



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:40 pm BST

PDB ID : 5CE3  
Title : The Yersinia YopO - actin complex with MgADP  
Authors : Lee, W.L.; Singaravelu, P.; Grimes, J.M.; Robinson, R.C.  
Deposited on : 2015-07-06  
Resolution : 2.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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

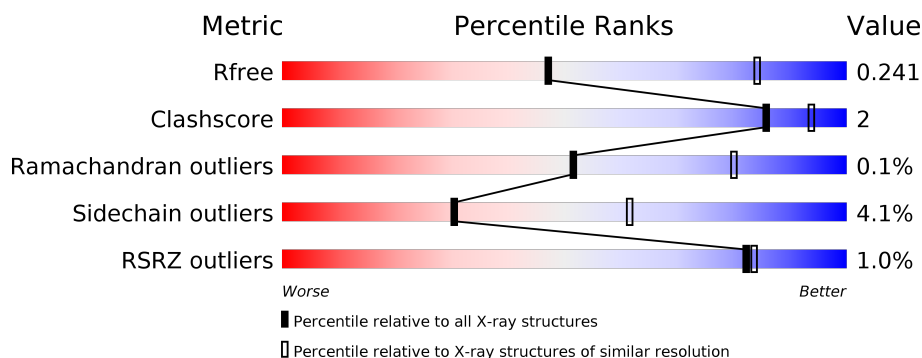
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	376	
1	C	376	
2	B	643	
2	D	643	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15121 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2786	1766	470	531	19			
1	C	358	Total	C	N	O	S	0	0	0
			2786	1766	470	531	19			

- Molecule 2 is a protein called Protein kinase YopO.

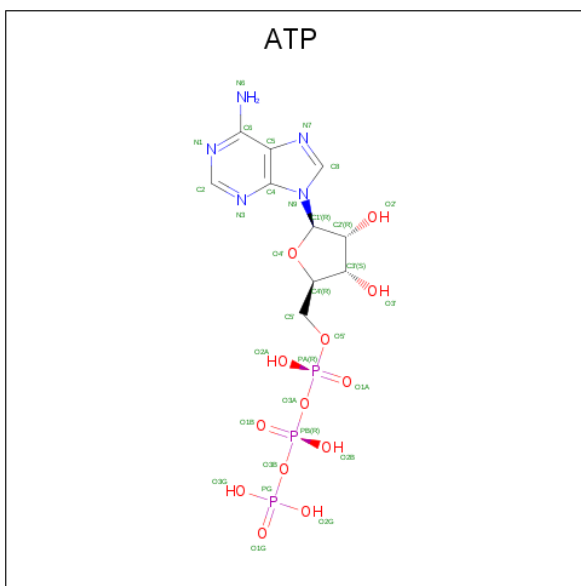
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	598	Total	C	N	O	S	0	0	0
			4710	2960	827	908	15			
2	D	598	Total	C	N	O	S	0	0	0
			4710	2960	827	908	15			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	GLY	-	expression tag	UNP Q93KQ6
B	88	PRO	-	expression tag	UNP Q93KQ6
B	205	TYR	LYS	engineered mutation	UNP Q93KQ6
B	206	TYR	GLU	engineered mutation	UNP Q93KQ6
B	207	TYR	GLU	engineered mutation	UNP Q93KQ6
B	440	TYR	LYS	engineered mutation	UNP Q93KQ6
B	441	TYR	LYS	engineered mutation	UNP Q93KQ6
D	87	GLY	-	expression tag	UNP Q93KQ6
D	88	PRO	-	expression tag	UNP Q93KQ6
D	205	TYR	LYS	engineered mutation	UNP Q93KQ6
D	206	TYR	GLU	engineered mutation	UNP Q93KQ6
D	207	TYR	GLU	engineered mutation	UNP Q93KQ6
D	440	TYR	LYS	engineered mutation	UNP Q93KQ6
D	441	TYR	LYS	engineered mutation	UNP Q93KQ6

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:

$\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).

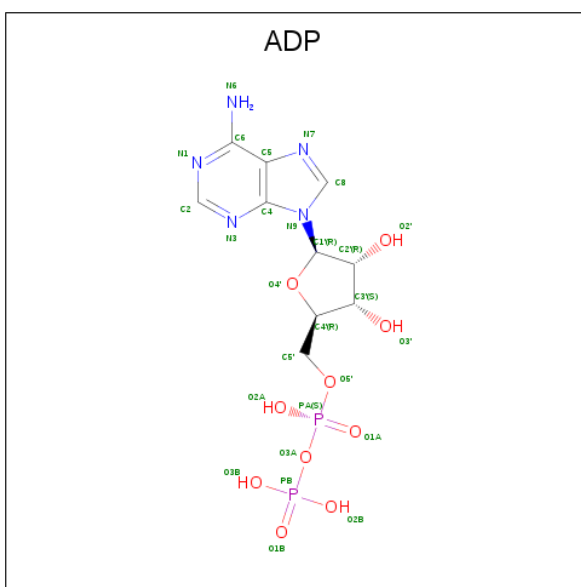


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

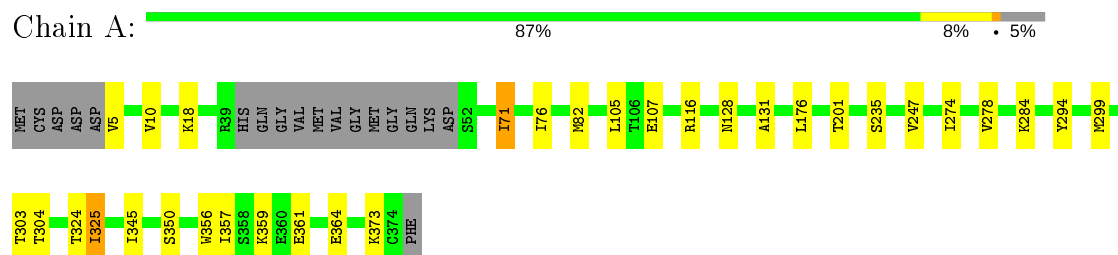
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		
7	B	3	Total	O	0	0
			3	3		
7	C	1	Total	O	0	0
			1	1		
7	D	2	Total	O	0	0
			2	2		

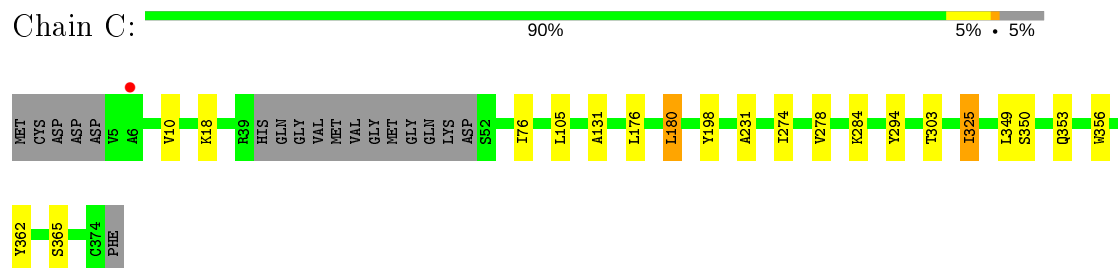
### 3 Residue-property plots [i](#)

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.

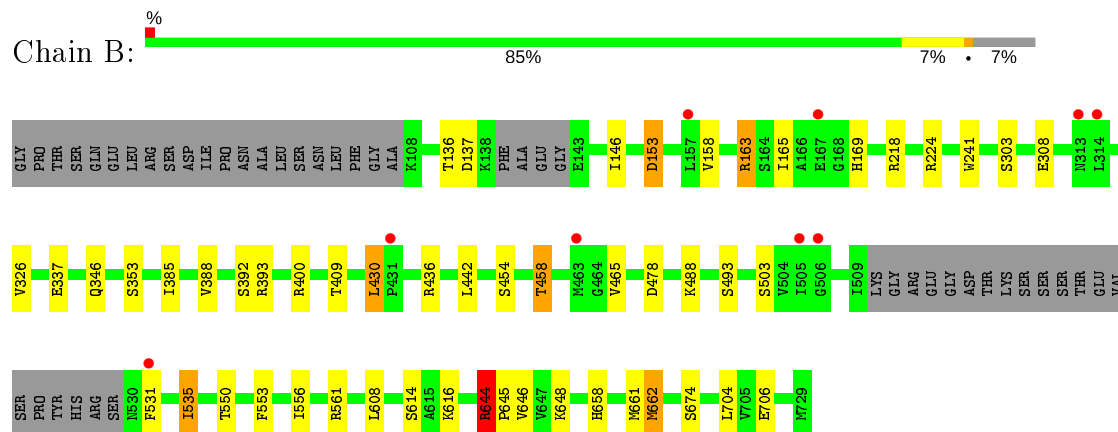
#### • Molecule 1: Actin



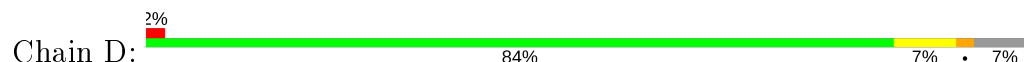
#### • Molecule 1: Actin

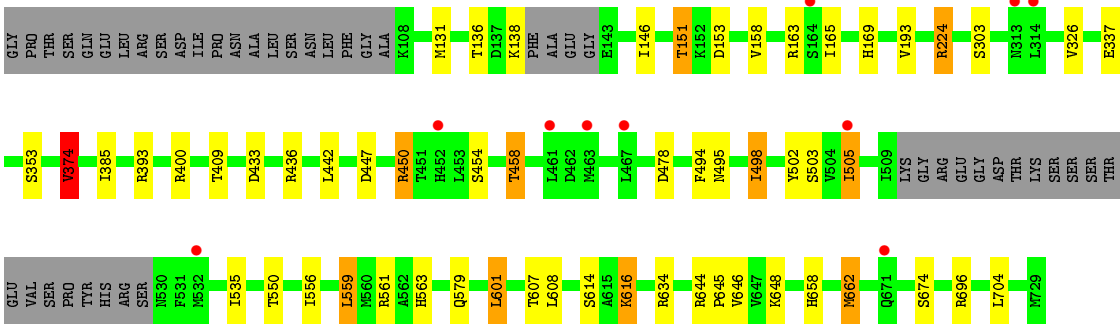


#### • Molecule 2: Protein kinase YopO



#### • Molecule 2: Protein kinase YopO





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.73Å 121.75Å 118.58Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	114.60 – 2.93 114.60 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.3 (114.60-2.93) 99.3 (114.60-2.93)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX 5.8.0107, REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.196 , 0.240 0.203 , 0.241	Depositor DCC
$R_{free}$ test set	3230 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	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 50.29 % 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 6.6078e-05. 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: ATP, MG, CA, 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	0.50	0/2846	0.72	0/3857
1	C	0.48	0/2846	0.71	0/3857
2	B	0.49	0/4796	0.74	7/6484 (0.1%)
2	D	0.49	0/4796	0.75	7/6484 (0.1%)
All	All	0.49	0/15284	0.73	14/20682 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	ASP	CB-CG-OD1	6.86	124.47	118.30
2	D	662	MET	CG-SD-CE	-6.19	90.29	100.20
2	B	662	MET	CG-SD-CE	-6.09	90.45	100.20
2	B	644	ARG	NE-CZ-NH1	5.87	123.24	120.30
2	B	163	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	D	224	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	D	374	VAL	CB-CA-C	-5.38	101.18	111.40
2	B	430	LEU	CA-CB-CG	5.31	127.51	115.30
2	D	450	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	B	436	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	D	634	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	D	498	ILE	CG1-CB-CG2	-5.11	100.16	111.40
2	D	400	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	B	400	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	2786	0	2762	15	0
1	C	2786	0	2762	13	0
2	B	4710	0	4701	22	0
2	D	4710	0	4701	22	0
3	A	31	0	12	0	0
3	C	31	0	12	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	B	27	0	12	1	0
5	D	27	0	12	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
All	All	15121	0	14974	67	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 2.

All (67) 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)
2:B:556:ILE:HD11	2:B:608:LEU:HB3	1.71	0.71
2:B:658:HIS:CE1	2:B:662:MET:HE3	2.27	0.69
2:D:658:HIS:CE1	2:D:662:MET:HE3	2.27	0.68
1:A:10:VAL:HG22	1:A:105:LEU:HD23	1.80	0.64
1:A:176:LEU:HD21	1:A:284:LYS:HE3	1.80	0.64
1:C:176:LEU:HD21	1:C:284:LYS:HE3	1.81	0.63
1:C:10:VAL:HG22	1:C:105:LEU:HD23	1.81	0.63
2:B:388:VAL:HG22	2:B:392:SER:HB2	1.81	0.63
2:B:326:VAL:HG21	2:B:385:ILE:HG21	1.82	0.59
2:D:494:PHE:O	2:D:498:ILE:HD12	2.01	0.59
2:D:326:VAL:HG21	2:D:385:ILE:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:ARG:HD3	2:B:337:GLU:OE2	2.02	0.58
2:D:224:ARG:HD3	2:D:337:GLU:OE2	2.03	0.58
1:A:247:VAL:HG11	2:B:644:ARG:NH2	2.19	0.58
1:C:274:ILE:O	1:C:278:VAL:HG23	2.03	0.58
1:A:274:ILE:O	1:A:278:VAL:HG23	2.03	0.57
1:A:299:MET:HE3	1:A:304:THR:HB	1.88	0.56
1:C:231:ALA:O	2:D:696:ARG:NH1	2.39	0.55
2:D:556:ILE:HD11	2:D:608:LEU:HB3	1.89	0.55
2:D:645:PRO:HA	2:D:662:MET:HE2	1.88	0.55
2:B:645:PRO:HA	2:B:662:MET:HE2	1.89	0.54
1:C:294:TYR:CD2	1:C:325:ILE:HG21	2.45	0.52
1:C:362:TYR:O	1:C:365:SER:O	2.27	0.52
2:D:146:ILE:HD13	5:D:801:ADP:O4'	2.09	0.51
2:D:146:ILE:CD1	5:D:801:ADP:O4'	2.58	0.51
2:B:531:PHE:CZ	2:B:535:ILE:HD11	2.45	0.51
2:D:478:ASP:OD1	2:D:561:ARG:NH2	2.44	0.50
1:A:294:TYR:CD2	1:A:325:ILE:HG21	2.46	0.50
2:B:531:PHE:O	2:B:535:ILE:HD13	2.12	0.50
2:D:495:ASN:HA	2:D:498:ILE:HD13	1.94	0.49
1:A:107:GLU:OE2	1:A:116:ARG:NH1	2.45	0.49
2:D:502:TYR:O	2:D:505:ILE:O	2.31	0.48
2:D:559:LEU:O	2:D:601:LEU:HD21	2.13	0.48
1:C:198:TYR:CD1	2:D:374:VAL:HG22	2.47	0.48
1:C:353:GLN:OE1	1:C:353:GLN:N	2.46	0.48
2:B:478:ASP:OD1	2:B:561:ARG:NH2	2.46	0.48
2:B:146:ILE:HG23	2:B:158:VAL:HG13	1.96	0.47
2:D:616:LYS:HG2	2:D:704:LEU:HD13	1.96	0.47
2:B:616:LYS:HG2	2:B:704:LEU:HD13	1.97	0.47
2:D:146:ILE:HG23	2:D:158:VAL:HG13	1.96	0.47
2:D:454:SER:O	2:D:458:THR:HG23	2.15	0.47
2:B:454:SER:O	2:B:458:THR:HG23	2.15	0.46
1:A:247:VAL:HG11	2:B:644:ARG:HH21	1.81	0.45
2:B:308:GLU:OE2	2:B:393:ARG:NH2	2.48	0.45
2:B:556:ILE:CD1	2:B:608:LEU:HB3	2.44	0.45
1:A:357:ILE:HG12	1:A:373:LYS:HD3	1.98	0.44
2:B:658:HIS:CE1	2:B:662:MET:CE	2.97	0.44
2:D:658:HIS:CE1	2:D:662:MET:CE	2.97	0.44
1:A:131:ALA:HB1	1:A:356:TRP:HB3	1.98	0.44
2:D:131:MET:HG2	2:D:151:THR:HB	2.00	0.44
1:C:131:ALA:HB1	1:C:356:TRP:HB3	1.98	0.43
2:B:648:LYS:HE2	2:B:658:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:648:LYS:HE2	2:D:658:HIS:CE1	2.54	0.43
2:B:218:ARG:NH1	5:B:801:ADP:O3'	2.52	0.42
2:B:388:VAL:O	2:B:393:ARG:NH1	2.53	0.41
1:A:201:THR:HG22	2:B:241:TRP:CE2	2.55	0.41
1:C:76:ILE:H	1:C:76:ILE:HD12	1.84	0.41
1:A:76:ILE:H	1:A:76:ILE:HD12	1.84	0.41
2:D:563:HIS:HB2	2:D:601:LEU:HD22	2.03	0.41
1:A:71:ILE:HD11	1:A:82:MET:CE	2.50	0.41
1:C:180:LEU:C	1:C:180:LEU:HD12	2.41	0.41
1:A:361:GLU:HA	1:A:364:GLU:HG2	2.03	0.41
1:C:303:THR:O	1:C:303:THR:HG22	2.21	0.41
2:B:553:PHE:O	2:B:556:ILE:HG12	2.20	0.40
1:A:303:THR:O	1:A:303:THR:HG22	2.21	0.40
1:C:349:LEU:O	1:C:353:GLN:OE1	2.39	0.40
2:D:447:ASP:OD1	2:D:450:ARG:NH1	2.53	0.40

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	354/376 (94%)	348 (98%)	6 (2%)	0	100	100
1	C	354/376 (94%)	347 (98%)	7 (2%)	0	100	100
2	B	592/643 (92%)	572 (97%)	19 (3%)	1 (0%)	47	76
2	D	592/643 (92%)	574 (97%)	17 (3%)	1 (0%)	47	76
All	All	1892/2038 (93%)	1841 (97%)	49 (3%)	2 (0%)	51	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	646	VAL
2	D	646	VAL

### 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	301/316 (95%)	291 (97%)	10 (3%)	38	69
1	C	301/316 (95%)	297 (99%)	4 (1%)	69	88
2	B	517/554 (93%)	493 (95%)	24 (5%)	27	57
2	D	517/554 (93%)	488 (94%)	29 (6%)	21	50
All	All	1636/1740 (94%)	1569 (96%)	67 (4%)	30	61

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	18	LYS
1	A	71	ILE
1	A	128	ASN
1	A	235	SER
1	A	324	THR
1	A	325	ILE
1	A	345	ILE
1	A	350	SER
1	A	359	LYS
2	B	136	THR
2	B	137	ASP
2	B	153	ASP
2	B	163	ARG
2	B	165	ILE
2	B	169	HIS
2	B	303	SER
2	B	346	GLN
2	B	353	SER
2	B	409	THR

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Mol	Chain	Res	Type
2	B	430	LEU
2	B	442	LEU
2	B	458	THR
2	B	465	VAL
2	B	488	LYS
2	B	493	SER
2	B	503	SER
2	B	535	ILE
2	B	550	THR
2	B	614	SER
2	B	644	ARG
2	B	661	MET
2	B	674	SER
2	B	706	GLU
1	C	18	LYS
1	C	180	LEU
1	C	325	ILE
1	C	350	SER
2	D	136	THR
2	D	138	LYS
2	D	151	THR
2	D	153	ASP
2	D	163	ARG
2	D	165	ILE
2	D	169	HIS
2	D	193	VAL
2	D	303	SER
2	D	353	SER
2	D	374	VAL
2	D	393	ARG
2	D	409	THR
2	D	433	ASP
2	D	436	ARG
2	D	442	LEU
2	D	458	THR
2	D	503	SER
2	D	505	ILE
2	D	535	ILE
2	D	550	THR
2	D	559	LEU
2	D	579	GLN
2	D	601	LEU

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Mol	Chain	Res	Type
2	D	607	THR
2	D	614	SER
2	D	616	LYS
2	D	644	ARG
2	D	674	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	256	ASN
2	B	397	ASN
2	B	530	ASN
2	B	638	GLN
2	D	155	GLN
2	D	460	GLN
2	D	530	ASN
2	D	546	HIS
2	D	638	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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	401	4	26,33,33	0.96	1 (3%)	31,52,52	1.40	4 (12%)
5	ADP	B	801	6	24,29,29	0.99	1 (4%)	29,45,45	1.38	4 (13%)
3	ATP	C	401	4	26,33,33	0.96	1 (3%)	31,52,52	1.41	4 (12%)
5	ADP	D	801	6	24,29,29	0.93	1 (4%)	29,45,45	1.44	6 (20%)

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	401	4	-	1/18/38/38	0/3/3/3
5	ADP	B	801	6	-	2/12/32/32	0/3/3/3
3	ATP	C	401	4	-	3/18/38/38	0/3/3/3
5	ADP	D	801	6	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	ADP	C5-C4	2.42	1.47	1.40
5	D	801	ADP	C5-C4	2.38	1.47	1.40
3	C	401	ATP	C5-C4	2.34	1.47	1.40
3	A	401	ATP	C5-C4	2.32	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	801	ADP	N3-C2-N1	-3.80	122.75	128.68
5	B	801	ADP	N3-C2-N1	-3.75	122.82	128.68
3	C	401	ATP	PA-O3A-PB	-3.56	120.61	132.83
3	A	401	ATP	PA-O3A-PB	-3.35	121.35	132.83
3	C	401	ATP	N3-C2-N1	-3.30	123.53	128.68
3	A	401	ATP	N3-C2-N1	-3.27	123.57	128.68
5	D	801	ADP	C4-C5-N7	-3.06	106.21	109.40
3	C	401	ATP	C4-C5-N7	-2.89	106.39	109.40
3	A	401	ATP	C4-C5-N7	-2.83	106.45	109.40
5	B	801	ADP	C1'-N9-C4	-2.78	121.75	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	801	ADP	C1'-N9-C4	-2.71	121.88	126.64
5	D	801	ADP	C3'-C2'-C1'	2.44	104.66	100.98
3	A	401	ATP	PB-O3B-PG	-2.32	124.86	132.83
5	B	801	ADP	C4-C5-N7	-2.30	107.00	109.40
5	B	801	ADP	C2-N1-C6	2.24	122.59	118.75
5	D	801	ADP	C2-N1-C6	2.10	122.34	118.75
3	C	401	ATP	C1'-N9-C4	-2.07	123.01	126.64
5	D	801	ADP	O2A-PA-O1A	2.01	122.17	112.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

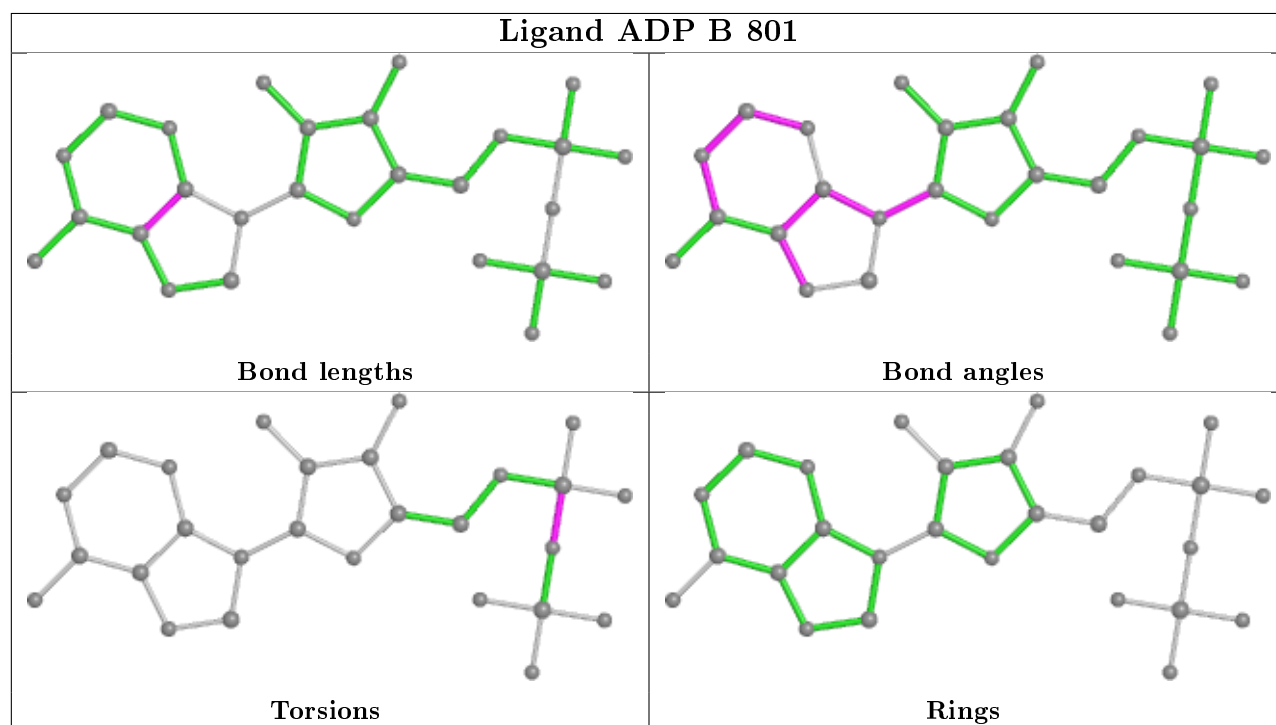
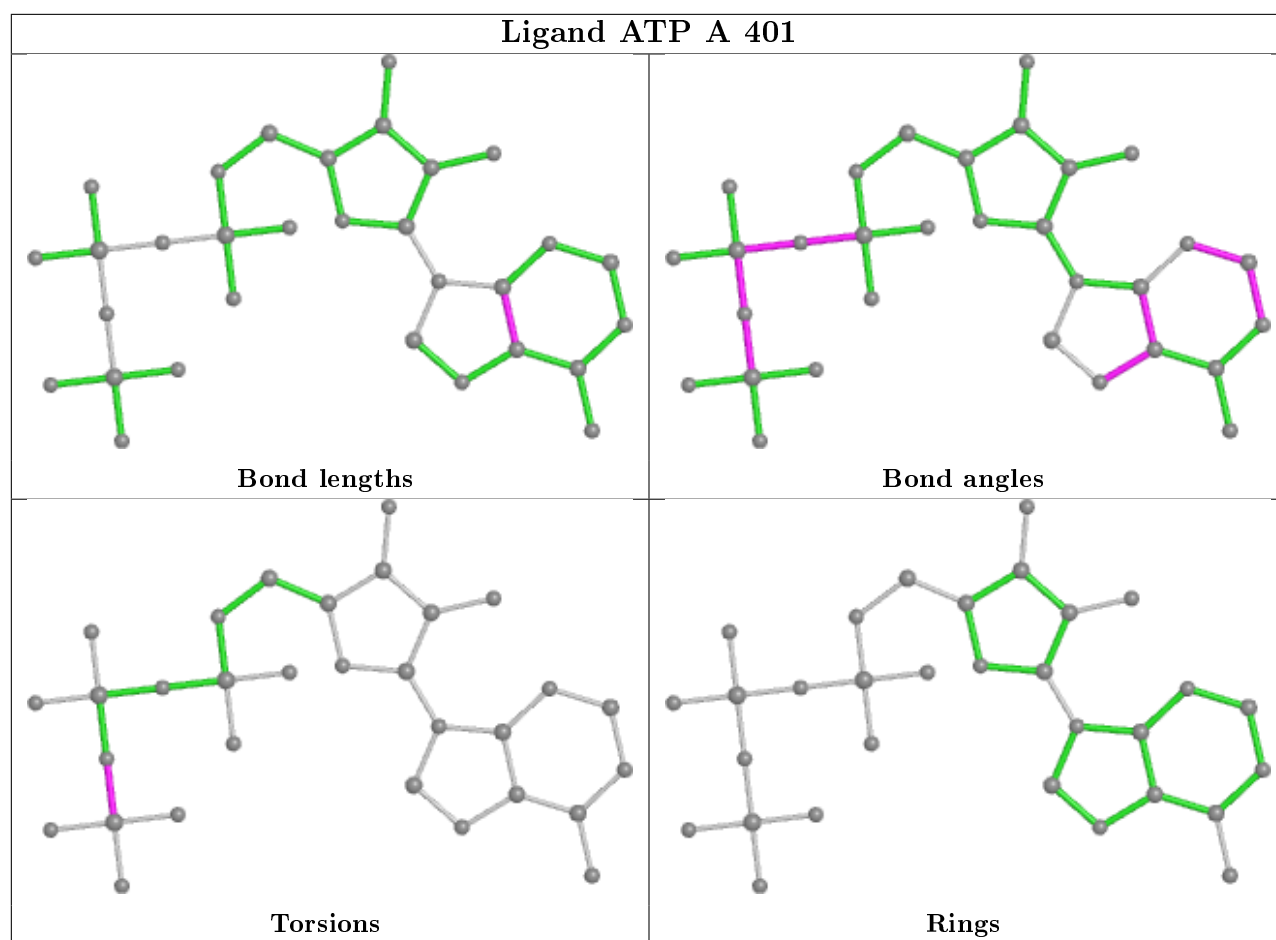
Mol	Chain	Res	Type	Atoms
3	C	401	ATP	PB-O3B-PG-O3G
3	C	401	ATP	PB-O3B-PG-O2G
5	B	801	ADP	PB-O3A-PA-O2A
5	D	801	ADP	PB-O3A-PA-O2A
3	C	401	ATP	PB-O3B-PG-O1G
3	A	401	ATP	PB-O3B-PG-O2G
5	B	801	ADP	PB-O3A-PA-O1A
5	D	801	ADP	PB-O3A-PA-O1A

There are no ring outliers.

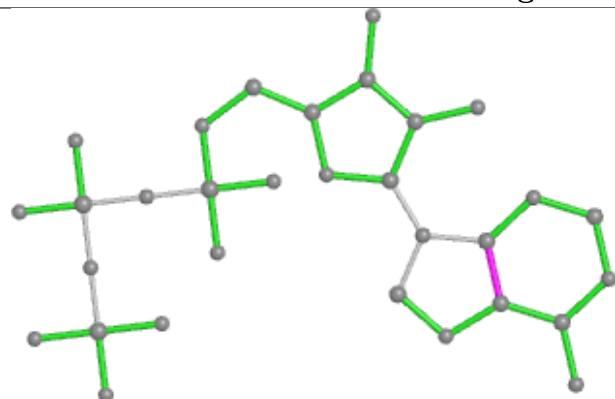
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	ADP	1	0
5	D	801	ADP	2	0

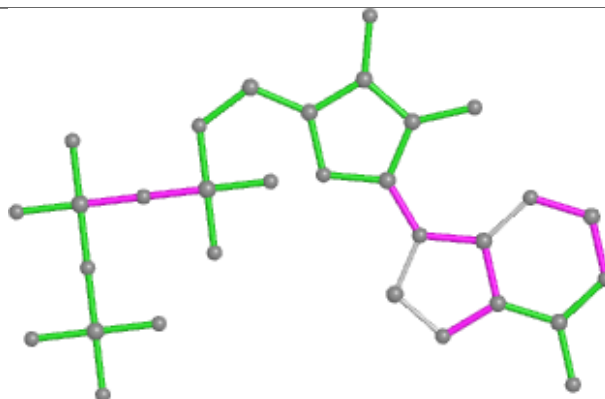
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



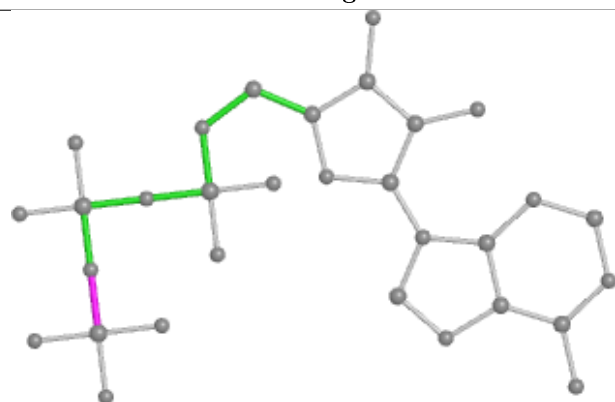
## Ligand ATP C 401



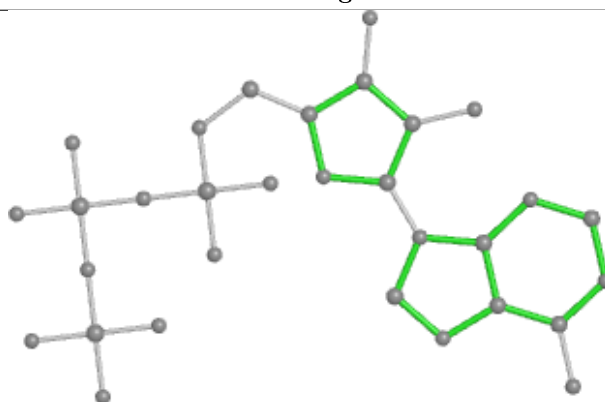
Bond lengths



Bond angles

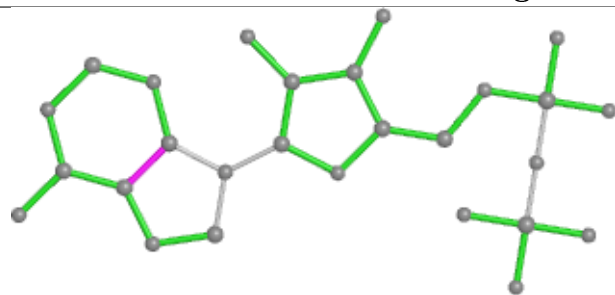


Torsions

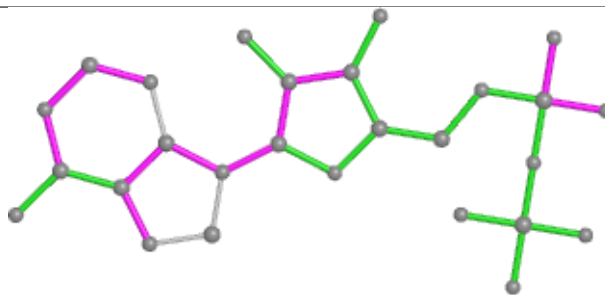


Rings

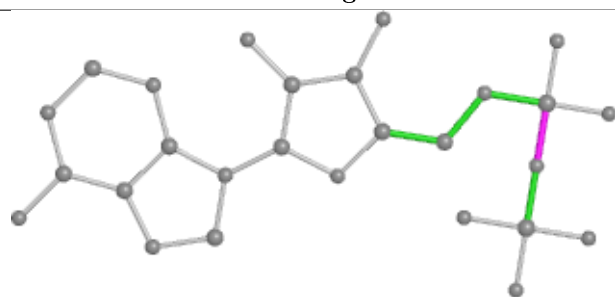
## Ligand ADP D 801



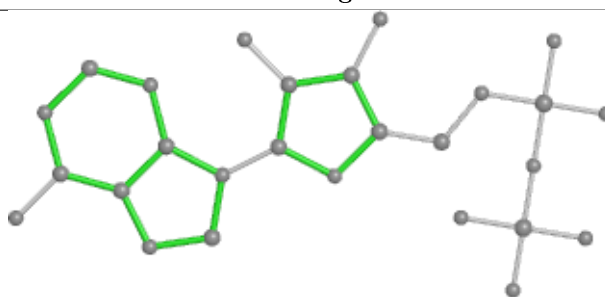
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	358/376 (95%)	0.10	0 100 100	49, 67, 102, 118	0
1	C	358/376 (95%)	0.09	1 (0%) 94 94	48, 68, 98, 112	0
2	B	598/643 (93%)	0.21	9 (1%) 73 75	50, 76, 113, 147	0
2	D	598/643 (93%)	0.23	10 (1%) 70 71	48, 76, 113, 138	0
All	All	1912/2038 (93%)	0.17	20 (1%) 82 83	48, 72, 108, 147	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	463	MET	3.4
2	D	164	SER	3.3
2	B	313	ASN	3.1
2	B	505	ILE	2.7
2	D	461	LEU	2.5
2	B	506	GLY	2.5
2	D	505	ILE	2.5
2	D	313	ASN	2.4
2	B	463	MET	2.4
2	D	467	LEU	2.3
2	B	431	PRO	2.3
1	C	6	ALA	2.3
2	B	314	LEU	2.2
2	B	157	LEU	2.2
2	B	167	GLU	2.1
2	D	532	MET	2.1
2	D	452	HIS	2.1
2	D	314	LEU	2.1
2	B	531	PHE	2.1
2	D	671	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

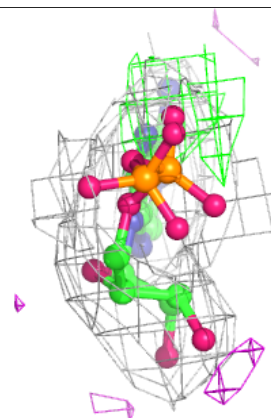
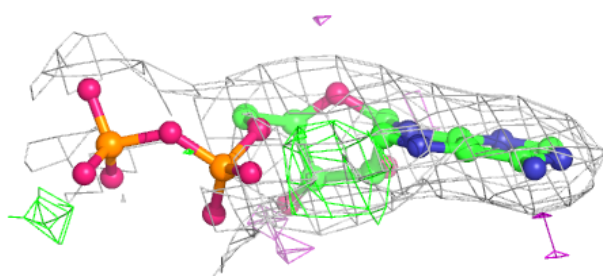
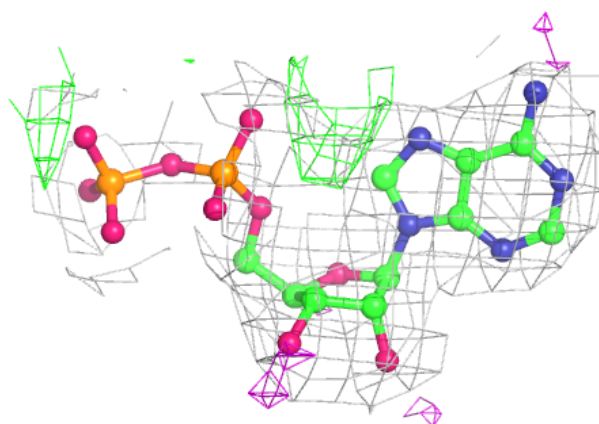
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	CA	C	402	1/1	0.96	0.25	66,66,66,66	0
5	ADP	D	801	27/27	0.96	0.18	52,57,66,71	0
5	ADP	B	801	27/27	0.97	0.18	51,56,66,68	0
6	MG	B	802	1/1	0.98	0.14	59,59,59,59	0
6	MG	D	802	1/1	0.98	0.21	51,51,51,51	0
3	ATP	A	401	31/31	0.99	0.18	48,54,59,62	0
4	CA	A	402	1/1	0.99	0.19	59,59,59,59	0
3	ATP	C	401	31/31	0.99	0.18	47,52,56,59	0

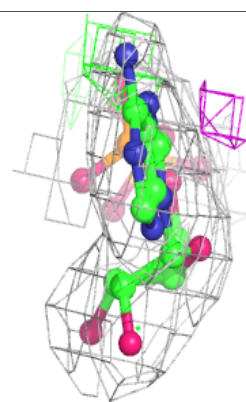
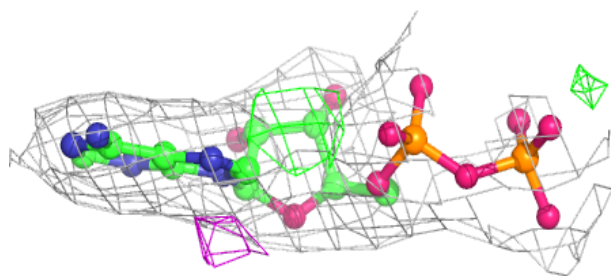
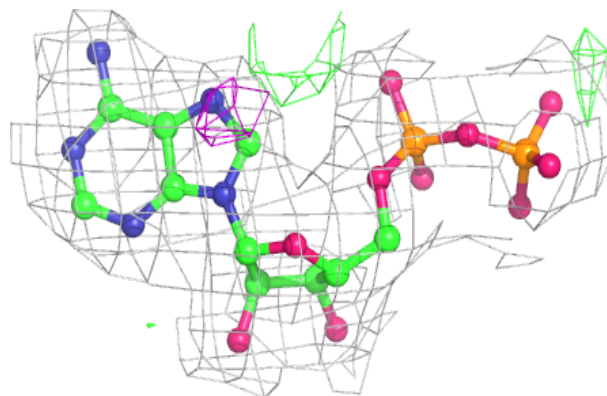
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP D 801:**

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

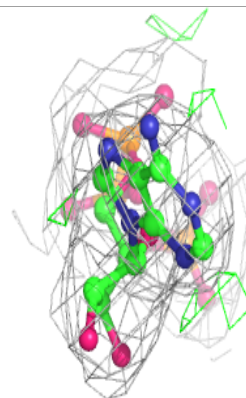
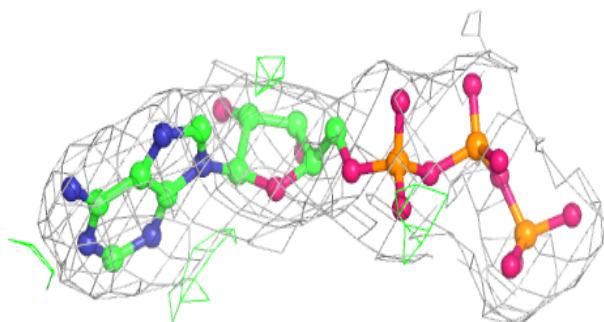
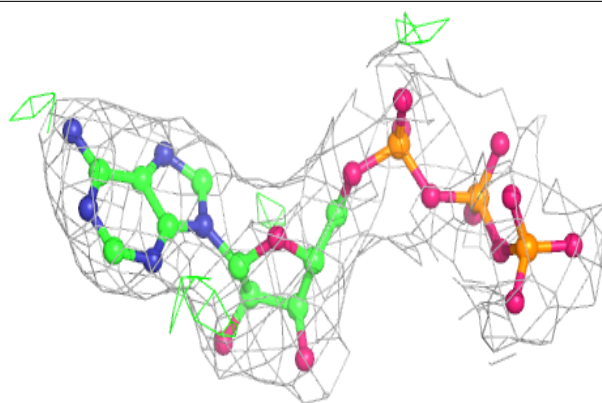
**Electron density around ADP B 801:**

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

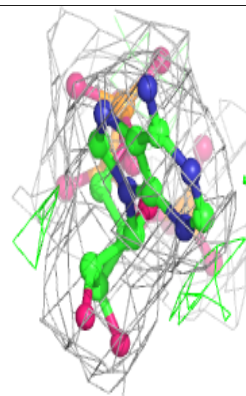
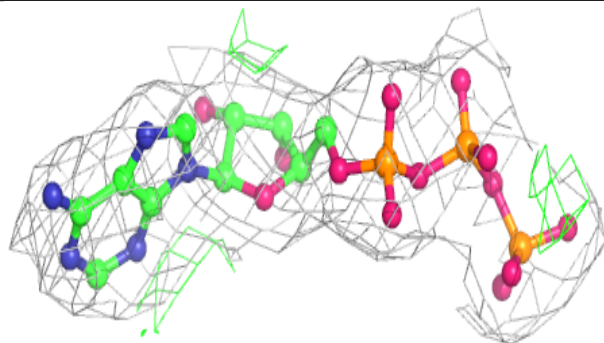
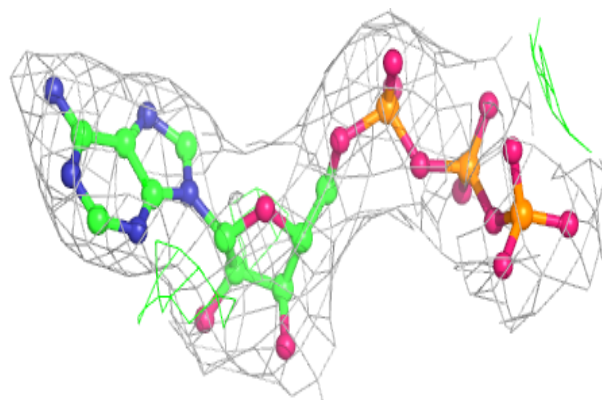


**Electron density around ATP A 401:**

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

**Electron density around ATP C 401:**

$2mF_o-DF_c$  (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.