



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:09 AM GMT

PDB ID : 2PK2  
Title : Cyclin box structure of the P-TEFb subunit Cyclin T1 derived from a fusion complex with EIAV Tat  
Authors : Anand, K.; Schulte, A.; Fujinaga, K.; Scheffzek, K.; Geyer, M.  
Deposited on : 2007-04-17  
Resolution : 2.67 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

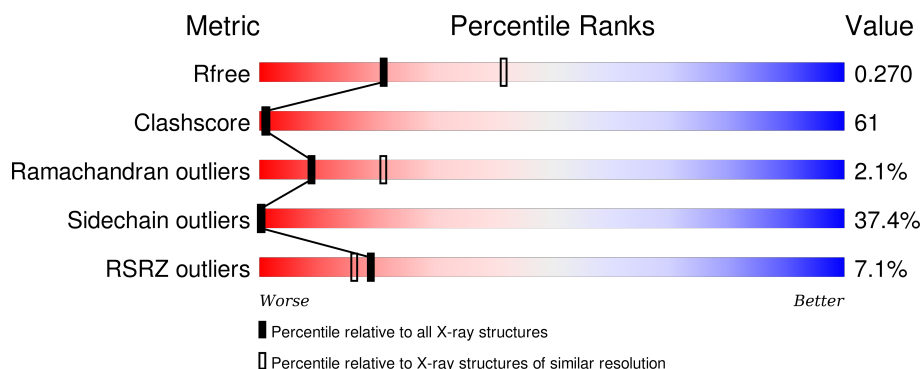
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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	358	<div> <div>4%</div> <div>13% 39% 19% 28%</div> </div>
1	B	358	<div> <div>6%</div> <div>13% 38% 20% 28%</div> </div>
1	C	358	<div> <div>5%</div> <div>12% 37% 22% 28%</div> </div>
1	D	358	<div> <div>6%</div> <div>13% 40% 17% 28%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8396 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 Cyclin-T1, Protein Tat.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2076	1331	360	375	10			
1	B	256	Total	C	N	O	S	0	0	0
			2080	1333	360	377	10			
1	C	256	Total	C	N	O	S	0	0	0
			2082	1334	361	377	10			
1	D	256	Total	C	N	O	S	0	0	0
			2079	1332	360	377	10			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ARG	GLN	SEE REMARK 999	UNP O60563
A	282	GLY	-	linker	UNP O60563
A	283	GLY	-	linker	UNP O60563
A	284	THR	-	linker	UNP O60563
A	285	GLY	-	linker	UNP O60563
A	286	GLY	-	linker	UNP O60563
A	287	GLY	-	linker	UNP O60563
A	288	SER	-	linker	UNP O60563
A	289	GLY	-	linker	UNP O60563
A	290	GLY	-	linker	UNP O60563
A	291	GLY	-	linker	UNP O60563
A	292	SER	-	linker	UNP O60563
A	293	GLY	-	linker	UNP O60563
A	294	GLY	-	linker	UNP O60563
A	295	GLY	-	linker	UNP O60563
A	296	SER	-	linker	UNP O60563
A	297	GLY	-	linker	UNP O60563
A	298	GLY	-	linker	UNP O60563
A	299	GLY	-	linker	UNP O60563
A	300	THR	-	linker	UNP O60563
A	301	SER	-	linker	UNP O60563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	77	ARG	GLN	SEE REMARK 999	UNP O60563
B	282	GLY	-	linker	UNP O60563
B	283	GLY	-	linker	UNP O60563
B	284	THR	-	linker	UNP O60563
B	285	GLY	-	linker	UNP O60563
B	286	GLY	-	linker	UNP O60563
B	287	GLY	-	linker	UNP O60563
B	288	SER	-	linker	UNP O60563
B	289	GLY	-	linker	UNP O60563
B	290	GLY	-	linker	UNP O60563
B	291	GLY	-	linker	UNP O60563
B	292	SER	-	linker	UNP O60563
B	293	GLY	-	linker	UNP O60563
B	294	GLY	-	linker	UNP O60563
B	295	GLY	-	linker	UNP O60563
B	296	SER	-	linker	UNP O60563
B	297	GLY	-	linker	UNP O60563
B	298	GLY	-	linker	UNP O60563
B	299	GLY	-	linker	UNP O60563
B	300	THR	-	linker	UNP O60563
B	301	SER	-	linker	UNP O60563
C	77	ARG	GLN	SEE REMARK 999	UNP O60563
C	282	GLY	-	linker	UNP O60563
C	283	GLY	-	linker	UNP O60563
C	284	THR	-	linker	UNP O60563
C	285	GLY	-	linker	UNP O60563
C	286	GLY	-	linker	UNP O60563
C	287	GLY	-	linker	UNP O60563
C	288	SER	-	linker	UNP O60563
C	289	GLY	-	linker	UNP O60563
C	290	GLY	-	linker	UNP O60563
C	291	GLY	-	linker	UNP O60563
C	292	SER	-	linker	UNP O60563
C	293	GLY	-	linker	UNP O60563
C	294	GLY	-	linker	UNP O60563
C	295	GLY	-	linker	UNP O60563
C	296	SER	-	linker	UNP O60563
C	297	GLY	-	linker	UNP O60563
C	298	GLY	-	linker	UNP O60563
C	299	GLY	-	linker	UNP O60563
C	300	THR	-	linker	UNP O60563
C	301	SER	-	linker	UNP O60563

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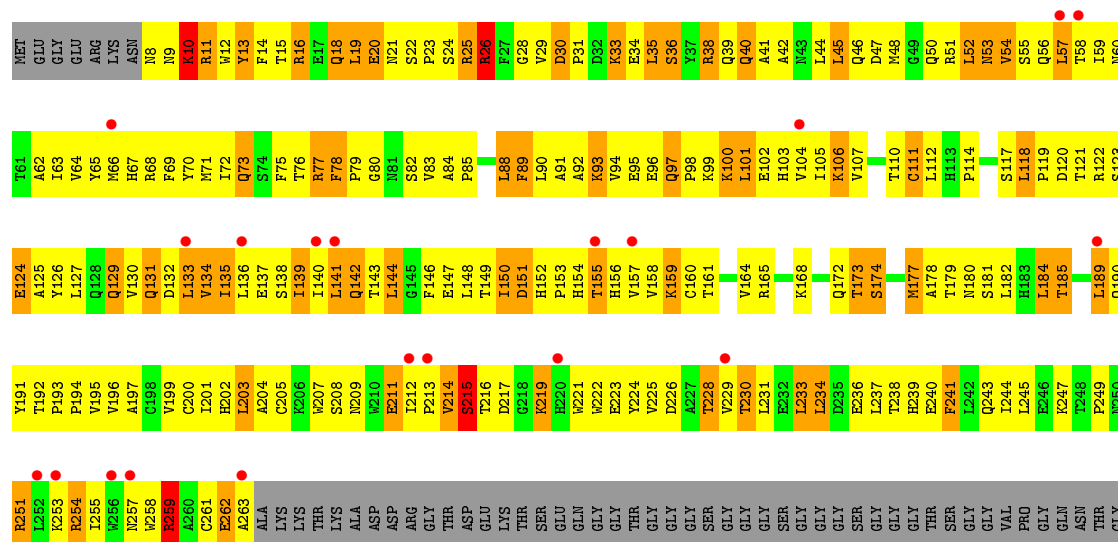
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Chain	Residue	Modelled	Actual	Comment	Reference
D	77	ARG	GLN	SEE REMARK 999	UNP O60563
D	282	GLY	-	linker	UNP O60563
D	283	GLY	-	linker	UNP O60563
D	284	THR	-	linker	UNP O60563
D	285	GLY	-	linker	UNP O60563
D	286	GLY	-	linker	UNP O60563
D	287	GLY	-	linker	UNP O60563
D	288	SER	-	linker	UNP O60563
D	289	GLY	-	linker	UNP O60563
D	290	GLY	-	linker	UNP O60563
D	291	GLY	-	linker	UNP O60563
D	292	SER	-	linker	UNP O60563
D	293	GLY	-	linker	UNP O60563
D	294	GLY	-	linker	UNP O60563
D	295	GLY	-	linker	UNP O60563
D	296	SER	-	linker	UNP O60563
D	297	GLY	-	linker	UNP O60563
D	298	GLY	-	linker	UNP O60563
D	299	GLY	-	linker	UNP O60563
D	300	THR	-	linker	UNP O60563
D	301	SER	-	linker	UNP O60563

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	25	Total O 25 25	0	0
2	B	16	Total O 16 16	0	0
2	C	21	Total O 21 21	0	0
2	D	17	Total O 17 17	0	0





GLY	GLN	GLU	ALA	ARG	PRO	ASN	TYR	HIS	CYS	GLN	LEU	CYS	PHE	LEU	ARG	SER	LEU	GLY	ILE	ASP	TYR	LEU	ASP	ALA	SER	LEU	ARG	LYS	LYS	ASN	LYS	GLN	ARG	LEU	LYS	ALA	ILE	GLN	GLN	GLY	ARG	GLN	PRO	GLN	TYR	LEU	LEU
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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.83Å 203.83Å 124.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.67 19.99 – 2.66	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.67) 99.2 (19.99-2.66)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.67Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.274 , 0.306 0.249 , 0.270	Depositor DCC
$R_{free}$ test set	1547 reflections (2.91%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.5	EDS
Estimated twinning fraction	0.188 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.186 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.186 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.437 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.437 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.429 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.187 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.30$ , $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	0 of 55259 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	8396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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

### 5.1 Standard geometry

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	0/2130	0.62	1/2904 (0.0%)
1	B	0.28	0/2134	0.66	3/2909 (0.1%)
1	C	0.25	0/2136	0.59	0/2911
1	D	0.28	0/2133	0.66	5/2908 (0.2%)
All	All	0.29	0/8533	0.63	9/11632 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	ARG	CA-CB-CG	7.41	129.70	113.40
1	A	26	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	18	GLN	C-N-CA	6.66	138.35	121.70
1	B	26	ARG	CD-NE-CZ	6.53	132.75	123.60
1	B	16	ARG	C-N-CA	5.96	136.60	121.70

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	2076	0	2043	259	0
1	B	2080	0	2045	241	0
1	C	2082	0	2052	323	0
1	D	2079	0	2045	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	0	6	0
2	B	16	0	0	4	0
2	C	21	0	0	3	0
2	D	17	0	0	0	0
All	All	8396	0	8185	1008	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 61.

The worst 5 of 1008 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:A:15:THR:HG23	1:A:18:GLN:HB2	1.38	1.03
1:D:215:SER:HG	1:D:224:TYR:HE1	1.04	1.02
1:A:177:MET:HB3	1:A:200:CYS:HB3	1.42	0.98
1:C:63:ILE:HG21	1:C:182:LEU:HB3	1.47	0.97
1:C:239:HIS:HA	1:C:242:LEU:HD12	1.47	0.97

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	254/358 (71%)	223 (88%)	26 (10%)	5 (2%)	9	22
1	B	254/358 (71%)	219 (86%)	30 (12%)	5 (2%)	9	22
1	C	254/358 (71%)	186 (73%)	63 (25%)	5 (2%)	9	22
1	D	254/358 (71%)	222 (87%)	26 (10%)	6 (2%)	7	17
All	All	1016/1432 (71%)	850 (84%)	145 (14%)	21 (2%)	9	21

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	THR
1	C	214	VAL
1	D	10	LYS
1	D	215	SER
1	A	38	ARG

### 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	227/307 (74%)	145 (64%)	82 (36%)	0	0
1	B	228/307 (74%)	145 (64%)	83 (36%)	0	0
1	C	229/307 (75%)	144 (63%)	85 (37%)	0	0
1	D	228/307 (74%)	137 (60%)	91 (40%)	0	0
All	All	912/1228 (74%)	571 (63%)	341 (37%)	0	0

5 of 341 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	230	THR
1	C	88	LEU
1	D	182	LEU
1	B	241	PHE
1	C	29	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	202	HIS
1	C	129	GLN
1	D	190	GLN
1	C	39	GLN
1	C	60	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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	256/358 (71%)	0.58	16 (6%) 23 21	23, 60, 69, 76	0
1	B	256/358 (71%)	0.62	20 (7%) 16 13	23, 60, 69, 76	0
1	C	256/358 (71%)	0.46	17 (6%) 22 19	22, 53, 67, 80	0
1	D	256/358 (71%)	0.63	20 (7%) 16 13	24, 61, 69, 76	0
All	All	1024/1432 (71%)	0.57	73 (7%) 19 16	22, 59, 69, 80	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	VAL	5.9
1	A	255	ILE	5.7
1	D	257	ASN	5.4
1	D	57	LEU	4.3
1	D	253	LYS	4.1

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.