



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 04:27 AM UTC

PDB ID : 4B1Z / pdb_00004b1z
Title : Structure of the Phactr1 RPEL domain bound to G-actin
Authors : Mouilleron, S.; Wiezlak, M.; O'Reilly, N.; Treisman, R.; McDonald, N.Q.
Deposited on : 2012-07-12
Resolution : 3.30 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

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>.

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)
Xtriage (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

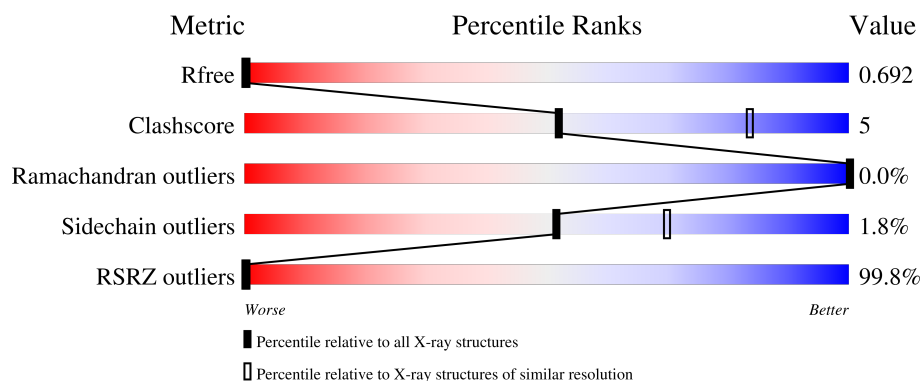
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 $\leq 5\%$. 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	376	89% 78% 10% • 11%
1	B	376	95% 84% 10% • 5%
1	C	376	98% 87% 10% ••
1	D	376	95% 82% 12% • 5%
1	E	376	95% 83% 12% • 5%

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Mol	Chain	Length	Quality of chain
1	F	376	95% 81% 13% • 5%
2	M	115	96% 74% 18% • •
2	N	115	93% 76% 15% • 7%

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	D	1376	-	-	-	X
5	GOL	A	1379	-	-	-	X
5	GOL	B	1378	-	-	-	X
5	GOL	C	1379	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17941 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.

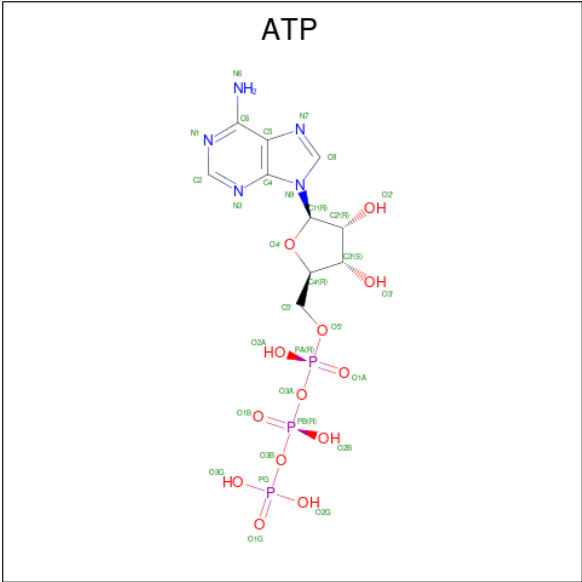
- Molecule 1 is a protein called ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2495	1588	415	474	18			
1	B	357	Total	C	N	O	S	0	0	0
			2711	1721	448	523	19			
1	C	370	Total	C	N	O	S	0	0	0
			2815	1787	476	532	20			
1	D	356	Total	C	N	O	S	0	0	0
			2648	1675	446	508	19			
1	E	359	Total	C	N	O	S	0	0	0
			2682	1701	450	512	19			
1	F	357	Total	C	N	O	S	0	0	0
			2682	1706	444	513	19			

- Molecule 2 is a protein called PHOSPHATASE AND ACTIN REGULATOR 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	110	Total	C	N	O	0	0	0
			846	517	166	163			
2	N	107	Total	C	N	O	0	0	0
			821	505	159	157			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

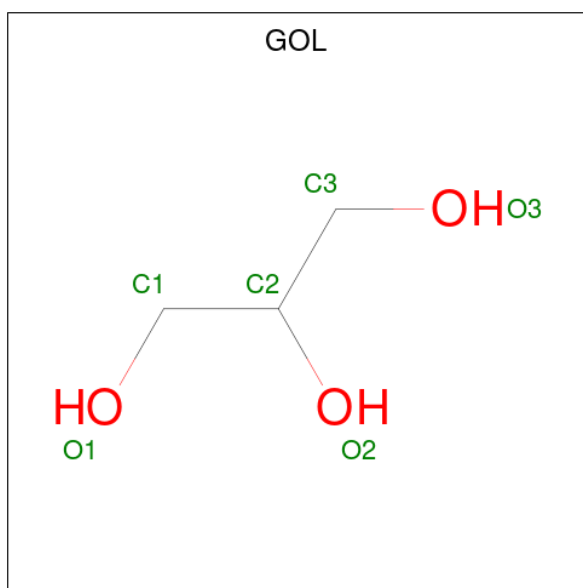


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	F	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		

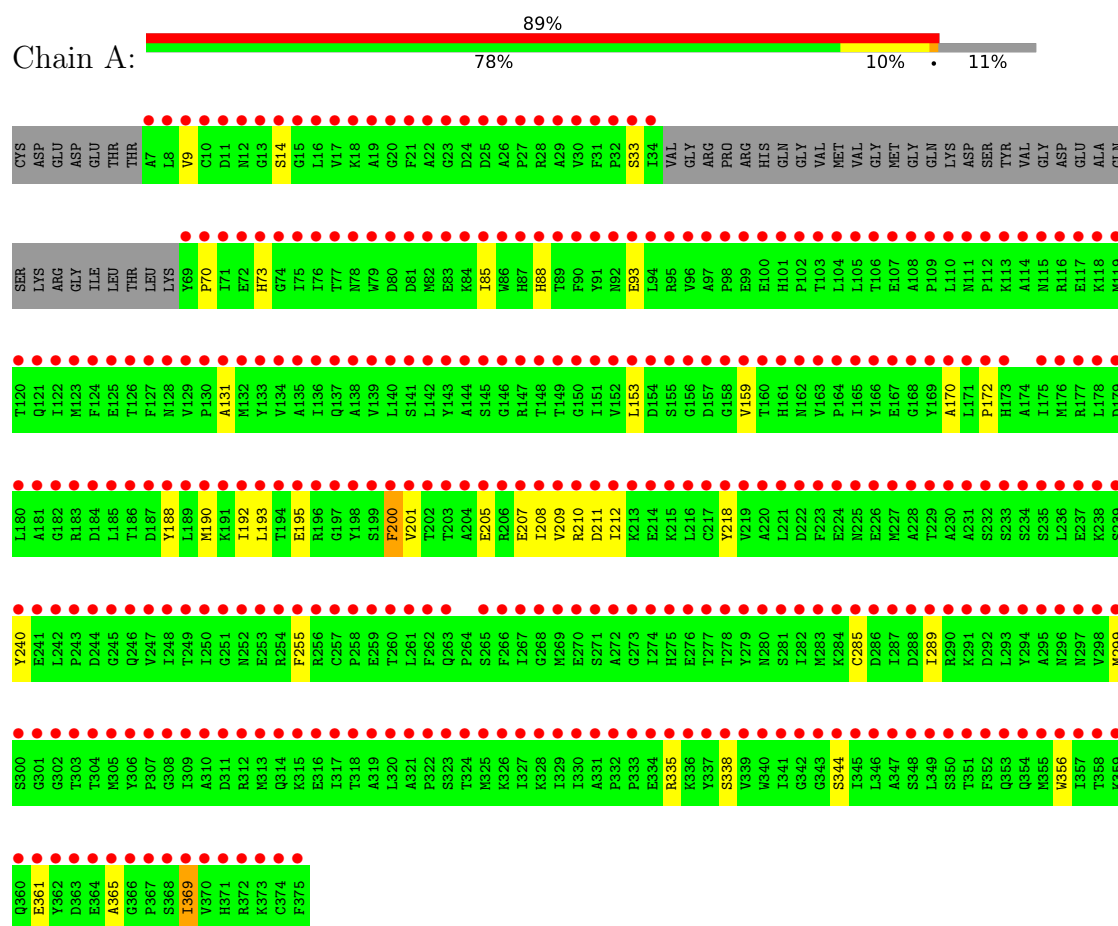
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	O	0	0
			1	1		

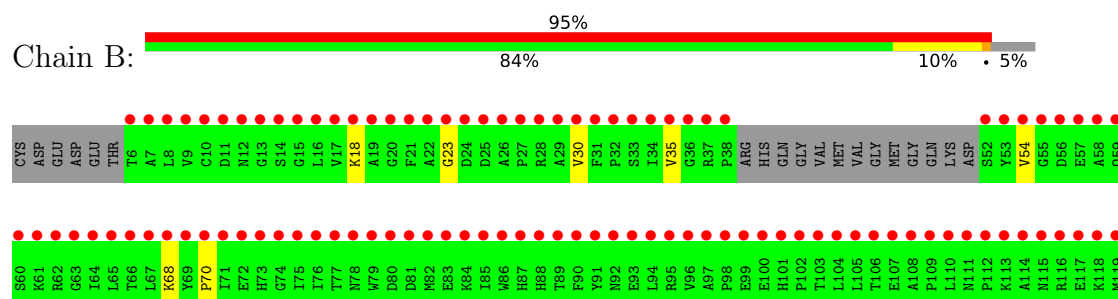
3 Residue-property plots

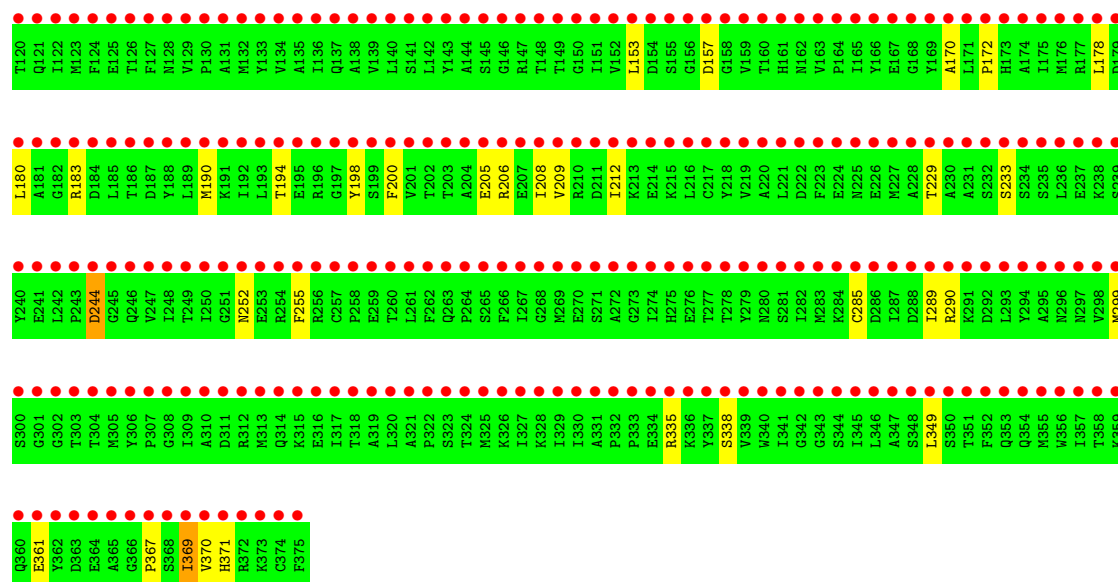
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

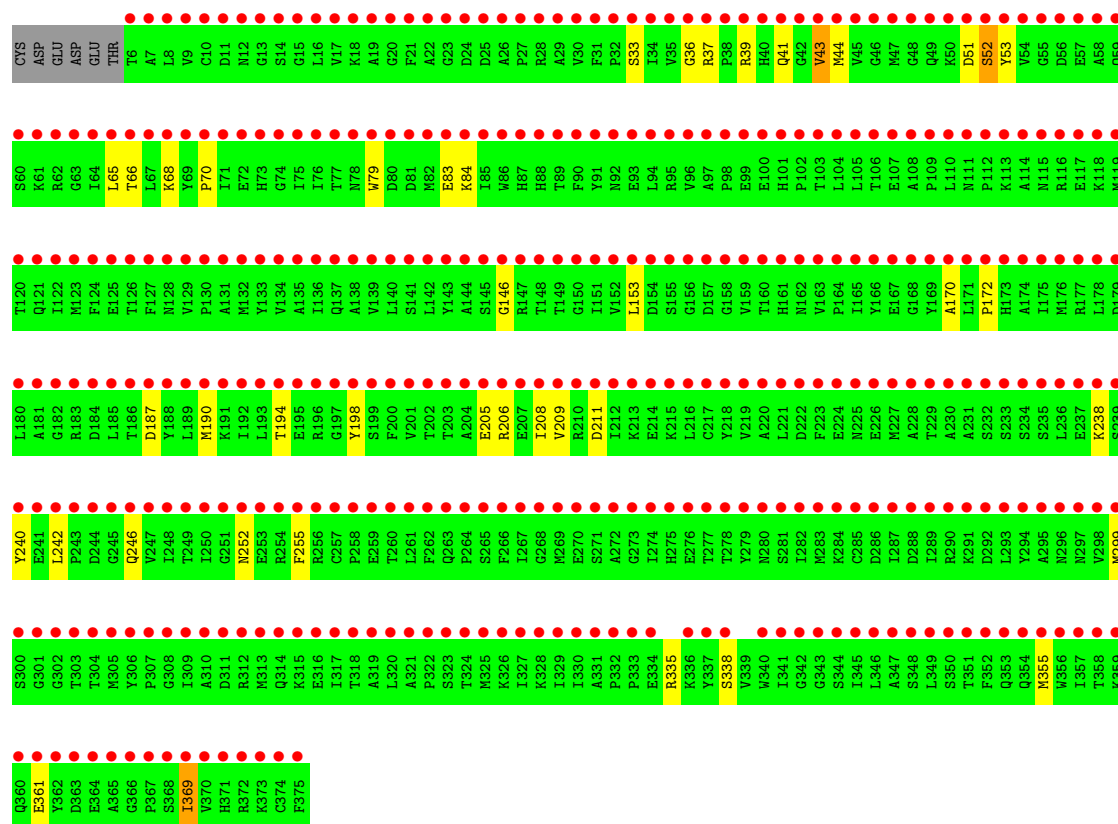
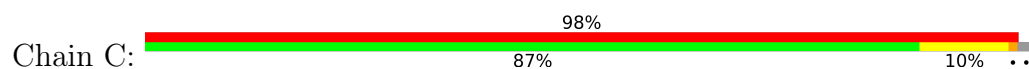


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

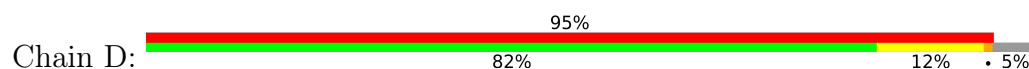


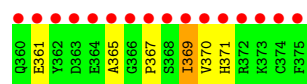


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

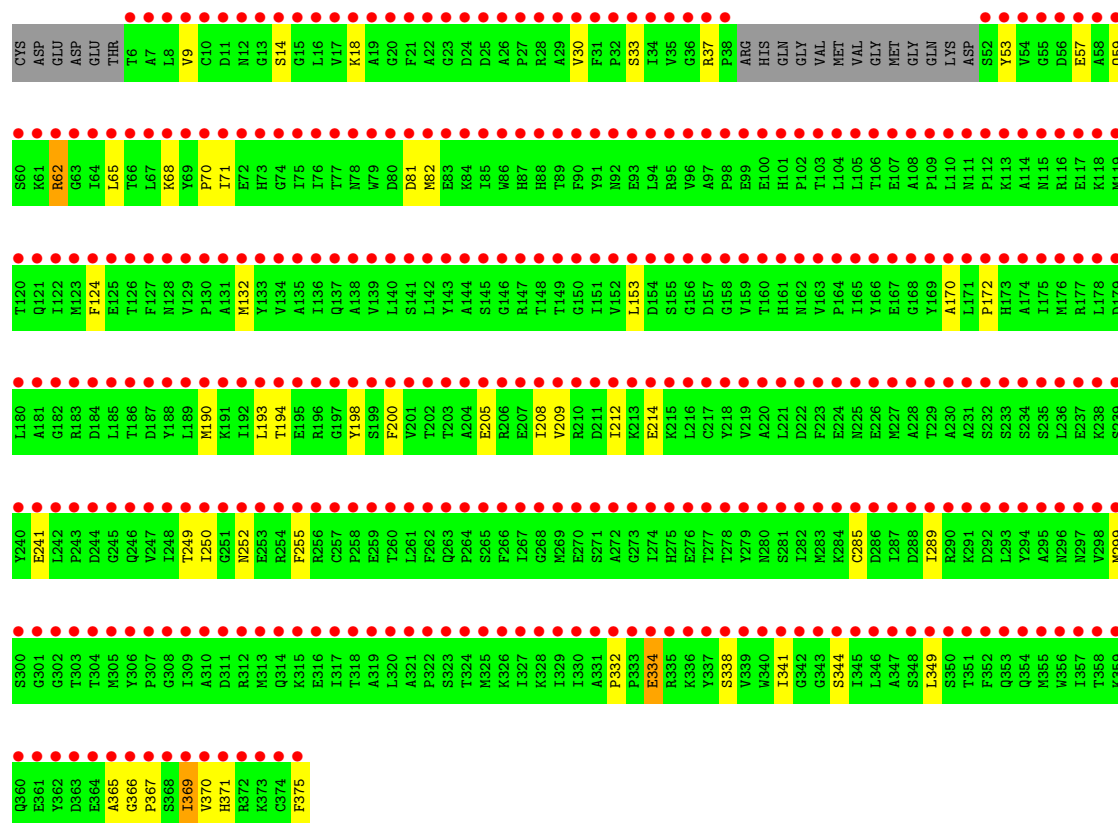
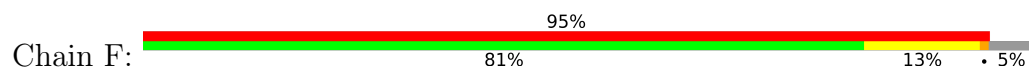


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

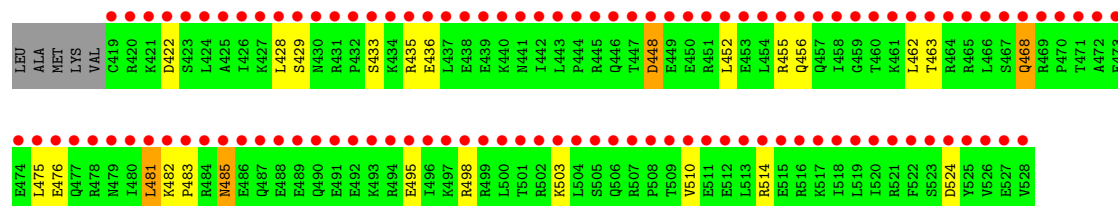




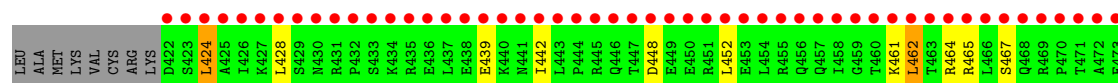
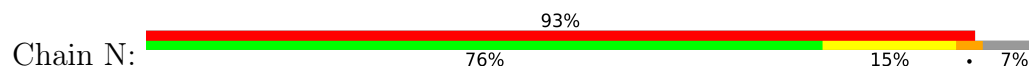
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1



• Molecule 2: PHOSPHATASE AND ACTIN REGULATOR 1



E474	E475	E476	Q477	R478	R479	I480	L481	K482	P483	R484	M485	E486	Q487	E488	E489	Q490	E491	E492	K493	R494	E495	I496	K497	R498	R499	L500	T501	R502	K503	L504	S505	Q506	R507	P508	T509	V510	E511	E512	L513	R514	E515	R516	K517	I518	L519	I520	R521	F522	S523	D524	Y525	V526	E527	V528
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.06Å 142.89Å 184.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.62 – 3.30 74.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (74.62-3.30) 96.7 (74.62-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.34 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.1_1168)	Depositor
R, R_{free}	0.213 , 0.236 0.685 , 0.692	Depositor DCC
R_{free} test set	2580 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.57	EDS
Total number of atoms	17941	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: GOL, ATP, MG

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	0.33	0/2552	0.83	2/3480 (0.1%)
1	B	0.33	0/2772	0.79	1/3774 (0.0%)
1	C	0.32	0/2878	0.80	0/3911
1	D	0.32	0/2706	0.84	4/3685 (0.1%)
1	E	0.34	0/2742	0.82	0/3738
1	F	0.34	0/2742	0.82	1/3736 (0.0%)
2	M	0.27	0/851	0.79	0/1148
2	N	0.26	0/827	0.77	0/1115
All	All	0.33	0/18070	0.81	8/24587 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	366	GLY	CA-C-N	6.57	126.26	119.56
1	D	366	GLY	C-N-CA	6.57	126.26	119.56
1	D	200	PHE	N-CA-C	5.68	117.32	109.54
1	A	200	PHE	N-CA-C	5.45	117.48	108.49
1	D	202	THR	N-CA-C	5.42	117.87	110.55

There are no chirality outliers.

There are no planarity outliers.

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	2495	0	2353	21	0
1	B	2711	0	2582	27	0
1	C	2815	0	2724	30	0
1	D	2648	0	2476	30	0
1	E	2682	0	2525	35	0
1	F	2682	0	2550	35	0
2	M	846	0	814	13	0
2	N	821	0	787	12	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	31	0	12	0	0
3	D	31	0	12	3	0
3	E	31	0	12	1	0
3	F	31	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	E	6	0	8	1	0
5	F	6	0	8	0	0
5	N	6	0	8	0	0
6	E	1	0	0	0	0
All	All	17941	0	16947	179	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 5.

The worst 5 of 179 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:E:146:GLY:O	2:N:465:ARG:NH1	2.04	0.89
1:F:371:HIS:HB3	2:N:527:GLU:HG3	1.58	0.84
1:D:62:ARG:HB2	1:D:67:LEU:HD11	1.63	0.80
1:C:41:GLN:O	1:E:28:ARG:NH2	2.14	0.80
1:C:39:ARG:HG2	1:C:66:THR:HG23	1.67	0.77

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	331/376 (88%)	326 (98%)	5 (2%)	0	100	100
1	B	353/376 (94%)	347 (98%)	6 (2%)	0	100	100
1	C	368/376 (98%)	359 (98%)	8 (2%)	1 (0%)	36	65
1	D	352/376 (94%)	346 (98%)	6 (2%)	0	100	100
1	E	355/376 (94%)	348 (98%)	7 (2%)	0	100	100
1	F	353/376 (94%)	346 (98%)	7 (2%)	0	100	100
2	M	108/115 (94%)	105 (97%)	3 (3%)	0	100	100
2	N	105/115 (91%)	102 (97%)	3 (3%)	0	100	100
All	All	2325/2486 (94%)	2279 (98%)	45 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	SER

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	251/319 (79%)	249 (99%)	2 (1%)	73	79
1	B	281/319 (88%)	279 (99%)	2 (1%)	76	80
1	C	292/319 (92%)	289 (99%)	3 (1%)	68	76
1	D	264/319 (83%)	263 (100%)	1 (0%)	84	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	270/319 (85%)	267 (99%)	3 (1%)	65	76
1	F	274/319 (86%)	271 (99%)	3 (1%)	65	76
2	M	83/111 (75%)	73 (88%)	10 (12%)	5	20
2	N	80/111 (72%)	71 (89%)	9 (11%)	5	21
All	All	1795/2136 (84%)	1762 (98%)	33 (2%)	51	70

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	452	LEU
2	N	461	LYS
2	N	527	GLU
1	F	334	GLU
1	F	62	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	297	ASN
1	F	353	GLN
1	E	263	GLN
2	N	446	GLN
1	F	162	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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
5	GOL	C	1379	-	5,5,5	0.37	0	5,5,5	0.33	0
3	ATP	F	1376	4	32,33,33	1.41	5 (15%)	48,52,52	1.72	9 (18%)
3	ATP	E	1376	4	32,33,33	1.42	5 (15%)	48,52,52	1.68	8 (16%)
5	GOL	A	1378	-	5,5,5	0.39	0	5,5,5	0.23	0
5	GOL	C	1378	-	5,5,5	0.38	0	5,5,5	0.34	0
3	ATP	D	1376	4	32,33,33	1.42	5 (15%)	48,52,52	1.70	9 (18%)
5	GOL	A	1379	-	5,5,5	0.38	0	5,5,5	0.32	0
3	ATP	C	1376	4	32,33,33	1.39	5 (15%)	48,52,52	1.72	9 (18%)
5	GOL	N	1529	-	5,5,5	0.38	0	5,5,5	0.33	0
5	GOL	B	1378	-	5,5,5	0.37	0	5,5,5	0.25	0
3	ATP	A	1376	4	32,33,33	1.40	5 (15%)	48,52,52	1.72	9 (18%)
3	ATP	B	1376	4	32,33,33	1.38	5 (15%)	48,52,52	1.74	10 (20%)
5	GOL	F	1378	-	5,5,5	0.38	0	5,5,5	0.25	0
5	GOL	E	1378	-	5,5,5	0.37	0	5,5,5	0.35	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
5	GOL	C	1379	-	-	4/4/4/4	-
3	ATP	F	1376	4	-	0/22/38/38	0/3/3/3
3	ATP	E	1376	4	-	3/22/38/38	0/3/3/3
5	GOL	A	1378	-	-	2/4/4/4	-
5	GOL	C	1378	-	-	2/4/4/4	-
3	ATP	D	1376	4	-	0/22/38/38	0/3/3/3
5	GOL	A	1379	-	-	0/4/4/4	-
3	ATP	C	1376	4	-	1/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	N	1529	-	-	2/4/4/4	-
5	GOL	B	1378	-	-	2/4/4/4	-
3	ATP	A	1376	4	-	0/22/38/38	0/3/3/3
3	ATP	B	1376	4	-	2/22/38/38	0/3/3/3
5	GOL	F	1378	-	-	2/4/4/4	-
5	GOL	E	1378	-	-	2/4/4/4	-

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1376	ATP	C5-C4	4.75	1.47	1.39
3	D	1376	ATP	C5-C4	4.72	1.47	1.39
3	C	1376	ATP	C5-C4	4.71	1.47	1.39
3	A	1376	ATP	C5-C4	4.69	1.47	1.39
3	F	1376	ATP	C5-C4	4.67	1.47	1.39

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1376	ATP	C5-C4-N3	-5.84	118.68	126.72
3	B	1376	ATP	C5-C4-N3	-5.82	118.70	126.72
3	C	1376	ATP	C5-C4-N3	-5.68	118.89	126.72
3	A	1376	ATP	C5-C4-N3	-5.65	118.94	126.72
3	D	1376	ATP	C5-C4-N3	-5.55	119.07	126.72

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1376	ATP	C5'-O5'-PA-O2A
5	A	1378	GOL	C1-C2-C3-O3
5	C	1378	GOL	C1-C2-C3-O3
5	C	1379	GOL	C1-C2-C3-O3
5	F	1378	GOL	C1-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 8 short contacts:

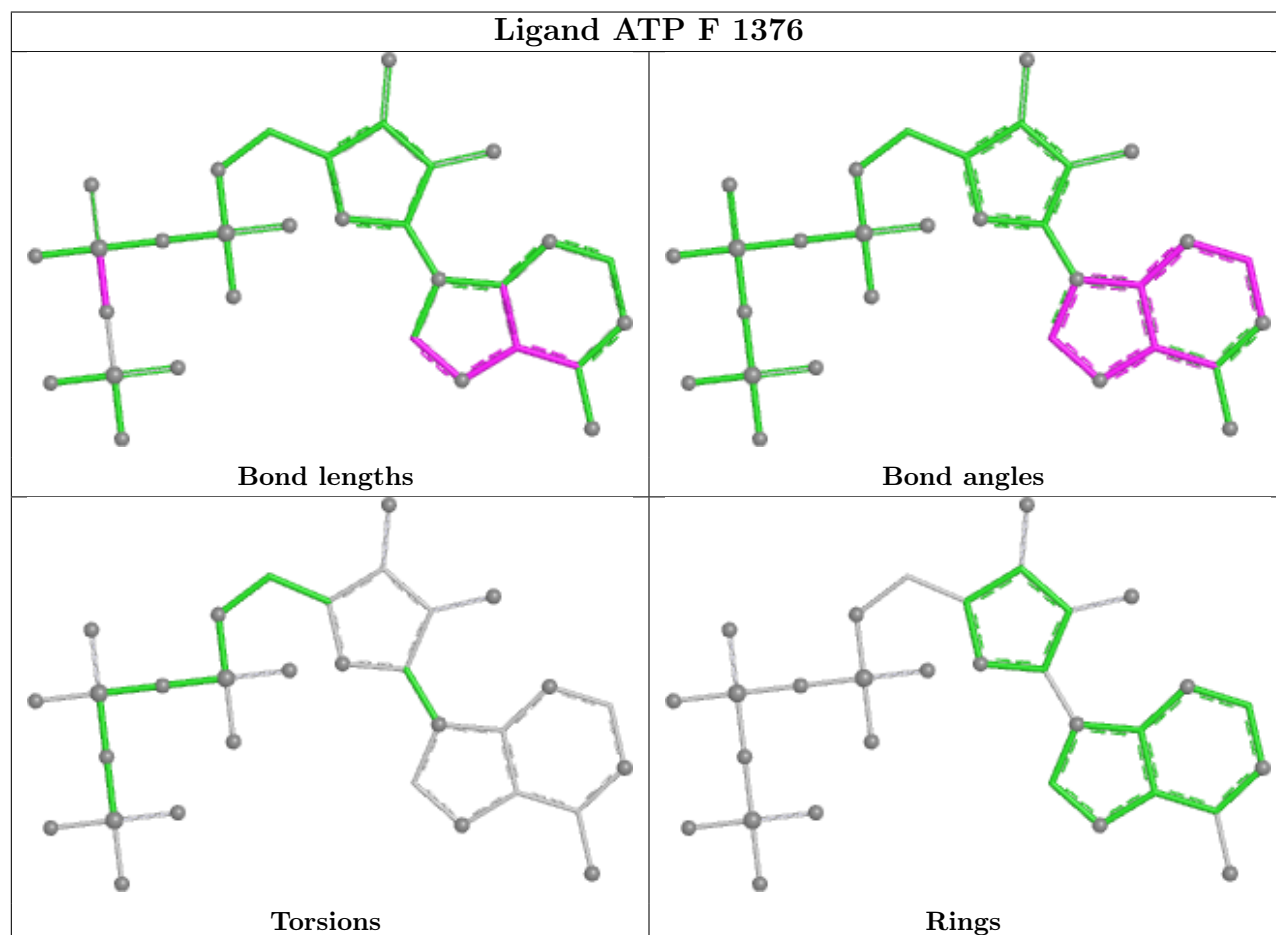
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1376	ATP	1	0

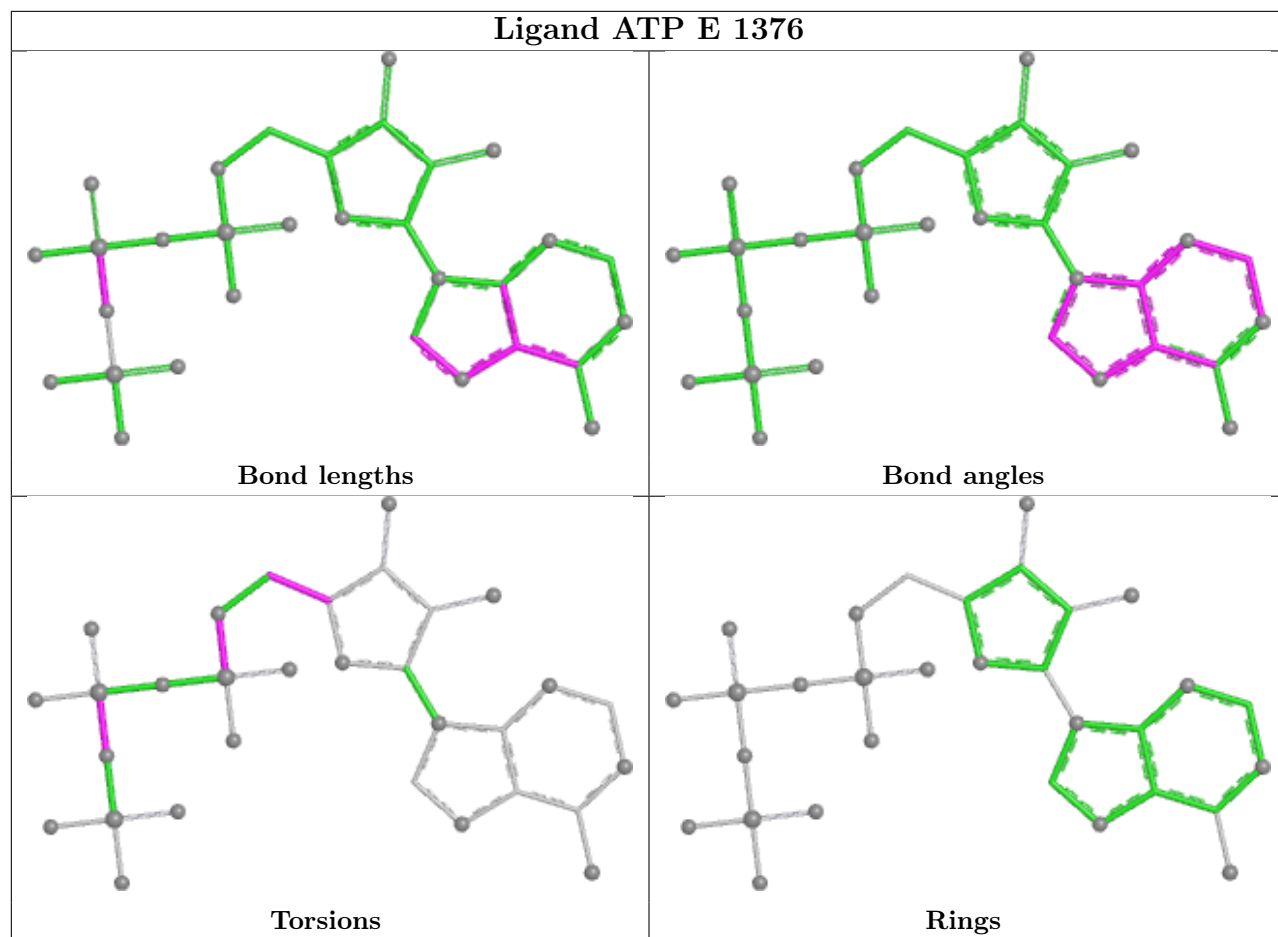
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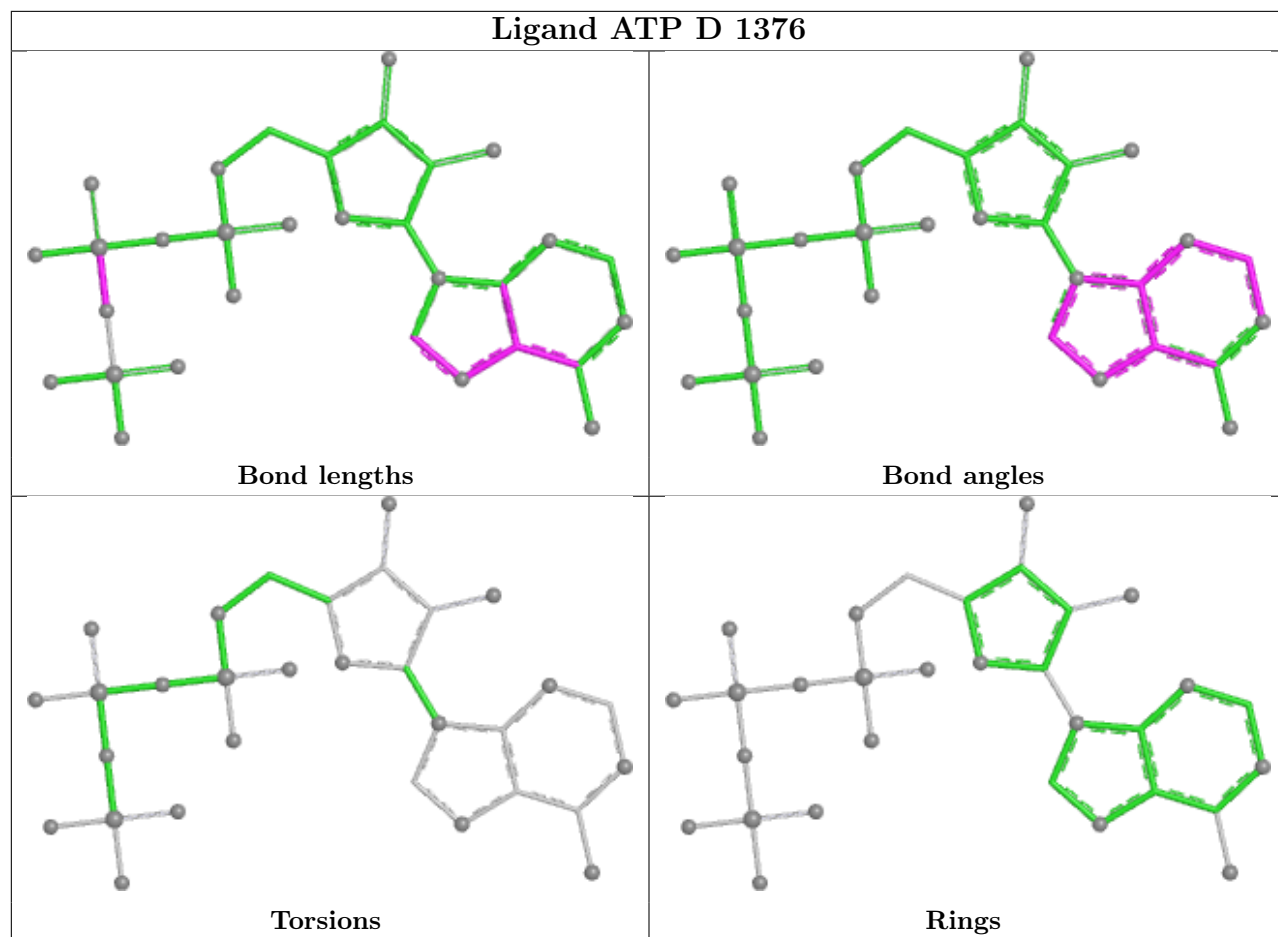
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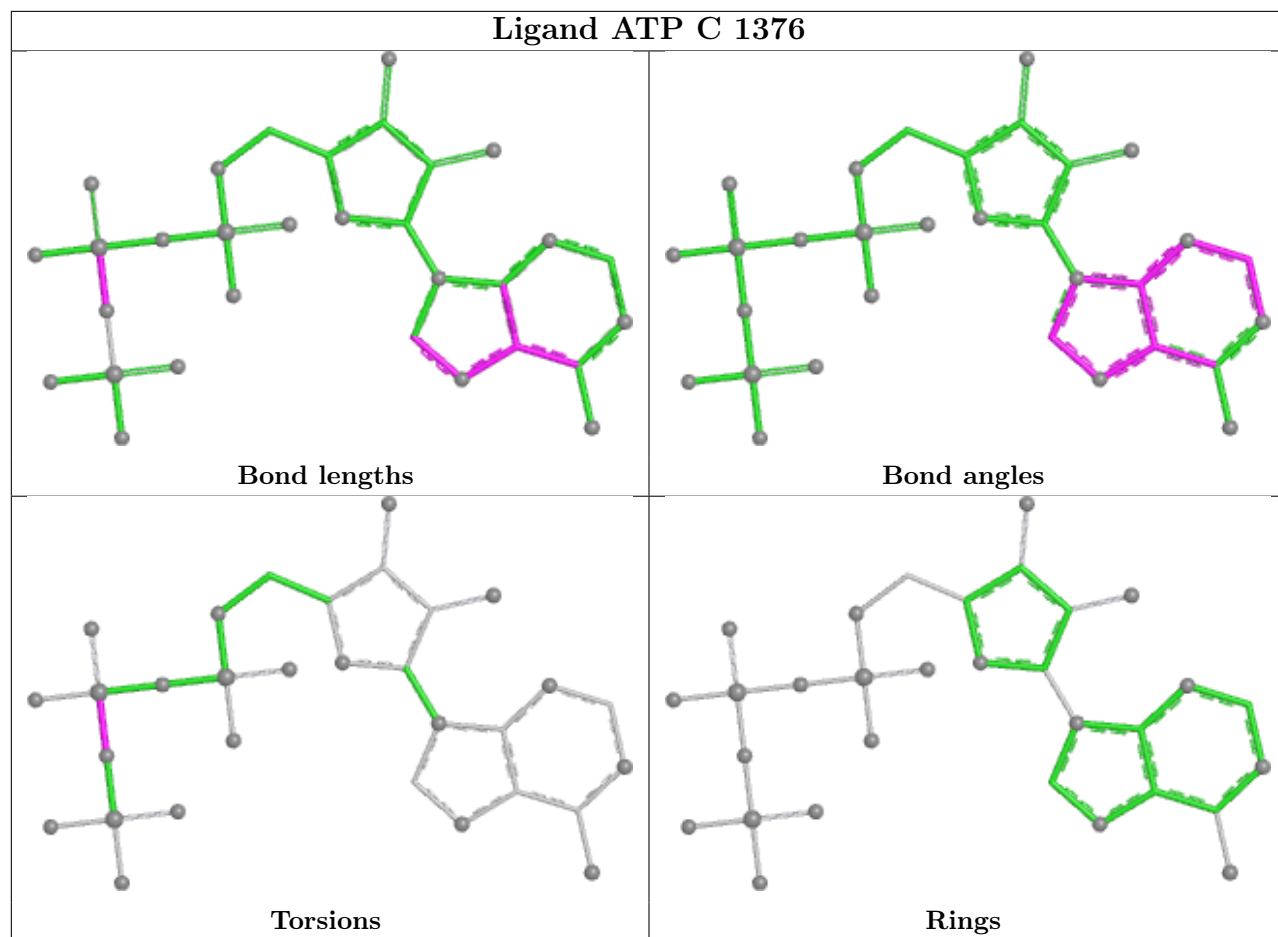
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1376	ATP	1	0
3	D	1376	ATP	3	0
3	A	1376	ATP	1	0
3	B	1376	ATP	1	0
5	E	1378	GOL	1	0

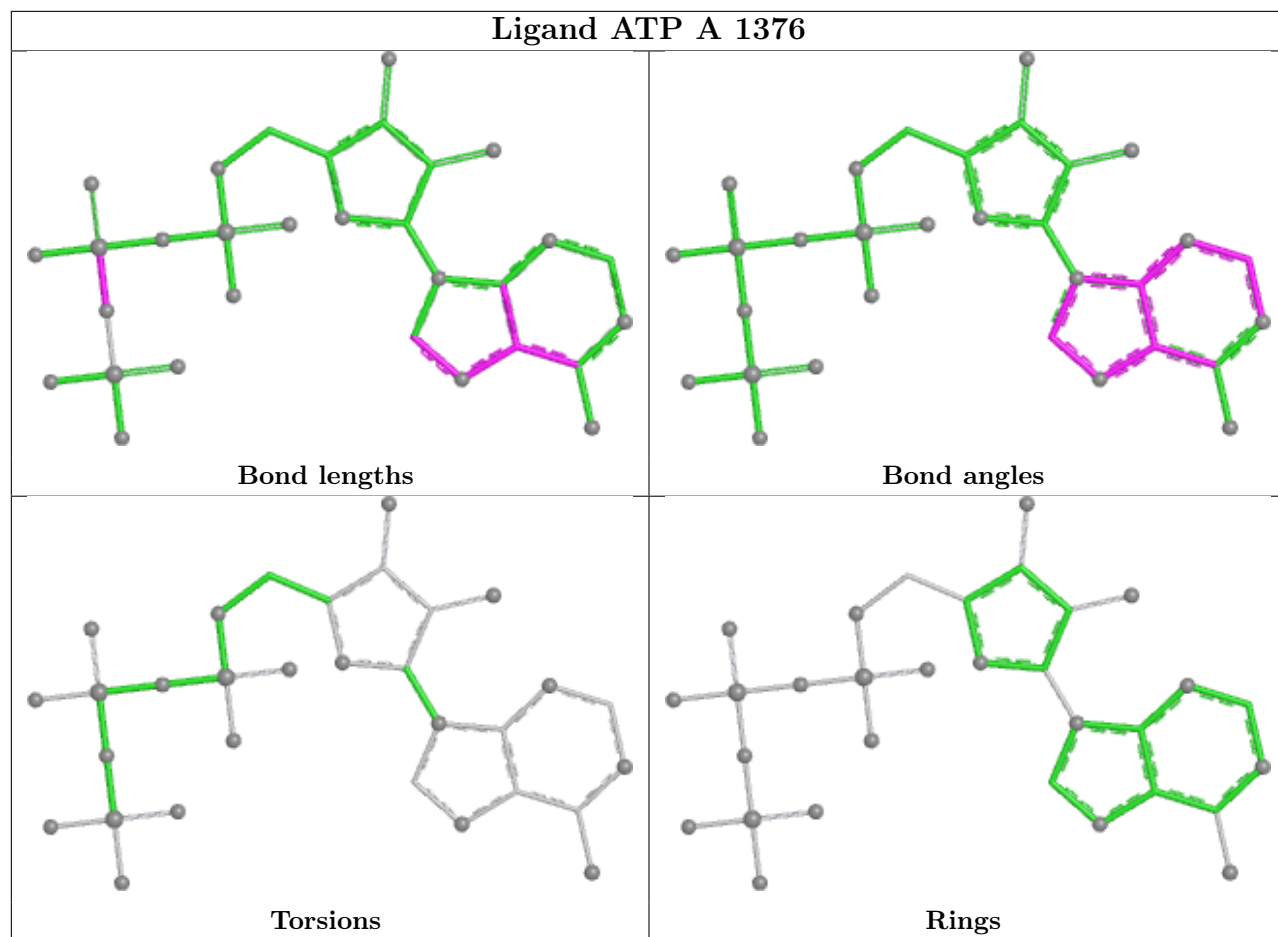
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

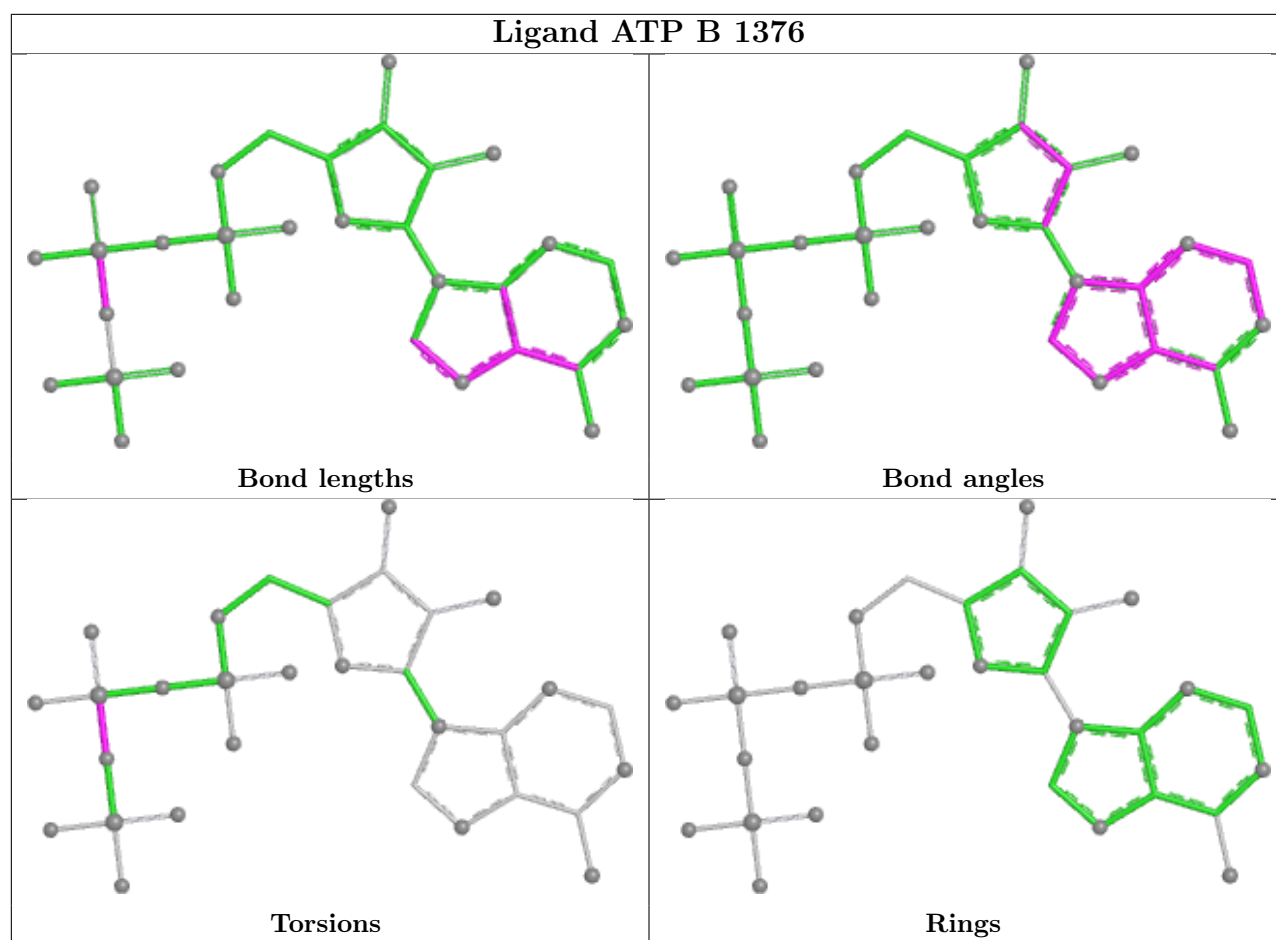












5.7 Other polymers [i](#)

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	A	335/376 (89%)	5.89	333 (99%) 0 0	57, 83, 142, 192	0
1	B	357/376 (94%)	5.73	357 (100%) 0 0	49, 78, 120, 162	0
1	C	370/376 (98%)	5.39	368 (99%) 0 0	55, 74, 107, 137	0
1	D	356/376 (94%)	6.19	356 (100%) 0 0	70, 98, 133, 162	0
1	E	359/376 (95%)	5.58	358 (99%) 0 0	58, 82, 118, 151	0
1	F	357/376 (94%)	5.54	357 (100%) 0 0	55, 82, 128, 166	0
2	M	110/115 (95%)	5.87	110 (100%) 0 0	61, 84, 128, 150	0
2	N	107/115 (93%)	5.83	107 (100%) 0 0	67, 88, 119, 133	0
All	All	2351/2486 (94%)	5.73	2346 (99%) 0 0	49, 84, 128, 192	0

The worst 5 of 2346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	15	GLY	17.8
1	D	25	ASP	15.5
2	M	487	GLN	14.8
1	F	354	GLN	14.4
2	M	436	GLU	13.5

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 ⓘ

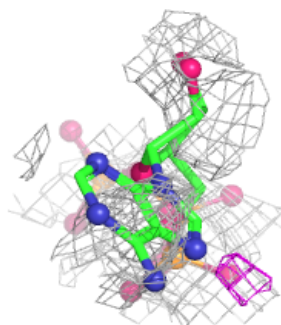
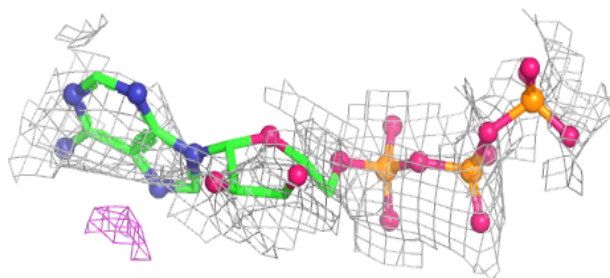
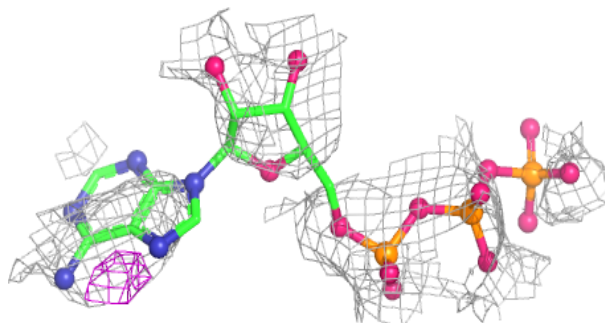
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	E	1378	6/6	0.33	0.36	82,82,82,82	0
3	ATP	D	1376	31/31	0.40	0.41	131,131,131,131	0
5	GOL	N	1529	6/6	0.40	0.39	99,99,99,99	0
3	ATP	F	1376	31/31	0.42	0.37	91,91,91,91	0
3	ATP	A	1376	31/31	0.45	0.37	99,99,99,99	0
5	GOL	B	1378	6/6	0.47	0.64	89,89,89,89	0
4	MG	F	1377	1/1	0.48	0.31	53,53,53,53	0
3	ATP	E	1376	31/31	0.49	0.35	112,112,112,112	0
3	ATP	C	1376	31/31	0.49	0.33	84,84,84,84	0
3	ATP	B	1376	31/31	0.49	0.36	81,81,81,81	0
5	GOL	F	1378	6/6	0.53	0.38	64,64,64,64	0
5	GOL	A	1379	6/6	0.53	0.50	89,89,89,89	0
4	MG	E	1377	1/1	0.56	0.29	50,50,50,50	0
5	GOL	C	1379	6/6	0.59	0.46	80,80,80,80	0
5	GOL	A	1378	6/6	0.59	0.37	73,73,73,73	0
4	MG	B	1377	1/1	0.60	0.20	39,39,39,39	0
5	GOL	C	1378	6/6	0.61	0.36	68,68,68,68	0
4	MG	A	1377	1/1	0.68	0.28	42,42,42,42	0
4	MG	D	1377	1/1	0.81	0.23	56,56,56,56	0
4	MG	C	1377	1/1	0.83	0.13	44,44,44,44	0

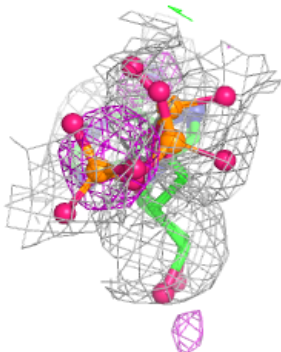
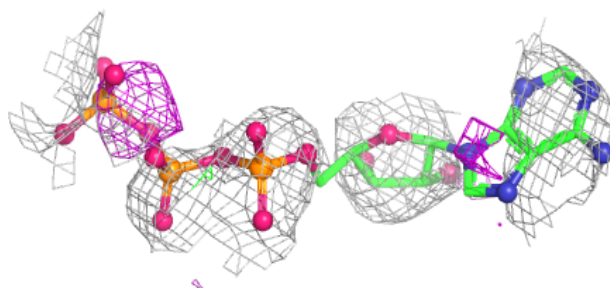
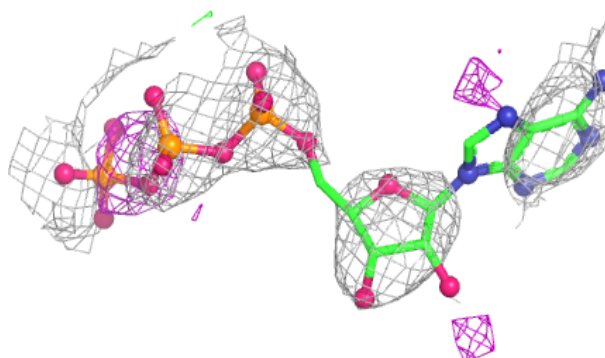
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP D 1376:

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

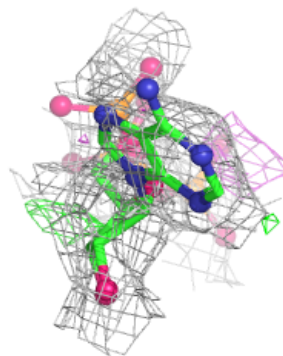
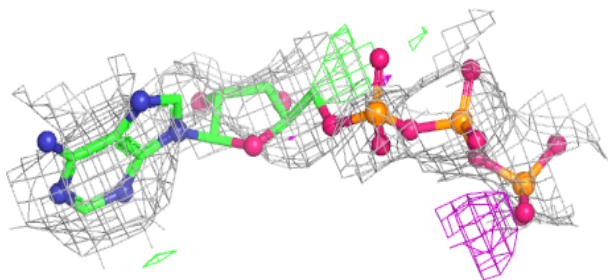
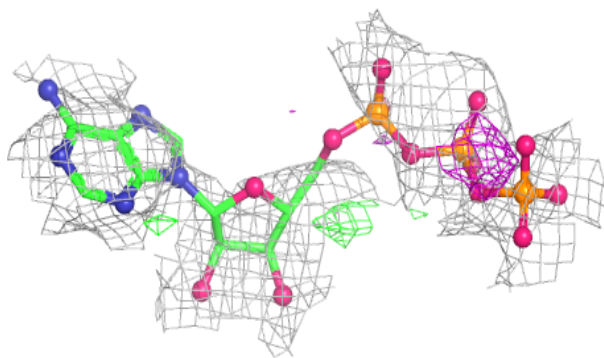
**Electron density around ATP F 1376:**

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

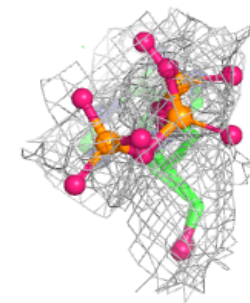
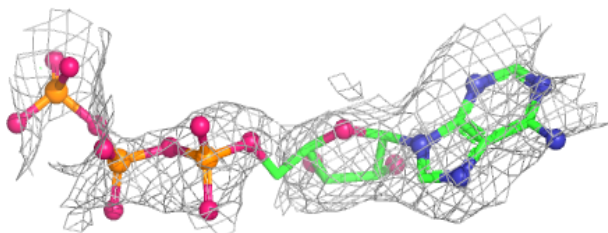
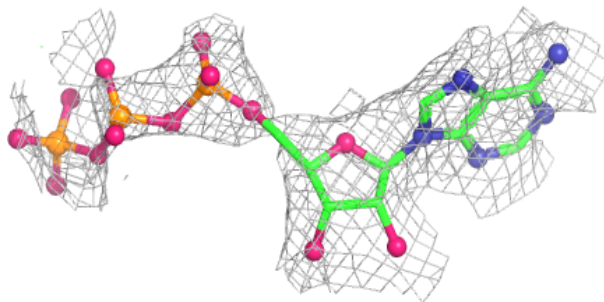


Electron density around ATP A 1376:

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

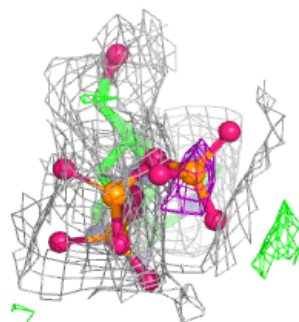
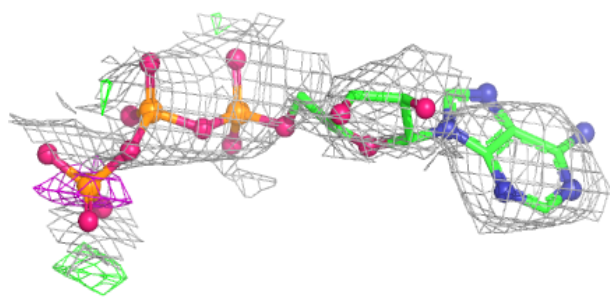
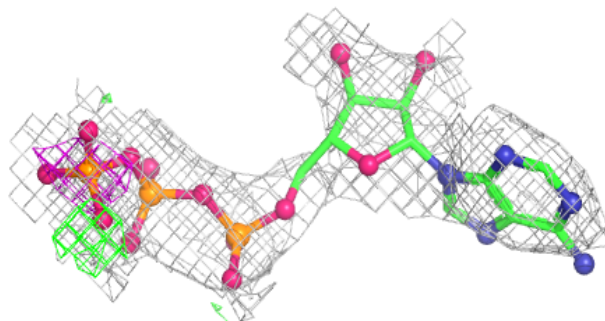
**Electron density around ATP E 1376:**

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

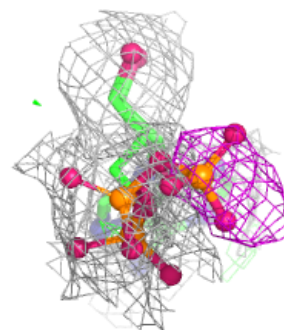
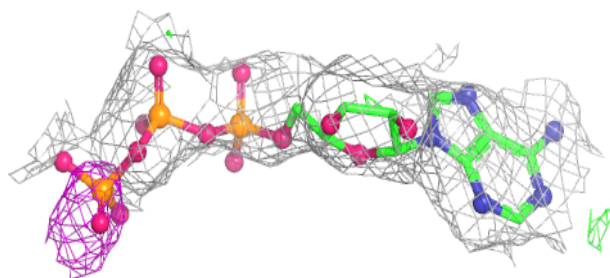
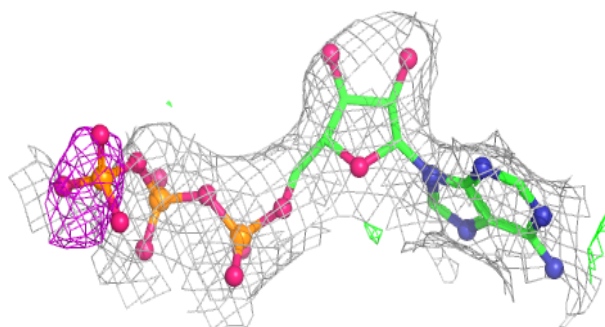


Electron density around ATP C 1376:

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

**Electron density around ATP B 1376:**

$2mF_o-DF_c$ (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.