

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

Nov 30, 2021 – 04:11 pm GMT

PDB ID : 7BCY

Title : X-ray structure of WDR5delta24 bound to the Kaposi's sarcoma herpesvirus

LANA win motif peptide

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Deposited on : 2020-12-21

Resolution : 1.50 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 (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: 1.8.4 (270009), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.23.2

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

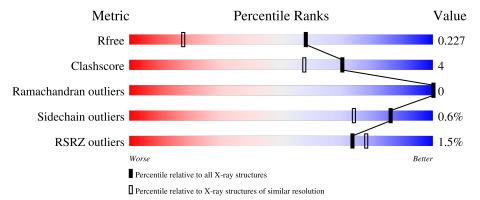
Validation Pipeline (wwPDB-VP) : 2.23.2

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.50 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	Similar resolution
Metric	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 <=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	314	89%	7%	-				
1	В	314	89%	8%	-				
2	Р	12	67% 33%		_				
2	Q	12	50% 17% 33%		_				



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10048 atoms, of which 4606 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 WD repeat-containing protein 5.

1 A 301 Total C H N O S 4559 1476 2250 382 440 11 0 3	Mo	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
	1	A	301		C 1476		N 382	O 440	S 11	0	3	0
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	В	303	Total	С	Н	N	О	S 12	0	4	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP P61964
A	22	PRO	-	expression tag	UNP P61964
A	23	GLY	-	expression tag	UNP P61964
A	24	TYR	-	expression tag	UNP P61964
В	21	GLY	-	expression tag	UNP P61964
В	22	PRO	-	expression tag	UNP P61964
В	23	GLY	-	expression tag	UNP P61964
В	24	TYR	-	expression tag	UNP P61964

• Molecule 2 is a protein called ORF 73.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
9	D	0	Total	С	Н	N	О	S	0	0	0
	Г	0	133	36	68	18	10	1	U	U	U
9	0	0	Total	С	Н	N	О	S	0	0	0
	Q	0	116	33	57	15	10	1			U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Р	22	ACE	-	acetylation	UNP Q76SB0
P	33	NH2	-	amidation	UNP Q76SB0
Q	22	ACE	-	acetylation	UNP Q76SB0
Q	33	NH2	-	amidation	UNP Q76SB0



### • Molecule 3 is water.

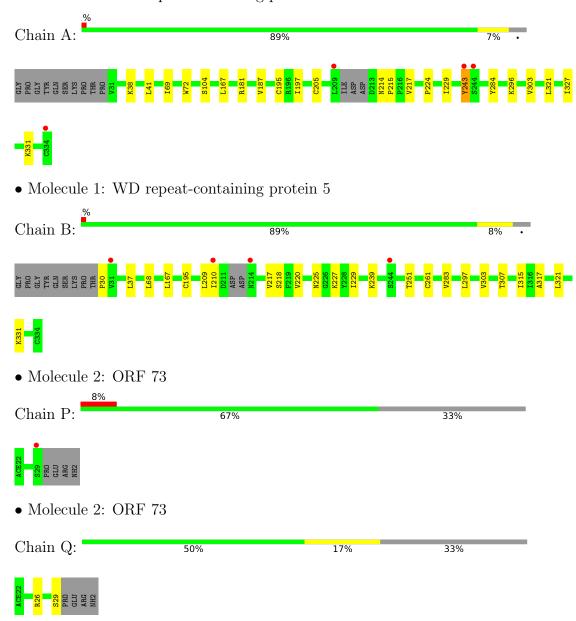
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	321	Total O 324 324	0	3
3	В	339	Total O 340 340	0	1
3	Р	16	Total O 16 16	0	0
3	Q	16	Total O 16 16	0	0



# 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: WD repeat-containing protein 5





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	46.31Å 53.17Å 65.12Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$72.58^{\circ}$ $89.75^{\circ}$ $73.16^{\circ}$	Depositor
Resolution (Å)	39.00 - 1.50	Depositor
resolution (A)	61.88 - 1.50	EDS
% Data completeness	86.2 (39.00-1.50)	Depositor
(in resolution range)	82.4 (61.88-1.50)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.77 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.19rc7_4070	Depositor
P. P.	0.193 , $0.227$	Depositor
$R, R_{free}$	0.194 , $0.227$	DCC
$R_{free}$ test set	3907 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.7	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning <sup>2</sup>	$  <  L  > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10048	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 22.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.6380e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  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: ACE

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
IVIOI	Chain	RMSZ	RMSZ $\# Z  > 5$		# Z  > 5
1	A	0.64	0/2374	0.75	0/3225
1	В	0.55	0/2385	0.73	$1/3247 \ (0.0\%)$
2	Р	0.63	0/62	0.96	0/79
2	Q	0.77	0/56	0.94	0/72
All	All	0.60	0/4877	0.75	1/6623 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
1	В	30	PRO	N-CA-CB	5.86	110.33	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	2309	2250	2242	17	0
1	В	2313	2231	2217	17	0
2	Р	65	68	71	0	0
2	Q	59	57	60	0	0
3	A	324	0	0	2	0
3	В	340	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Р	16	0	0	0	0
3	Q	16	0	0	0	0
All	All	5442	4606	4590	34	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 4.

The worst 5 of 34 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
1:B:195[B]:CYS:SG	1:B:210:ILE:HD12	2.31	0.70
1:B:195[B]:CYS:SG	1:B:217:VAL:HG11	2.35	0.66
1:B:68:LEU:HD12	3:B:418:HOH:O	1.97	0.63
1:B:239:LYS:HG2	1:B:251:THR:HG22	1.82	0.61
1:A:69:ILE:HD11	1:A:104:SER:HB3	1.83	0.60

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	A	300/314~(96%)	286 (95%)	14 (5%)	0	100	100
1	В	304/314~(97%)	293 (96%)	11 (4%)	0	100	100
2	Р	6/12 (50%)	6 (100%)	0	0	100	100
2	Q	6/12 (50%)	6 (100%)	0	0	100	100
All	All	$616/652 \ (94\%)$	591 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.



#### 5.3.2 Protein sidechains (i)

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	Perce	ntiles
1	A	254/274~(93%)	253 (100%)	1 (0%)	91	82
1	В	252/274 (92%)	252 (100%)	0	100	100
2	Р	7/10 (70%)	7 (100%)	0	100	100
2	Q	6/10 (60%)	4 (67%)	2 (33%)	0	0
All	All	519/568 (91%)	516 (99%)	3 (1%)	86	74

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	TYR
2	Q	26	ARG
2	Q	29	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	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 monosaccharides 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,  $95^{th}$  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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	301/314~(95%)	-0.15	4 (1%) 77 81	9, 14, 26, 37	0
1	В	303/314 (96%)	-0.22	4 (1%) 77 81	8, 13, 25, 45	0
2	Р	7/12 (58%)	0.40	1 (14%) 2 2	11, 21, 34, 53	0
2	Q	7/12 (58%)	0.39	0 100 100	12, 22, 45, 55	0
All	All	$618/652 \ (94\%)$	-0.17	9 (1%) 73 78	8, 14, 28, 55	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	210	ILE	4.1
1	A	244	SER	3.4
1	A	243	TYR	2.8
1	В	31	VAL	2.5
2	Р	29	SER	2.5

### 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 monosaccharides 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.

