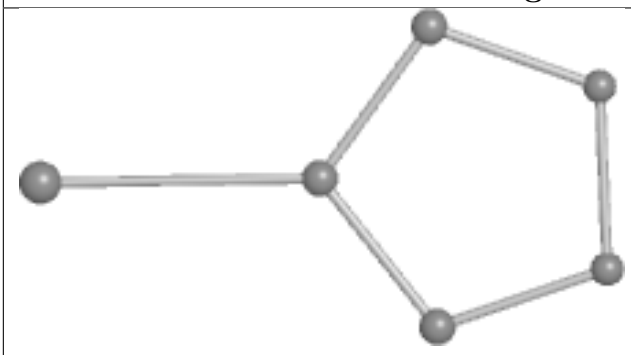


Torsions

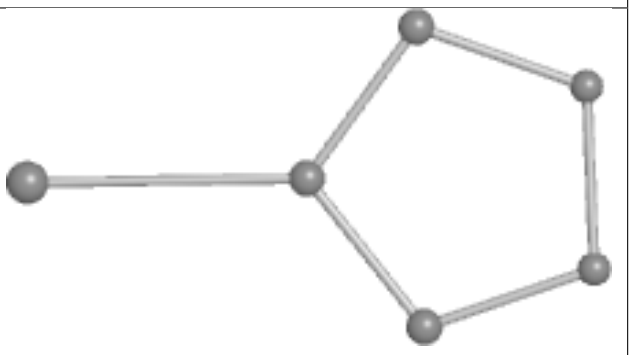


Rings

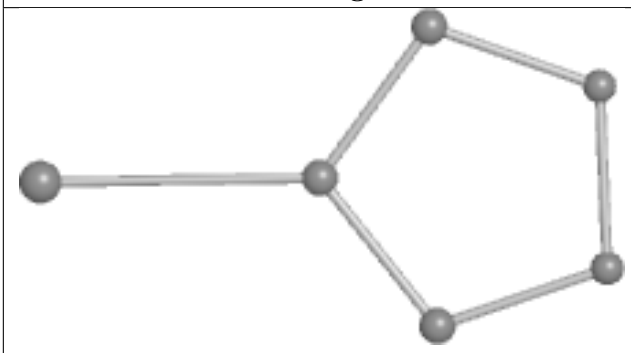
Ligand PYZ C 502



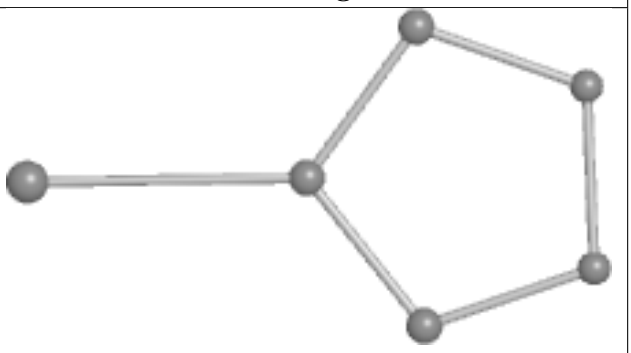
Bond lengths



Bond angles

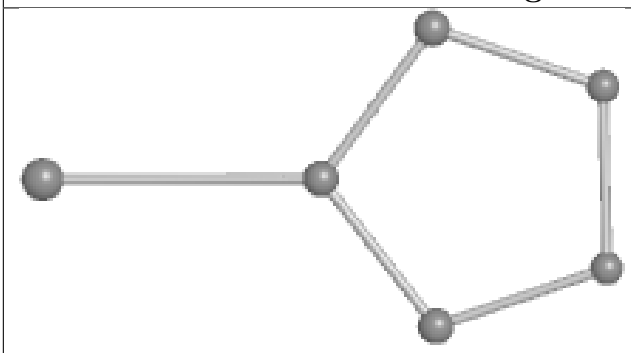


Torsions

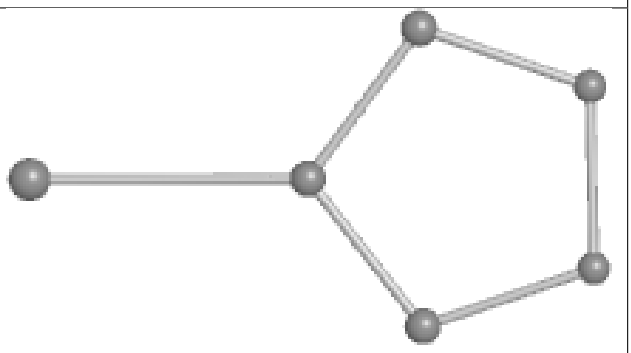


Rings

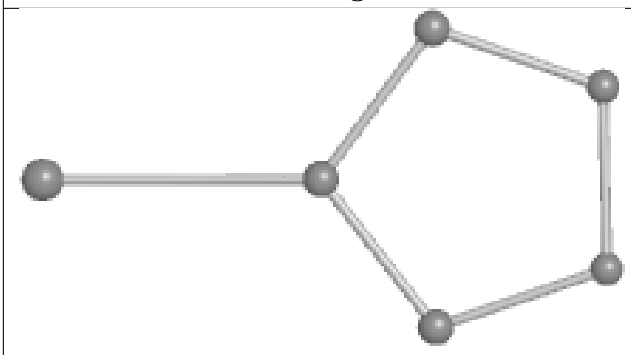
Ligand PYZ C 504



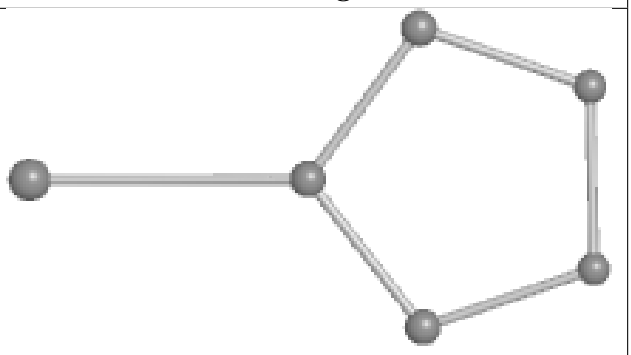
Bond lengths



Bond angles



Torsions



Rings

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

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	B	268/268 (100%)	-0.07	2 (0%)	84	85	26, 39, 66, 95	0
1	D	262/268 (97%)	0.29	8 (3%)	51	53	26, 50, 84, 107	0
2	A	300/302 (99%)	-0.12	12 (4%)	43	44	19, 34, 74, 120	1 (0%)
2	C	284/302 (94%)	0.37	18 (6%)	27	30	28, 46, 80, 110	0
All	All	1114/1140 (97%)	0.11	40 (3%)	46	48	19, 42, 80, 120	1 (0%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	241	PRO	4.4
2	C	254	PRO	4.4
2	C	225	VAL	4.1
2	A	-2	PRO	4.1
1	D	432	VAL	3.8

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

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
2	TPO	C	160	11/12	0.97	0.07	31,35,38,39	0
2	TPO	A	160	11/12	0.98	0.07	35,36,37,39	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

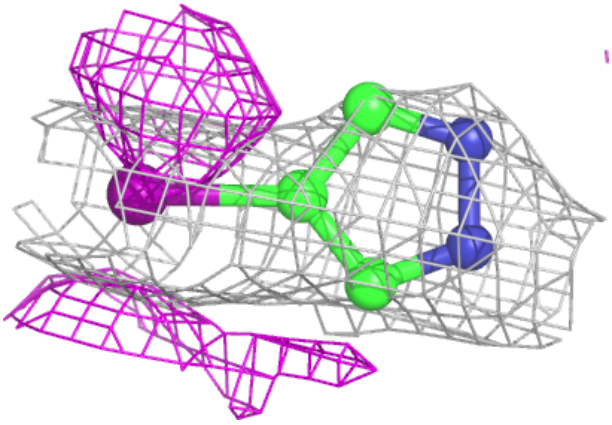
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

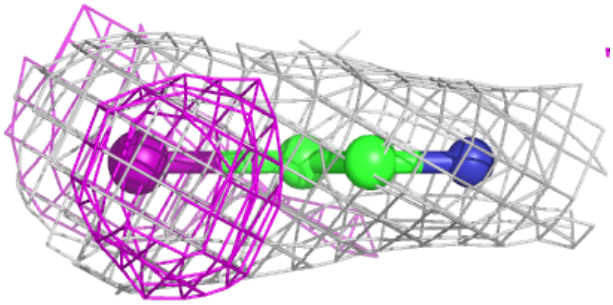
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PYZ	B	503	6/6	0.84	0.18	84,93,108,143	0
3	PYZ	B	504[A]	6/6	0.85	0.40	30,30,30,30	6
3	PYZ	B	504[B]	6/6	0.85	0.40	65,71,78,100	6
4	EPE	C	505	15/15	0.86	0.19	70,83,99,101	0
3	PYZ	A	604[B]	6/6	0.93	0.20	66,70,73,99	6
3	PYZ	B	502	6/6	0.93	0.19	70,72,77,103	0
3	PYZ	A	604[A]	6/6	0.93	0.20	51,53,55,72	6
3	PYZ	A	606	6/6	0.96	0.13	70,76,78,89	0
3	PYZ	B	501	6/6	0.97	0.14	91,94,99,102	0
3	PYZ	C	501[A]	6/6	0.98	0.13	25,25,26,33	6
3	PYZ	C	501[B]	6/6	0.98	0.13	40,41,41,47	6
3	PYZ	A	601	6/6	0.98	0.17	55,56,60,68	0
3	PYZ	A	602[B]	6/6	0.99	0.05	34,35,35,35	6
3	PYZ	D	501	6/6	0.99	0.10	67,69,80,86	0
3	PYZ	C	502	6/6	0.99	0.08	69,73,76,76	0
3	PYZ	C	504	6/6	0.99	0.09	60,61,63,67	0
3	PYZ	A	602[A]	6/6	0.99	0.05	34,35,36,36	6

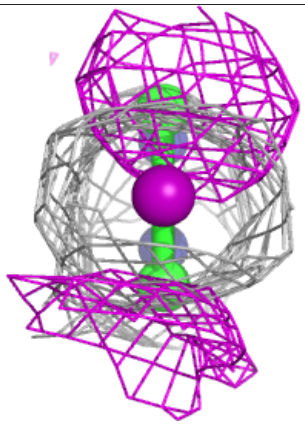
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PYZ B 503:

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

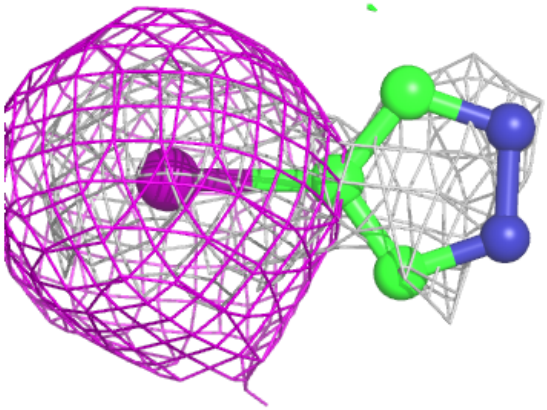


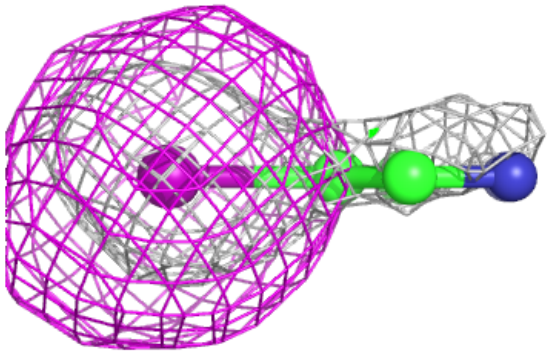


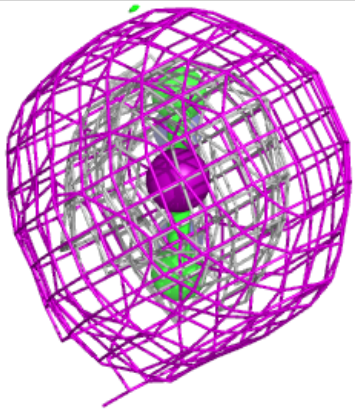


Electron density around PYZ B 504 (A):

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

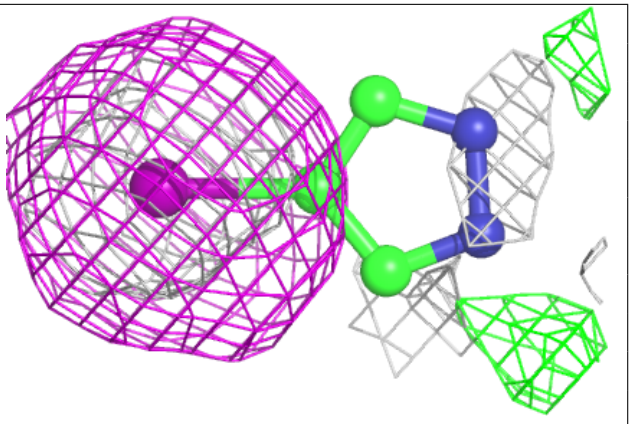


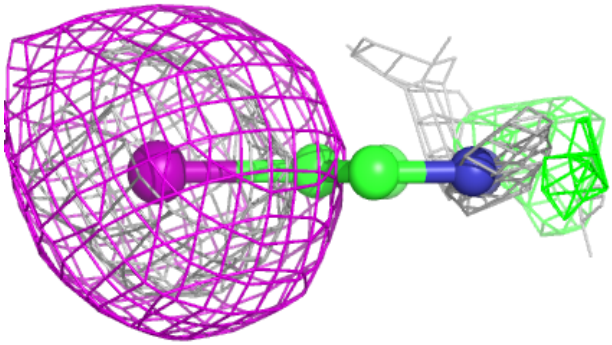


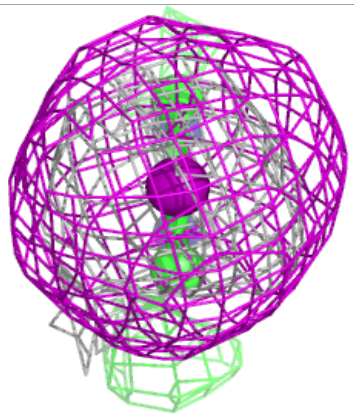


Electron density around PYZ B 504 (B):

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

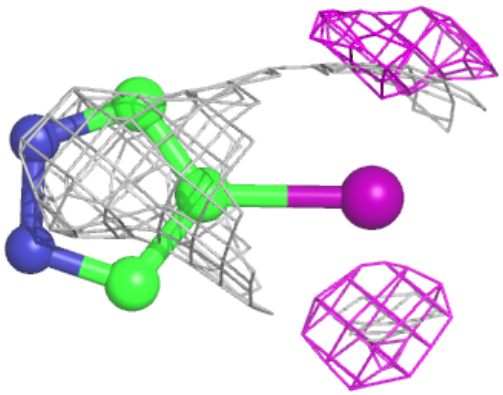


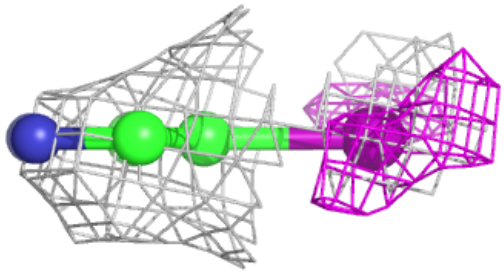


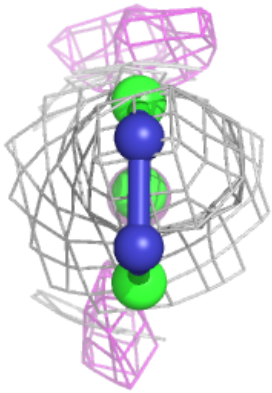


Electron density around PYZ A 604 (B):

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

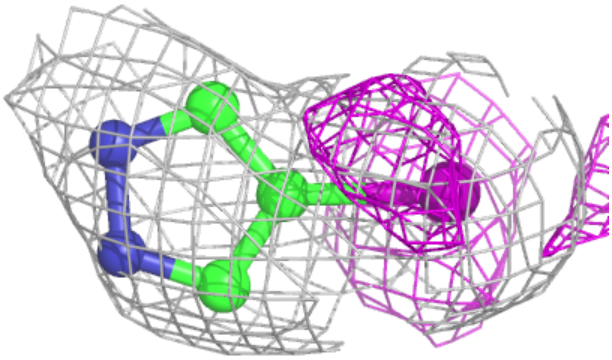


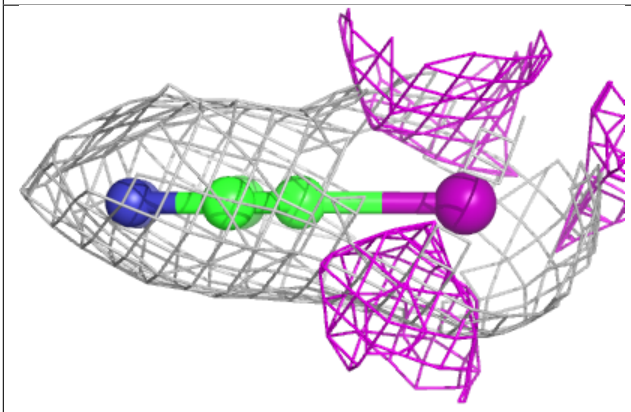


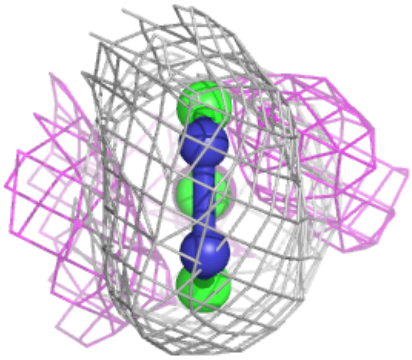


Electron density around PYZ B 502:

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

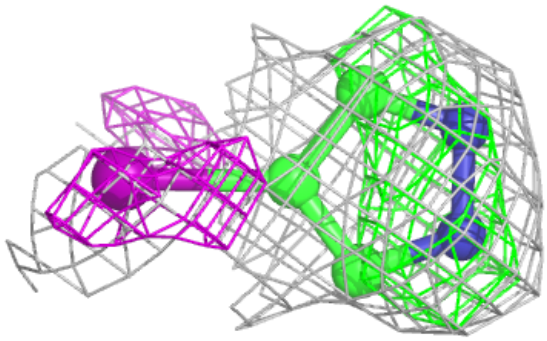


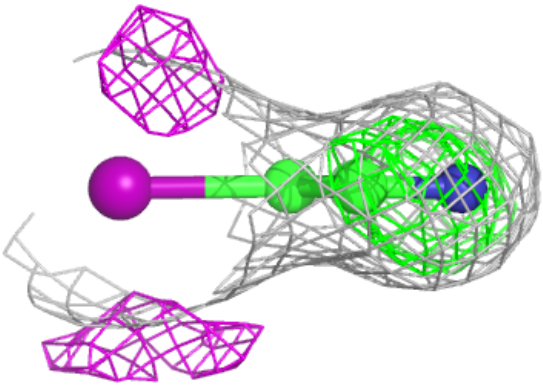


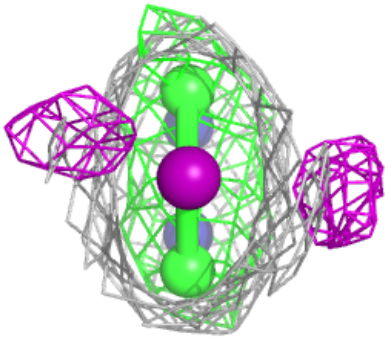


Electron density around PYZ A 604 (A):

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

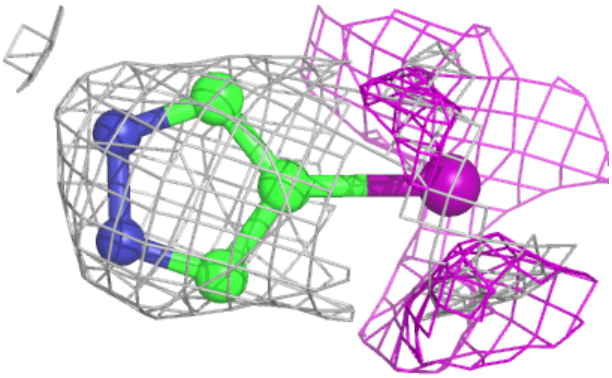


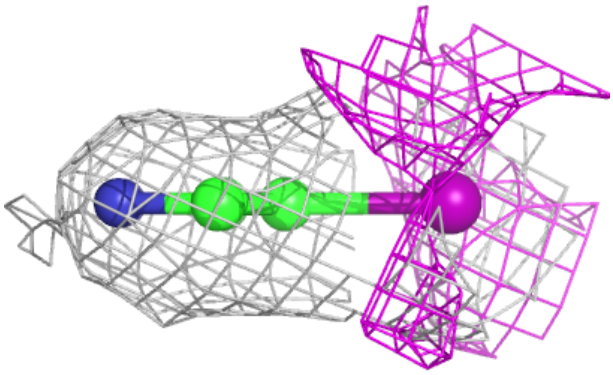


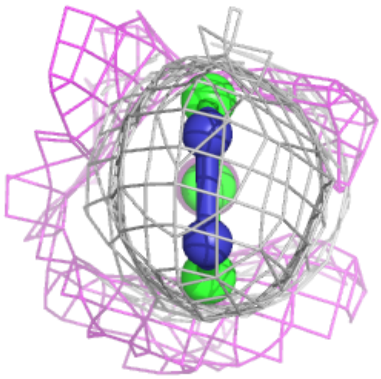


Electron density around PYZ A 606:

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

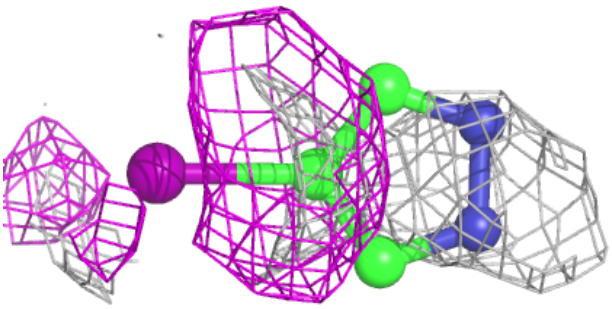


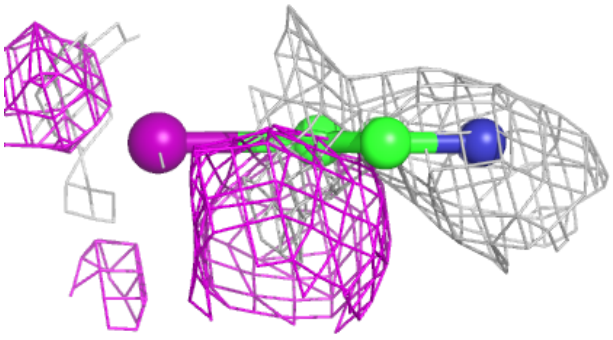


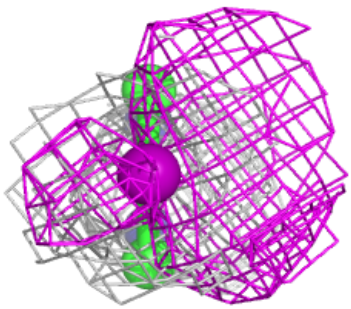


Electron density around PYZ B 501:

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

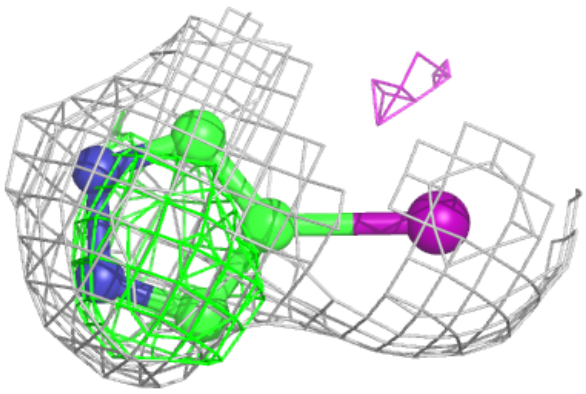


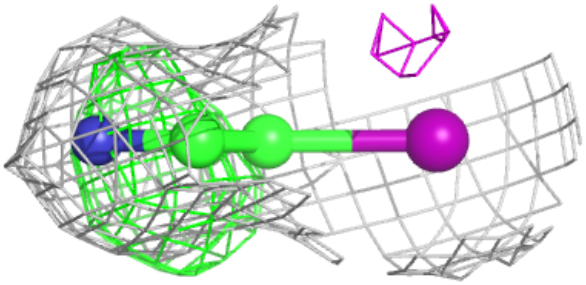


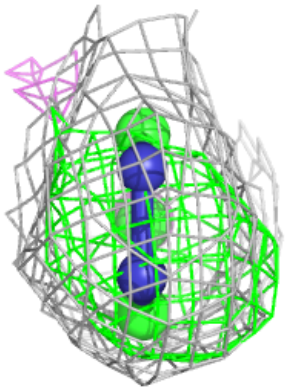


Electron density around PYZ C 501 (A):

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

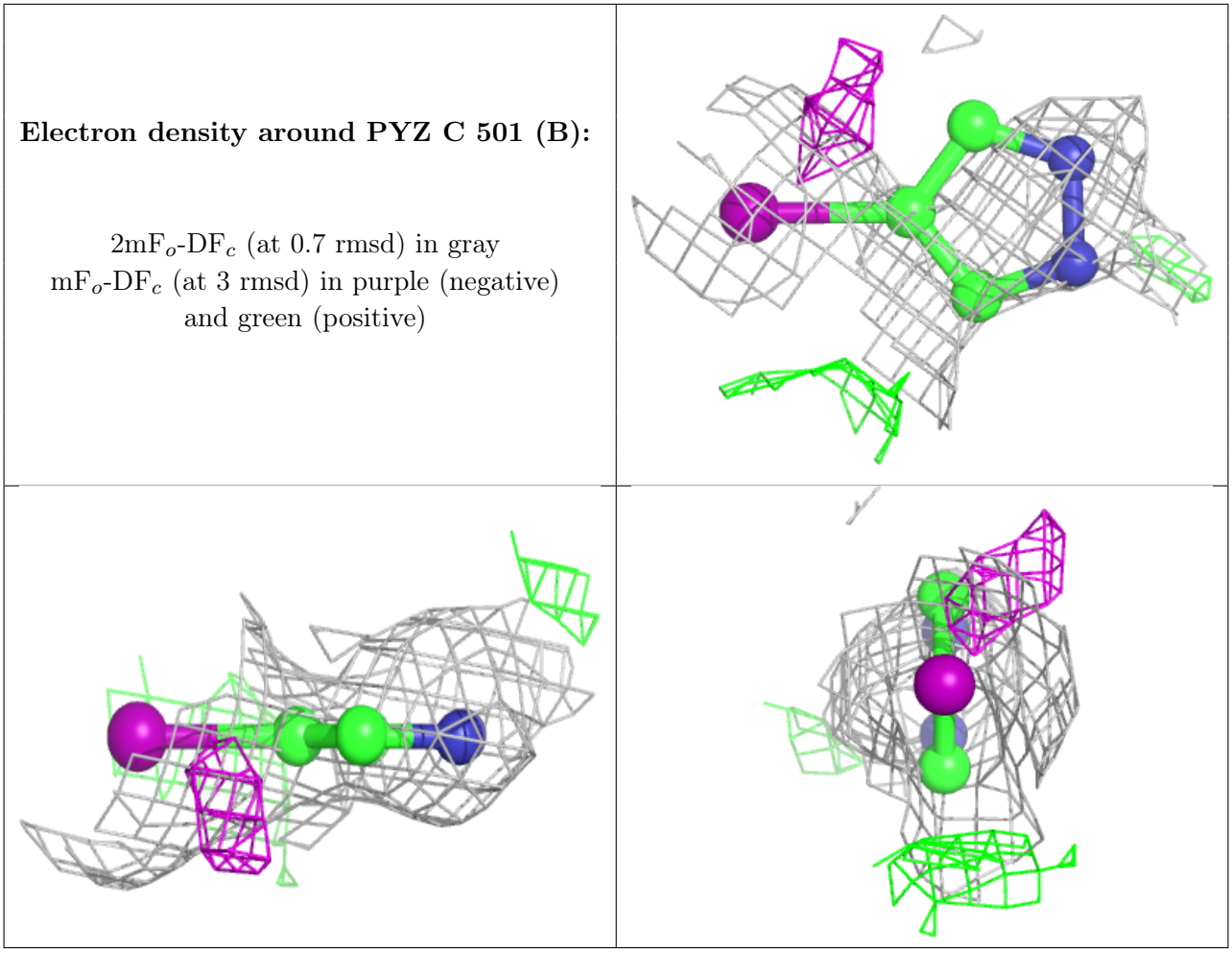






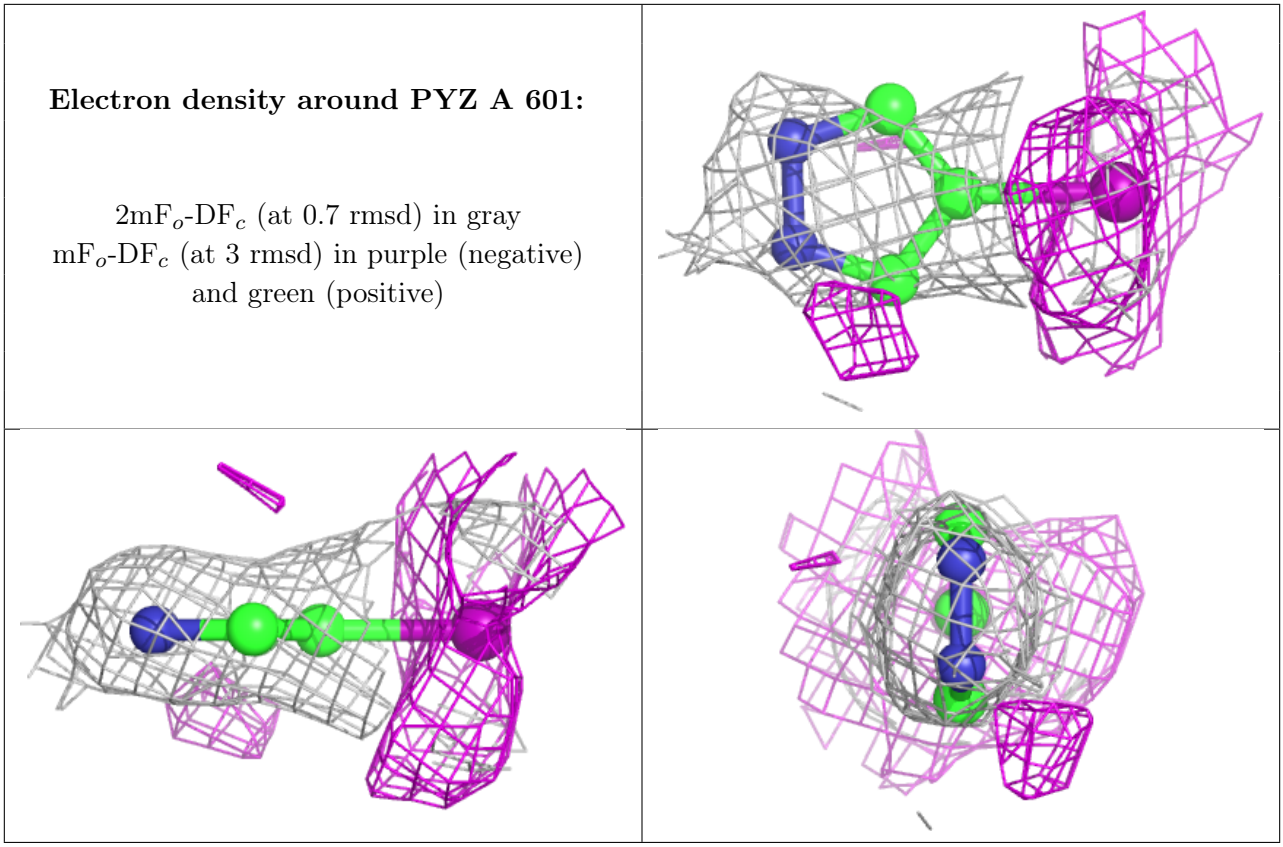
Electron density around PYZ C 501 (B):

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



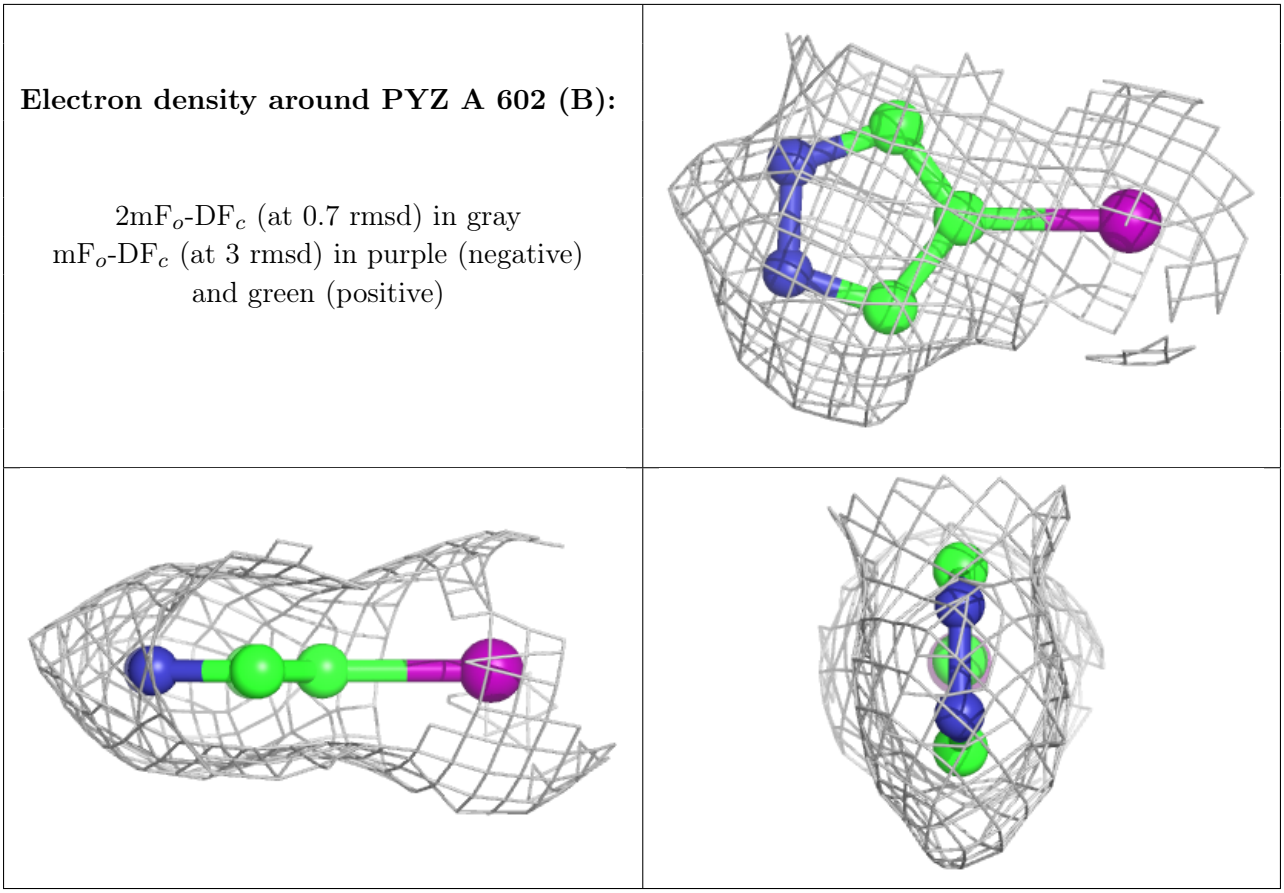
Electron density around PYZ A 601:

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



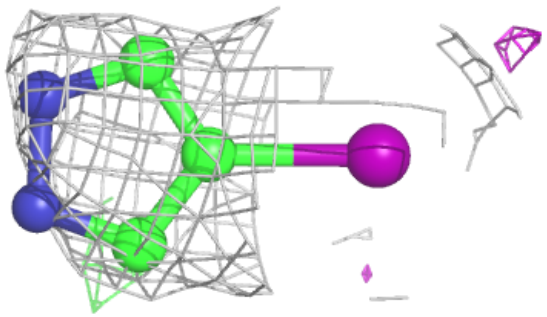
Electron density around PYZ A 602 (B):

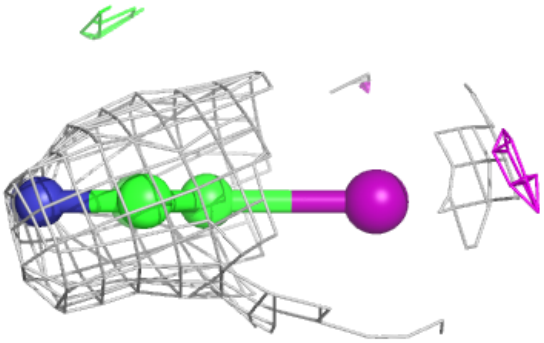
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

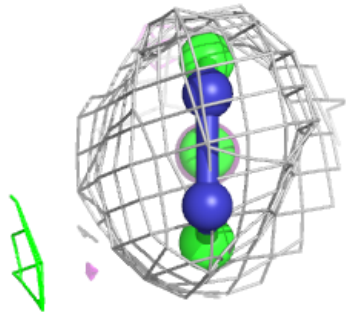


Electron density around PYZ D 501:

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

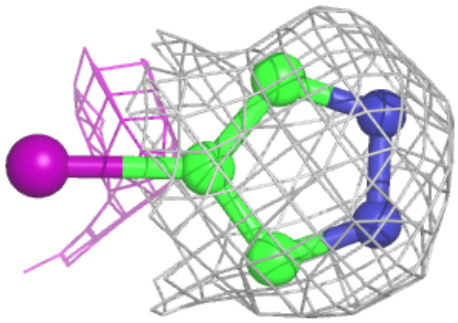


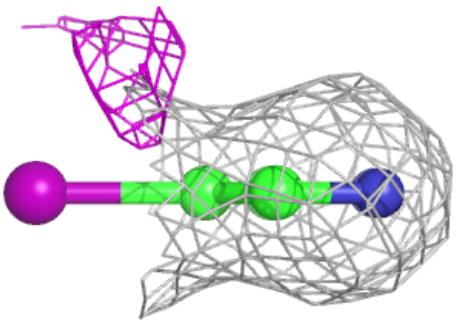


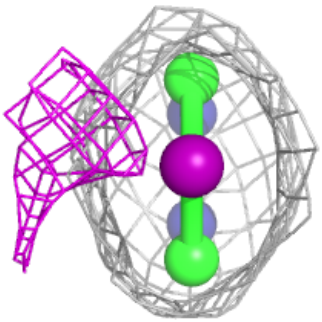


Electron density around PYZ C 502:

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

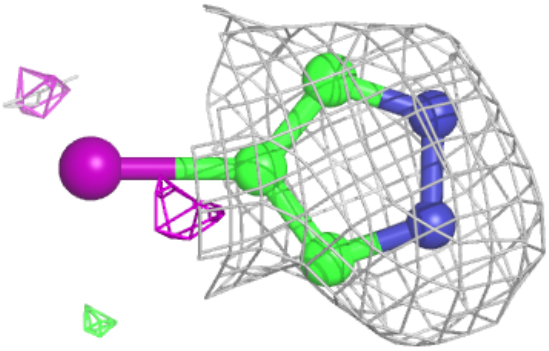


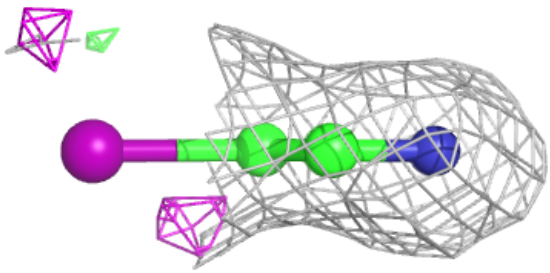


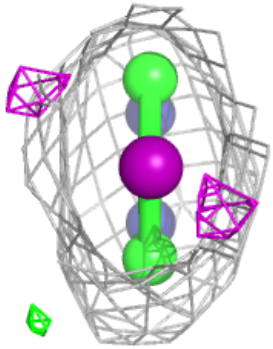


Electron density around PYZ C 504:

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

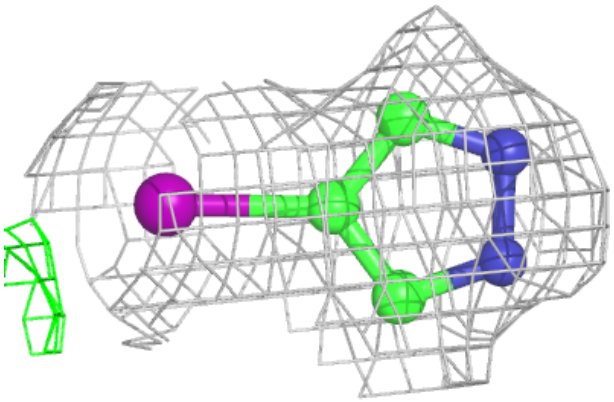


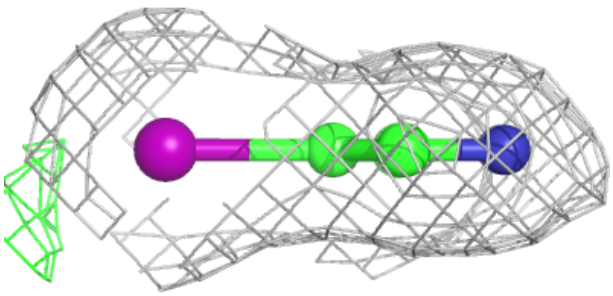


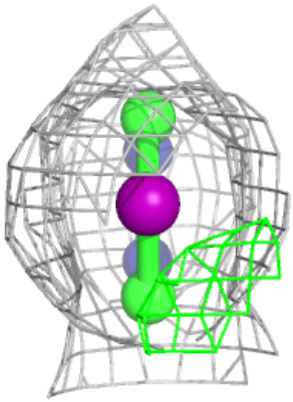


Electron density around PYZ A 602 (A):

$2mF_o$-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 (i)

There are no such residues in this entry.