



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 09:30 pm BST

PDB ID : 1RFQ
Title : Actin Crystal Dynamics: Structural Implications for F-actin Nucleation, Polymerization and Branching Mediated by the Anti-parallel Dimer
Authors : Reutzell, 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

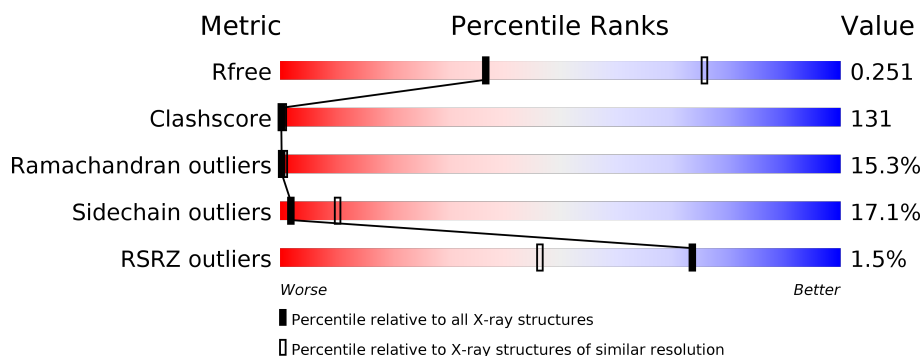
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

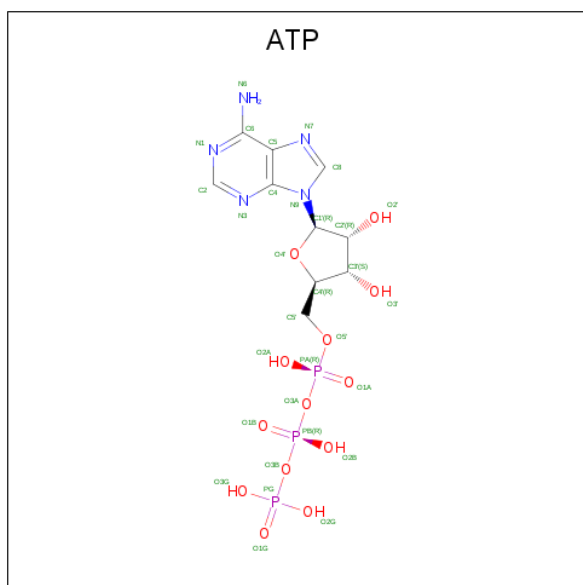
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

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

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

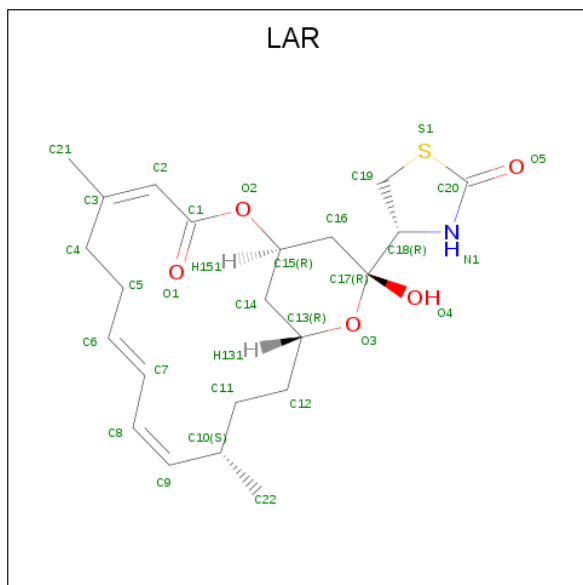
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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 (three-letter code: 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		

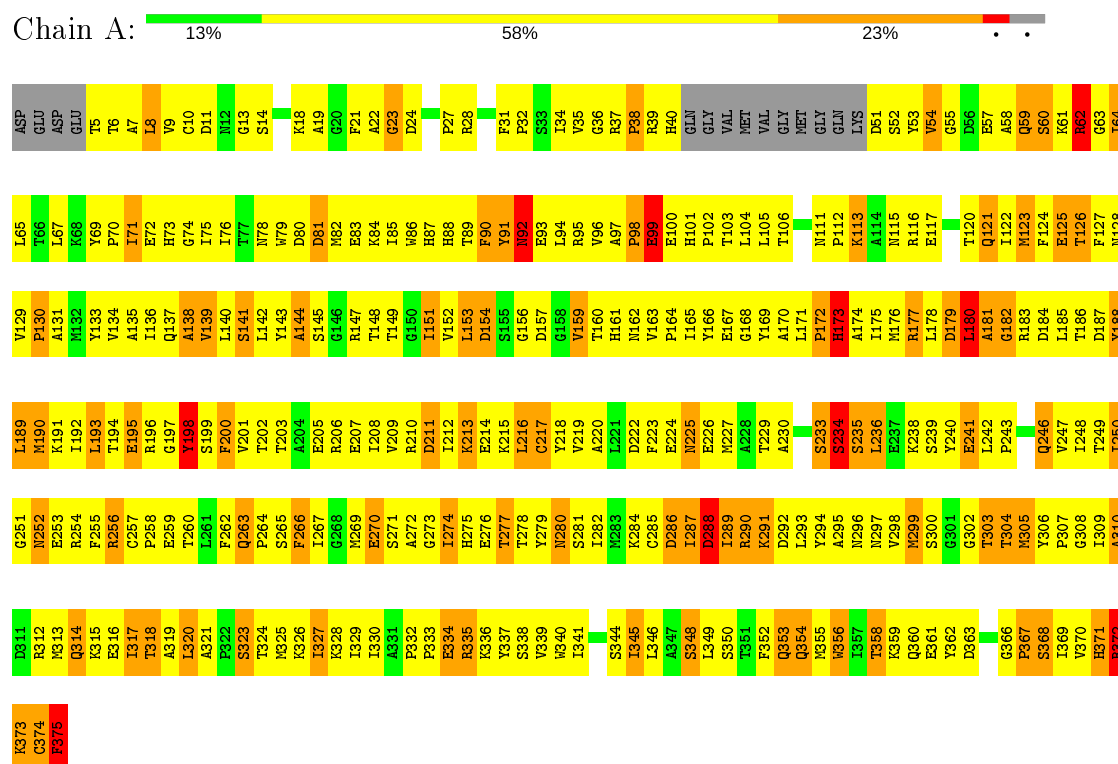
- Molecule 5 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Actin, alpha skeletal muscle



D363	E364	A365	G366	P367	S368	I369	V370	H371	R372	K373	C374	P375																																															
T303	R304	P305	T306	P307	G308	I309	A310	R311	R312	P313	G314	P315	E316	I317	T318	A319	I320	A321	P322	S323	T324	P325	R326	K327	K328	I329	I330	A331	P332	P333	E334	R335	K336	T337	S338	V339	K340	I341	G342	G343	S344	I345	I346	A347	S348	S350	T351	P352	G353	Q354	P355	K356	I357	T358	K359	G360	E361	Y362	
P243	D244	G245	Q246	V247	I248	T249	I250	G251	N252	E253	R254	P255	N256	C257	P258	E259	T260	L261	F262	Q263	P264	S265	F266	I267	G268	N269	E270	S271	A272	G273	I274	R275	E276	T277	T278	Y279	N280	S281	I282	N283	I284	C285	D286	I287	D288	I289	R290	K291	D292	L293	Y294	A295	N296	I297	V298	N299	S300	G301	G302
G182	R183	D184	L185	T186	D187	Y188	L189	M190	K191	T192	L193	T194	E195	R196	G197	Y198	S199	F200	V201	T202	T203	A204	E205	R206	E207	I208	V209	R210	D211	I212	K213	E214	K215	L216	Q217	Y218	V219	A220	L221	D222	F223	E224	R225	E226	N227	A228	T229	A230	A231	S232	S233	S234	S235	L236	F237	K238	S239	L242	

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	101.50Å 101.50Å 104.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 46.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 98.6 (46.35-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.261 0.205 , 0.251	Depositor DCC
R_{free} test set	2858 reflections (13.57%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 125.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	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	0.93	EDS
Total number of atoms	5824	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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, ATP, 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	0.63	2/2891 (0.1%)	1.03	20/3919 (0.5%)
1	B	0.64	2/2891 (0.1%)	1.02	18/3919 (0.5%)
All	All	0.63	4/5782 (0.1%)	1.02	38/7838 (0.5%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	SER	N-CA	16.41	1.79	1.46
1	B	200	PHE	N-CA	11.99	1.70	1.46
1	B	25	ASP	C-N	-6.15	1.20	1.34
1	A	374	CYS	CB-SG	-5.57	1.72	1.81

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	PHE	CB-CG-CD1	12.53	129.57	120.80
1	B	200	PHE	CB-CG-CD2	-11.75	112.57	120.80
1	A	272	ALA	C-N-CA	-10.81	99.61	122.30
1	A	200	PHE	CB-CG-CD2	9.51	127.46	120.80
1	A	270	GLU	N-CA-CB	9.40	127.52	110.60

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

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	703	0
1	B	2829	0	2793	838	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	5673	1501	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 131.

The worst 5 of 1501 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
1:A:235:SER:CA	1:A:235:SER:N	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	1

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%)	261 (85%)	46 (15%)	3	14
1	B	307/318 (96%)	248 (81%)	59 (19%)	1	8
All	All	614/636 (96%)	509 (83%)	105 (17%)	2	10

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	99	GLU
1	B	311	ASP
1	B	56	ASP
1	B	72	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	B	59	GLN
1	B	354	GLN
1	A	371	HIS
1	B	73	HIS

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 carbohydrates 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
3	ATP	A	376	2	26,33,33	2.23	9 (34%)	31,52,52	2.99	8 (25%)
4	LAR	B	387	-	30,31,31	1.28	5 (16%)	32,43,43	1.59	3 (9%)
4	LAR	A	377	-	30,31,31	1.30	4 (13%)	32,43,43	1.64	4 (12%)
3	ATP	B	386	2	26,33,33	2.20	10 (38%)	31,52,52	3.13	8 (25%)

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
3	ATP	A	376	2	-	2/18/38/38	0/3/3/3
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	-	2/18/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	376	ATP	O4'-C1'	5.54	1.48	1.41
3	B	386	ATP	O5'-C5'	-4.82	1.26	1.44
3	B	386	ATP	O4'-C1'	4.80	1.47	1.41
3	A	376	ATP	O5'-C5'	-4.69	1.26	1.44
3	B	386	ATP	C4-N3	3.92	1.41	1.35

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	386	ATP	O5'-C5'-C4'	12.12	150.71	108.99
3	A	376	ATP	O5'-C5'-C4'	11.13	147.30	108.99
3	B	386	ATP	O5'-PA-O1A	-7.25	80.74	109.07
3	A	376	ATP	O5'-PA-O1A	-7.13	81.21	109.07
3	A	376	ATP	PA-O5'-C5'	5.90	156.26	121.68

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	387	LAR	O3-C17-C18-C19
4	B	387	LAR	O2-C1-C2-C3

Continued on next page...

Continued from previous page...

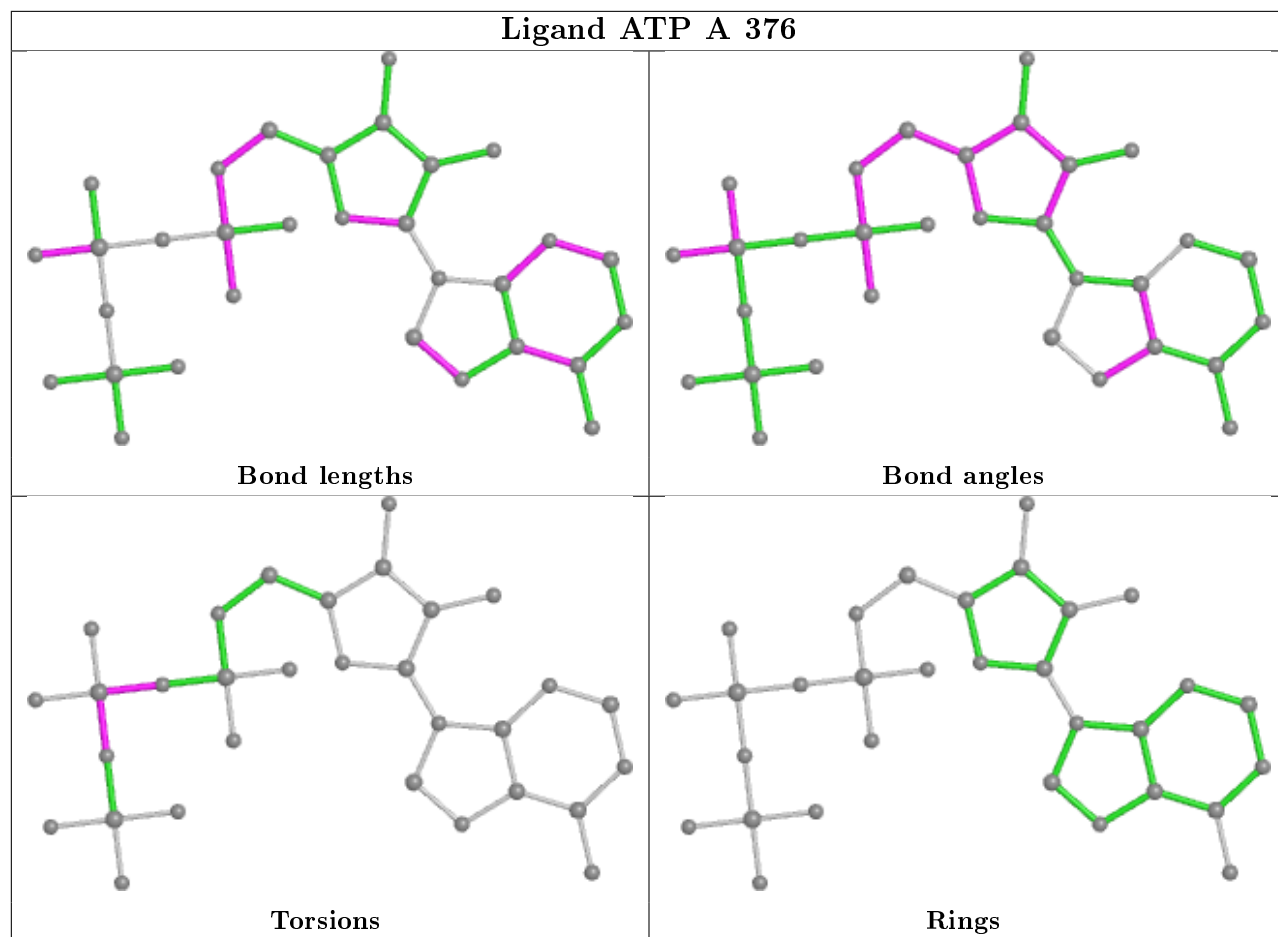
Mol	Chain	Res	Type	Atoms
3	A	376	ATP	PG-O3B-PB-O2B
3	B	386	ATP	PG-O3B-PB-O2B
3	B	386	ATP	PA-O3A-PB-O2B

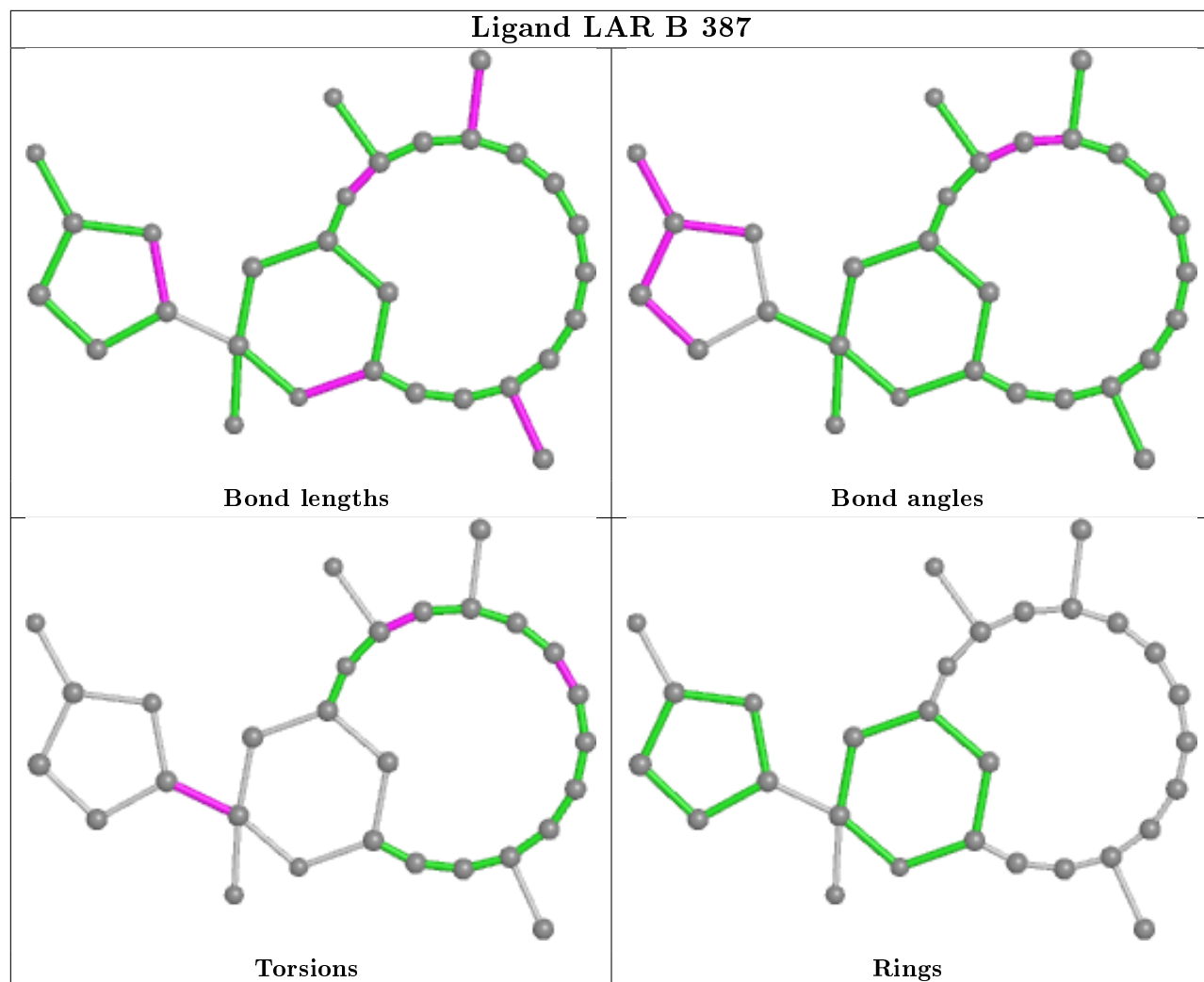
There are no ring outliers.

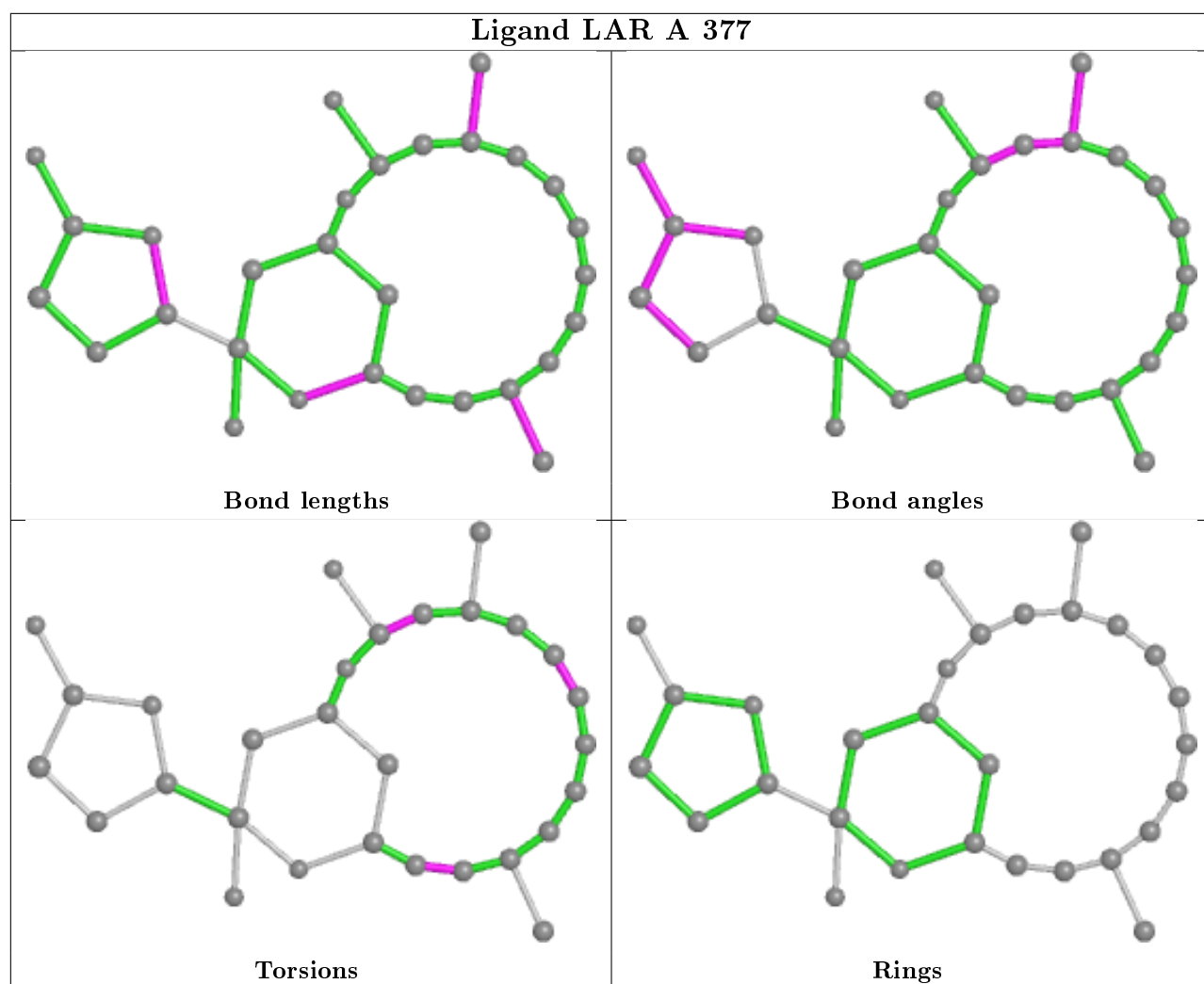
4 monomers are involved in 31 short contacts:

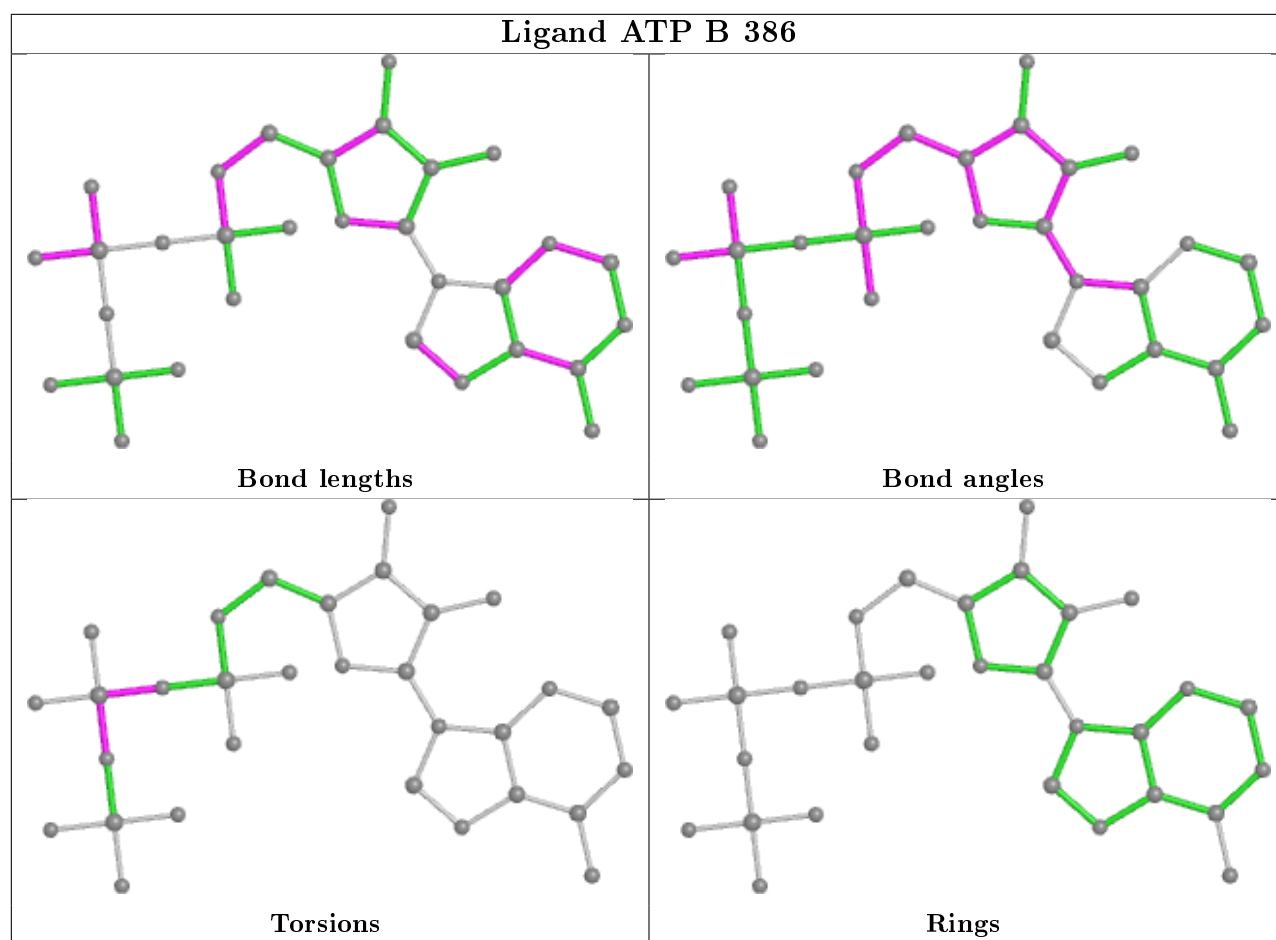
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	376	ATP	9	0
4	B	387	LAR	10	0
4	A	377	LAR	2	0
3	B	386	ATP	10	0

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, 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	A	361/375 (96%)	0.05	0 100 100	38, 57, 75, 82	0
1	B	361/375 (96%)	0.22	11 (3%) 50 22	42, 68, 83, 96	0
All	All	722/750 (96%)	0.13	11 (1%) 73 46	38, 63, 80, 96	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	ILE	3.5
1	B	33	SER	3.0
1	B	228	ALA	2.9
1	B	104	LEU	2.8
1	B	178	LEU	2.8

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](#)

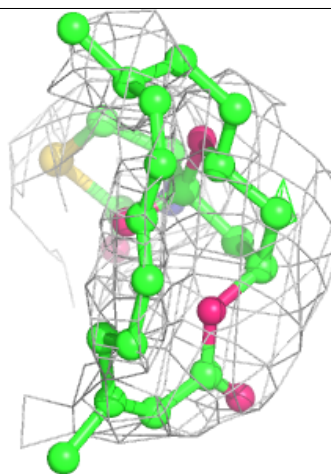
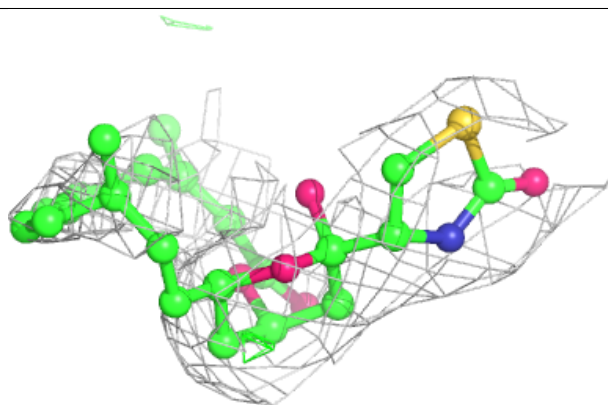
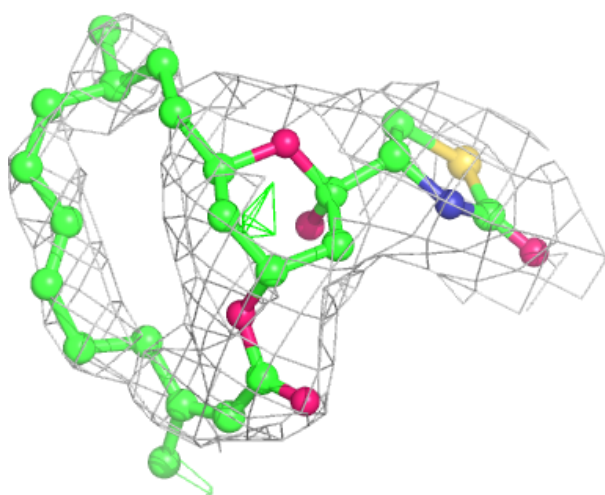
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	388	1/1	0.84	0.25	42,42,42,42	0
4	LAR	B	387	29/29	0.89	0.31	66,71,78,78	0
4	LAR	A	377	29/29	0.92	0.38	61,67,74,75	0
2	MG	A	378	1/1	0.93	0.26	36,36,36,36	0
3	ATP	B	386	31/31	0.93	0.19	53,57,61,62	0
3	ATP	A	376	31/31	0.95	0.22	37,50,55,56	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.

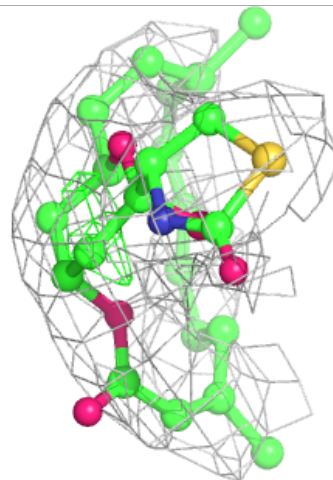
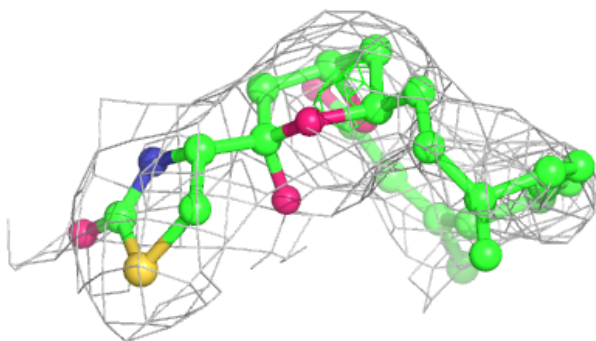
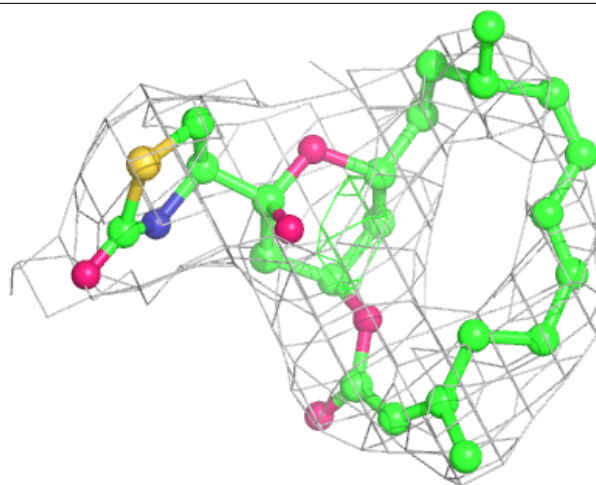
Electron density around LAR B 387:

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



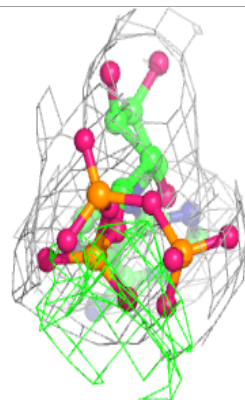
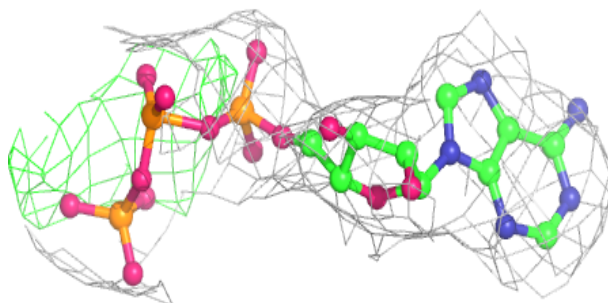
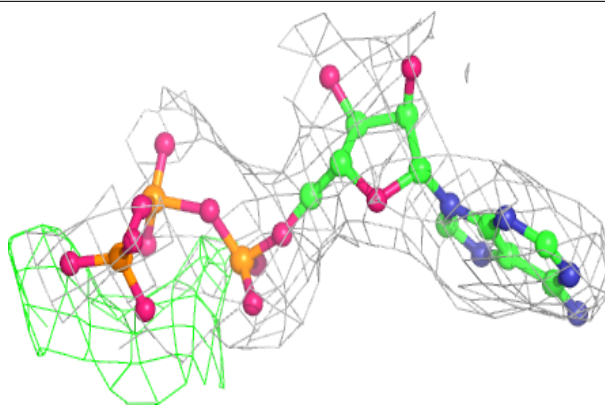
Electron density around LAR A 377:

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

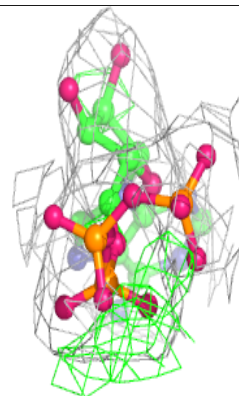
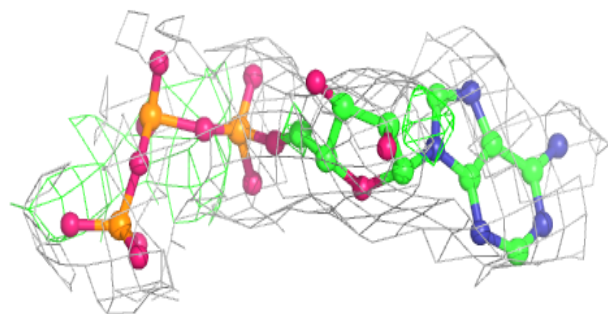
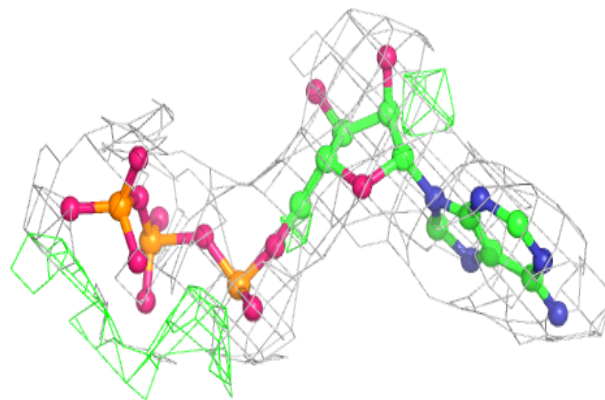


Electron density around ATP B 386:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.