



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:39 PM GMT

PDB ID : 4CFF  
Title : Structure of full length human AMPK in complex with a small molecule activator, a thienopyridone derivative (A-769662)  
Authors : Xiao, B.; Sanders, M.J.; Carmena, D.; Bright, N.J.; Haire, L.F.; Underwood, E.; Patel, B.R.; Heath, R.B.; Walker, P.A.; Hallen, S.; Giordanetto, F.; Martin, S.R.; Carling, D.; Gamblin, S.J.  
Deposited on : 2013-11-14  
Resolution : 3.92 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

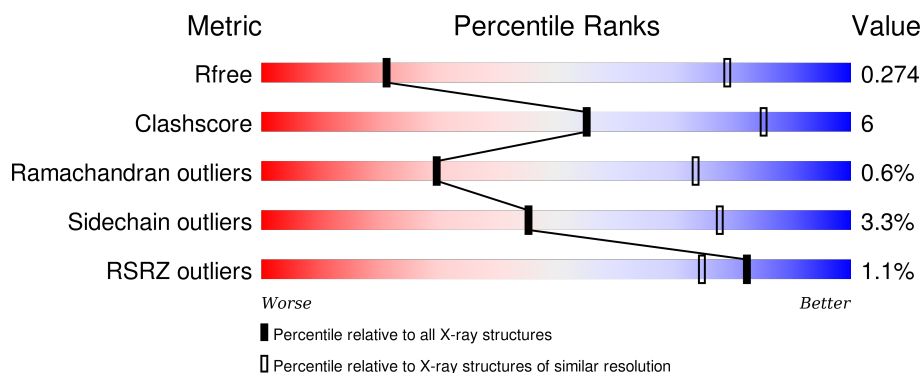
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.92 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))
$R_{free}$	91344	1047 (4.32-3.52)
Clashscore	102246	1008 (4.26-3.58)
Ramachandran outliers	100387	1044 (4.30-3.54)
Sidechain outliers	100360	1035 (4.30-3.54)
RSRZ outliers	91569	1002 (4.30-3.54)

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. 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	571	<div> <div>60%</div> <div>13%</div> <div>•</div> <div>26%</div> </div>
1	C	571	<div> <div>61%</div> <div>13%</div> <div>•</div> <div>26%</div> </div>
2	B	286	<div> <div>2%</div> <div>48%</div> <div>12%</div> <div>•</div> <div>40%</div> </div>
2	D	286	<div> <div>2%</div> <div>48%</div> <div>12%</div> <div>•</div> <div>40%</div> </div>
3	E	331	<div> <div>•</div> <div>70%</div> <div>18%</div> <div>•</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	331	<div><div><div>%</div><div><div></div><div></div><div></div></div><div>69%18%12%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14484 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-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	P	S	0	0	0
			3403	2187	592	601	1	22			
1	C	423	Total	C	N	O	P	S	0	0	0
			3394	2182	590	599	1	22			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	EXPRESSION TAG	UNP P54646
A	-17	SER	-	EXPRESSION TAG	UNP P54646
A	-16	HIS	-	EXPRESSION TAG	UNP P54646
A	-15	HIS	-	EXPRESSION TAG	UNP P54646
A	-14	HIS	-	EXPRESSION TAG	UNP P54646
A	-13	HIS	-	EXPRESSION TAG	UNP P54646
A	-12	HIS	-	EXPRESSION TAG	UNP P54646
A	-11	HIS	-	EXPRESSION TAG	UNP P54646
A	-10	SER	-	EXPRESSION TAG	UNP P54646
A	-9	SER	-	EXPRESSION TAG	UNP P54646
A	-8	GLY	-	EXPRESSION TAG	UNP P54646
A	-7	LEU	-	EXPRESSION TAG	UNP P54646
A	-6	GLU	-	EXPRESSION TAG	UNP P54646
A	-5	VAL	-	EXPRESSION TAG	UNP P54646
A	-4	LEU	-	EXPRESSION TAG	UNP P54646
A	-3	PHE	-	EXPRESSION TAG	UNP P54646
A	-2	GLN	-	EXPRESSION TAG	UNP P54646
A	-1	GLY	-	EXPRESSION TAG	UNP P54646
A	0	PRO	-	EXPRESSION TAG	UNP P54646
C	-18	MET	-	EXPRESSION TAG	UNP P54646
C	-17	SER	-	EXPRESSION TAG	UNP P54646
C	-16	HIS	-	EXPRESSION TAG	UNP P54646
C	-15	HIS	-	EXPRESSION TAG	UNP P54646
C	-14	HIS	-	EXPRESSION TAG	UNP P54646

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	EXPRESSION TAG	UNP P54646
C	-12	HIS	-	EXPRESSION TAG	UNP P54646
C	-11	HIS	-	EXPRESSION TAG	UNP P54646
C	-10	SER	-	EXPRESSION TAG	UNP P54646
C	-9	SER	-	EXPRESSION TAG	UNP P54646
C	-8	GLY	-	EXPRESSION TAG	UNP P54646
C	-7	LEU	-	EXPRESSION TAG	UNP P54646
C	-6	GLU	-	EXPRESSION TAG	UNP P54646
C	-5	VAL	-	EXPRESSION TAG	UNP P54646
C	-4	LEU	-	EXPRESSION TAG	UNP P54646
C	-3	PHE	-	EXPRESSION TAG	UNP P54646
C	-2	GLN	-	EXPRESSION TAG	UNP P54646
C	-1	GLY	-	EXPRESSION TAG	UNP P54646
C	0	PRO	-	EXPRESSION TAG	UNP P54646

- Molecule 2 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	P	S	0	0	0
			1351	872	227	246	1	5			
2	D	172	Total	C	N	O	P	S	0	0	0
			1356	875	228	247	1	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	EXPRESSION TAG	UNP Q9Y478
B	-14	GLY	-	EXPRESSION TAG	UNP Q9Y478
B	-13	LEU	-	EXPRESSION TAG	UNP Q9Y478
B	-12	ASN	-	EXPRESSION TAG	UNP Q9Y478
B	-11	ASP	-	EXPRESSION TAG	UNP Q9Y478
B	-10	ILE	-	EXPRESSION TAG	UNP Q9Y478
B	-9	PHE	-	EXPRESSION TAG	UNP Q9Y478
B	-8	GLU	-	EXPRESSION TAG	UNP Q9Y478
B	-7	ALA	-	EXPRESSION TAG	UNP Q9Y478
B	-6	GLN	-	EXPRESSION TAG	UNP Q9Y478
B	-5	LYS	-	EXPRESSION TAG	UNP Q9Y478
B	-4	ILE	-	EXPRESSION TAG	UNP Q9Y478
B	-3	GLU	-	EXPRESSION TAG	UNP Q9Y478
B	-2	TRP	-	EXPRESSION TAG	UNP Q9Y478
B	-1	HIS	-	EXPRESSION TAG	UNP Q9Y478

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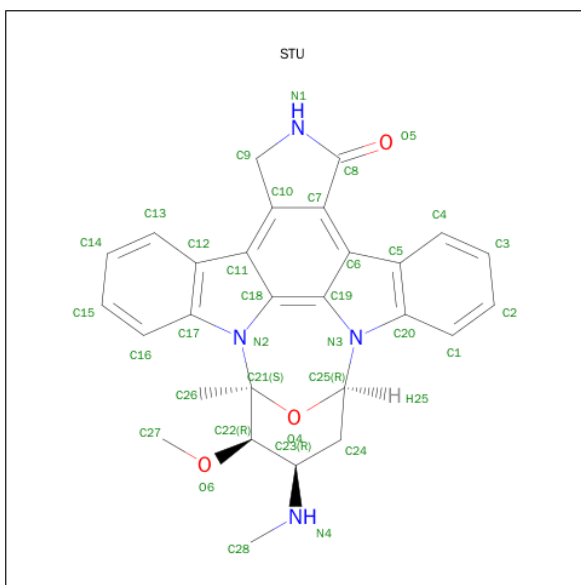
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLU	-	EXPRESSION TAG	UNP Q9Y478
D	-15	MET	-	EXPRESSION TAG	UNP Q9Y478
D	-14	GLY	-	EXPRESSION TAG	UNP Q9Y478
D	-13	LEU	-	EXPRESSION TAG	UNP Q9Y478
D	-12	ASN	-	EXPRESSION TAG	UNP Q9Y478
D	-11	ASP	-	EXPRESSION TAG	UNP Q9Y478
D	-10	ILE	-	EXPRESSION TAG	UNP Q9Y478
D	-9	PHE	-	EXPRESSION TAG	UNP Q9Y478
D	-8	GLU	-	EXPRESSION TAG	UNP Q9Y478
D	-7	ALA	-	EXPRESSION TAG	UNP Q9Y478
D	-6	GLN	-	EXPRESSION TAG	UNP Q9Y478
D	-5	LYS	-	EXPRESSION TAG	UNP Q9Y478
D	-4	ILE	-	EXPRESSION TAG	UNP Q9Y478
D	-3	GLU	-	EXPRESSION TAG	UNP Q9Y478
D	-2	TRP	-	EXPRESSION TAG	UNP Q9Y478
D	-1	HIS	-	EXPRESSION TAG	UNP Q9Y478
D	0	GLU	-	EXPRESSION TAG	UNP Q9Y478

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

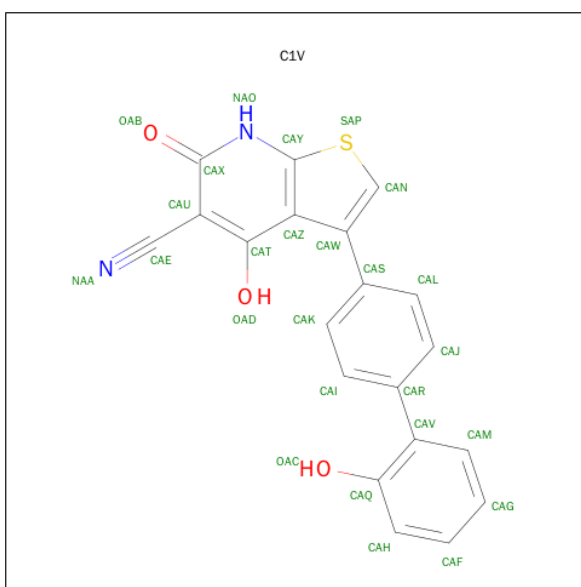
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	299	Total	C	N	O	S	0	0	0
			2412	1568	400	437	7			
3	F	292	Total	C	N	O	S	0	0	0
			2354	1531	391	425	7			

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: C<sub>28</sub>H<sub>26</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	4	3		
4	C	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 5 is 3-[4-(2-HYDROXYPHENYL)PHENYL]-4-OXIDANYL-6-OXIDANYLIDEN E-7H-THIENO[2,3-B]PYRIDINE-5-CARBONITRILE (three-letter code: C1V) (formula: C<sub>20</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>S).



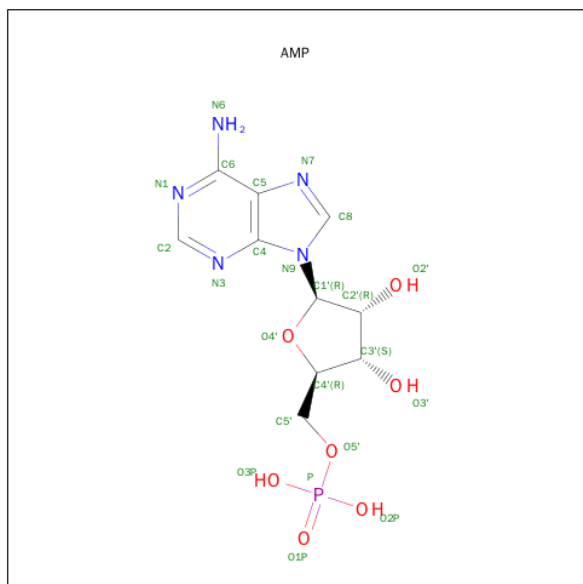
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	S	0	0
			26	20	2	3	1		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



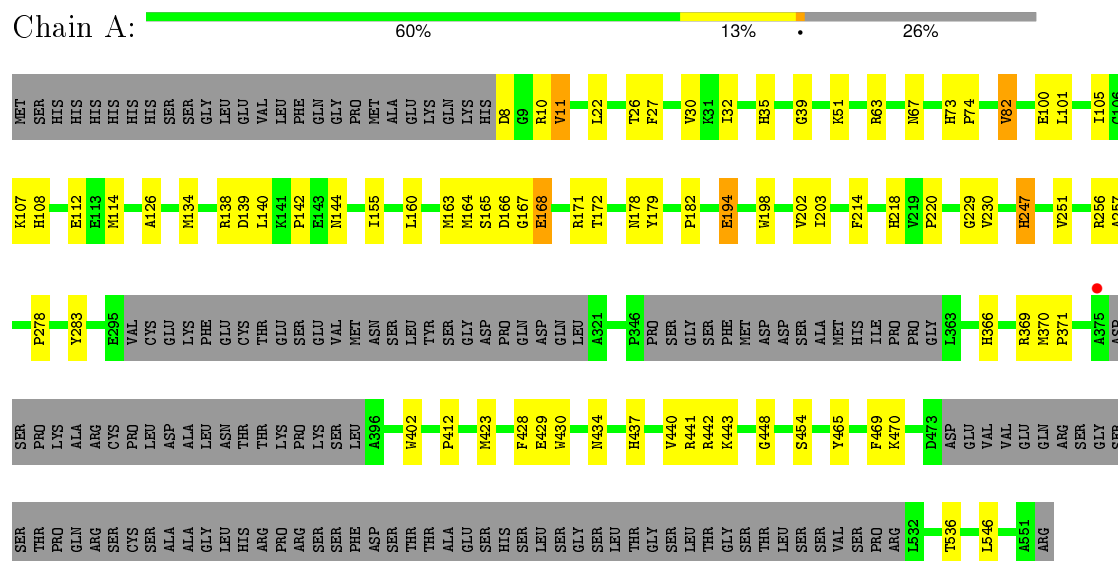
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		



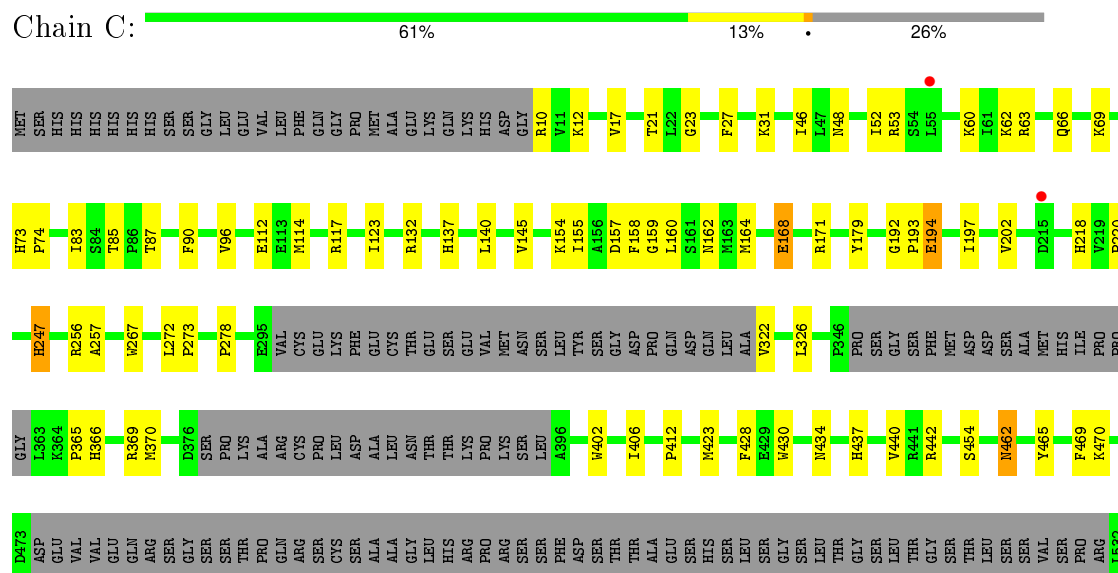
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-2

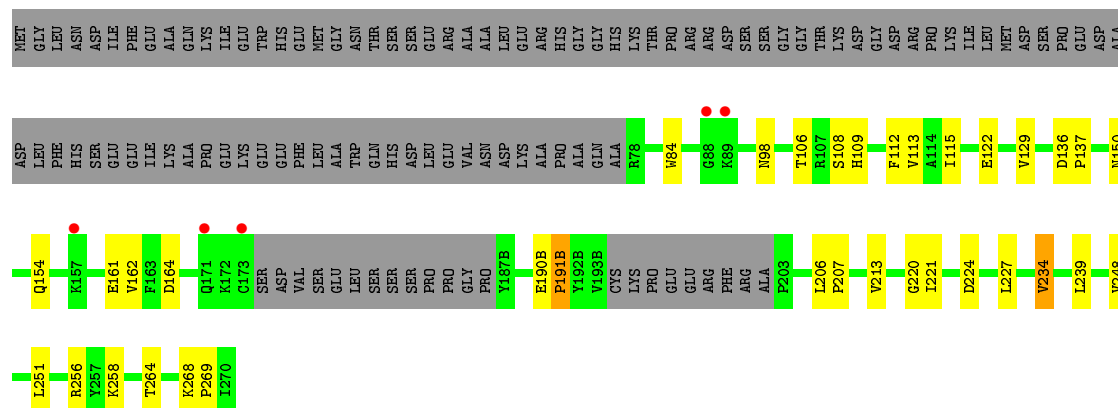


#### • Molecule 1: 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-2

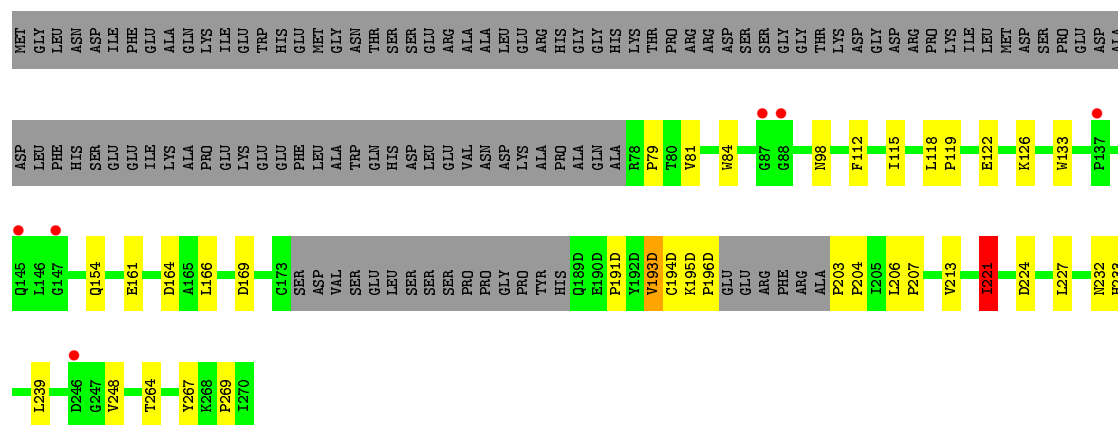




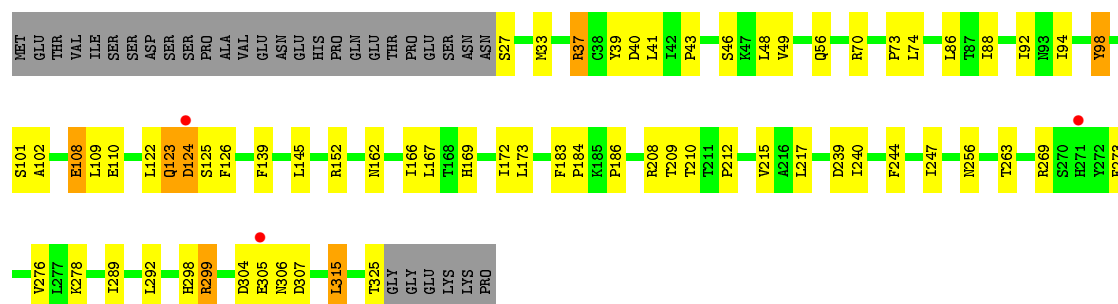
• Molecule 2: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-1



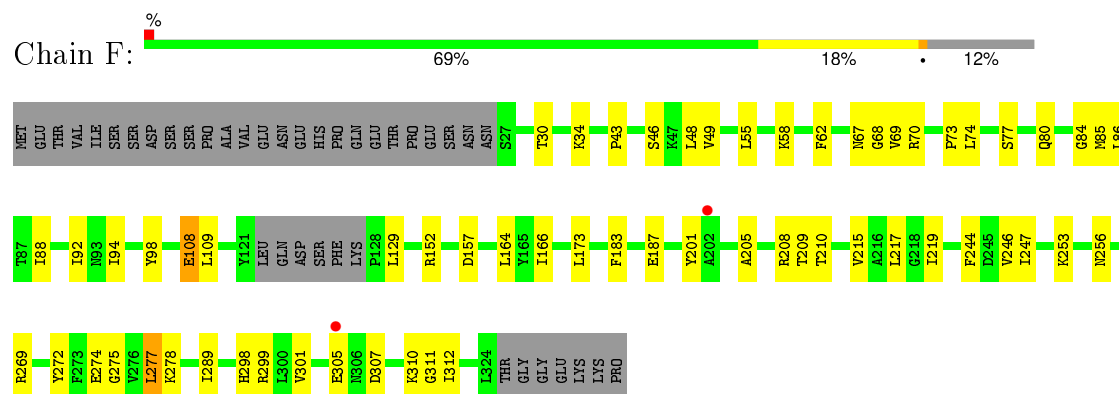
• Molecule 2: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-1



• Molecule 3: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1



• Molecule 3: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.02Å 134.79Å 141.29Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	19.93 – 3.92 19.93 – 3.92	Depositor EDS
% Data completeness (in resolution range)	94.1 (19.93-3.92) 94.2 (19.93-3.92)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.94Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.208 , 0.264 0.234 , 0.274	Depositor DCC
$R_{free}$ test set	1208 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	124.8	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 31.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 23932 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, STU, SEP, C1V, AMP

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	0.23	0/3470	0.39	0/4687
1	C	0.22	0/3461	0.37	0/4675
2	B	0.23	0/1376	0.44	1/1872 (0.1%)
2	D	0.24	0/1381	0.46	2/1879 (0.1%)
3	E	0.26	0/2463	0.43	0/3344
3	F	0.23	0/2403	0.40	0/3261
All	All	0.23	0/14554	0.41	3/19718 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	191(D)	PRO	N-CA-CB	5.86	110.33	103.30
2	B	191(B)	PRO	N-CA-CB	5.71	110.16	103.30
2	D	196(D)	PRO	N-CA-CB	5.53	109.94	103.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3403	0	3394	46	0
1	C	3394	0	3386	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1351	0	1328	22	0
2	D	1356	0	1329	23	0
3	E	2412	0	2483	35	0
3	F	2354	0	2426	30	0
4	A	35	0	26	3	0
4	C	35	0	26	3	0
5	B	26	0	12	1	0
5	C	26	0	12	0	0
6	E	46	0	24	1	0
6	F	46	0	24	2	0
All	All	14484	0	14470	183	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 183 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:C:370:MET:HG3	3:F:68:GLY:HA2	1.66	0.77
1:A:179:TYR:HA	1:A:202:VAL:HG11	1.73	0.71
1:C:430:TRP:HB3	1:C:440:VAL:HA	1.71	0.70
2:D:122:GLU:HG2	2:D:154:GLN:HG2	1.74	0.70
1:C:402:TRP:HB2	2:D:213:VAL:HG11	1.74	0.69

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	414/571 (72%)	388 (94%)	26 (6%)	0	100	100
1	C	412/571 (72%)	390 (95%)	21 (5%)	1 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	164/286 (57%)	157 (96%)	5 (3%)	2 (1%)	16	61
2	D	165/286 (58%)	153 (93%)	9 (6%)	3 (2%)	11	54
3	E	297/331 (90%)	278 (94%)	15 (5%)	4 (1%)	15	60
3	F	288/331 (87%)	275 (96%)	12 (4%)	1 (0%)	46	82
All	All	1740/2376 (73%)	1641 (94%)	88 (5%)	11 (1%)	30	73

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	191(B)	PRO
1	C	159	GLY
3	E	184	PRO
3	F	277	LEU
2	D	193(D)	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	364/503 (72%)	354 (97%)	10 (3%)	52	80
1	C	364/503 (72%)	355 (98%)	9 (2%)	55	82
2	B	149/253 (59%)	145 (97%)	4 (3%)	52	80
2	D	149/253 (59%)	147 (99%)	2 (1%)	76	90
3	E	275/304 (90%)	260 (94%)	15 (6%)	27	66
3	F	268/304 (88%)	257 (96%)	11 (4%)	37	73
All	All	1569/2120 (74%)	1518 (97%)	51 (3%)	45	78

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	98	ASN
3	E	123	GLN

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Mol	Chain	Res	Type
3	F	269	ARG
3	E	37	ARG
3	E	124	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	336	GLN
3	F	223	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TPO	A	172	1	8,10,11	0.83	0	7,14,16	1.19	0
2	SEP	B	108	2	8,9,10	0.85	0	8,12,14	1.01	1 (12%)
1	TPO	C	172	1	8,10,11	0.83	0	7,14,16	1.18	0
2	SEP	D	108	2	8,9,10	0.86	0	8,12,14	1.02	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
1	TPO	A	172	1	-	0/8/11/13	0/0/0/0
2	SEP	B	108	2	-	0/6/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	172	1	-	0/8/11/13	0/0/0/0
2	SEP	D	108	2	-	0/6/8/10	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	SEP	O-C-CA	-2.15	119.90	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	TPO	1	0
2	B	108	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	STU	A	1552	-	27,42,42	0.84	1 (3%)	23,68,68	1.51	4 (17%)
5	C1V	B	1271	-	27,29,29	2.62	8 (29%)	29,42,42	3.68	7 (24%)
4	STU	C	1552	-	27,42,42	0.80	0	23,68,68	1.40	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	C1V	C	1553	-	27,29,29	2.66	7 (25%)	29,42,42	3.78	6 (20%)
6	AMP	E	1326	-	20,25,25	0.97	1 (5%)	22,38,38	1.81	2 (9%)
6	AMP	E	1327	-	20,25,25	0.99	1 (5%)	22,38,38	1.70	2 (9%)
6	AMP	F	1325	-	20,25,25	0.92	1 (5%)	22,38,38	1.85	2 (9%)
6	AMP	F	1326	-	20,25,25	0.94	1 (5%)	22,38,38	1.73	2 (9%)

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	STU	A	1552	-	-	0/4/42/42	0/0/8/8
5	C1V	B	1271	-	-	0/9/10/10	0/4/4/4
4	STU	C	1552	-	-	0/4/42/42	0/0/8/8
5	C1V	C	1553	-	-	0/9/10/10	0/4/4/4
6	AMP	E	1326	-	-	0/6/26/26	0/3/3/3
6	AMP	E	1327	-	-	0/6/26/26	0/3/3/3
6	AMP	F	1325	-	-	0/6/26/26	0/3/3/3
6	AMP	F	1326	-	-	0/6/26/26	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1552	STU	C10-C11	-2.15	1.39	1.42
5	B	1271	C1V	CAX-CAU	-2.12	1.39	1.44
5	B	1271	C1V	OAC-CAQ	2.66	1.41	1.36
5	C	1553	C1V	OAC-CAQ	2.70	1.42	1.36
6	F	1326	AMP	C5-C4	3.01	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1553	C1V	CAW-CAN-SAP	-16.59	107.90	112.53
5	B	1271	C1V	CAW-CAN-SAP	-15.69	108.15	112.53
6	F	1325	AMP	N3-C2-N1	-6.96	123.57	128.89
6	E	1326	AMP	N3-C2-N1	-6.82	123.67	128.89
6	E	1327	AMP	N3-C2-N1	-6.28	124.09	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1552	STU	3	0
5	B	1271	C1V	1	0
4	C	1552	STU	3	0
6	E	1326	AMP	1	0
6	F	1325	AMP	1	0
6	F	1326	AMP	1	0

## 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, 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	424/571 (74%)	-0.17	1 (0%) 95 94	32, 79, 136, 159	0
1	C	422/571 (73%)	-0.16	2 (0%) 91 88	50, 92, 140, 161	0
2	B	170/286 (59%)	0.11	5 (2%) 55 42	48, 100, 152, 182	0
2	D	171/286 (59%)	0.05	6 (3%) 48 36	58, 101, 145, 173	0
3	E	299/331 (90%)	-0.34	3 (1%) 84 77	29, 68, 140, 192	0
3	F	292/331 (88%)	-0.40	2 (0%) 89 84	44, 73, 124, 147	0
All	All	1778/2376 (74%)	-0.19	19 (1%) 82 75	29, 83, 141, 192	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	124	ASP	5.3
2	B	89	LYS	4.5
2	B	88	GLY	4.4
2	B	171	GLN	3.2
1	A	375	ALA	3.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPO	C	172	11/12	0.94	0.12	-	66,92,95,95	0
1	TPO	A	172	11/12	0.93	0.13	-	54,71,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SEP	D	108	10/11	0.94	0.18	-	83,98,109,111	0
2	SEP	B	108	10/11	0.91	0.18	-	93,103,114,115	0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	C1V	C	1553	26/26	0.93	0.24	0.06	92,96,108,110	0
4	STU	C	1552	35/35	0.93	0.20	-0.50	119,122,127,127	0
5	C1V	B	1271	26/26	0.92	0.21	-0.55	90,90,94,94	0
4	STU	A	1552	35/35	0.94	0.21	-0.56	102,107,111,114	0
6	AMP	F	1326	23/23	0.95	0.16	-0.91	52,55,62,64	0
6	AMP	E	1326	23/23	0.93	0.20	-0.97	80,83,99,101	0
6	AMP	E	1327	23/23	0.94	0.16	-1.01	71,75,79,81	0
6	AMP	F	1325	23/23	0.96	0.16	-1.07	52,59,69,74	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.