



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 06:31 PM UTC

PDB ID : 2Y8L / pdb_00002y8l
Title : Structure of the regulatory fragment of mammalian aMPK in complex with two ADP
Authors : Xiao, B.; Sanders, M.J.; Underwood, E.; Heath, R.; Mayer, F.; Carmena, D.; Jing, C.; Walker, P.A.; Eccleston, J.F.; Haire, L.F.; Saiu, P.; Howell, S.A.; Aasland, R.; Martin, S.R.; Carling, D.; Gamblin, S.J.
Deposited on : 2011-02-07
Resolution : 2.50 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](#) ①) 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

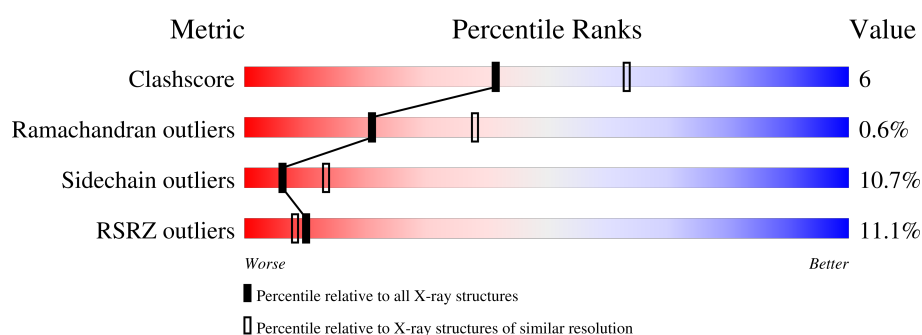
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	173	4% 45% 13% • 40%
2	B	87	18% 66% 6% 6% • 21%
3	E	330	9% 73% 17% • 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4045 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 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUB-UNIT ALPHA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			855	539	152	157	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	MET	-	expression tag	UNP P54645
A	379	SER	-	expression tag	UNP P54645
A	380	HIS	-	expression tag	UNP P54645
A	381	HIS	-	expression tag	UNP P54645
A	382	HIS	-	expression tag	UNP P54645
A	383	HIS	-	expression tag	UNP P54645
A	384	HIS	-	expression tag	UNP P54645
A	385	HIS	-	expression tag	UNP P54645
A	386	SER	-	expression tag	UNP P54645
A	387	GLY	-	expression tag	UNP P54645
A	388	LEU	-	expression tag	UNP P54645
A	389	VAL	-	expression tag	UNP P54645
A	390	PRO	-	expression tag	UNP P54645
A	391	ARG	-	expression tag	UNP P54645
A	392	GLY	-	expression tag	UNP P54645
A	393	SER	-	cloning artifact	UNP P54645
A	394	MET	-	cloning artifact	UNP P54645
A	395	ALA	-	cloning artifact	UNP P54645
A	545	ASN	-	cloning artifact	UNP P54645
A	546	SER	-	cloning artifact	UNP P54645
A	547	CYS	-	cloning artifact	UNP P54645
A	548	THR	-	cloning artifact	UNP P54645
A	549	VAL	-	cloning artifact	UNP P54645
A	550	ASN	-	cloning artifact	UNP P54645

- Molecule 2 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-

2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			570	374	97	96	3			

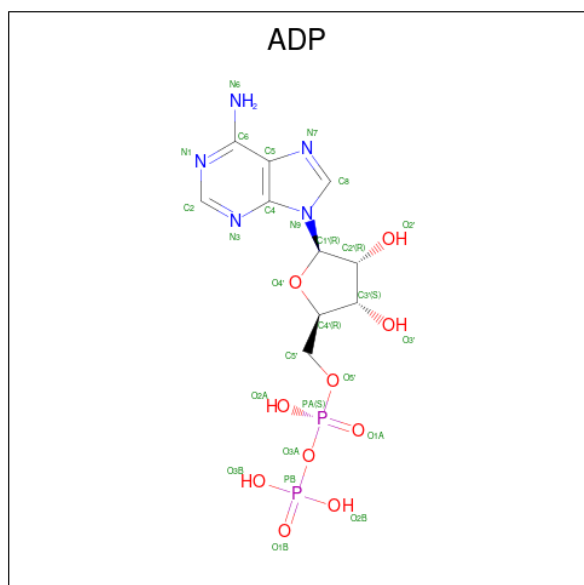
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	186	MET	-	cloning artifact	UNP O43741

- Molecule 3 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1.

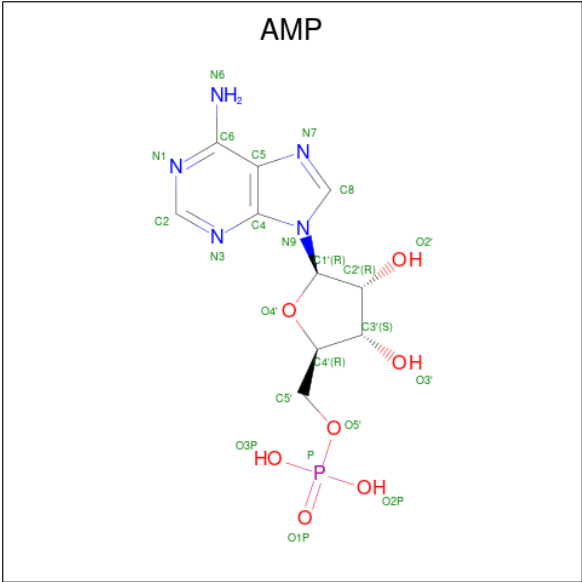
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	305	Total	C	N	O	S	0	0	1
			2442	1584	408	443	7			

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	17	Total	O	0	0
			17	17		
6	E	61	Total	O	0	0
			61	61		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.57Å 121.46Å 125.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.42 – 2.50 87.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (87.42-2.50) 97.8 (87.42-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.228 , 0.253 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4045	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: AMP, 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	0.58	0/873	0.83	1/1178 (0.1%)
2	B	0.60	0/585	0.98	4/789 (0.5%)
3	E	0.63	1/2494 (0.0%)	0.90	1/3386 (0.0%)
All	All	0.61	1/3952 (0.0%)	0.90	6/5353 (0.1%)

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
2	B	0	1
3	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	326	GLY	C-N	-6.90	1.23	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	237	MET	N-CA-C	-7.26	104.31	113.02
2	B	209	PRO	N-CA-C	7.14	119.42	110.70
3	E	182	PHE	N-CA-C	5.92	122.88	109.81
1	A	428	ASN	CB-CA-C	-5.61	100.69	109.22
2	B	201	ARG	N-CA-C	-5.45	106.67	113.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	209	PRO	Peptide
3	E	182	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	855	0	845	25	0
2	B	570	0	595	9	0
3	E	2442	0	2506	26	0
4	E	54	0	24	1	0
5	E	23	0	12	0	0
6	A	23	0	0	0	0
6	B	17	0	0	0	0
6	E	61	0	0	0	0
All	All	4045	0	3982	51	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 6.

The worst 5 of 51 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:208:LEU:O	2:B:210:PRO:HD3	1.44	1.14
3:E:84:MET:HE3	3:E:153:PRO:HG3	1.63	0.79
1:A:410:MET:HE2	1:A:410:MET:HA	1.66	0.77
1:A:416:ALA:HB2	1:A:546:SER:HB3	1.70	0.72
2:B:208:LEU:O	2:B:210:PRO:CD	2.36	0.65

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	100/173 (58%)	98 (98%)	2 (2%)	0	100	100
2	B	65/87 (75%)	57 (88%)	7 (11%)	1 (2%)	8	16
3	E	303/330 (92%)	287 (95%)	14 (5%)	2 (1%)	18	34
All	All	468/590 (79%)	442 (94%)	23 (5%)	3 (1%)	21	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	236	VAL
3	E	122	GLN
3	E	182	PHE

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	97/157 (62%)	91 (94%)	6 (6%)	16	34
2	B	65/81 (80%)	60 (92%)	5 (8%)	12	25
3	E	277/299 (93%)	241 (87%)	36 (13%)	4	8
All	All	439/537 (82%)	392 (89%)	47 (11%)	6	13

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	232	GLU
3	E	275	VAL
3	E	246	ILE
3	E	251	GLU
3	E	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	161	ASN
3	E	168	HIS
3	E	297	HIS
3	E	222	HIS
3	E	24	ASN

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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	E	1327	-	28,29,29	1.41	3 (10%)	43,45,45	1.97	11 (25%)
5	AMP	E	1329	-	25,25,25	1.43	3 (12%)	37,38,38	1.91	11 (29%)
4	ADP	E	1328	-	28,29,29	1.39	4 (14%)	43,45,45	1.80	9 (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
4	ADP	E	1327	-	-	4/16/32/32	0/3/3/3
5	AMP	E	1329	-	-	0/10/26/26	0/3/3/3
4	ADP	E	1328	-	-	7/16/32/32	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1329	AMP	C5-C4	4.89	1.47	1.39
4	E	1328	ADP	C5-C4	4.76	1.47	1.39
4	E	1327	ADP	C5-C4	4.65	1.47	1.39
4	E	1327	ADP	C5-C6	3.03	1.49	1.41
5	E	1329	AMP	C5-C6	2.72	1.48	1.41

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1327	ADP	C5-C4-N3	-5.57	119.04	126.72
5	E	1329	AMP	C5-C4-N3	-5.43	119.24	126.72
4	E	1328	ADP	C5-C4-N3	-5.05	119.76	126.72
4	E	1327	ADP	N3-C4-N9	4.58	134.96	127.17
5	E	1329	AMP	N3-C4-N9	4.45	134.74	127.17

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1328	ADP	PA-O3A-PB-O3B
4	E	1328	ADP	C5'-O5'-PA-O1A
4	E	1328	ADP	C5'-O5'-PA-O2A
4	E	1328	ADP	C5'-O5'-PA-O3A

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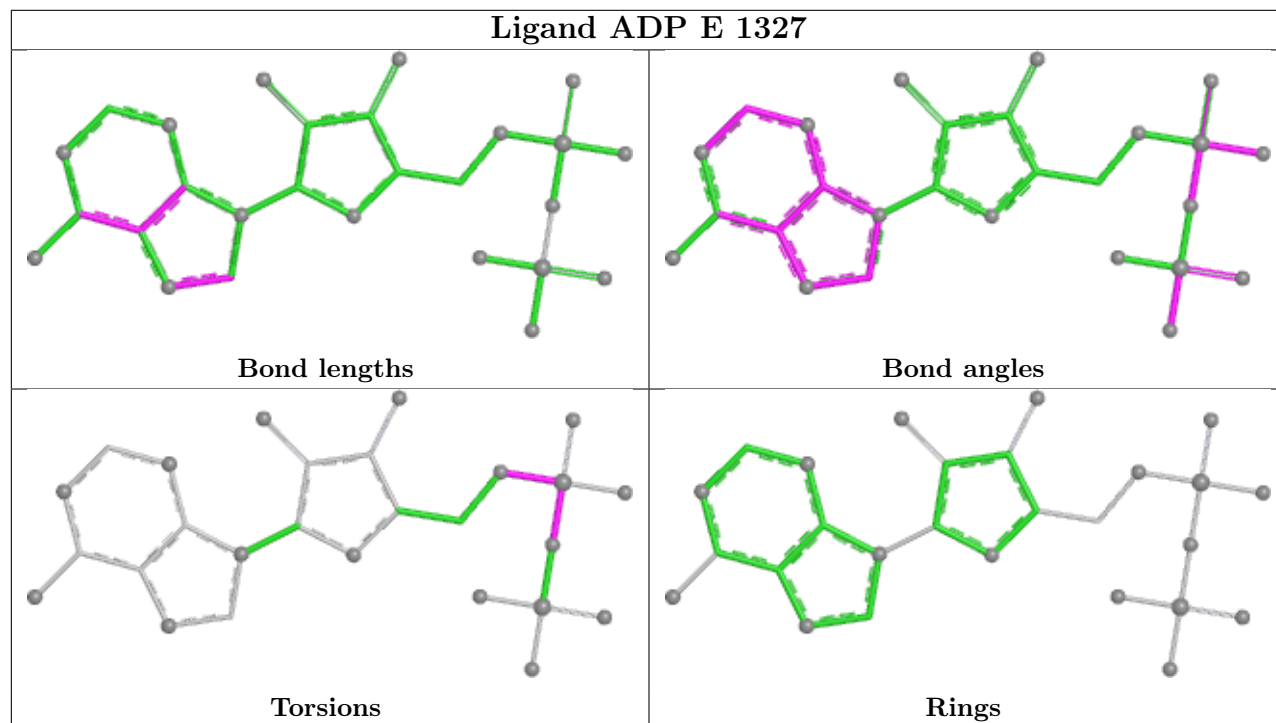
Mol	Chain	Res	Type	Atoms
4	E	1328	ADP	O4'-C4'-C5'-O5'

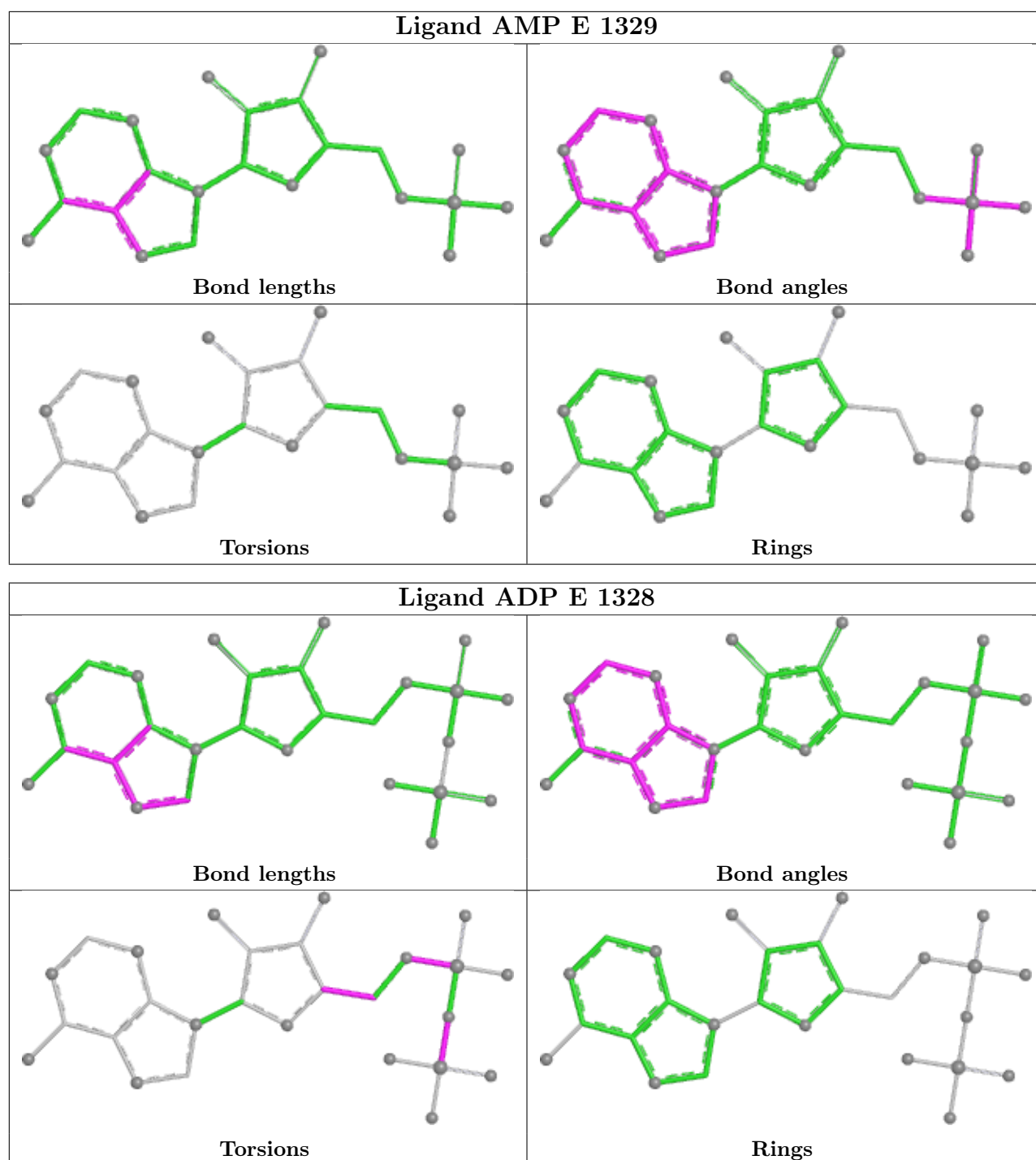
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1328	ADP	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	104/173 (60%)	0.42	7 (6%) 24 21	30, 54, 91, 111	0
2	B	69/87 (79%)	1.11	16 (23%) 2 1	32, 80, 102, 119	0
3	E	305/330 (92%)	0.40	30 (9%) 13 11	28, 50, 111, 199	0
All	All	478/590 (81%)	0.51	53 (11%) 10 8	28, 53, 105, 199	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	182	PHE	5.9
3	E	252	LYS	5.8
3	E	249	ALA	5.5
3	E	326	GLY	5.5
1	A	524	VAL	5.4

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](#)

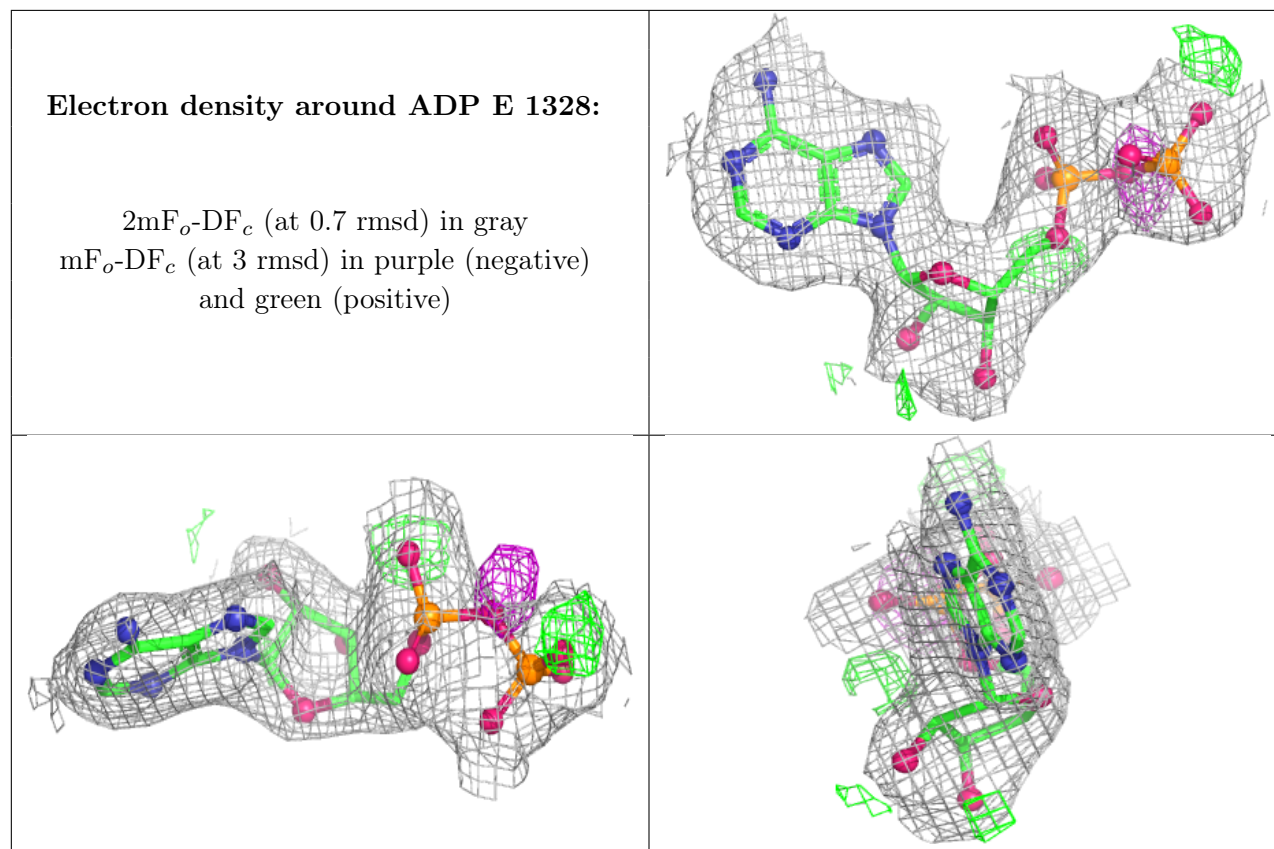
There are no oligosaccharides in this entry.

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, 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.

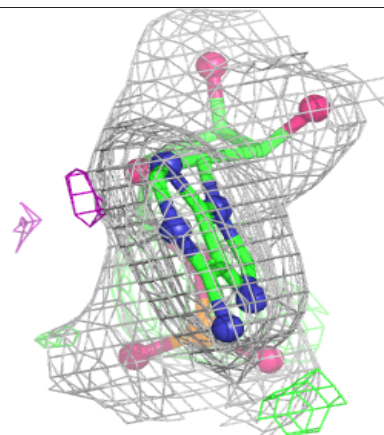
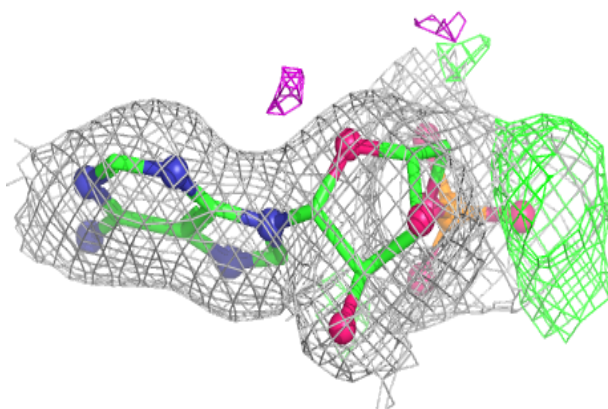
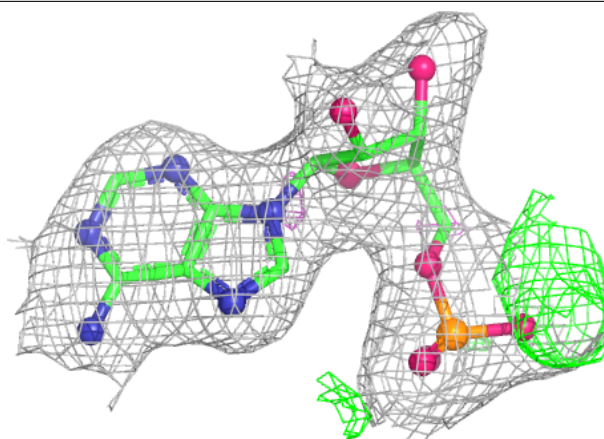
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	E	1328	27/27	0.89	0.09	52,62,71,73	0
5	AMP	E	1329	23/23	0.91	0.09	37,44,47,49	0
4	ADP	E	1327	27/27	0.98	0.06	39,43,47,51	0

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.



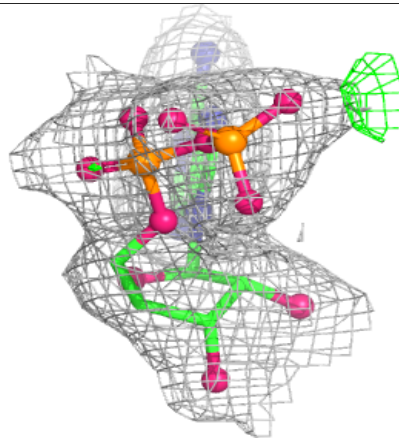
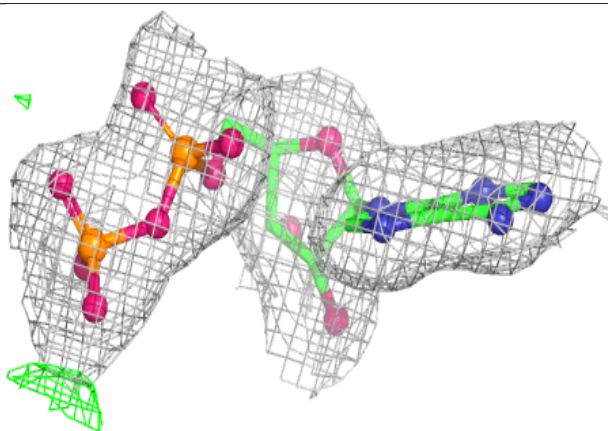
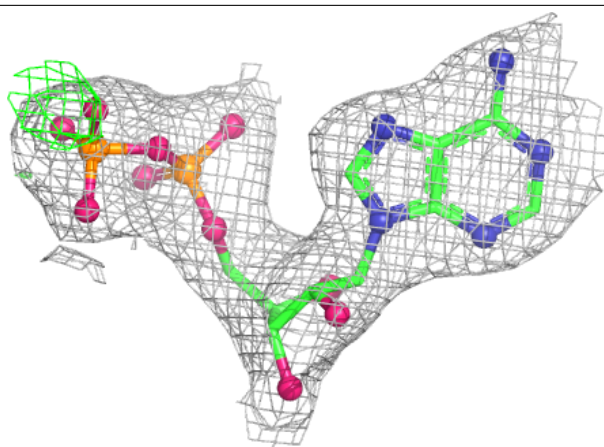
Electron density around AMP E 1329:

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



Electron density around ADP E 1327:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.