



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:40 AM UTC

PDB ID : 1RFQ / pdb\_00001rfq  
Title : Actin Crystal Dynamics: Structural Implications for F-actin Nucleation, Polymerization and Branching Mediated by the Anti-parallel Dimer  
Authors : Reutzel, R.; Yoshioka, C.; Govindasamy, L.; Yarmola, E.G.; Agbandje-McKenna, M.; Bubb, M.R.; McKenna, R.  
Deposited on : 2003-11-10  
Resolution : 3.00 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

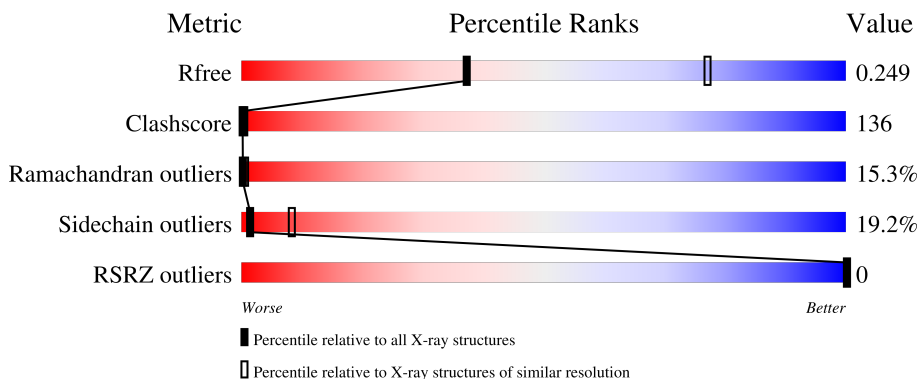
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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  $\geq 3$ , 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	375	
1	B	375	

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	ATP	A	376	-	-	X	-
3	ATP	B	386	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5824 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.

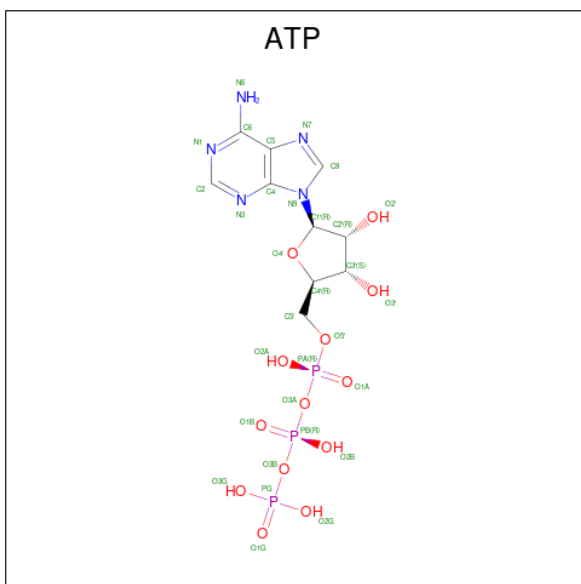
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	Total 2829	C 1794	N 476	O 540	S 19	0	0	0
1	B	361	Total 2829	C 1794	N 476	O 540	S 19	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

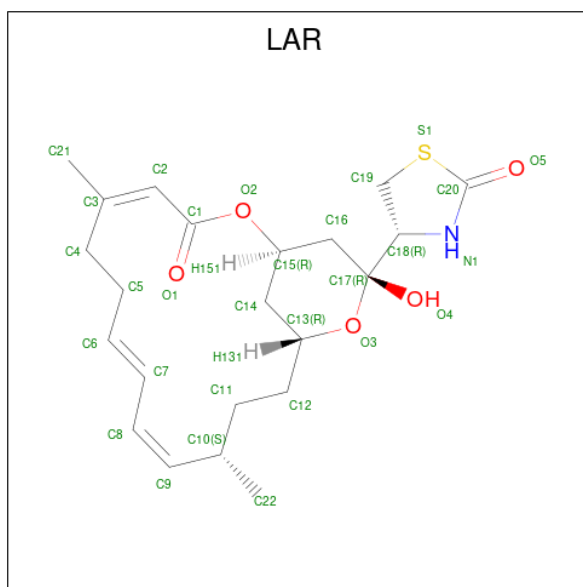
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0
2	B	1	Total 1	Mg 1	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is LATRUNCULIN A (CCD ID: LAR) (formula:  $C_{22}H_{31}NO_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			29	22	1	5	1		
4	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	22	Total	O	0	0
			22	22		



D863	T803	G182
E564	T804	R183
A365	M305	D184
G366	Y306	L185
P367	P307	Q246
S368	G308	V247
I369	I309	T248
V370	A310	Y188
H371	D311	L189
K372	R312	M190
K373	M313	E253
G374	Q314	L192
F375	K315	L193
	E316	T194
	I317	E195
	T318	R196
	A319	G197
	L320	Y198
	A321	S199
	P322	L261
	S323	F262
	T324	Q263
	M325	P264
	K326	S265
	I327	F266
	K328	I267
	I329	G268
	L330	M269
	A331	E270
	P332	S271
	P333	A272
	E334	G273
	R335	I274
	K336	R275
	Y337	E276
	S338	T277
	V339	T278
	M340	Y279
	I341	M280
	G342	S281
	G343	I282
	S344	M283
	I345	K284
	L346	C285
	A347	D286
	S348	I287
	L349	D288
	S350	I289
	T351	R290
	F352	K291
	G353	D292
	Q354	L293
	M355	Y294
	W356	A295
	I357	N296
	T358	M297
	K359	V298
	Q360	M299
	E361	S300
	Y362	G301
		G302
		L242

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.50Å 101.50Å 104.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 98.6 (50.00-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.193 , 0.261 0.205 , 0.249	Depositor DCC
$R_{free}$ test set	2858 reflections (13.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.2	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 205.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.089 for -h,-l,-k 0.088 for -h,l,k 0.094 for l,-k,h 0.096 for -l,-k,-h 0.368 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, LAR

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	0.87	4/2891 (0.1%)	1.49	58/3919 (1.5%)
1	B	0.92	10/2891 (0.3%)	1.48	70/3919 (1.8%)
All	All	0.89	14/5782 (0.2%)	1.48	128/7838 (1.6%)

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	4
1	B	0	1
All	All	0	5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	SER	N-CA	25.57	1.79	1.46
1	B	200	PHE	N-CA	18.71	1.70	1.46
1	B	25	ASP	C-N	-9.97	1.20	1.33
1	A	298	VAL	CA-C	-8.89	1.45	1.52
1	B	26	ALA	C-N	-8.26	1.26	1.33

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	PHE	CA-CB-CG	-21.42	92.38	113.80
1	B	200	PHE	CA-CB-CG	17.30	131.10	113.80
1	A	270	GLU	N-CA-C	-12.84	89.86	109.24
1	A	272	ALA	CA-C-N	-12.80	99.61	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	ALA	C-N-CA	-12.80	99.61	123.03

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	TYR	Sidechain
1	A	234	SER	Mainchain,Peptide
1	A	372	ARG	Mainchain
1	B	91	TYR	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2829	0	2794	726	0
1	B	2829	0	2794	876	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	9	0
3	B	31	0	12	10	0
4	A	29	0	31	2	0
4	B	29	0	31	10	0
5	A	22	0	0	6	0
5	B	22	0	0	6	0
All	All	5824	0	5674	1562	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 136.

The worst 5 of 1562 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:373:LYS:NZ	1:B:373:LYS:CA	1.67	1.54
1:B:200:PHE:N	1:B:200:PHE:CA	1.70	1.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:SER:N	1:A:235:SER:CA	1.79	1.44
1:B:103:THR:O	1:B:356:TRP:CZ3	1.71	1.44
1:B:21:PHE:CB	1:B:24:ASP:OD2	1.65	1.43

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	357/375 (95%)	223 (62%)	84 (24%)	50 (14%)	0	1
1	B	357/375 (95%)	210 (59%)	88 (25%)	59 (16%)	0	0
All	All	714/750 (95%)	433 (61%)	172 (24%)	109 (15%)	0	0

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	TYR
1	A	92	ASN
1	A	99	GLU
1	A	138	ALA
1	A	139	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	A	307/318 (96%)	257 (84%)	50 (16%)	2	12
1	B	307/318 (96%)	239 (78%)	68 (22%)	1	5
All	All	614/636 (96%)	496 (81%)	118 (19%)	1	8

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	ILE
1	B	324	THR
1	B	132	MET
1	B	318	THR
1	B	274	ILE

Sometimes 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	73	HIS
1	B	115	ASN
1	B	354	GLN
1	B	101	HIS
1	B	121	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	LAR	B	387	-	30,31,31	1.29	5 (16%)	32,43,43	1.47	3 (9%)
4	LAR	A	377	-	30,31,31	1.33	4 (13%)	32,43,43	1.56	3 (9%)
3	ATP	B	386	2	32,33,33	2.44	9 (28%)	48,52,52	3.01	14 (29%)
3	ATP	A	376	2	32,33,33	2.19	11 (34%)	48,52,52	2.91	14 (29%)

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	LAR	B	387	-	-	4/23/51/51	0/2/3/3
4	LAR	A	377	-	-	3/23/51/51	0/2/3/3
3	ATP	B	386	2	-	3/22/38/38	0/3/3/3
3	ATP	A	376	2	-	2/22/38/38	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	386	ATP	PB-O3A	8.78	1.69	1.59
3	A	376	ATP	PB-O3A	5.74	1.65	1.59
3	B	386	ATP	O5'-C5'	-4.85	1.26	1.44
3	A	376	ATP	O5'-C5'	-4.72	1.26	1.44
3	B	386	ATP	C5-C6	4.03	1.52	1.41

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	386	ATP	O5'-C5'-C4'	12.25	150.71	108.99
3	A	376	ATP	O5'-C5'-C4'	11.25	147.30	108.99
3	A	376	ATP	O3A-PB-O1B	-7.40	88.44	110.70
3	B	386	ATP	O3A-PB-O1B	-7.28	88.80	110.70
3	B	386	ATP	O5'-PA-O1A	-7.11	80.74	108.94

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

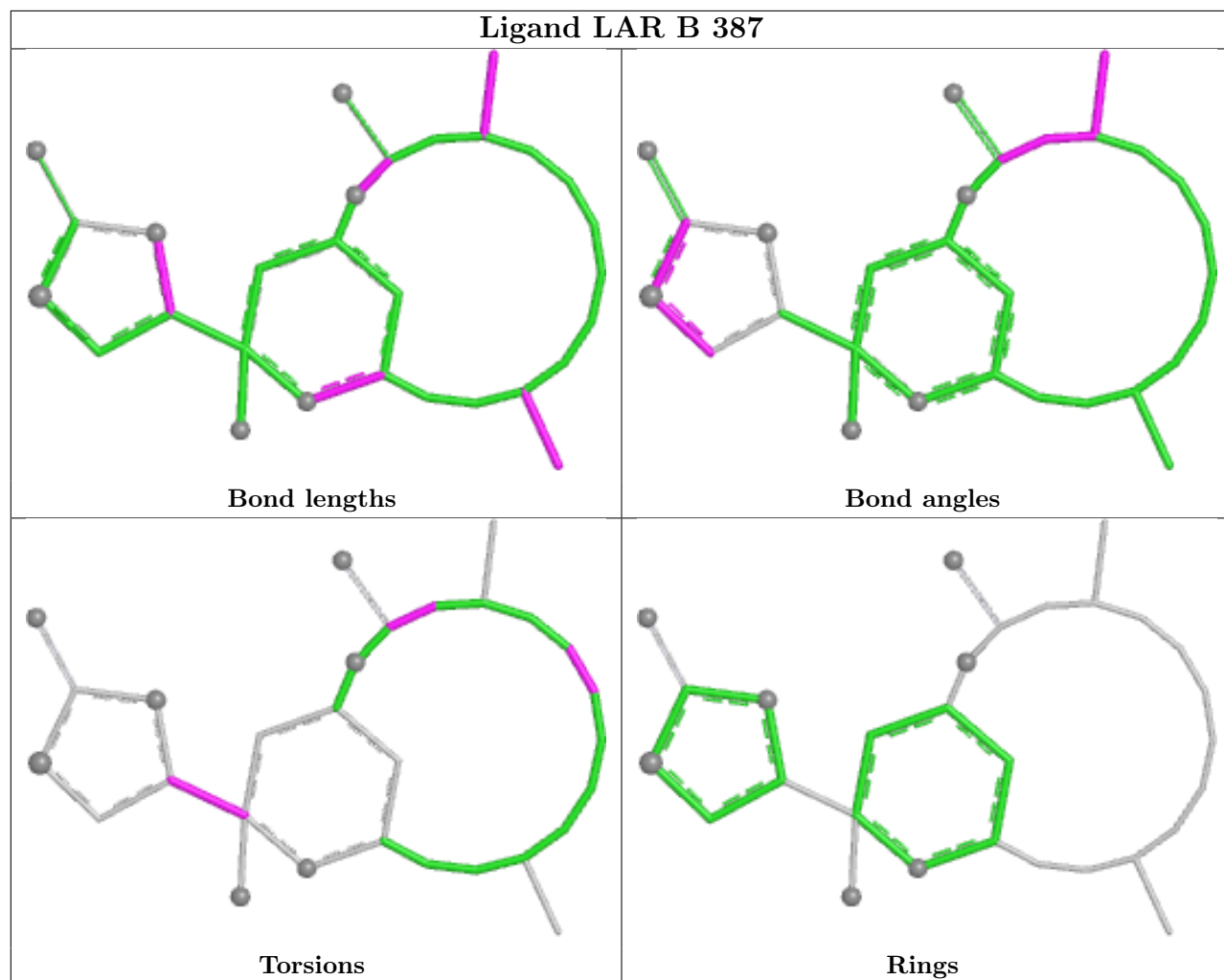
Mol	Chain	Res	Type	Atoms
4	B	387	LAR	O3-C17-C18-C19
3	A	376	ATP	PG-O3B-PB-O2B
3	B	386	ATP	PG-O3B-PB-O2B
4	B	387	LAR	O2-C1-C2-C3
3	B	386	ATP	PA-O3A-PB-O2B

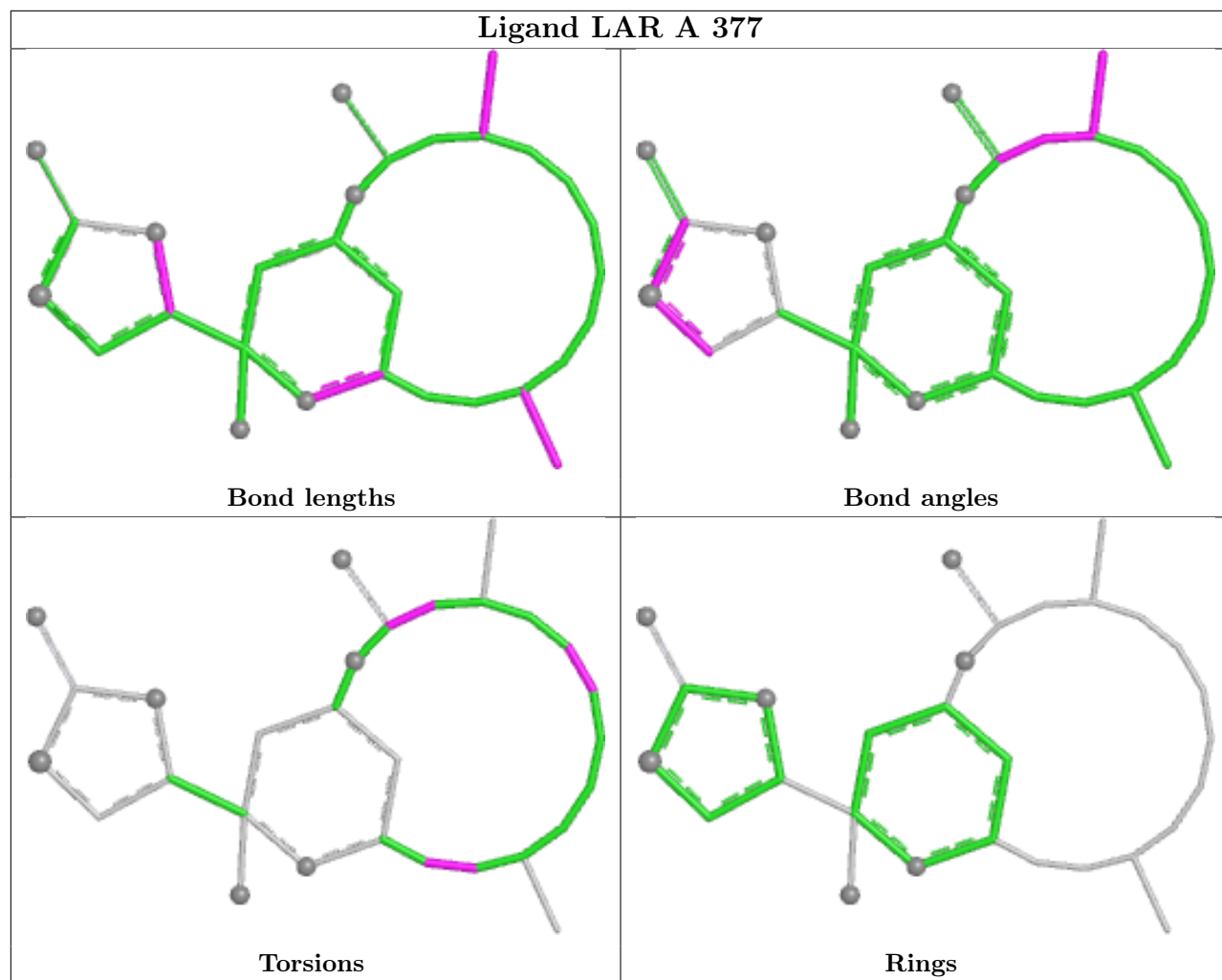
There are no ring outliers.

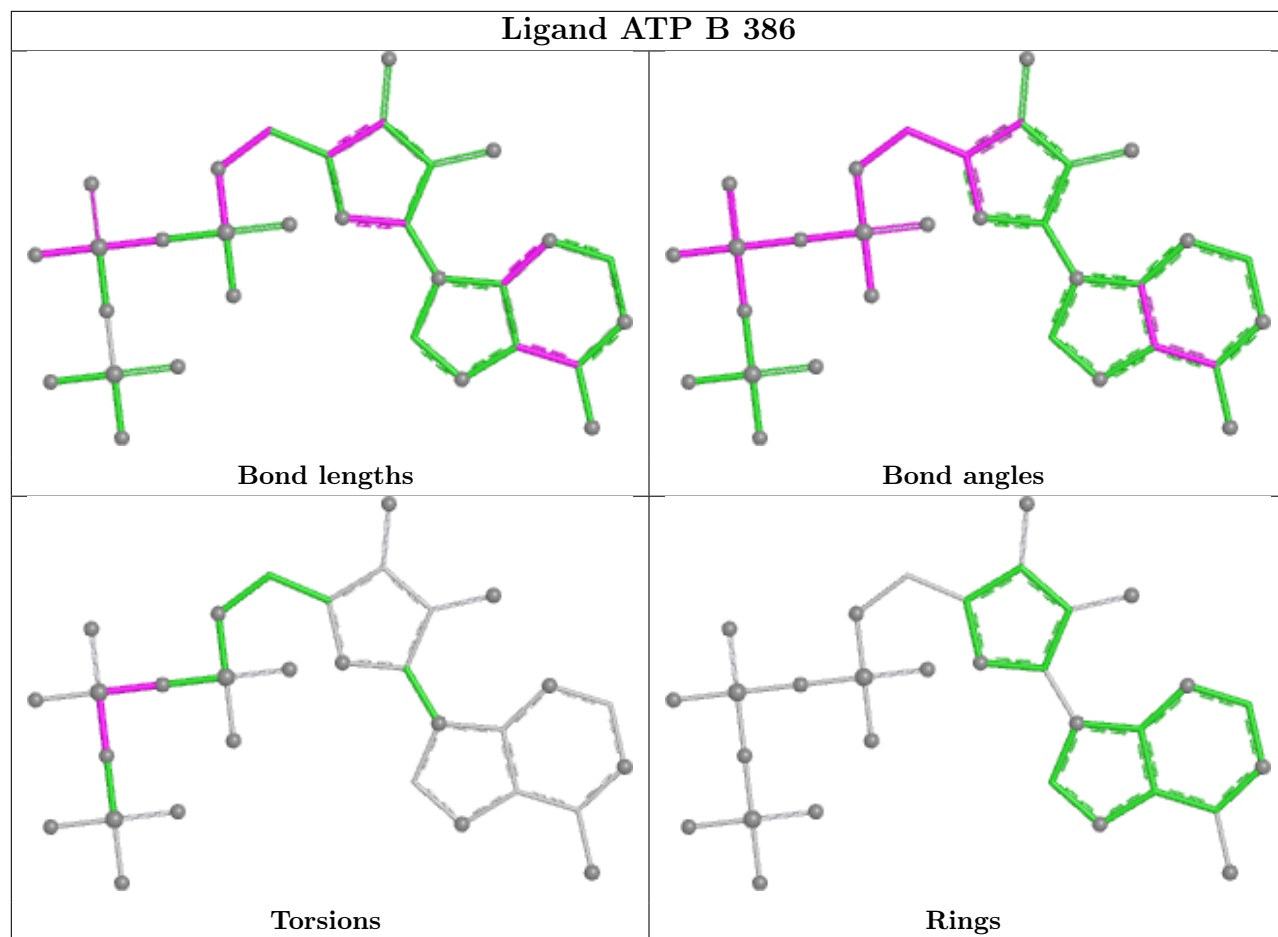
4 monomers are involved in 31 short contacts:

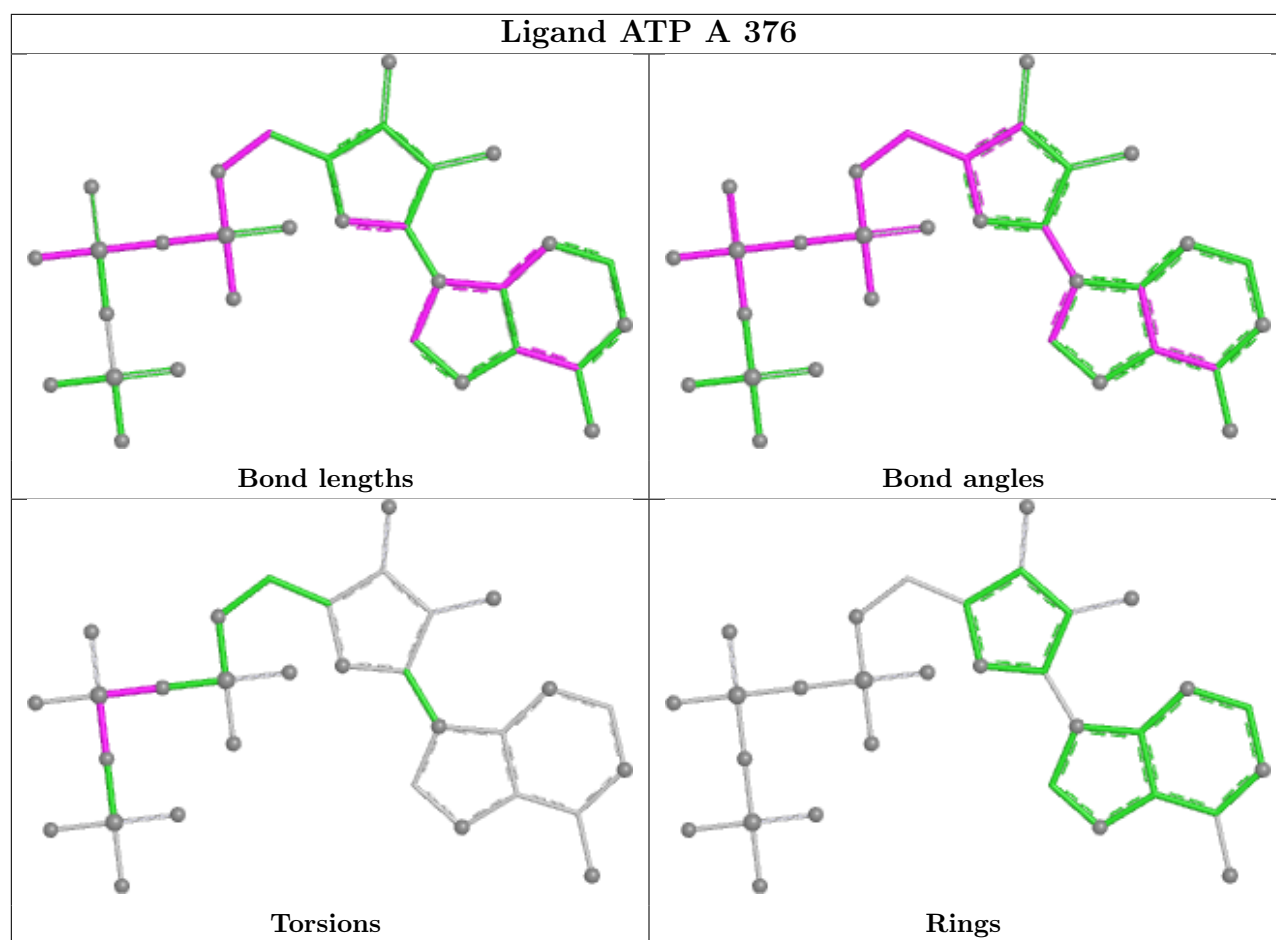
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	387	LAR	10	0
4	A	377	LAR	2	0
3	B	386	ATP	10	0
3	A	376	ATP	9	0

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.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	25:ASP	C	26:ALA	N	1.19

## 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	361/375 (96%)	-1.26	0 100 100	38, 57, 75, 82	0
1	B	361/375 (96%)	-1.12	0 100 100	42, 68, 83, 96	0
All	All	722/750 (96%)	-1.19	0 100 100	38, 63, 80, 96	0

There are no RSRZ outliers to report.

### 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](#)

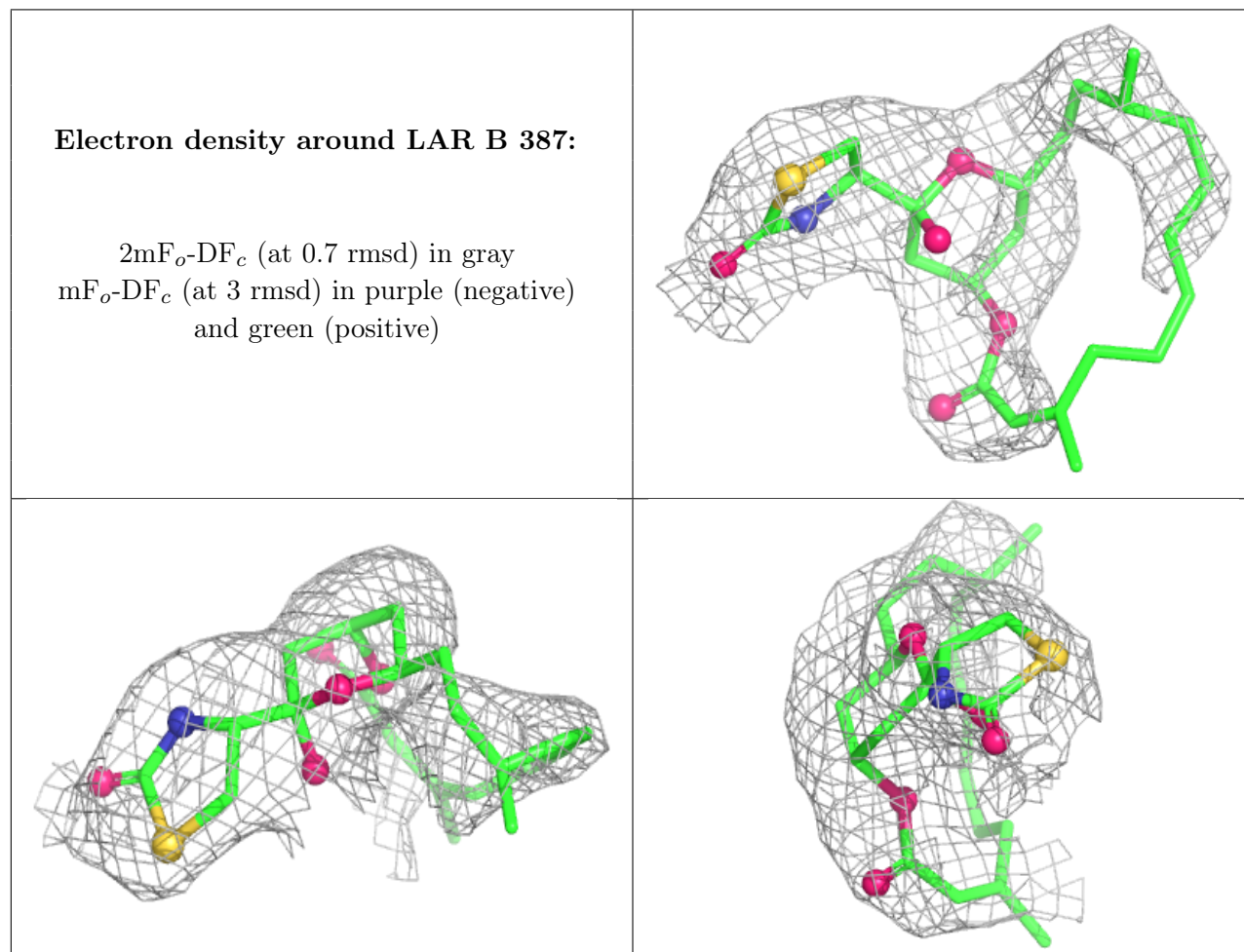
There are no oligosaccharides in this entry.

### 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.

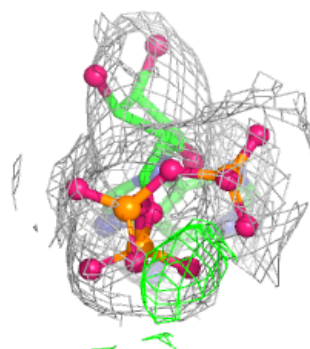
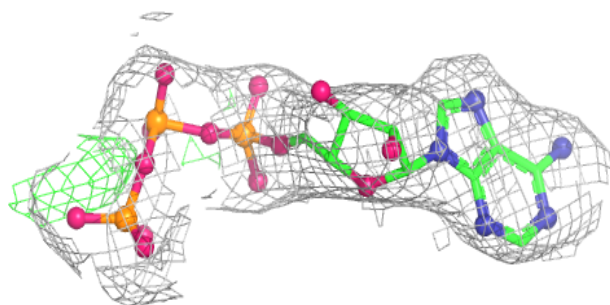
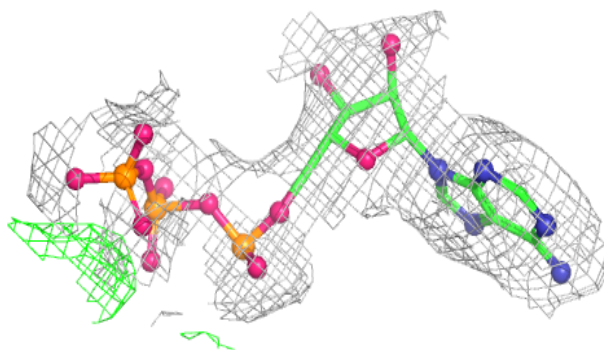
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	LAR	B	387	29/29	0.98	0.07	66,71,78,78	0
2	MG	B	388	1/1	0.99	0.04	42,42,42,42	0
3	ATP	A	376	31/31	0.99	0.03	37,50,55,56	0
3	ATP	B	386	31/31	0.99	0.03	53,57,61,62	0
4	LAR	A	377	29/29	0.99	0.05	61,67,74,75	0
2	MG	A	378	1/1	0.99	0.05	36,36,36,36	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.

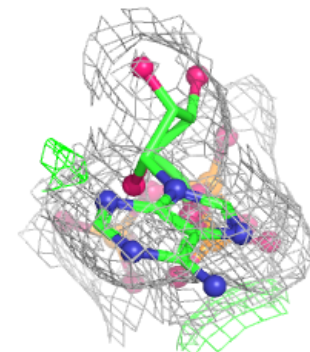
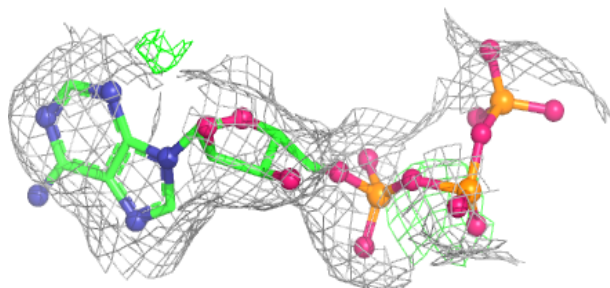
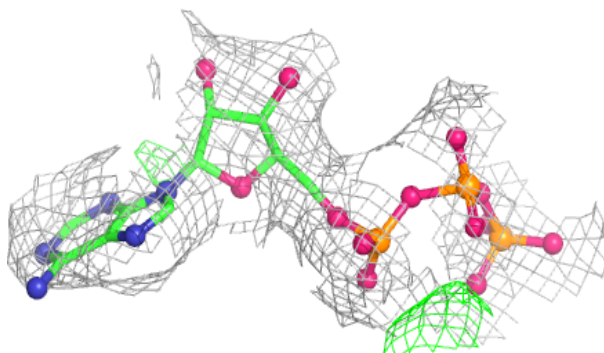


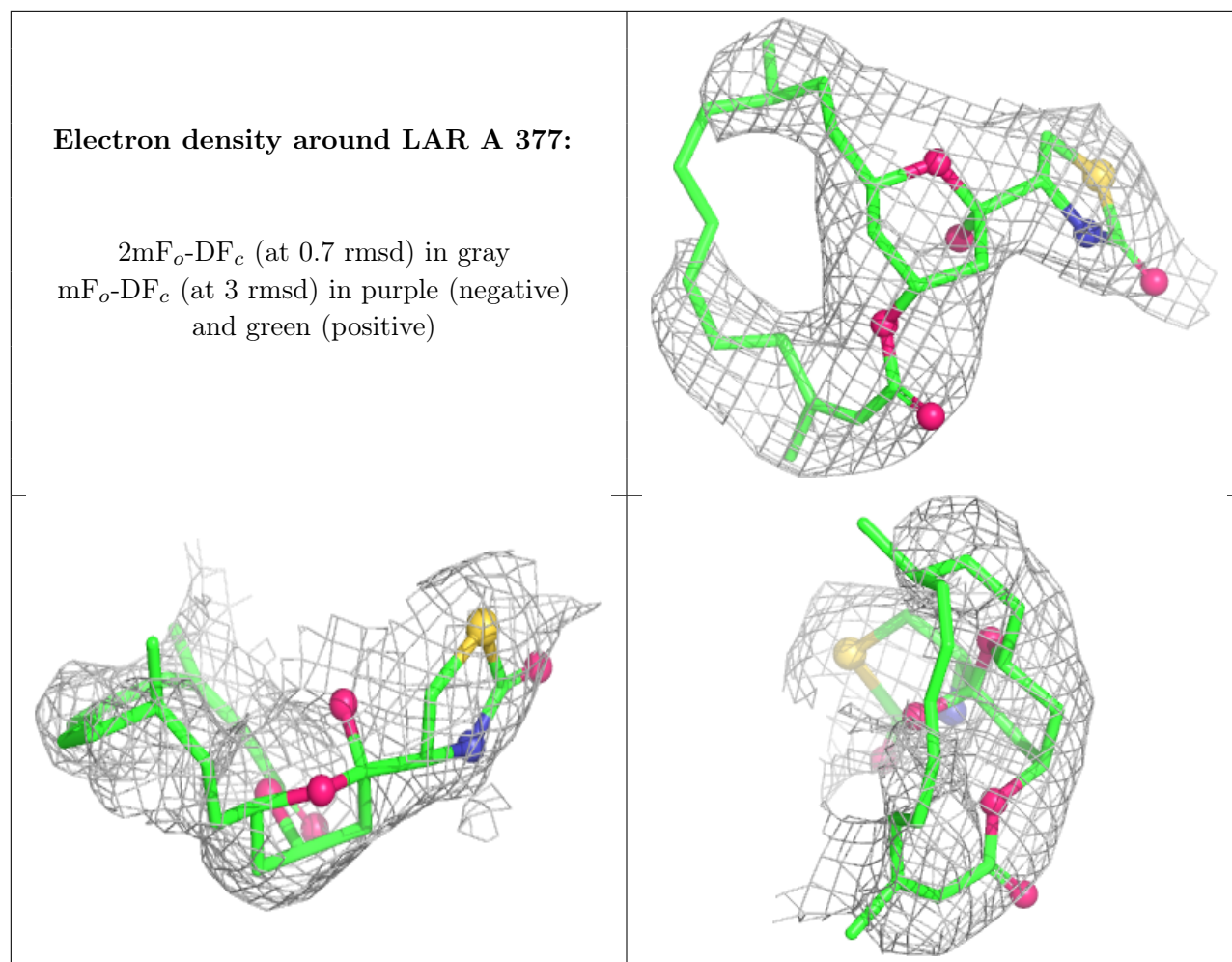
**Electron density around ATP A 376:**

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

**Electron density around ATP B 386:**

$2mF_o-DF_c$  (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.