

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

#### May 28, 2020 – 08:08 pm BST

PDB ID	:	6YIE
$\operatorname{Title}$	:	Structure of a Borealin-INCENP-Survivin complex
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Deposited on		
Resolution	:	3.49 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:

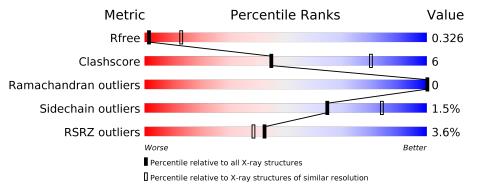
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 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 3.49 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 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	Q	uality of chain		
-1		144	3%			
	A	144	799	%	15%	6%
1	D	144	3%		16%	8%
2	В	100	54%	8%	38%	
2	Е	100	2% <b>52%</b>	8%	40%	
3	С	60	3% 58%	8%	33%	
3	F	60	5%	20%	28%	



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6808 atoms, of which 3225 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 Baculoviral IAP repeat-containing protein 5.

Mol	Chain	Residues			Aton	ıs			ZeroOcc	AltConf	Trace
1	А	135	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
		100	1966	658	939	177	185	7	0	0	0
1	а	133	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0	0
		100	1899	643	887	171	191	7	0		0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-1	GLY	-	expression tag	UNP 015392
А	0	PRO	-	expression tag	UNP 015392
D	-1	GLY	-	expression tag	UNP 015392
D	0	PRO	-	expression tag	UNP 015392

#### • Molecule 2 is a protein called Borealin.

Mol	Chain	Residues		A	Atom	s			ZeroOcc	AltConf	Trace
9	в	62	Total	С	Η	Ν	Ο	S	0	0	0
	D	02	883	299	418	83	82	1	0	0	0
0	Г	60	Total	С	Η	Ν	Ο	S	0	0	0
		00	874	297	416	75	85	1	0	U	U

• Molecule 3 is a protein called Inner centromere protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	С	40	Total 574	0	Н 275	÷ '	~	S 5	0	0	0
3	F	43	Total 610	C 205	Н 290	N 51	O 59	${ m S}{ m 5}$	0	0	0

There are 4 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP Q9NQS7
С	0	PRO	-	expression tag	UNP Q9NQS7
F	-1	GLY	-	expression tag	UNP Q9NQS7
F	0	PRO	-	expression tag	UNP Q9NQS7

• Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0



SLY MET NHR THR THR

# 3 Residue-property plots (i)

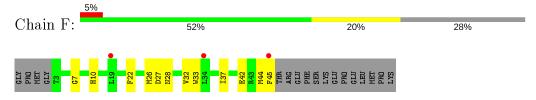
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Chain A: 79% 15% 6% GLY PRO GLY GLY ALA PRO • Molecule 1: Baculoviral IAP repeat-containing protein 5 Chain D: 76% 16% 8% ALA AET ASP • Molecule 2: Borealin Chain B: 54% 38% 8% LYS GLN GLEU GLEU GLU GLU GLU ALA ALA ASP ASP THR THR ASN ALA ALA ALA ALA VAL ALA LYS THR ASN SP • Molecule 2: Borealin Chain E: 52% 8% 40% VAL ALA LYS ASN SER LEU • Molecule 3: Inner centromere protein Chain C: 58% 8% 33%

• Molecule 1: Baculoviral IAP repeat-containing protein 5



• Molecule 3: Inner centromere protein





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	59.54Å 78.82Å 125.17Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	66.70 - 3.49	Depositor
Resolution (A)	66.70 - 3.49	EDS
% Data completeness	87.2 (66.70-3.49)	Depositor
(in resolution range)	87.7(66.70-3.49)	EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.84 (at 3.49 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
B B.	0.269 , $0.324$	Depositor
$R, R_{free}$	0.271 , $0.326$	DCC
$R_{free}$ test set	339 reflections $(4.90%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	61.0	Xtriage
Anisotropy	1.164	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $23.1$	EDS
L-test for $twinning^2$	$ \langle L  \rangle = 0.41, \langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6808	wwPDB-VP
Average B, all atoms $(Å^2)$	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 19.53% 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: ZN

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
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.33	0/1056	0.55	0/1434
1	D	0.30	0/1041	0.54	0/1418
2	В	0.24	0/472	0.45	0/643
2	Е	0.25	0/465	0.44	0/635
3	С	0.26	0/304	0.47	0/412
3	F	0.27	0/326	0.50	0/444
All	All	0.29	0/3664	0.51	0/4986

There are no bond length outliers.

There are no bond angle outliers.

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	1027	939	939	13	2
1	D	1012	887	887	19	2
2	В	465	418	418	4	0
2	Е	458	416	415	7	0
3	С	299	275	274	3	0
3	F	320	290	290	7	0
4	А	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
All	All	3583	3225	3223	44	2

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 44 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:21:THR:HG21	1:A:44:ILE:HG23	1.71	0.71
3:F:7:GLY:O	3:F:10:HIS:ND1	2.29	0.66
1:D:98:LEU:HD23	2:E:65:LEU:O	1.95	0.65
1:D:44:ILE:HD11	1:D:58:PHE:HB3	1.79	0.64
1:A:21:THR:HG21	1:A:44:ILE:CG2	2.27	0.63

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:OE1	1:D:133:ARG:HH12[2_455]	1.41	0.19
1:A:95:GLU:OE1	1:D:133:ARG:NH1[2_455]	2.14	0.06

## 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	А	133/144~(92%)	127~(96%)	6 (4%)	0	100 100
1	D	131/144~(91%)	126 (96%)	5(4%)	0	100 100
2	В	60/100~(60%)	60 (100%)	0	0	100 100
2	Е	58/100~(58%)	58 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	С	38/60~(63%)	38~(100%)	0	0	100	100
3	F	41/60~(68%)	41 (100%)	0	0	100	100
All	All	461/608~(76%)	450 (98%)	11 (2%)	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 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	А	100/124~(81%)	99~(99%)	1 (1%)	76 88
1	D	98/124~(79%)	97~(99%)	1 (1%)	76 88
2	В	41/88~(47%)	40~(98%)	1 (2%)	49 76
2	Е	43/88~(49%)	42 (98%)	1 (2%)	50 77
3	С	29/55~(53%)	29~(100%)	0	100 100
3	F	32/55~(58%)	31~(97%)	1 (3%)	40 70
All	All	343/534~(64%)	338~(98%)	5(2%)	65 84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	70	ASP
2	В	24	PHE
1	D	46	CYS
2	Е	24	PHE
3	F	27	ASP

Some 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)

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)

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 $>$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{A}^2)$	Q<0.9
1	А	135/144~(93%)	0.23	5 (3%) 41 37	26, 51, 80, 101	0
1	D	133/144~(92%)	0.32	5 (3%) 40 36	48, 71, 117, 145	0
2	В	62/100~(62%)	0.14	0 100 100	43, 66, 98, 111	0
2	Е	60/100~(60%)	0.19	2 (3%) 46 41	26, 53, 82, 87	0
3	С	40/60~(66%)	0.28	2 (5%) 28 25	46, 64, 90, 104	0
3	F	43/60~(71%)	0.35	3 (6%) 16 16	46, 70, 93, 113	0
All	All	473/608~(77%)	0.26	17 (3%) 42 38	26,63,100,145	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	RSRZ
1	А	24	ASN	4.7
3	С	19	LEU	3.7
3	С	7	GLY	3.5
1	А	111	ASN	3.1
1	D	31	CYS	3.0

## 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)

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	ZN	D	201	1/1	0.99	0.11	$23,\!23,\!23,\!23$	0
4	ZN	А	201	1/1	1.00	0.14	$30,\!30,\!30,\!30$	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

