

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

#### Aug 15, 2024 – 01:17 pm BST

PDB ID	:	8S31
Title	:	Crystal structure of human PLK1 Polo-Box Domain in complex with
		Mis18BP1
Authors	:	Jeyaprakash, A.A.; Medina-Pritchard, B.
Deposited on	:	2024-02-19
Resolution	:	2.13  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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

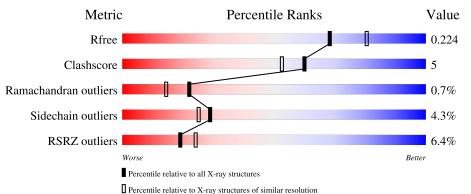
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 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 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	А	242	5%		83%		10%	• 6%
1	В	242	6%	79	9%		14%	•• 6%
2	С	11	18%	55%		18%	27%	
2	D	11	18%	55%		27%	18	3%



#### $\mathbf{2}$ Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4013 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	Δ	227	Total	С	Ν	0	S	0	0	0
1	А	221	1833	1161	318	343	11	0	0	0
1	D	227	Total	С	Ν	0	S	0	0	0
1	D	221	1827	1157	314	345	11	U	U	U

• Molecule 1 is a protein called Serine/threenine-protein kinase PLK1.

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ARG	-	expression tag	UNP P53350
А	363	SER	-	expression tag	UNP P53350
А	364	MET	-	expression tag	UNP P53350
В	362	ARG	-	expression tag	UNP P53350
В	363	SER	-	expression tag	UNP P53350
В	364	MET	-	expression tag	UNP P53350

• Molecule 2 is a protein called Mis18-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
0	C	0	Total	Total C N O P S	N O P S O	0	0				
	U	0	69	42	10	15	1	1	0	0	0
0	Л	0	Total	С	Ν	Ο	Р	S	0	0	0
	D	9	73	45	10	16	1	1	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	99	Total O 99 99	0	0
3	В	93	Total O 93 93	0	0
3	С	12	Total         O           12         12	0	0

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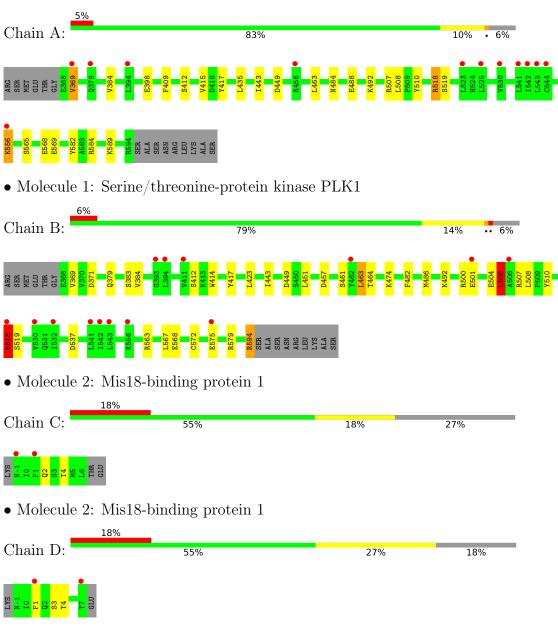
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	7	Total O 7 7	0	0



# 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: Serine/threonine-protein kinase PLK1



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	67.15Å 67.15Å 254.54Å	Denesiten
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	29.08 - 2.13	Depositor
Resolution (A)	29.69 - 2.13	EDS
% Data completeness	99.2 (29.08-2.13)	Depositor
(in resolution range)	99.2 (29.69-2.13)	EDS
R <sub>merge</sub>	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.79 (at 2.14 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
$R, R_{free}$	0.195 , $0.224$	Depositor
II, Ilfree	0.194 , $0.224$	DCC
$R_{free}$ test set	2001  reflections  (5.28%)	wwPDB-VP
Wilson B-factor $(Å^2)$	34.7	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.38,44.0	EDS
L-test for $twinning^2$	$<  L  > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4013	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 4.00% 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

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	Bo	nd lengths	Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.46	1/1871~(0.1%)	0.75	5/2532~(0.2%)	
1	В	0.45	0/1865	0.74	4/2526~(0.2%)	
2	С	0.35	0/57	0.61	0/73	
2	D	0.41	0/61	0.52	0/79	
All	All	0.46	1/3854~(0.0%)	0.74	9/5210~(0.2%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	369	VAL	CB-CG1	6.72	1.67	1.52

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	589	LYS	CB-CG-CD	-9.36	87.26	111.60
1	В	518	ARG	CB-CG-CD	-7.72	91.53	111.60
1	А	589	LYS	CG-CD-CE	7.42	134.16	111.90
1	А	589	LYS	CA-CB-CG	7.25	129.36	113.40
1	В	575	GLU	CA-CB-CG	5.70	125.95	113.40
1	А	556	LYS	CA-CB-CG	-5.70	100.87	113.40
1	А	556	LYS	CD-CE-NZ	-5.61	98.80	111.70
1	В	423	LEU	CA-CB-CG	5.54	128.05	115.30
1	В	505	LEU	CA-CB-CG	5.10	127.03	115.30

All (9) bond angle outliers are listed below:

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	1833	0	1809	11	0
1	В	1827	0	1791	24	0
2	С	69	0	67	0	0
2	D	73	0	70	1	0
3	А	99	0	0	2	0
3	В	93	0	0	2	0
3	С	12	0	0	0	0
3	D	7	0	0	0	0
All	All	4013	0	3737	35	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 5.

All (35) 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:518:ARG:HD2	1:B:519:SER:N	2.12	0.63
1:B:518:ARG:HE	1:B:518:ARG:H	1.45	0.63
1:A:443:ILE:HD11	1:A:510:TYR:HB3	1.79	0.63
1:B:443:ILE:HD11	1:B:510:TYR:HB3	1.81	0.62
1:A:507:ARG:NH2	3:A:701:HOH:O	2.36	0.56
1:B:500:ARG:NH2	3:B:702:HOH:O	2.34	0.56
1:B:518:ARG:HD2	1:B:519:SER:H	1.70	0.56
1:A:384:VAL:HA	1:A:568:GLU:HG3	1.88	0.54
1:B:384:VAL:HA	1:B:568:GLU:HG2	1.90	0.54
1:B:518:ARG:HD2	1:B:518:ARG:N	2.22	0.53
1:B:449:ASP:OD1	1:B:464:THR:HB	2.09	0.53
1:B:518:ARG:H	1:B:518:ARG:NE	2.09	0.50
1:B:567:LEU:HD22	1:B:572:CYS:HB3	1.94	0.50
1:A:518:ARG:HD2	1:A:519:SER:N	2.27	0.49
1:B:482:PHE:O	1:B:486:MET:HG3	2.14	0.47
1:B:474:LYS:HB2	1:B:474:LYS:HE3	1.43	0.46
1:A:518:ARG:NH1	1:A:582:TYR:OH	2.49	0.45
1:B:518:ARG:N	1:B:518:ARG:CD	2.79	0.45
1:A:556:LYS:HA	1:A:556:LYS:HD3	1.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:PHE:CE1	1:A:508:LEU:HD12	2.53	0.44
1:B:414:TRP:CD1	2:D:3:SER:HB3	2.53	0.44
1:B:379:GLN:NE2	1:B:383:SER:OG	2.52	0.43
1:B:504:GLU:O	1:B:505:LEU:CB	2.66	0.43
1:A:484:ASN:O	1:A:488:GLU:HG3	2.18	0.42
1:A:412:SER:HB2	1:A:492:LYS:HG3	2.01	0.42
1:B:451:LEU:HB2	1:B:463:LEU:HG	2.01	0.42
1:B:443:ILE:HG21	1:B:508:LEU:CD2	2.50	0.42
1:B:412:SER:HB2	1:B:492:LYS:HG2	2.02	0.41
1:B:371:ASP:OD1	1:B:594:ARG:HD3	2.20	0.41
1:B:504:GLU:O	1:B:505:LEU:HB2	2.20	0.41
1:A:398:GLU:HB3	3:A:771:HOH:O	2.20	0.41
1:B:537:ASP:OD2	1:B:579:ARG:NH2	2.51	0.41
1:B:518:ARG:HE	1:B:518:ARG:HB3	1.58	0.40
1:A:565:SER:O	1:A:568:GLU:HB2	2.21	0.40
1:B:563:ARG:HG3	3:B:716:HOH:O	2.20	0.40

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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	225/242~(93%)	221 (98%)	4(2%)	0	100	100
1	В	225/242~(93%)	216 (96%)	6 (3%)	3~(1%)	12	6
2	$\mathbf{C}$	5/11~(46%)	4 (80%)	1 (20%)	0	100	100
2	D	6/11~(54%)	5 (83%)	1 (17%)	0	100	100
All	All	461/506~(91%)	446 (97%)	12 (3%)	3~(1%)	22	14

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	505	LEU
1	В	457	ASP
1	В	507	ARG

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentile	es
1	А	203/218~(93%)	194~(96%)	9~(4%)	28 24	
1	В	202/218~(93%)	195~(96%)	7 (4%)	36 33	
2	С	7/10~(70%)	6 (86%)	1 (14%)	3 1	
2	D	7/10 (70%)	6 (86%)	1 (14%)	3 1	
All	All	419/456~(92%)	401 (96%)	18 (4%)	29 25	

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	369	VAL
1	А	415	VAL
1	А	417	TYR
1	А	435	LEU
1	А	449	ASP
1	А	463	LEU
1	А	518	ARG
1	А	569	GLU
1	А	584	ARG
1	В	369	VAL
1	В	417	TYR
1	В	461	SER
1	В	463	LEU
1	В	501	GLU
1	В	518	ARG
1	В	594	ARG
2	С	2	GLN
2	D	1	PHE



Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	В	379	GLN
2	С	2	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	Turne	Chain Bog Link		be Chain Res Link Bond lengths $(1 + D)                                       $				В	ond ang	les
NIOI	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	TPO	С	4	2	8,10,11	1.64	1 (12%)	10,14,16	1.31	1 (10%)
2	TPO	D	4	2	8,10,11	1.68	2 (25%)	10,14,16	1.34	1 (10%)

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	4	2	-	0/9/11/13	-
2	TPO	D	4	2	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	D	4	TPO	P-O1P	3.26	1.61	1.50
2	С	4	TPO	P-O1P	3.23	1.61	1.50
2	D	4	TPO	P-OG1	2.15	1.63	1.59



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	4	TPO	P-OG1-CB	-3.51	112.60	123.21
2	D	4	TPO	P-OG1-CB	-3.31	113.21	123.21

All (2) bond angle outliers are listed below:

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	227/242~(93%)	0.04	12 (5%) 26 33	27, 37, 55, 69	0
1	В	227/242 (93%)	0.10	14 (6%) 20 25	29, 39, 57, 73	0
2	С	7/11~(63%)	0.81	2 (28%) 0 0	36, 44, 53, 58	0
2	D	8/11 (72%)	1.58	2 (25%) 0 0	38, 49, 60, 66	0
All	All	469/506~(92%)	0.10	30 (6%) 19 24	27, 38, 57, 73	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	7	THR	7.9
1	В	393	GLY	3.9
2	С	-1	ASN	3.7
2	С	1	PHE	3.7
1	А	542	ILE	3.4
1	А	525	LEU	2.9
1	В	543	LEU	2.8
1	А	556	LYS	2.8
2	D	1	PHE	2.7
1	А	394	LEU	2.7
1	А	530	VAL	2.7
1	В	556	LYS	2.7
1	А	543	LEU	2.6
1	А	541	LEU	2.5
1	В	394	LEU	2.5
1	В	532	ILE	2.5
1	В	530	VAL	2.5
1	В	518	ARG	2.4
1	В	542	ILE	2.4
1	В	575	GLU	2.4
1	В	462	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	В	501	GLU	2.3
1	В	411	VAL	2.2
1	А	523	LEU	2.2
1	А	544	CYS	2.2
1	А	456	ARG	2.1
1	В	541	LEU	2.1
1	A	369	VAL	2.1
1	В	506	ALA	2.1
1	A	379	GLN	2.0

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### 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	TPO	D	4	11/12	0.97	0.08	32,34,39,41	0
2	TPO	С	4	11/12	0.98	0.07	36,38,41,41	0

#### 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.

