



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 03:58 am GMT

PDB ID : 2OOX
Title : Crystal structure of the adenylate sensor from AMP-activated protein kinase complexed with AMP
Authors : Townley, R.; Shapiro, L.
Deposited on : 2007-01-26
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

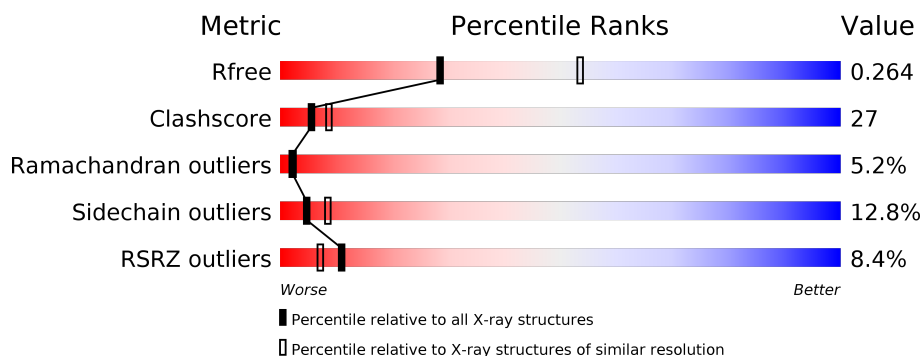
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	137	<div> <div>10%</div> <div> <div>53%</div> <div>31%</div> <div>9%</div> <div>7%</div> </div> </div>
1	C	137	<div> <div>16%</div> <div> <div>49%</div> <div>31%</div> <div>12%</div> <div>7%</div> </div> </div>
2	B	97	<div> <div>12%</div> <div> <div>52%</div> <div>29%</div> <div>12%</div> <div>•</div> </div> </div>
2	D	97	<div> <div>12%</div> <div> <div>45%</div> <div>30%</div> <div>15%</div> <div>5%</div> <div>•</div> </div> </div>
3	E	333	<div> <div>6%</div> <div> <div>63%</div> <div>30%</div> <div>6%</div> <div>•</div> </div> </div>
3	G	333	<div> <div>4%</div> <div> <div>57%</div> <div>30%</div> <div>10%</div> <div>•</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9329 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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			1025	657	178	180	10			
1	C	128	Total	C	N	O	S	0	0	0
			1003	646	173	175	9			

- Molecule 2 is a protein called SPCC1919.03c protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	93	Total	C	N	O	S	0	0	0
			733	467	125	139	2			
2	D	93	Total	C	N	O	S	6	0	0
			733	467	125	139	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	MET	-	CLONING ARTIFACT	UNP P78789
D	202	MET	-	CLONING ARTIFACT	UNP P78789

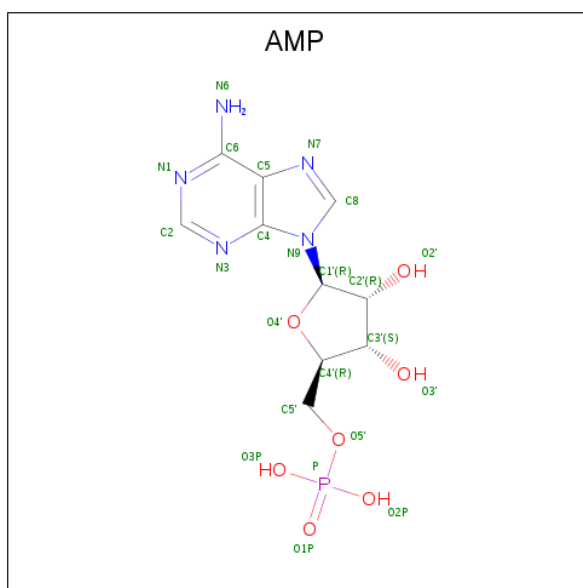
- Molecule 3 is a protein called Hypothetical protein C1556.08c in chromosome I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	324	Total	C	N	O	S	0	1	0
			2548	1629	426	478	15			
3	E	333	Total	C	N	O	S	0	0	0
			2589	1649	433	492	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	MET	-	CLONING ARTIFACT	UNP Q10343
G	2	MET	-	CLONING ARTIFACT	UNP Q10343

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

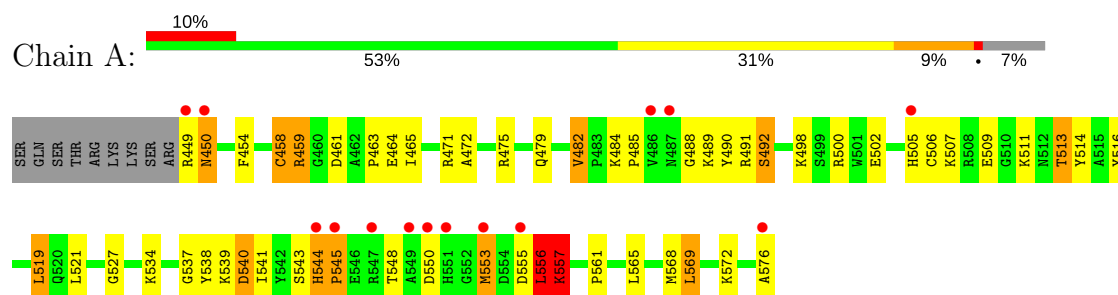
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total	O	0	0
			94	94		
5	B	78	Total	O	0	0
			78	78		
5	G	217	Total	O	0	0
			217	217		
5	C	66	Total	O	0	0
			66	66		
5	D	51	Total	O	0	0
			51	51		
5	E	146	Total	O	0	0
			146	146		

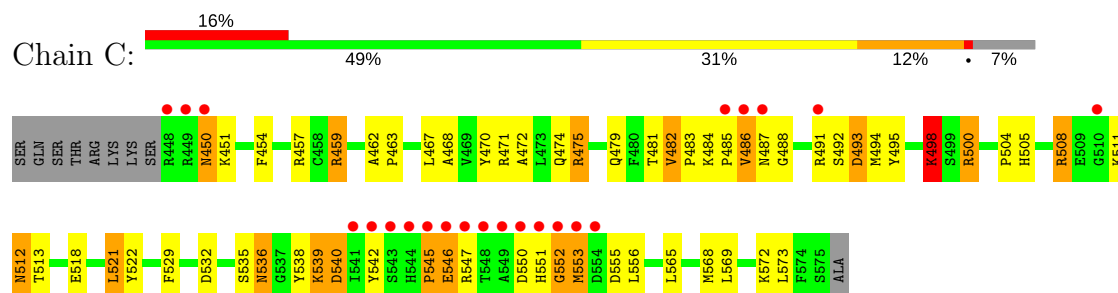
3 Residue-property plots

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

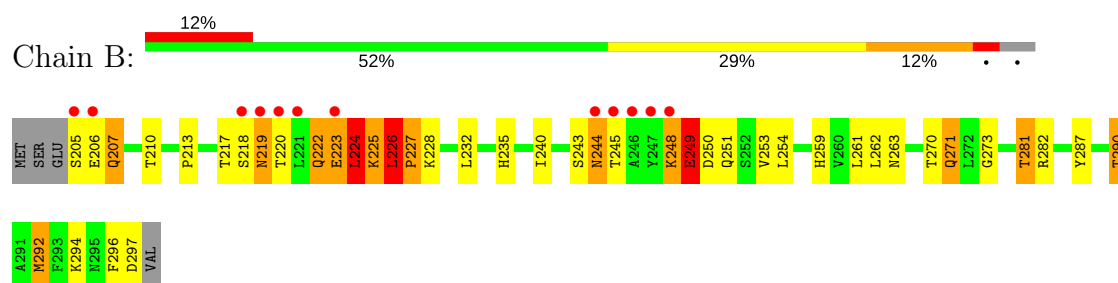
• Molecule 1: SNF1-like protein kinase ssp2



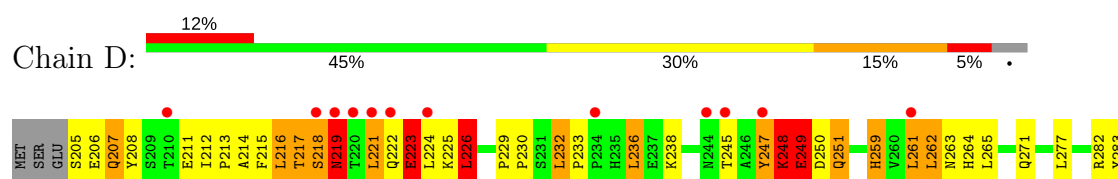
• Molecule 1: SNF1-like protein kinase ssp2

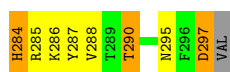


• Molecule 2: SPCC1919.03c protein

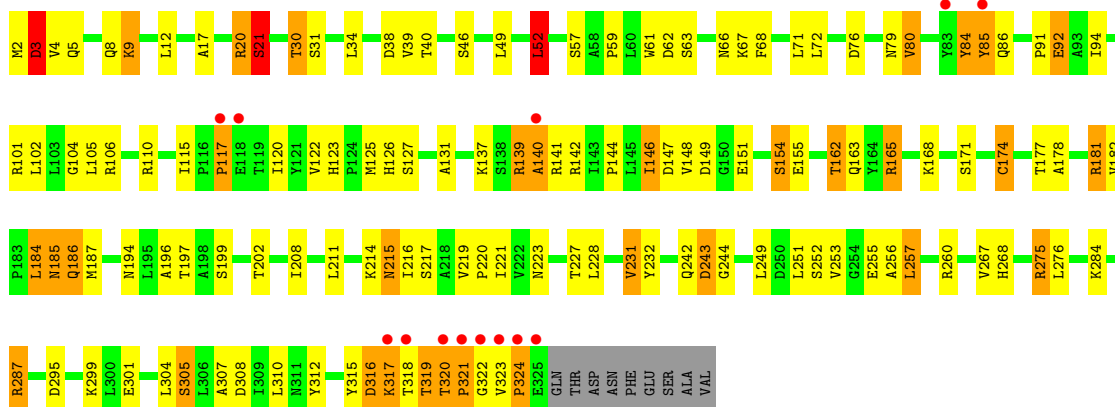


• Molecule 2: SPCC1919.03c protein

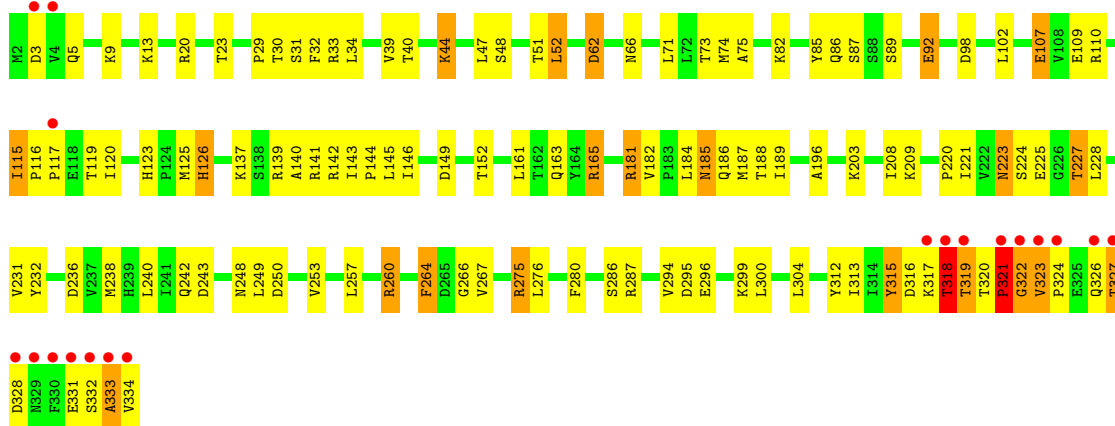




• Molecule 3: Hypothetical protein C1556.08c in chromosome I



• Molecule 3: Hypothetical protein C1556.08c in chromosome I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.46Å 97.39Å 168.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 29.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.60) 99.9 (29.69-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.91 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.273 0.200 , 0.264	Depositor DCC
R_{free} test set	1903 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9329	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

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	0.79	0/1053	0.93	4/1420 (0.3%)
1	C	0.77	2/1030 (0.2%)	0.82	1/1393 (0.1%)
2	B	0.74	0/751	0.89	1/1026 (0.1%)
2	D	1.03	3/751 (0.4%)	0.96	2/1026 (0.2%)
3	E	0.74	0/2631	0.83	3/3565 (0.1%)
3	G	0.76	1/2596 (0.0%)	0.85	2/3521 (0.1%)
All	All	0.78	6/8812 (0.1%)	0.86	13/11951 (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
1	A	0	2
1	C	0	1
2	D	0	2
3	E	0	2
3	G	0	2
All	All	0	9

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	218	SER	CB-OG	16.16	1.63	1.42
2	D	284	HIS	CA-CB	-10.79	1.30	1.53
1	C	481	THR	C-N	-10.41	1.10	1.34
2	D	286	LYS	C-N	-8.59	1.14	1.34
1	C	482	VAL	C-N	6.38	1.46	1.34

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	285	ARG	O-C-N	-8.71	108.77	122.70
3	E	321	PRO	N-CA-CB	7.76	112.61	103.30
1	A	519	LEU	CA-CB-CG	6.15	129.45	115.30
1	A	459	ARG	NE-CZ-NH1	-6.07	117.27	120.30
3	G	52	LEU	CA-CB-CG</			

