



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2020 – 09:19 pm BST

PDB ID : 2GM1  
Title : Crystal structure of the mitotic kinesin eg5 in complex with mg-adp and n-(3-aminopropyl)-n-((3-benzyl-5-chloro-4-oxo-3,4-dihydropyrrolo[2,1-f][1,2,4]triazin-2-yl)(cyclopropyl)methyl)-4-methylbenzamide  
Authors : Sheriff, S.  
Deposited on : 2006-04-05  
Resolution : 2.30 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

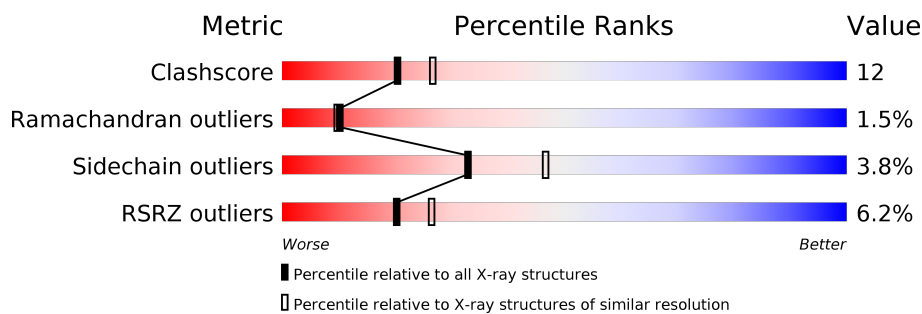
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	368	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	368	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>••</div> <div>13%</div> </div> </div>
1	D	368	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	368	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>•</div> <div>12%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10443 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.

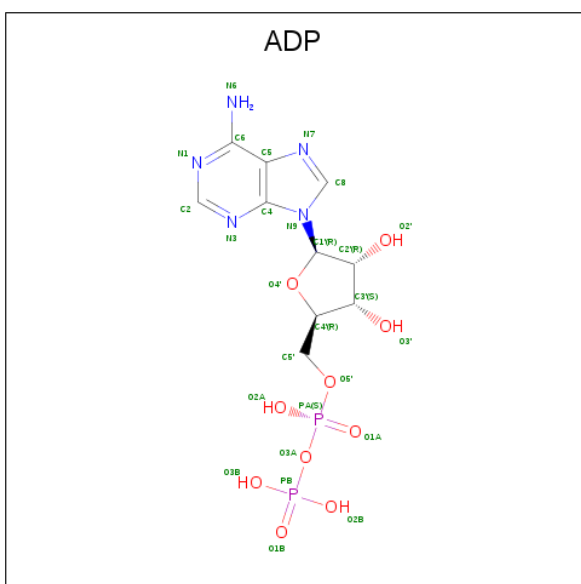
- Molecule 1 is a protein called KINESIN-RELATED MOTOR PROTEIN EG5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	1
			2505	1570	435	490	10			
1	B	321	Total	C	N	O	S	0	0	1
			2467	1550	427	480	10			
1	D	325	Total	C	N	O	S	0	0	1
			2483	1561	432	480	10			
1	E	323	Total	C	N	O	S	0	0	1
			2492	1563	436	483	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		

- Molecule 3 is N-(3-AMINOPROPYL)-N-[(R)-(3-BENZYL-5-CHLORO-4-OXO-3,4-DIHYDROPIRROLO[2,1-F][1,2,4]TRIAZIN-2-YL)(CYCLOPROPYL)METHYL]-4-METHYLBENZAMIDE (three-letter code: 2AZ) (formula: C<sub>28</sub>H<sub>30</sub>ClN<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

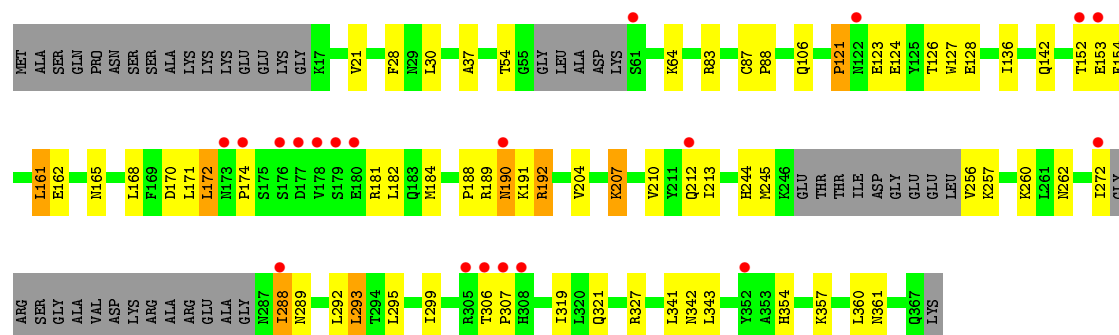
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	69	Total	O	0	0
			69	69		
5	B	44	Total	O	0	0
			44	44		
5	D	55	Total	O	0	0
			55	55		
5	E	68	Total	O	0	0
			68	68		



- Molecule 1: KINESIN-RELATED MOTOR PROTEIN EG5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.70Å 112.60Å 108.10Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	49.86 – 2.30 49.85 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.86-2.30) 96.3 (49.85-2.31)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.95 (at 2.32Å)	Xtriage
Refinement program	CNS, CNX 2005	Depositor
R, $R_{free}$	0.230 , 0.269 0.228 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 17.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.002 for -h,-l,-k 0.000 for -h,l,k 0.167 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 28.25 % 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 1.9059e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MG, 2AZ, ADP

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	0.31	0/2542	0.49	0/3447
1	B	0.31	0/2504	0.49	0/3394
1	D	0.32	0/2520	0.50	0/3416
1	E	0.32	0/2529	0.50	0/3427
All	All	0.31	0/10095	0.50	0/13684

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	D	0	1
1	E	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	GLU	Peptide
1	B	123	GLU	Peptide
1	B	124	GLU	Peptide
1	D	124	GLU	Peptide
1	E	124	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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	2505	0	2460	69	0
1	B	2467	0	2446	62	0
1	D	2483	0	2460	64	0
1	E	2492	0	2470	59	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
3	A	36	0	30	1	0
3	B	36	0	30	1	0
3	D	36	0	30	0	0
3	E	36	0	30	1	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	2	0
5	A	69	0	0	2	0
5	B	44	0	0	0	0
5	D	55	0	0	1	0
5	E	68	0	0	5	0
All	All	10443	0	10004	251	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 12.

The worst 5 of 251 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:A:152:THR:HG22	1:A:153:GLU:H	1.19	1.08
1:B:152:THR:HG22	1:B:153:GLU:H	1.20	1.07
1:E:152:THR:HG22	1:E:153:GLU:H	1.20	1.04
1:D:152:THR:HG22	1:D:153:GLU:H	1.20	1.04
1:D:60:LYS:HA	1:D:61:SER:CB	1.88	1.03

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	320/368 (87%)	306 (96%)	7 (2%)	7 (2%)	6	5
1	B	315/368 (86%)	303 (96%)	7 (2%)	5 (2%)	9	9
1	D	317/368 (86%)	304 (96%)	8 (2%)	5 (2%)	9	9
1	E	315/368 (86%)	304 (96%)	9 (3%)	2 (1%)	25	31
All	All	1267/1472 (86%)	1217 (96%)	31 (2%)	19 (2%)	10	10

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	62	SER
1	B	60	LYS
1	B	62	SER
1	B	191	LYS

### 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	274/322 (85%)	265 (97%)	9 (3%)	38	53
1	B	271/322 (84%)	259 (96%)	12 (4%)	28	39
1	D	272/322 (84%)	263 (97%)	9 (3%)	38	53
1	E	275/322 (85%)	264 (96%)	11 (4%)	31	44
All	All	1092/1288 (85%)	1051 (96%)	41 (4%)	33	47

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	292	LEU
1	D	30	LEU
1	E	288	ILE
1	B	293	LEU
1	B	343	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	GLN
1	D	205	HIS
1	E	321	GLN
1	B	342	ASN
1	D	190	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 ⓘ

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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
4	ADP	D	372	2	24,29,29	1.32	2 (8%)	29,45,45	1.94	5 (17%)
4	ADP	B	372	2	24,29,29	1.42	3 (12%)	29,45,45	2.02	4 (13%)
3	2AZ	B	371	-	35,40,40	1.73	7 (20%)	39,57,57	1.47	6 (15%)
4	ADP	E	372	2	24,29,29	1.39	3 (12%)	29,45,45	1.89	4 (13%)
3	2AZ	E	371	-	35,40,40	1.64	7 (20%)	39,57,57	1.47	5 (12%)
4	ADP	A	372	2	24,29,29	1.49	3 (12%)	29,45,45	2.02	4 (13%)
3	2AZ	A	371	-	35,40,40	1.78	8 (22%)	39,57,57	1.49	4 (10%)
3	2AZ	D	371	-	35,40,40	1.68	6 (17%)	39,57,57	1.48	5 (12%)

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	ADP	D	372	2	-	2/12/32/32	0/3/3/3
4	ADP	B	372	2	-	2/12/32/32	0/3/3/3
3	2AZ	B	371	-	-	4/24/30/30	0/5/5/5
4	ADP	E	372	2	-	2/12/32/32	0/3/3/3
3	2AZ	E	371	-	-	5/24/30/30	0/5/5/5
4	ADP	A	372	2	-	3/12/32/32	0/3/3/3
3	2AZ	A	371	-	-	5/24/30/30	0/5/5/5
3	2AZ	D	371	-	-	5/24/30/30	0/5/5/5

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	371	2AZ	C11-C9	4.75	1.57	1.50
3	B	371	2AZ	C11-C9	4.70	1.57	1.50
3	A	371	2AZ	C11-N12	4.64	1.38	1.31
3	D	371	2AZ	C11-N12	4.42	1.37	1.31
3	B	371	2AZ	C11-N12	4.24	1.37	1.31

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	372	ADP	N3-C2-N1	-7.70	116.65	128.68
4	B	372	ADP	N3-C2-N1	-7.47	117.00	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	372	ADP	N3-C2-N1	-7.12	117.54	128.68
4	E	372	ADP	N3-C2-N1	-6.87	117.94	128.68
3	B	371	2AZ	C14-C21-N22	-5.05	115.11	120.30

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

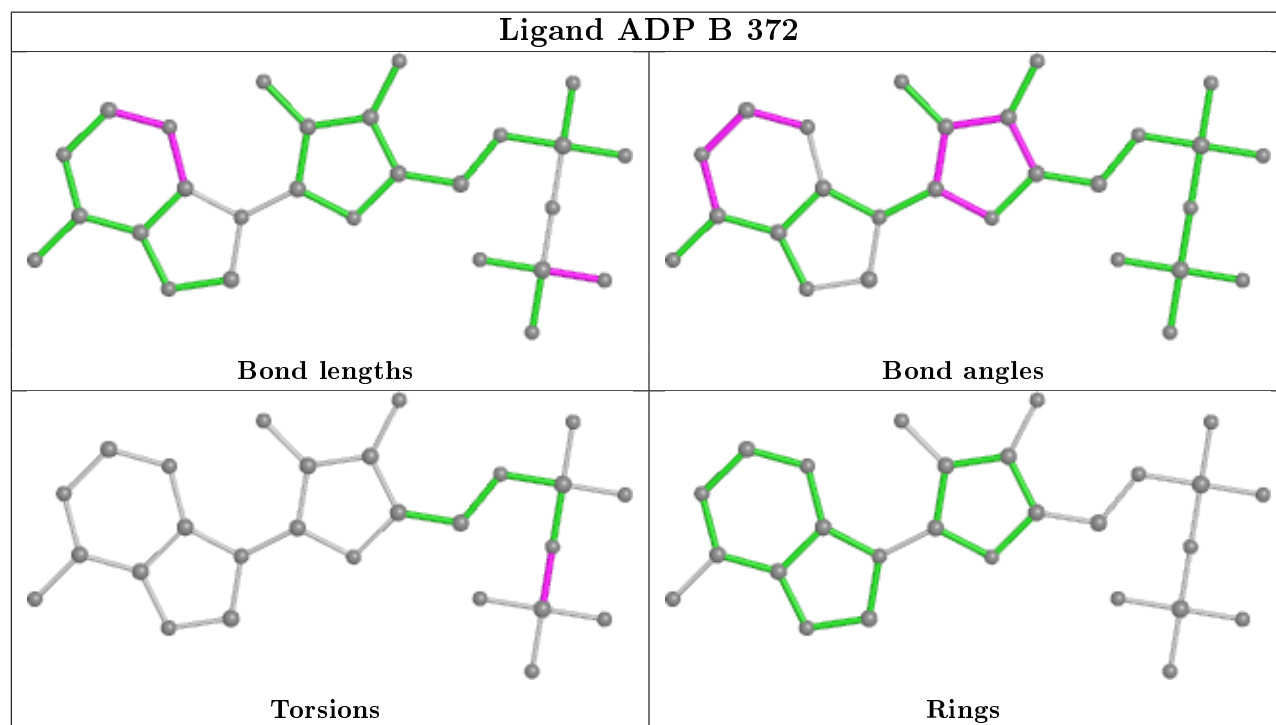
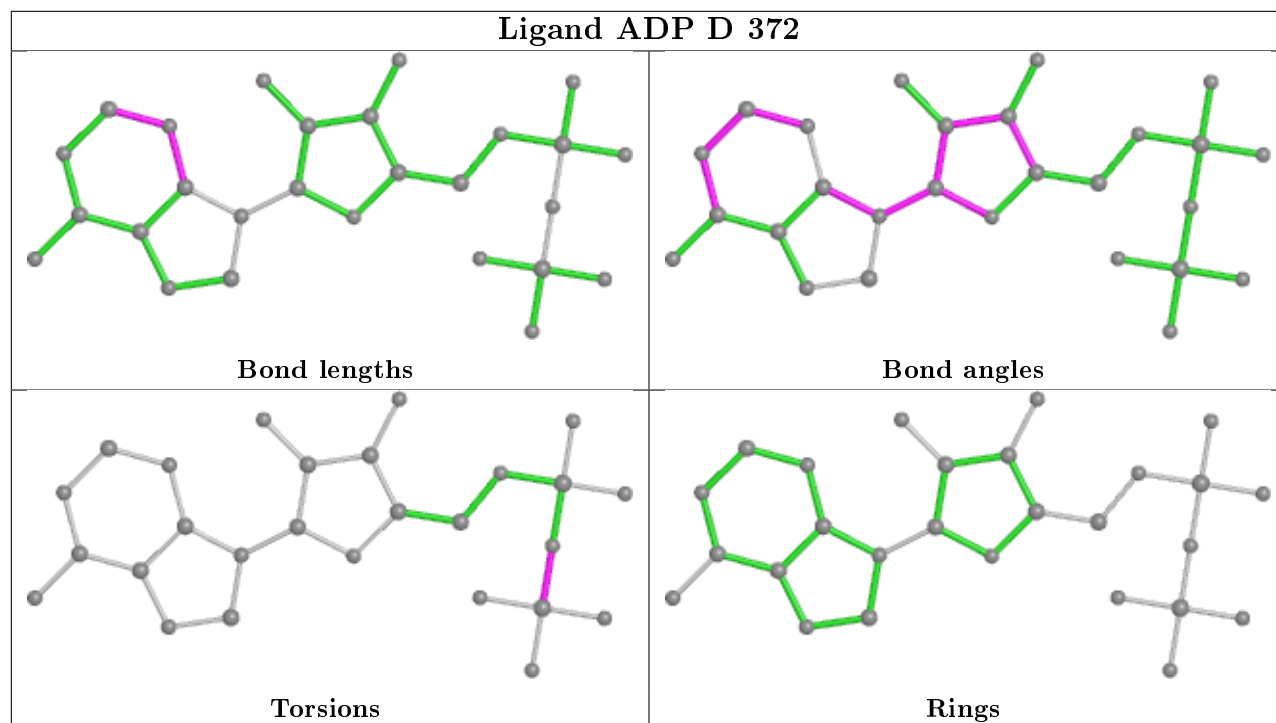
Mol	Chain	Res	Type	Atoms
4	D	372	ADP	PA-O3A-PB-O2B
4	D	372	ADP	PA-O3A-PB-O3B
4	B	372	ADP	PA-O3A-PB-O2B
4	B	372	ADP	PA-O3A-PB-O3B
3	E	371	2AZ	C42-C39-N38-C51

There are no ring outliers.

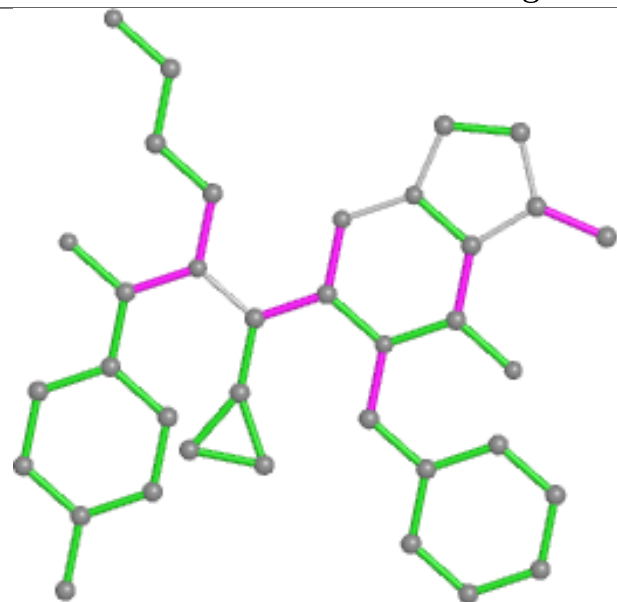
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	372	ADP	1	0
4	B	372	ADP	1	0
3	B	371	2AZ	1	0
4	E	372	ADP	2	0
3	E	371	2AZ	1	0
4	A	372	ADP	1	0
3	A	371	2AZ	1	0

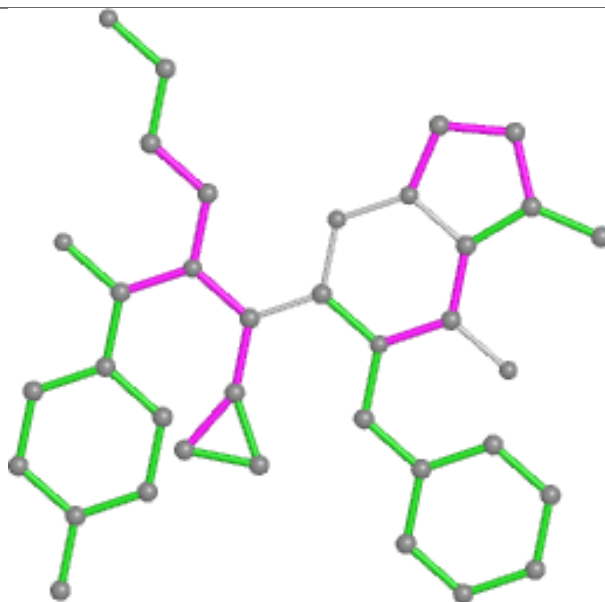
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



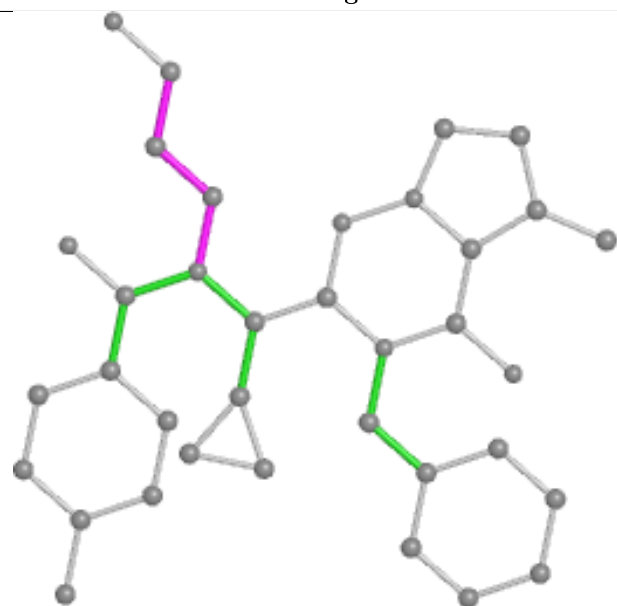
## Ligand 2AZ B 371



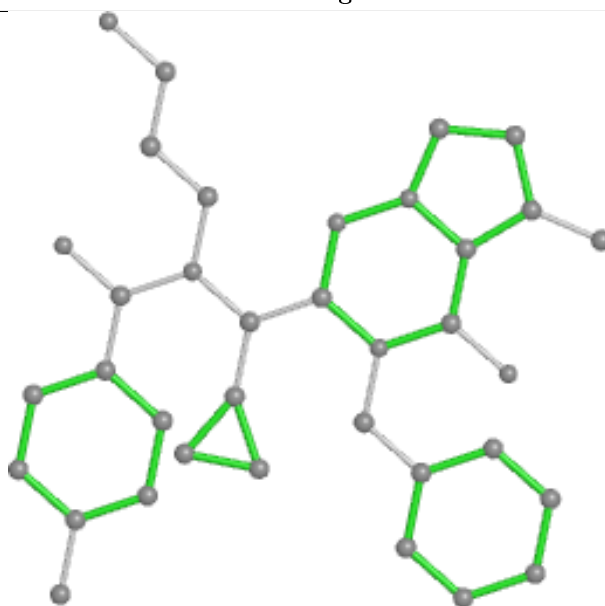
Bond lengths



Bond angles

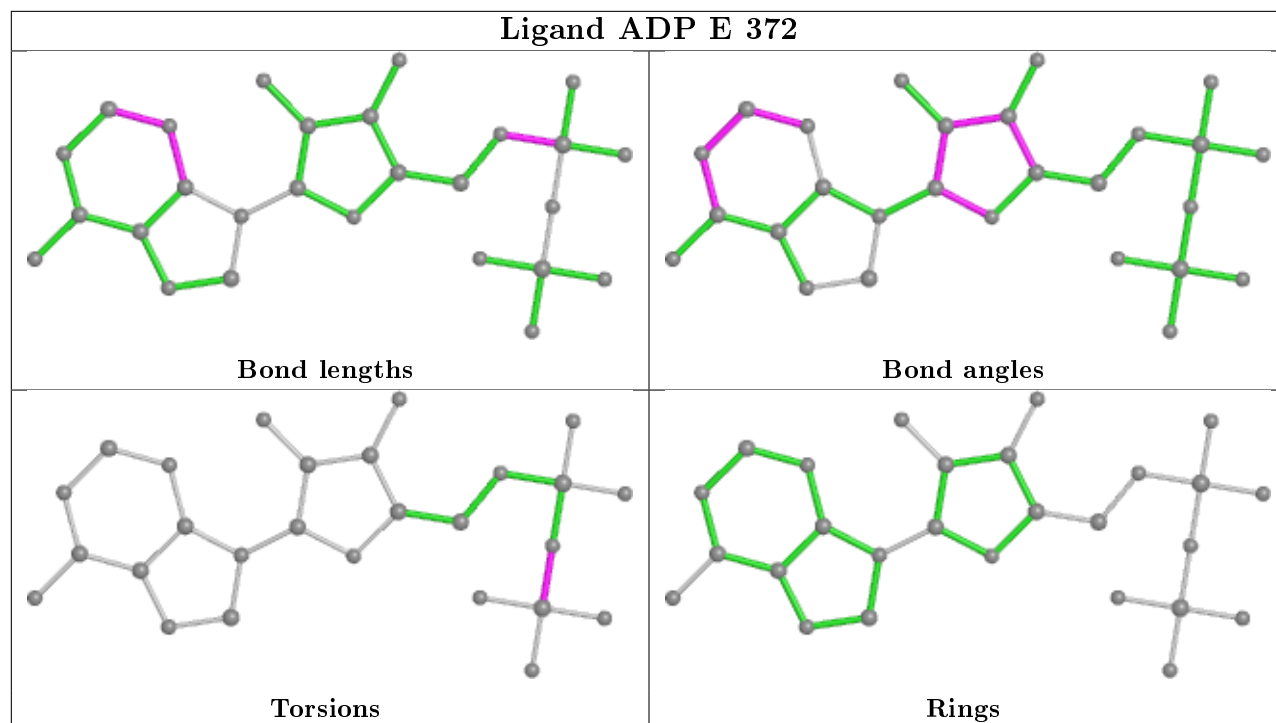


Torsions

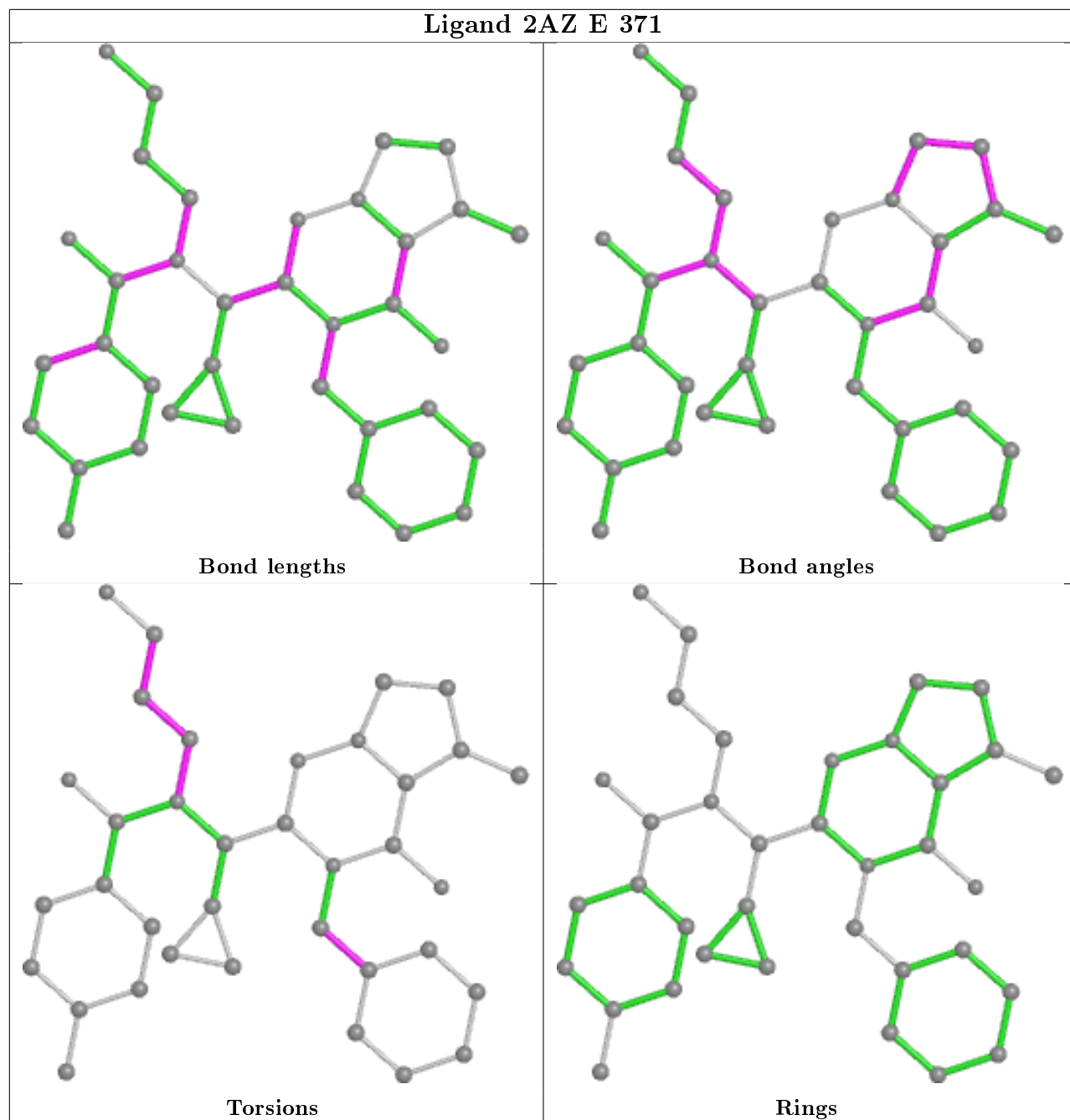


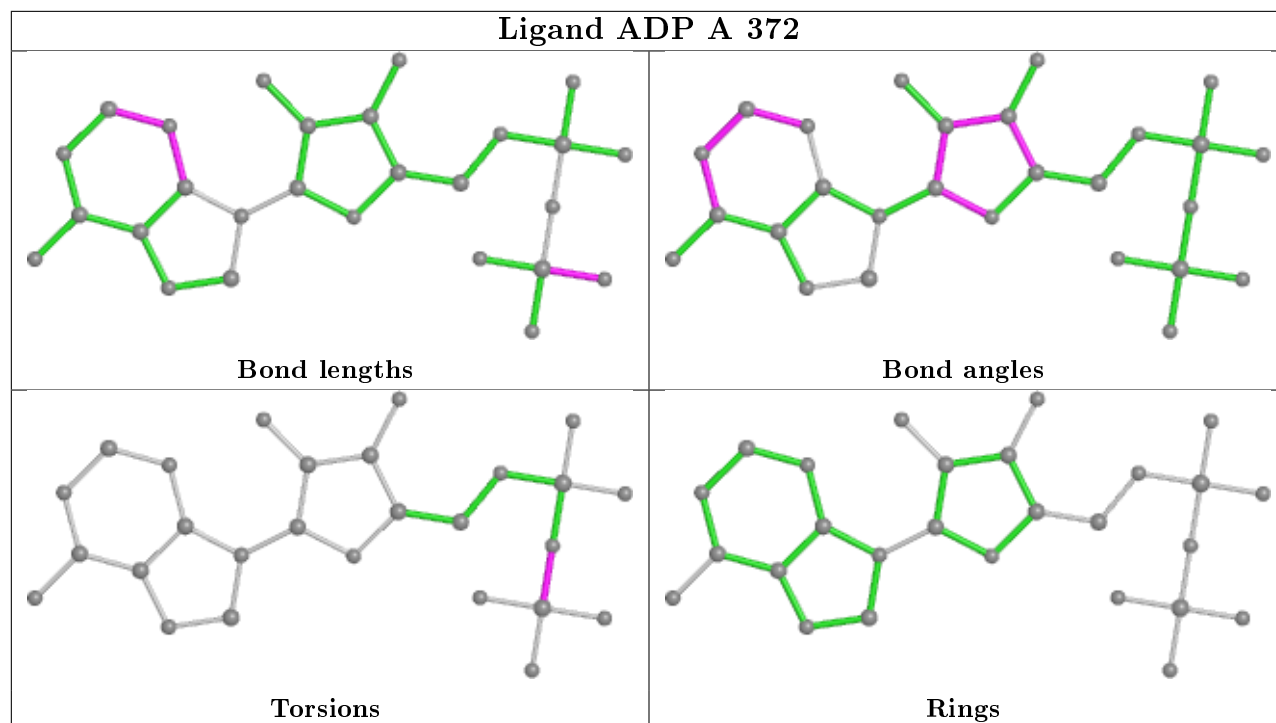
Rings



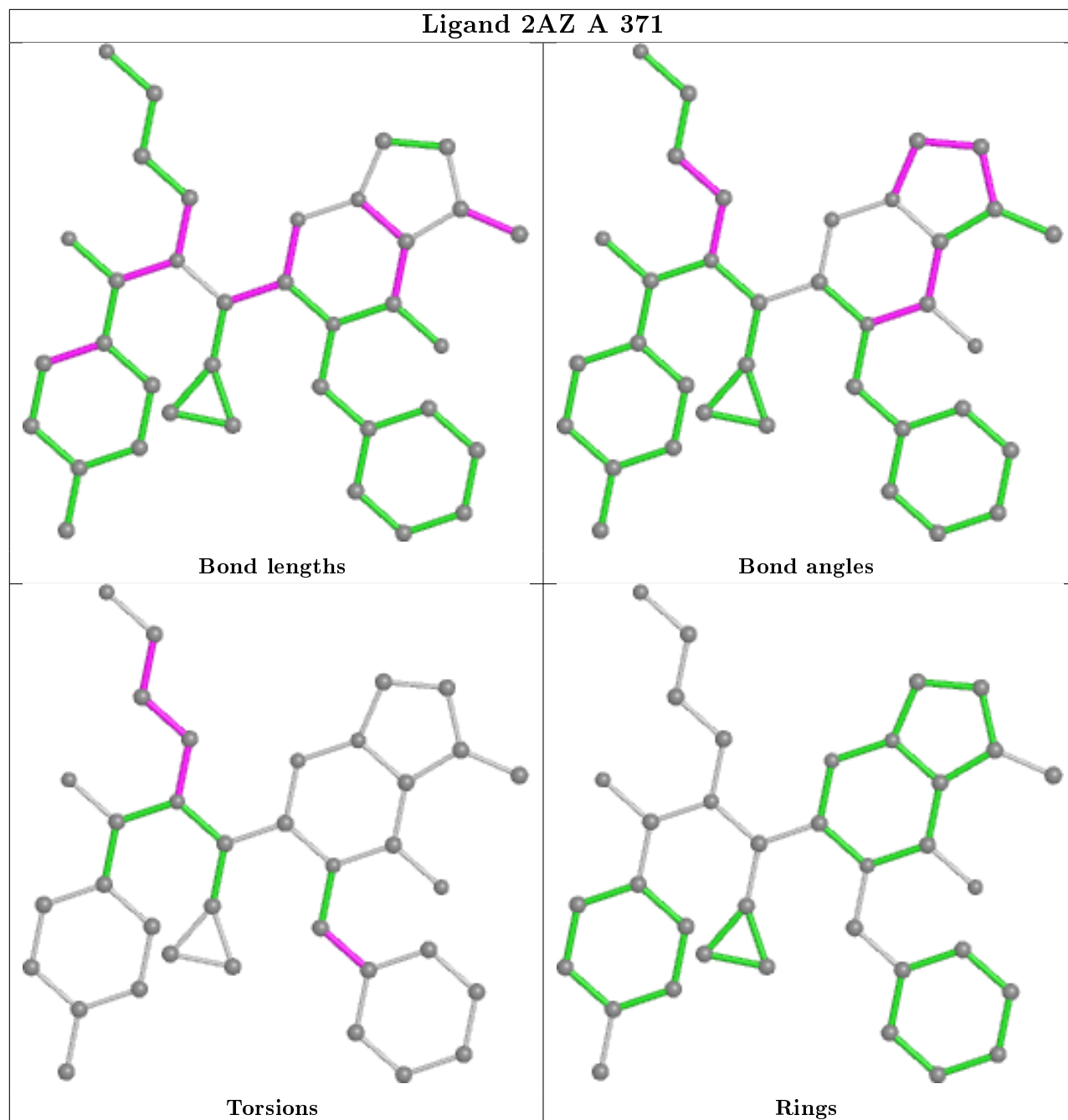


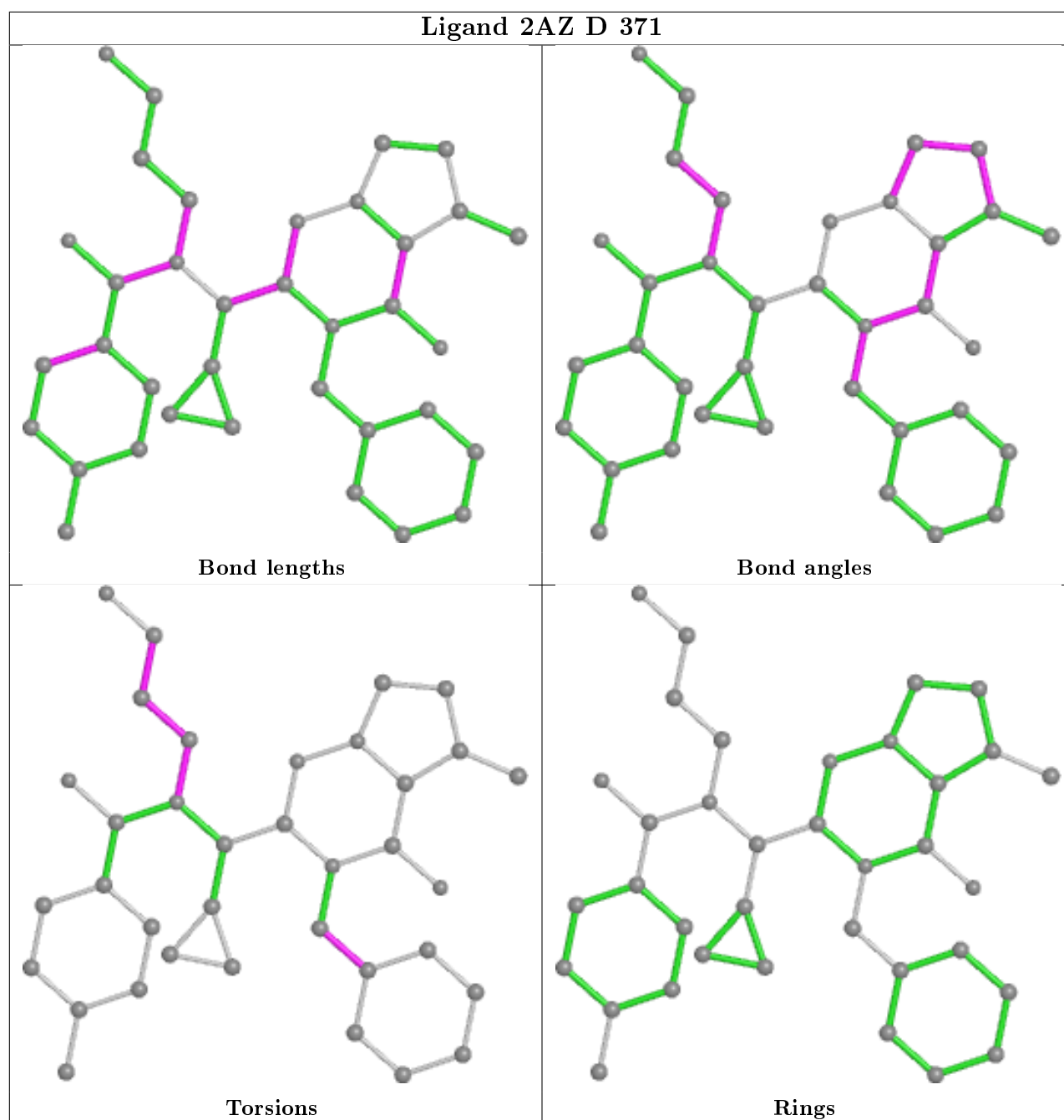
## Ligand 2AZ E 371





## Ligand 2AZ A 371





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	328/368 (89%)	0.14	17 (5%) 27 34	13, 30, 61, 70	0
1	B	321/368 (87%)	0.16	21 (6%) 18 24	12, 32, 60, 72	0
1	D	325/368 (88%)	0.14	22 (6%) 17 22	13, 31, 61, 73	0
1	E	323/368 (87%)	0.25	20 (6%) 20 26	13, 30, 57, 69	0
All	All	1297/1472 (88%)	0.17	80 (6%) 20 26	12, 31, 60, 73	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	178	VAL	11.7
1	D	178	VAL	10.3
1	D	175	SER	8.3
1	B	58	ALA	7.3
1	D	179	SER	5.9

### 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](#)

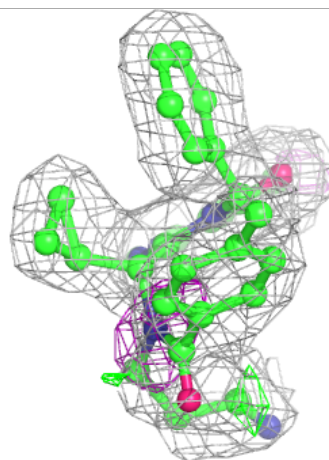
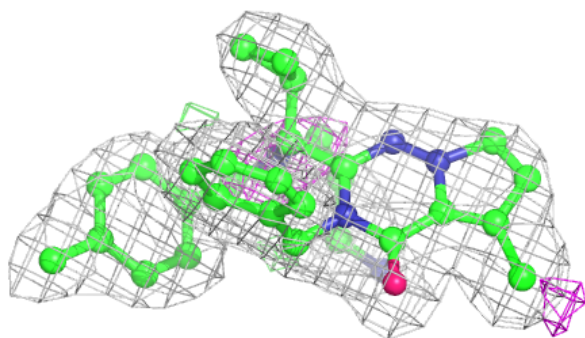
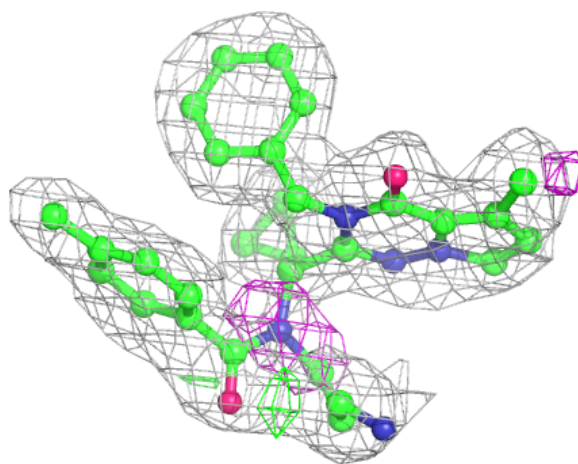
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	370	1/1	0.84	0.14	41,41,41,41	0
2	MG	B	370	1/1	0.88	0.13	51,51,51,51	0
3	2AZ	B	371	36/36	0.90	0.15	18,25,34,34	0
2	MG	E	370	1/1	0.91	0.08	39,39,39,39	0
3	2AZ	A	371	36/36	0.91	0.14	19,25,35,36	0
3	2AZ	E	371	36/36	0.92	0.14	16,23,33,33	0
3	2AZ	D	371	36/36	0.92	0.15	16,22,34,35	0
2	MG	A	370	1/1	0.94	0.12	41,41,41,41	0
2	MG	A	369	1/1	0.97	0.14	19,19,19,19	0
4	ADP	B	372	27/27	0.98	0.10	14,15,18,20	0
4	ADP	E	372	27/27	0.98	0.10	12,16,18,20	0
2	MG	E	369	1/1	0.98	0.14	22,22,22,22	0
2	MG	D	369	1/1	0.98	0.16	24,24,24,24	0
4	ADP	D	372	27/27	0.98	0.11	13,15,16,21	0
2	MG	B	369	1/1	0.98	0.16	23,23,23,23	0
4	ADP	A	372	27/27	0.98	0.10	11,14,17,19	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 2AZ B 371:**

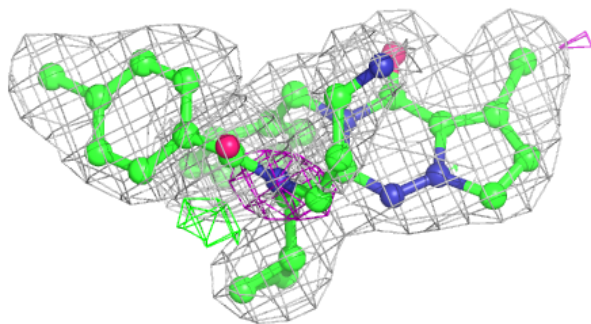
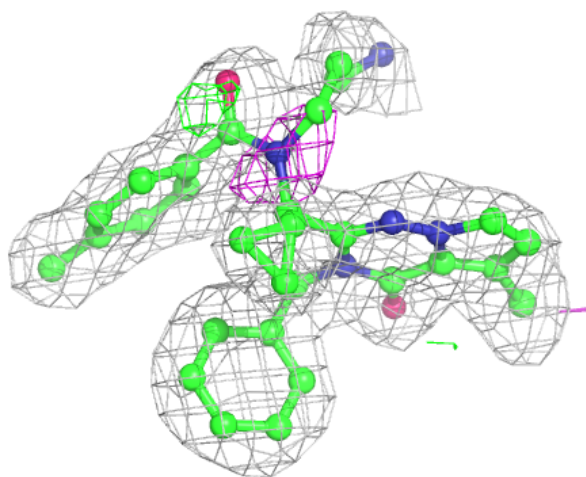
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





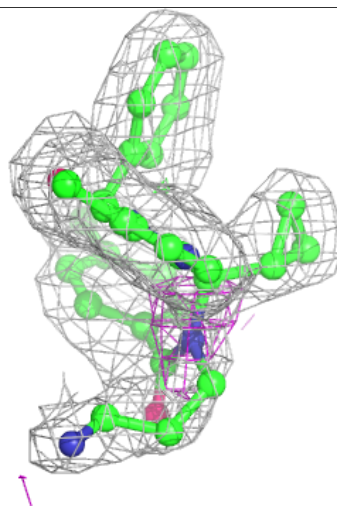
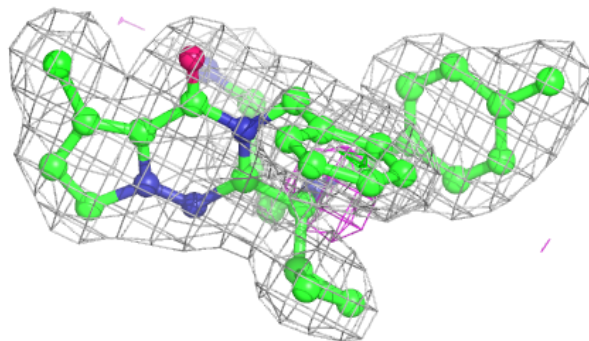
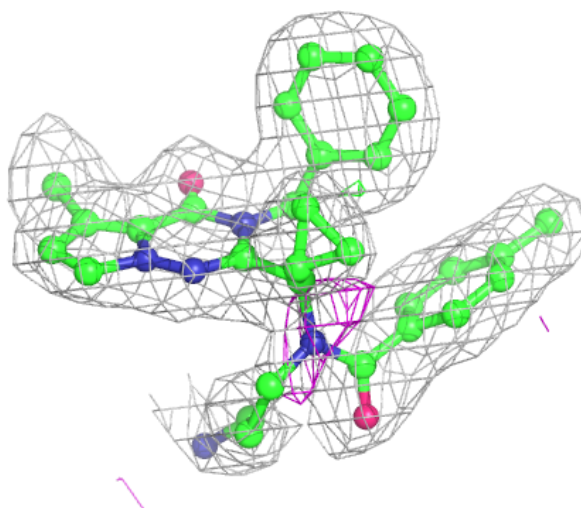
**Electron density around 2AZ A 371:**

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



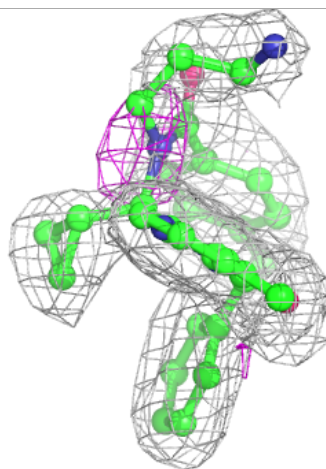
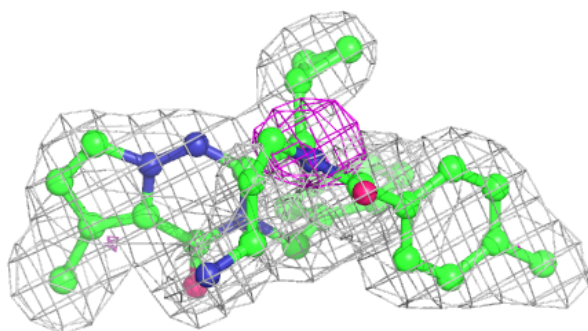
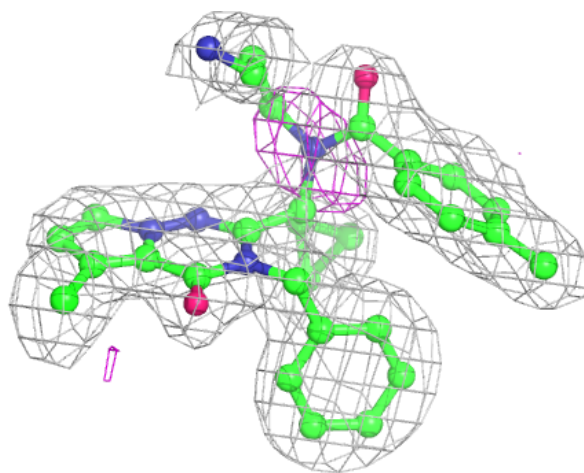
**Electron density around 2AZ E 371:**

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



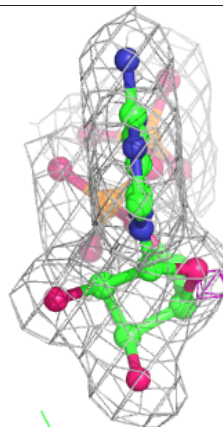
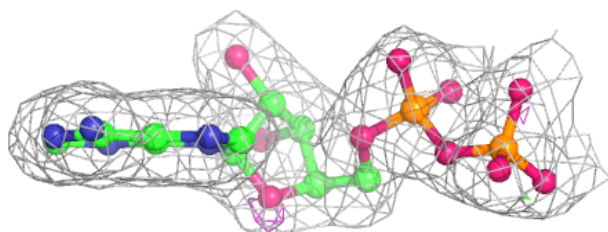
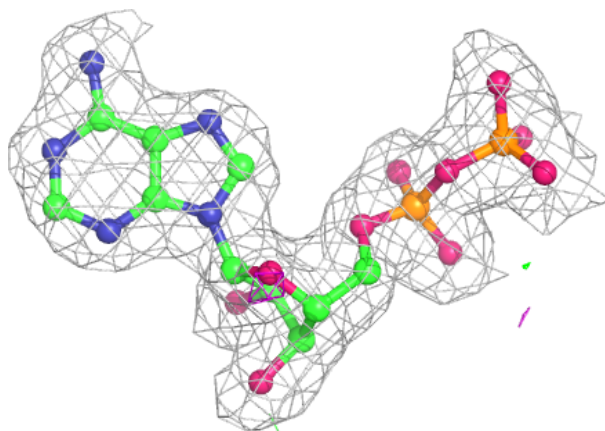
**Electron density around 2AZ D 371:**

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



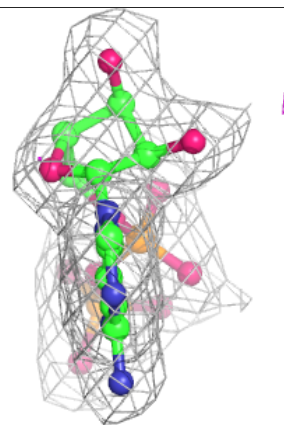
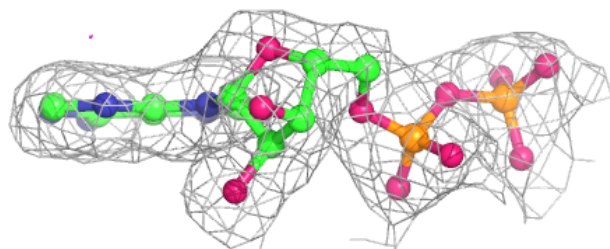
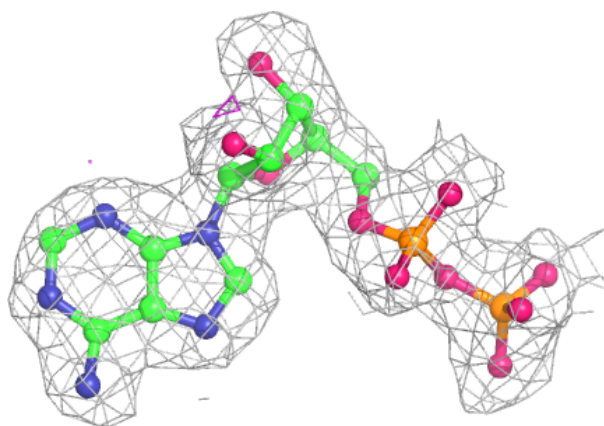
**Electron density around ADP B 372:**

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

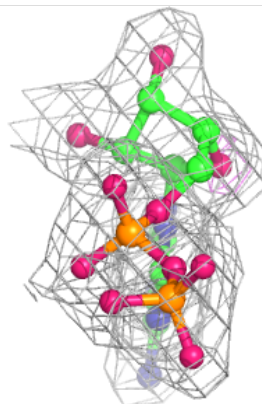
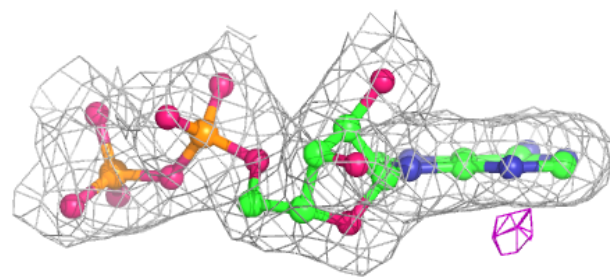
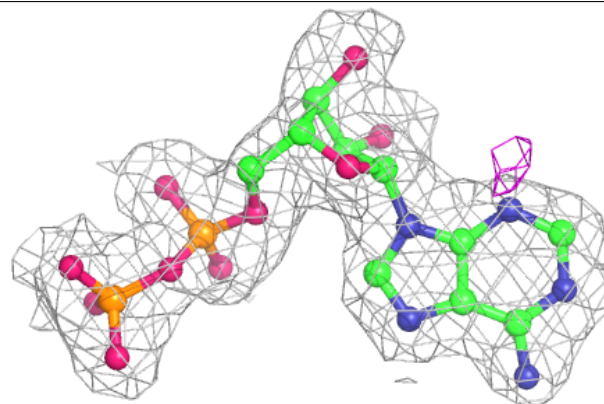


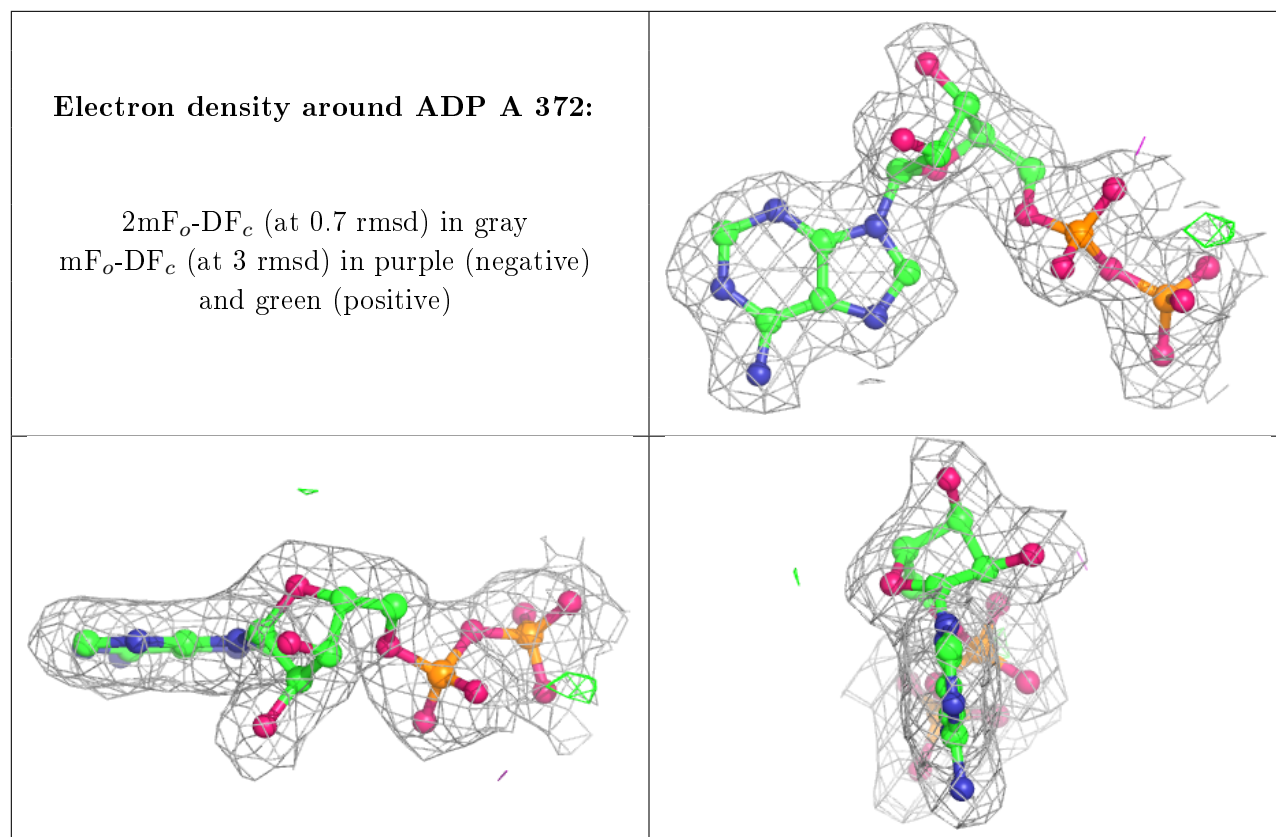
**Electron density around ADP E 372:**

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

**Electron density around ADP D 372:**

$2mF_o-DF_c$  (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.