

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 3, 2022 – 10:06 AM EST

PDB ID	:	7LBK
Title	:	Crystal structure of human Survivin bound to histone H3 T3phK4me3 peptide
Authors	:	Niedziałkowska, E.; Minor, W.; Stukenberg, P.T.
Deposited on		
Resolution	:	2.70 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

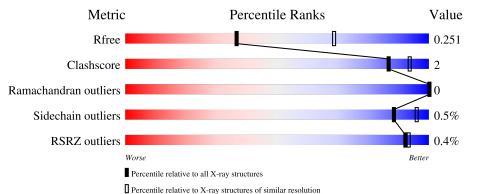
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.25
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.25

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.70 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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			Qı	uality of chain		
1	А	146				88%	5%	6%
1	В	146				88%	5%	7%
2	С	12	33%		8%	58%		
2	D	12	25%	8%	8%	58%		_



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## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2286 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	р	136	Total	С	Ν	0	S	0	0	0
ГБ	130	1088	695	182	204	$\overline{7}$	0	0	0	
1	Δ	137	Total	С	Ν	0	S	0	0	0
	A	137	1080	692	181	200	$\overline{7}$			U

• Molecule 1 is a protein called Baculoviral IAP repeat-containing protein 5.

There are 8 discrepancies between the modelled and reference sequences	
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Chain	Residue	Modelled	Actual	Comment	Reference
В	-3	GLY	-	expression tag	UNP O15392
В	-2	SER	-	expression tag	UNP O15392
В	-1	HIS	-	expression tag	UNP O15392
В	0	GLU	-	expression tag	UNP O15392
A	-3	GLY	-	expression tag	UNP O15392
А	-2	SER	-	expression tag	UNP O15392
А	-1	HIS	-	expression tag	UNP O15392
А	0	GLU	-	expression tag	UNP O15392

• Molecule 2 is a protein called histone H3 T3phK4me3 peptide.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
0	Л	Б	Total	С	Ν	Ο	Р	0	0	0
	5	44	25	9	9	1	0	0	0	
0	С	Б	Total	С	Ν	Ο	Р	0	0	0
	2 C	Э	38	22	6	9	1	U		0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

M	Iol	Chain	Residues	Atoms	ZeroOcc	AltConf
:	3	В	1	Total Zn 1 1	0	0
	3	А	1	Total Zn 1 1	0	0



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	19	Total O 19 19	0	0
4	А	15	Total         O           15         15	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Baculoviral IAP repeat-containing protein 5

Chain B:		88%		5%	7%
GLY SER HIS GLU GLU ALA ALA PRO LIS PRO LIS P7	q11 P12 R18 F27 L28 Q92	E95 A140 MET ASP			
• Molecule 1: Ba	aculoviral IA	P repeat-cont	aining protein 5		
Chain A:		88%		5%	6%
GLY SER HIS GLU GLU MET GLY ALA ALA THR THR THR LIG	P26 F27 L28 R37 S82 S82 1113	R133 D142			
• Molecule 2: his	stone H3 T3 <sub>1</sub>	phK4me3 pep	tide		
Chain D:	25% 8%	% 8%	58%		
A1 13 K4 K4 ALA ALA ARG LYS SIER SIER SIER CLY					
• Molecule 2: his	stone H3 T3 <sub>1</sub>	phK4me3 pep	tide		
Chain C:					
Unann U:	33%	8%	58%		
A1 T3 K4 H4 A1A A1A A1A A1A A1A C1Y S1A C1Y C1Y					



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	114.29Å 71.37Å 82.55Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $129.33^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	41.04 - 2.70	Depositor
Resolution (A)	41.01 - 2.70	EDS
% Data completeness	87.2 (41.04-2.70)	Depositor
(in resolution range)	87.4 (41.01-2.70)	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.66 (at 2.69 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
D D	0.212 , $0.253$	Depositor
$R, R_{free}$	0.215 , $0.251$	DCC
$R_{free}$ test set	623 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	35.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.31, 28.1	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2286	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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, ZN, M3L

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	Bo	nd angles
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.73	0/1109	0.81	2/1499~(0.1%)
1	В	0.77	0/1117	0.84	1/1508~(0.1%)
2	С	0.77	0/14	0.76	0/18
2	D	0.72	0/20	0.83	0/25
All	All	0.75	0/2260	0.83	3/3050~(0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$\operatorname{Ideal}(^{o})$
1	В	18	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	А	133	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	А	133	ARG	NE-CZ-NH2	-5.08	117.76	120.30

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	А	1080	0	999	5	0
1	В	1088	0	1025	4	0
2	С	38	0	36	0	0
2	D	44	0	47	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	1	0	0	0	0
3	В	1	0	0	0	0
4	А	15	0	0	1	0
4	В	19	0	0	0	0
All	All	2286	0	2107	9	0

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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 (9) 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:B:7:PRO:HG3	1:A:7:PRO:HG3	1.96	0.47
1:B:11:GLN:HB2	1:B:12:PRO:HD3	1.97	0.45
1:A:26:PRO:HG2	1:A:27:PHE:CD2	2.52	0.45
2:D:3:TPO:O	2:D:4:M3L:C	2.65	0.44
1:B:92:GLN:HB2	1:B:95:GLU:OE1	2.18	0.43
1:A:37:ARG:NE	4:A:301:HOH:O	2.52	0.43
1:B:27:PHE:O	1:B:28:LEU:HD23	2.18	0.42
1:A:113:ILE:HD13	1:A:113:ILE:HA	1.94	0.40
1:A:27:PHE:O	1:A:28:LEU:HD23	2.20	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	Perce	ntiles
1	А	135/146~(92%)	131 (97%)	4(3%)	0	100	100
1	В	134/146~(92%)	131 (98%)	3~(2%)	0	100	100
2	С	1/12~(8%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	1/12~(8%)	1 (100%)	0	0	100 100
All	All	271/316~(86%)	264 (97%)	7 (3%)	0	100 100

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There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	106/126~(84%)	105~(99%)	1 (1%)	78 92		
1	В	112/126~(89%)	112 (100%)	0	100 100		
2	D	1/7~(14%)	1 (100%)	0	100 100		
All	All	219/259~(85%)	218 (100%)	1 (0%)	88 96		

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	82	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	Bo	Bond lengths			Bond angles		
	Tor Type Chain Re	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2		
2	TPO	С	3	2	8,10,11	0.81	0	10, 14, 16	1.34	2 (20%)	
2	TPO	D	3	2	8,10,11	0.62	0	10,14,16	1.85	4 (40%)	
2	M3L	С	4	2	10,11,12	0.60	0	9,14,16	0.31	0	
2	M3L	D	4	2	10,11,12	0.56	0	9,14,16	0.65	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
2	TPO	С	3	2	-	1/9/11/13	-
2	TPO	D	3	2	-	2/9/11/13	-
2	M3L	С	4	2	-	4/9/10/12	-
2	M3L	D	4	2	-	5/9/10/12	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	D	3	TPO	OG1-P-O1P	-3.25	96.83	109.39
2	D	3	TPO	O3P-P-O1P	2.47	120.34	110.68
2	С	3	TPO	OG1-P-O1P	-2.24	100.74	109.39
2	С	3	TPO	O2P-P-O1P	2.15	119.11	110.68
2	D	3	TPO	O3P-P-OG1	-2.15	96.37	105.99
2	D	3	TPO	O2P-P-OG1	2.09	115.36	105.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	TPO	O-C-CA-CB
2	D	4	M3L	C-CA-CB-CG
2	С	4	M3L	N-CA-CB-CG
2	С	4	M3L	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	D	4	M3L	CG-CD-CE-NZ
2	D	4	M3L	CA-CB-CG-CD
2	С	4	M3L	CE-CD-CG-CB
2	С	4	M3L	CA-CB-CG-CD
2	D	4	M3L	N-CA-CB-CG
2	D	4	M3L	CE-CD-CG-CB
2	D	3	TPO	CB-OG1-P-O2P
2	С	3	TPO	O-C-CA-CB

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There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	TPO	1	0
2	D	4	M3L	1	0

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 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,  $95^{th}$  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	А	137/146~(93%)	-0.14	0 100 100	18, 42, 75, 99	0
1	В	136/146~(93%)	-0.30	0 100 100	18, 34, 62, 93	0
2	С	3/12~(25%)	1.34	1 (33%) 0 0	60, 60, 62, 77	0
2	D	3/12~(25%)	0.03	0 100 100	35, 35, 50, 52	0
All	All	279/316~(88%)	-0.20	1 (0%) 92 93	18, 37, 73, 99	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	С	5	GLN	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. The B-factors column lists the minimum, median,  $95^{th}$  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	$B-factors(Å^2)$	Q<0.9
2	M3L	С	4	12/13	0.90	0.29	67,73,84,94	0
2	TPO	С	3	11/12	0.91	0.17	54,59,70,84	0
2	M3L	D	4	12/13	0.95	0.18	42,52,64,64	0
2	TPO	D	3	11/12	0.96	0.11	35,39,45,46	0

#### 6.3 Carbohydrates (i)

There are no monosaccharides 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	ZN	А	201	1/1	0.99	0.04	$23,\!23,\!23,\!23$	0
3	ZN	В	201	1/1	1.00	0.05	22,22,22,22	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

