Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 07:54 am GMT

PDB ID	:	6IA9
Title	:	urate oxidase under 2000 bar (220 MPa) of argon
Authors	:	Prange, T.; Colloc'h, N.; Carpentier, P.
Deposited on	:	2018-11-26
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

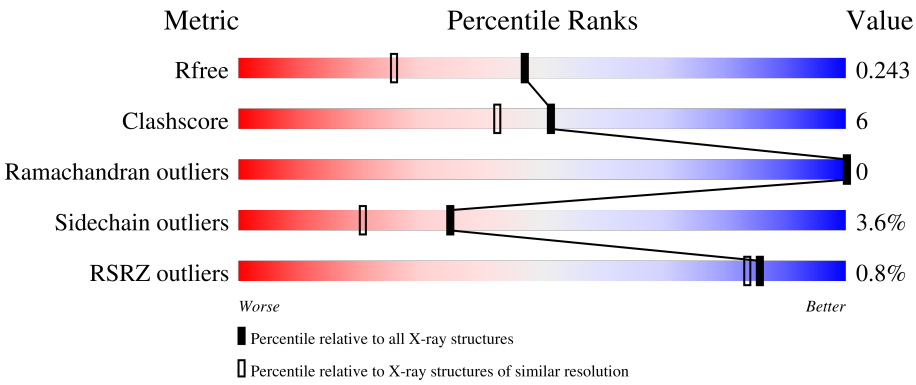
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	aaa	295	% 97% .
1	aba	295	% 96% .

2 Entry composition (i)

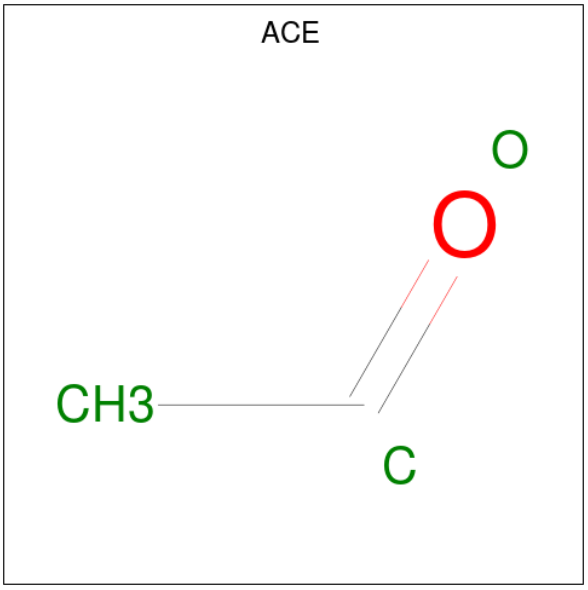
There are 6 unique types of molecules in this entry. The entry contains 5338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uricase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	aaa	295	2408	1525	418	457	8	0	9	0
1	aba	295	2379	1502	412	456	9	0	4	0

- Molecule 2 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O).

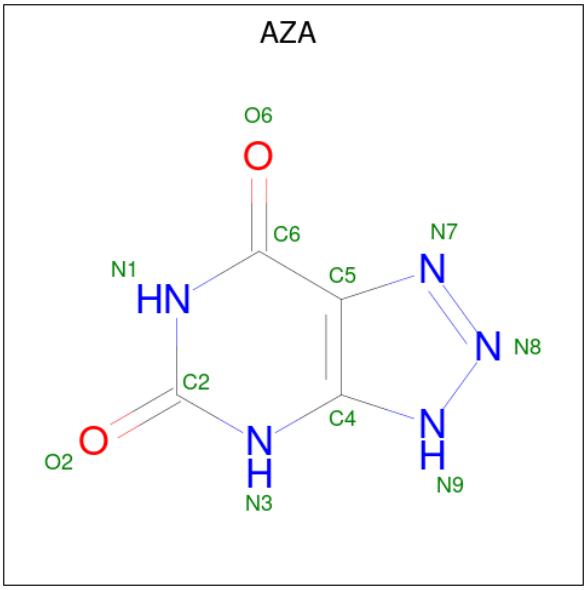


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	aaa	1	3	2	1	0	0
2	aba	1	3	2	1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	aaa	1	Total Na 1 1	0	0
3	aba	1	Total Na 1 1	0	0

- Molecule 4 is 8-AZAXANTHINE (three-letter code: AZA) (formula: $C_4H_3N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	aaa	1	Total C N O 11 4 5 2	0	0
4	aaa	1	Total C N O 11 4 5 2	0	0
4	aba	1	Total C N O 11 4 5 2	0	0
4	aba	1	Total C N O 11 4 5 2	0	0

- Molecule 5 is ARGON (three-letter code: AR) (formula: Ar).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	aaa	2	Total Ar 2 2	0	0
5	aba	2	Total Ar 2 2	0	0

- Molecule 6 is water.

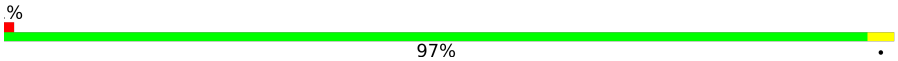
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	aaa	217	219	219	0	2
			Total	O		
6	aba	274	276	276	0	2

3 Residue-property plots (i)

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

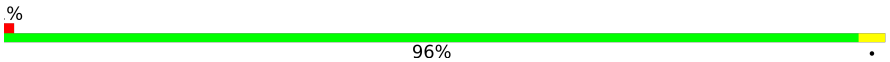
- Molecule 1: Uricase

Chain aaa:



- Molecule 1: Uricase

Chain aba:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	78.55Å 96.68Å 105.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.33 – 1.80 46.33 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (46.33-1.80) 96.0 (46.33-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.243 0.209 , 0.243	Depositor DCC
R_{free} test set	3583 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5338	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0947e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: AR, AZA, NA, ACE

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	aaa	0.40	0/2489	0.74	0/3373
1	aba	0.43	1/2443 (0.0%)	0.78	1/3314 (0.0%)
All	All	0.41	1/4932 (0.0%)	0.76	1/6687 (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	aba	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	aba	125	GLU	CD-OE2	5.49	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	aba	236	GLU	CB-CA-C	5.62	121.65	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	aba	223	ASN	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	aaa	2408	0	2393	0	0
1	aba	2379	0	2334	0	0
2	aaa	3	0	3	0	0
2	aba	3	0	3	0	0
3	aaa	1	0	0	0	0
3	aba	1	0	0	0	0
4	aaa	22	0	6	0	0
4	aba	22	0	6	0	0
5	aaa	2	0	0	0	0
5	aba	2	0	0	0	0
6	aaa	219	0	0	0	0
6	aba	276	0	0	0	0
All	All	5338	0	4745	0	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 6.

There are no clashes within the asymmetric unit.

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	aaa	302/295 (102%)	292 (97%)	10 (3%)	0	100	100
1	aba	297/295 (101%)	292 (98%)	5 (2%)	0	100	100
All	All	599/590 (102%)	584 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aaa	270/261 (103%)	258 (96%)	12 (4%)	28	14
1	aba	265/261 (102%)	255 (96%)	10 (4%)	33	18
All	All	535/522 (102%)	513 (96%)	22 (4%)	35	16

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	aaa	22	GLU
1	aaa	23[A]	LYS
1	aaa	23[B]	LYS
1	aaa	52	SER
1	aaa	122	ARG
1	aaa	125	GLU
1	aaa	171[A]	LYS
1	aaa	171[B]	LYS
1	aaa	194	LEU
1	aaa	216	LEU
1	aaa	252	LEU
1	aaa	294	ARG
1	aba	114	LYS
1	aba	124	SER
1	aba	125	GLU
1	aba	138	LYS
1	aba	187[A]	GLN
1	aba	187[B]	GLN
1	aba	194	LEU
1	aba	216	LEU
1	aba	244	LEU
1	aba	252	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	ACE	aaa	301	1	1,2,2	0.15	0	1,1,1	0.50	0
4	AZA	aaa	304	-	9,12,12	1.39	1 (11%)	4,17,17	6.44	2 (50%)
4	AZA	aba	306	-	9,12,12	1.51	1 (11%)	4,17,17	6.43	3 (75%)
4	AZA	aba	305	-	9,12,12	1.55	1 (11%)	4,17,17	6.73	2 (50%)
4	AZA	aaa	303	-	9,12,12	1.37	1 (11%)	4,17,17	6.53	2 (50%)
2	ACE	aba	301	1	1,2,2	0.19	0	1,1,1	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AZA	aba	305	-	-	-	0/2/2/2
4	AZA	aaa	303	-	-	-	0/2/2/2
4	AZA	aaa	304	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AZA	aba	306	-	-	-	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	aba	305	AZA	C6-N1	4.22	1.40	1.33
4	aba	306	AZA	C6-N1	4.06	1.40	1.33
4	aaa	304	AZA	C6-N1	3.97	1.39	1.33
4	aaa	303	AZA	C6-N1	3.93	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	aba	305	AZA	C2-N1-C6	11.24	124.63	115.14
4	aaa	304	AZA	C2-N1-C6	10.93	124.37	115.14
4	aba	306	AZA	C2-N1-C6	10.89	124.34	115.14
4	aaa	303	AZA	C2-N1-C6	10.85	124.30	115.14
4	aba	305	AZA	C5-C6-N1	-7.16	113.64	123.43
4	aaa	303	AZA	C5-C6-N1	-7.13	113.67	123.43
4	aaa	304	AZA	C5-C6-N1	-6.60	114.40	123.43
4	aba	306	AZA	C5-C6-N1	-6.52	114.51	123.43
4	aba	306	AZA	N9-N8-N7	-2.01	108.64	111.25

There are no chirality outliers.

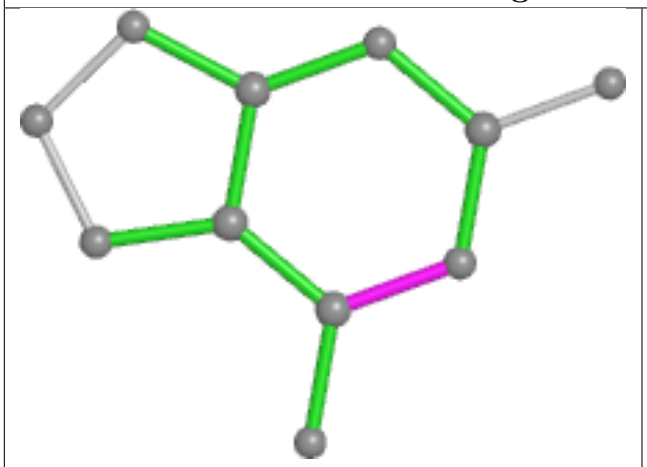
There are no torsion outliers.

There are no ring outliers.

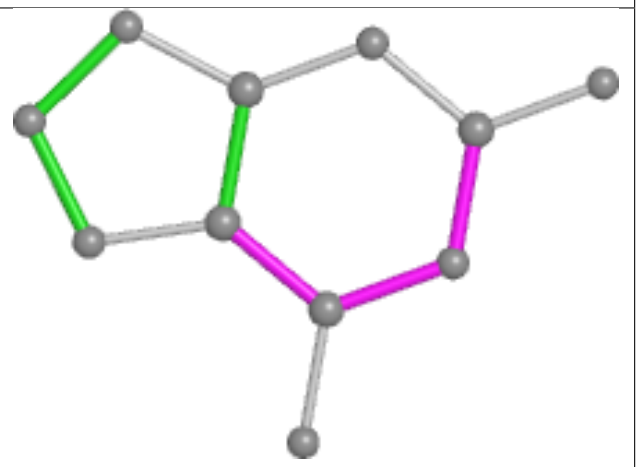
No monomer is involved in short contacts.

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.

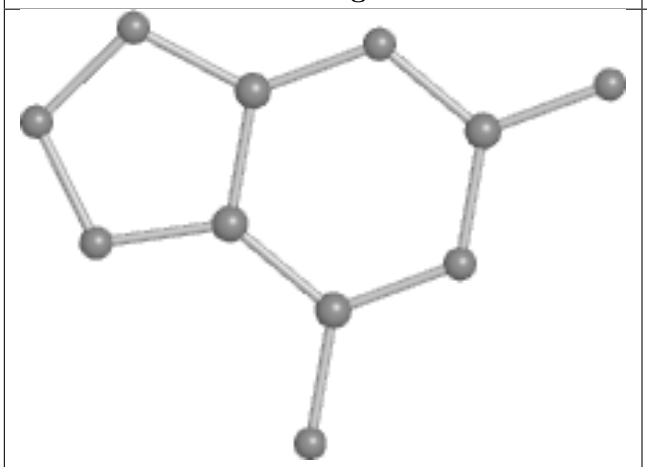
Ligand AZA aaa 304



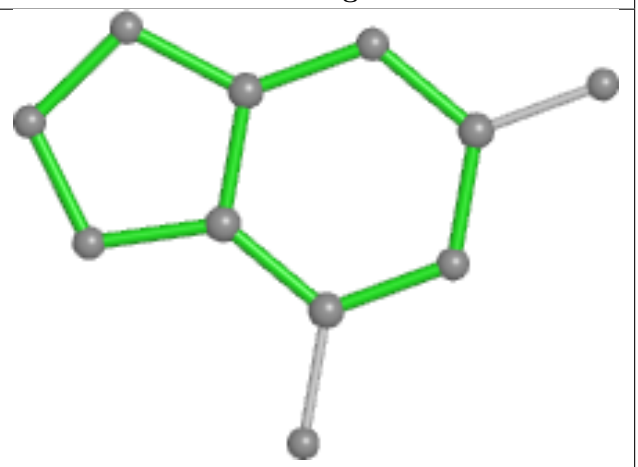
Bond lengths



Bond angles

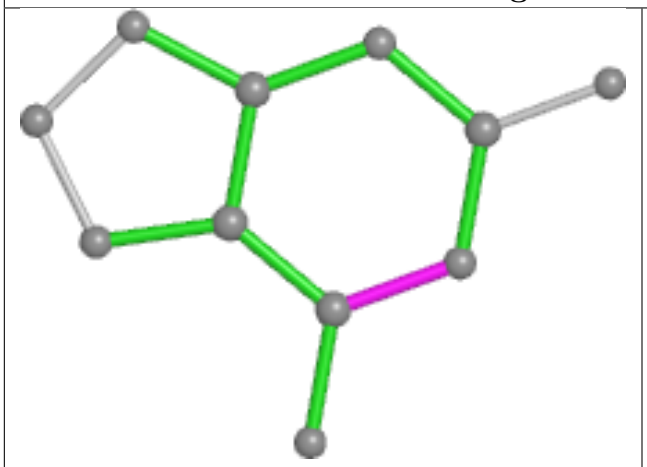


Torsions



Rings

Ligand AZA aba 306



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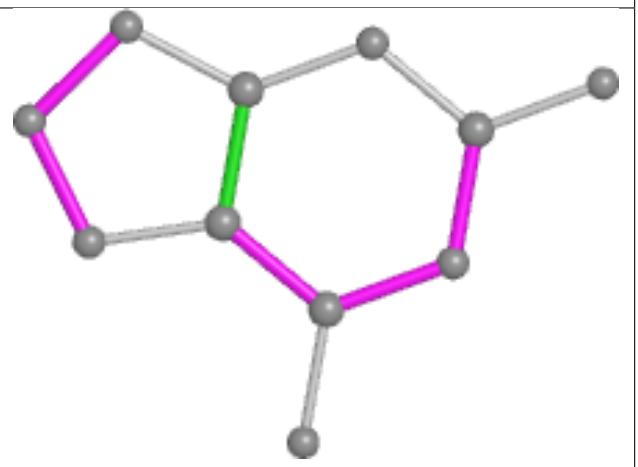

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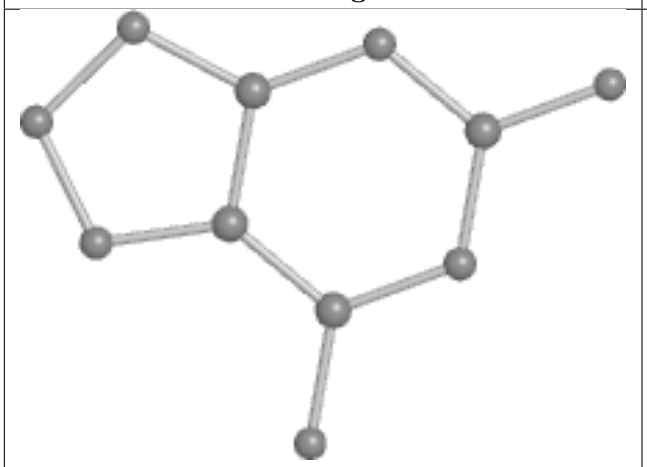
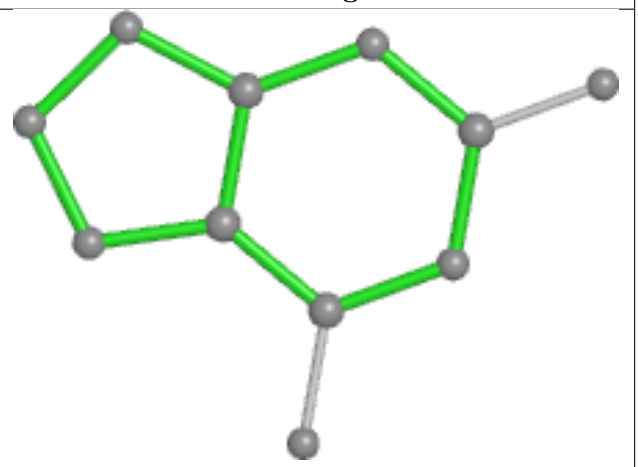
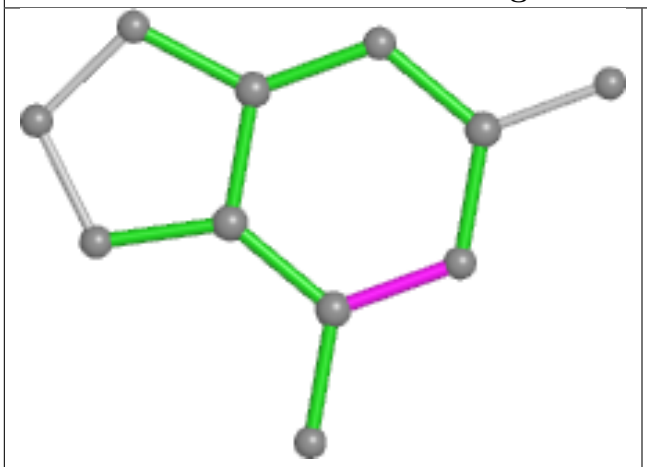


Torsions

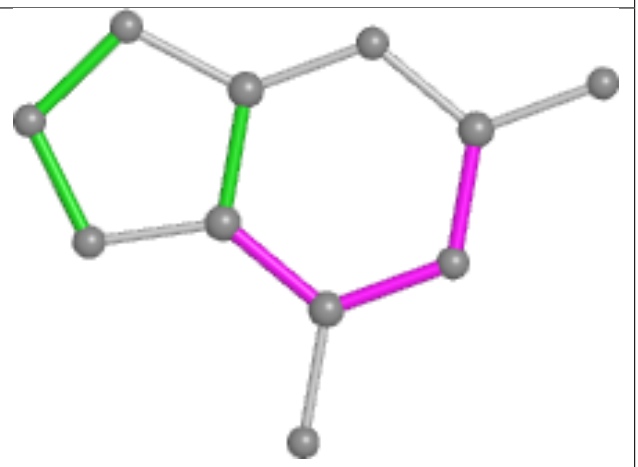


Rings

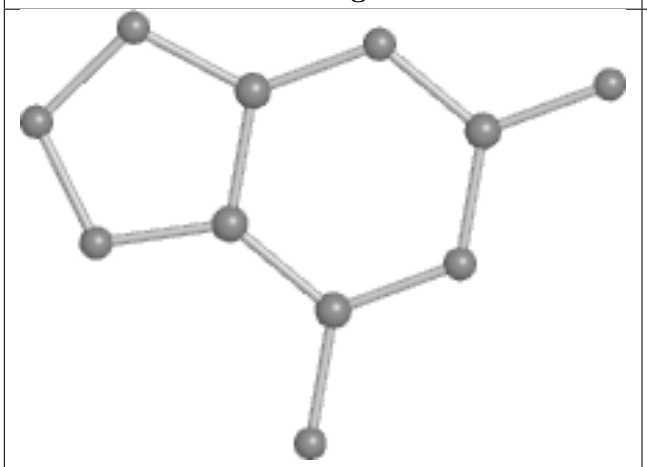
Ligand AZA aba 305



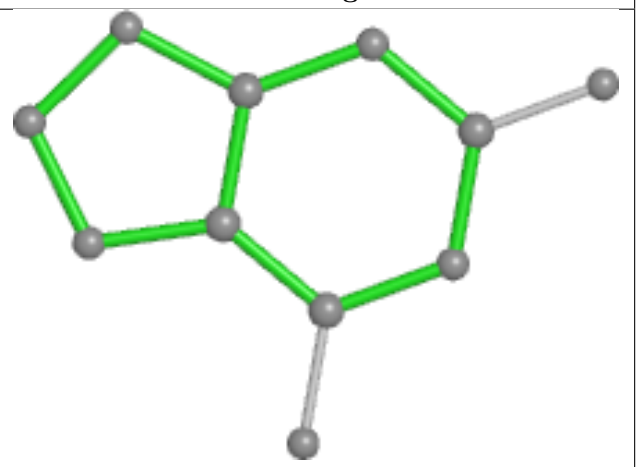
Bond lengths



Bond angles

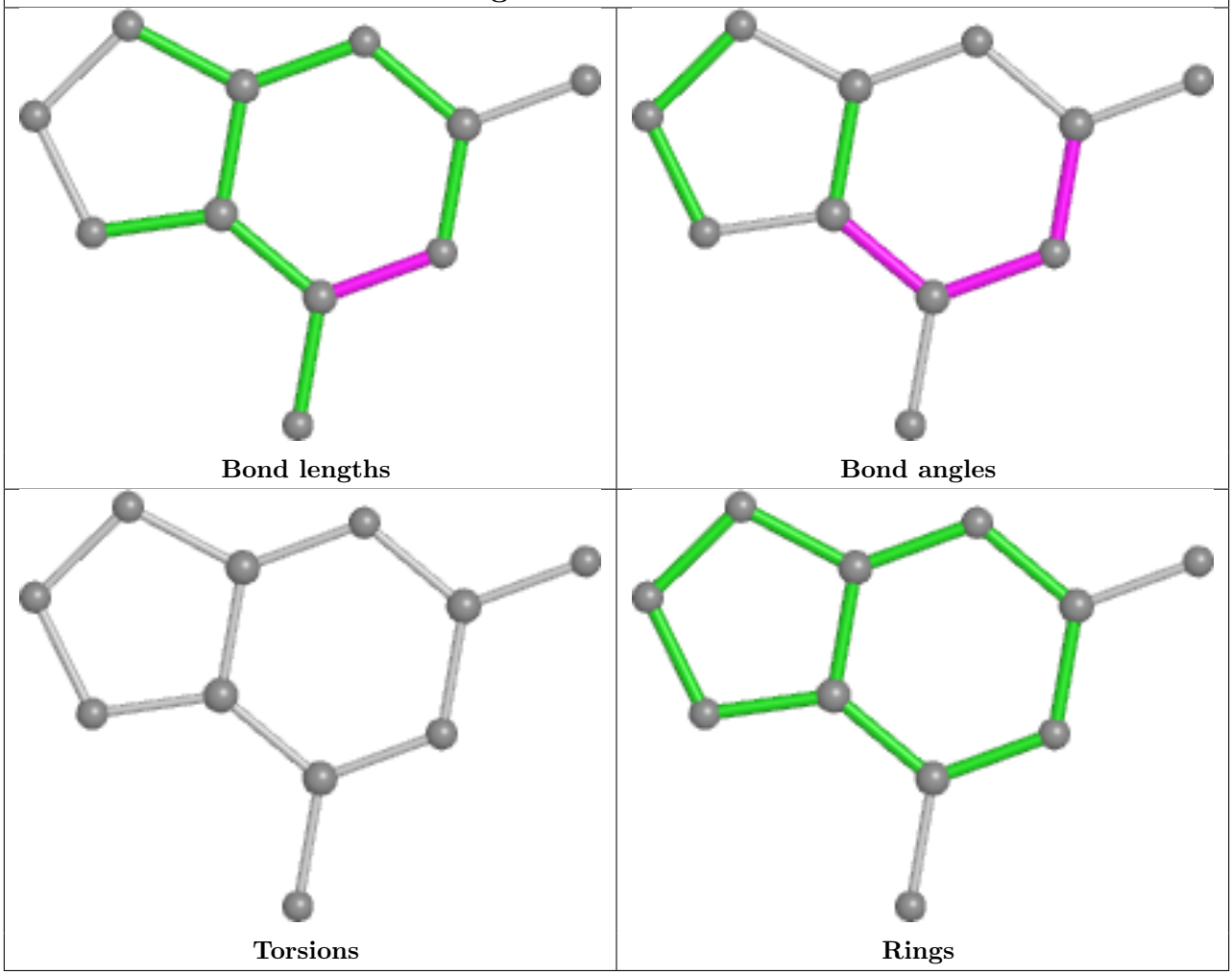


Torsions



Rings

Ligand AZA aaa 303



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	aaa	295/295 (100%)	-0.28	2 (0%)	87	86	22, 35, 54, 80	0
1	aba	295/295 (100%)	-0.39	3 (1%)	82	80	19, 29, 48, 79	0
All	All	590/590 (100%)	-0.34	5 (0%)	86	84	19, 32, 52, 80	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	aaa	22	GLU	4.0
1	aba	23	LYS	2.6
1	aba	22	GLU	2.3
1	aaa	23[A]	LYS	2.2
1	aba	295	SER	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

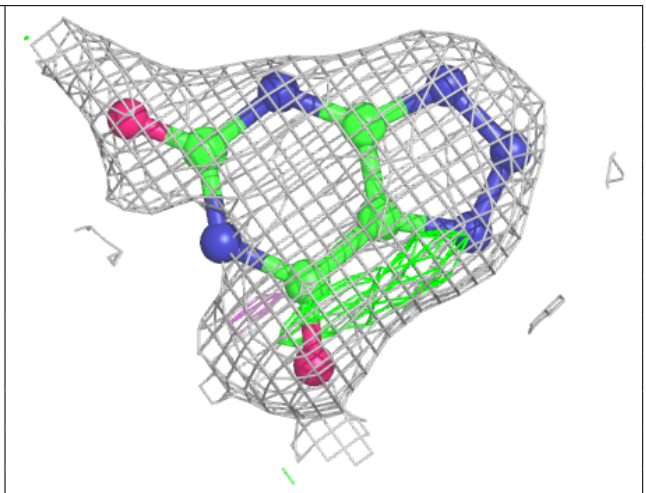
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

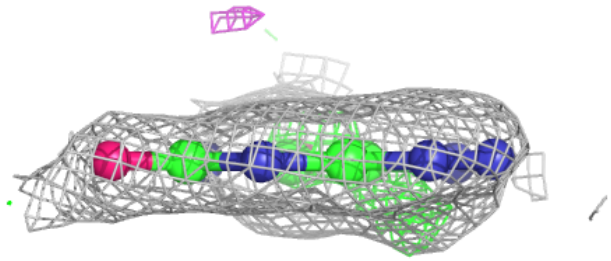
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	AZA	aaa	304	11/11	0.84	0.22	34,38,45,50	11
4	AZA	aba	306	11/11	0.85	0.22	26,37,41,59	11
5	AR	aaa	305	1/1	0.89	0.18	56,56,56,56	1
3	NA	aba	302	1/1	0.90	0.06	38,38,38,38	0
5	AR	aaa	306	1/1	0.90	0.39	44,44,44,44	1
3	NA	aaa	302	1/1	0.92	0.11	46,46,46,46	0
2	ACE	aaa	301	3/3	0.94	0.29	58,58,61,65	0
2	ACE	aba	301	3/3	0.95	0.23	55,55,61,64	0
5	AR	aba	303	1/1	0.96	0.08	57,57,57,57	0
5	AR	aba	304	1/1	0.96	0.19	42,42,42,42	1
4	AZA	aaa	303	11/11	0.97	0.09	25,28,29,30	0
4	AZA	aba	305	11/11	0.98	0.10	20,23,26,26	0

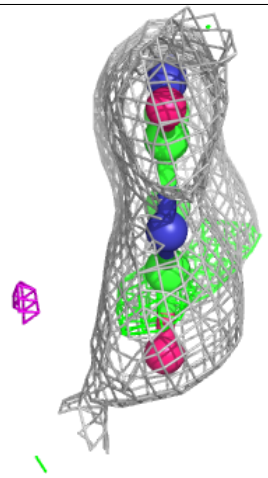
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AZA aaa 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

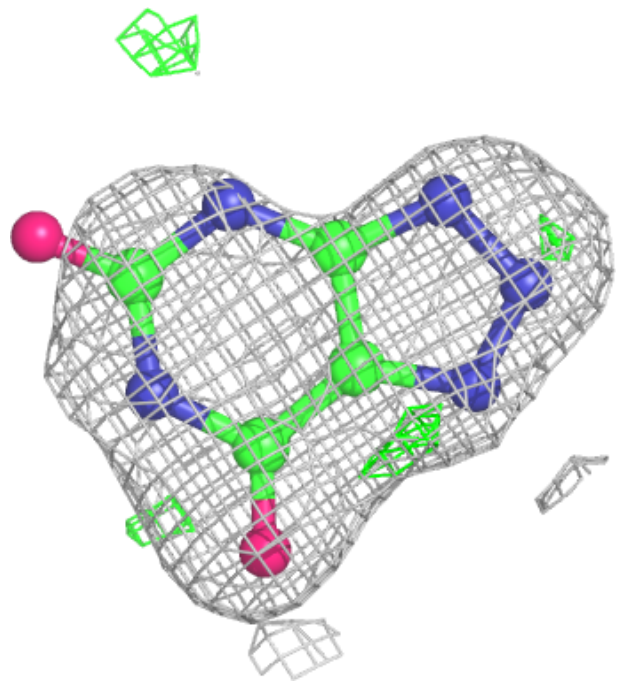


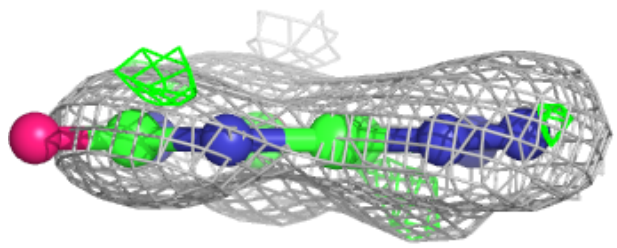


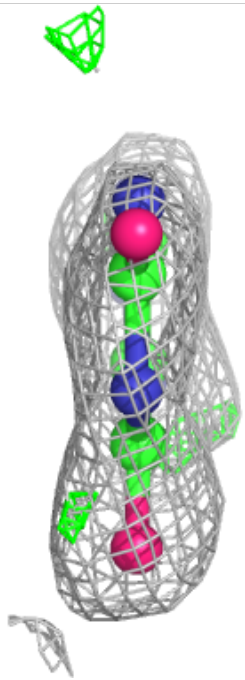


Electron density around AZA aba 306:

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

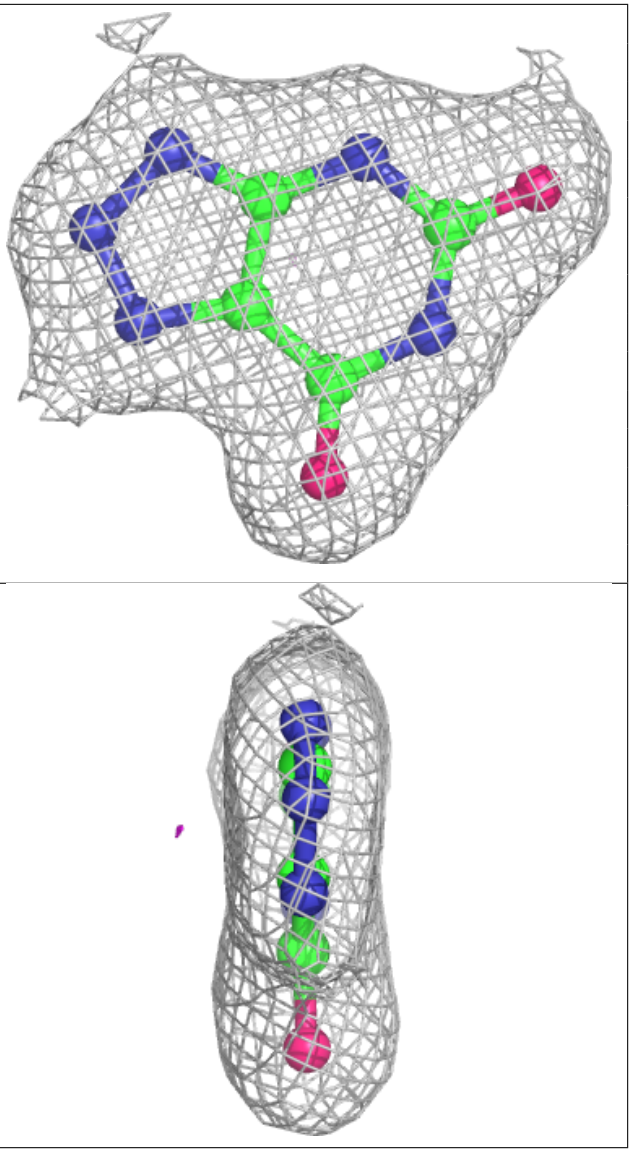






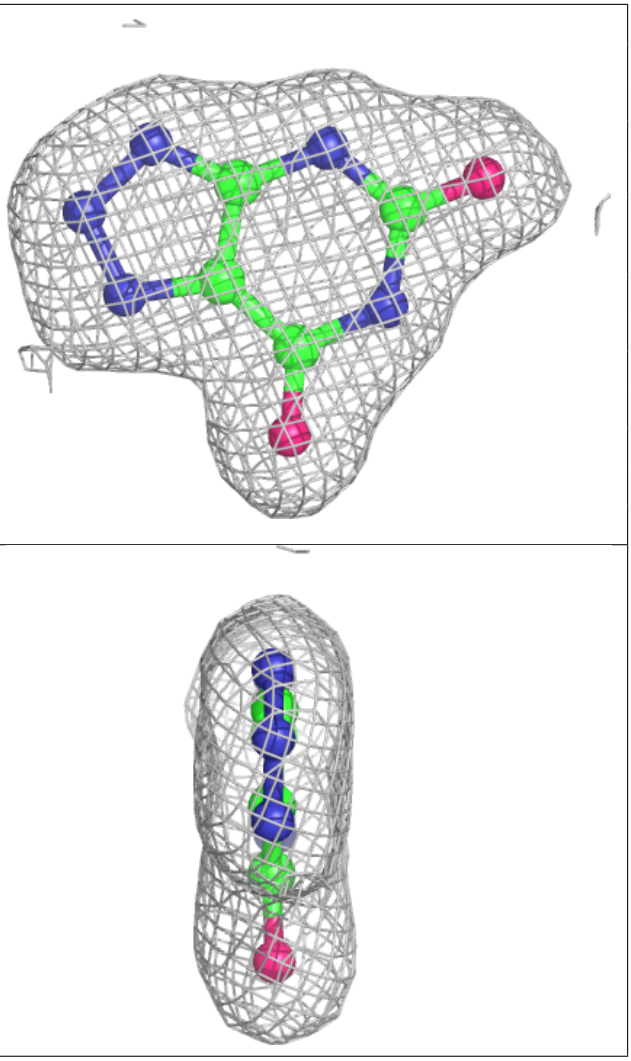
Electron density around AZA aaa 303:

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



Electron density around AZA aba 305:

$2mF_o$-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.