Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2023 – 10:24 PM EDT

PDB ID	:	6N46
Title	:	Crystal structure of the cryptic polo box domain of a human activated Plk4
Authors	:	Park, J.-E.; DiMaio, F.; Zhang, L.; Lee, K.S.
Deposited on	:	2018-11-17
Resolution	:	3.71 Å(reported)

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

MolProbity	:	FAILED
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.71 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 14000 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 Serine/threonine-protein kinase PLK4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1750	1118	294	332	6			
1	B	212	Total	C	N	O	S	0	0	0
			1750	1118	294	332	6			
1	C	212	Total	C	N	O	S	0	0	0
			1750	1118	294	332	6			
1	D	212	Total	C	N	O	S	0	0	0
			1750	1118	294	332	6			
1	E	212	Total	C	N	O	S	0	0	0
			1750	1118	294	332	6			
1	F	212	Total	C	N	O	S	0	0	0
			1750	1118	294	332	6			
1	G	212	Total	C	N	O	S	0	0	0
			1750	1118	294	332	6			
1	H	212	Total	C	N	O	S	0	0	0
			1750	1118	294	332	6			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	initiating methionine	UNP O00444
A	-24	GLY	-	expression tag	UNP O00444
A	-23	SER	-	expression tag	UNP O00444
A	-22	SER	-	expression tag	UNP O00444
A	-21	HIS	-	expression tag	UNP O00444
A	-20	HIS	-	expression tag	UNP O00444
A	-19	HIS	-	expression tag	UNP O00444
A	-18	HIS	-	expression tag	UNP O00444
A	-17	HIS	-	expression tag	UNP O00444
A	-16	HIS	-	expression tag	UNP O00444
A	-15	SER	-	expression tag	UNP O00444
A	-14	SER	-	expression tag	UNP O00444
A	-13	GLY	-	expression tag	UNP O00444

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	LEU	-	expression tag	UNP O00444
A	-11	VAL	-	expression tag	UNP O00444
A	-10	PRO	-	expression tag	UNP O00444
A	-9	ARG	-	expression tag	UNP O00444
A	-8	GLY	-	expression tag	UNP O00444
A	-7	SER	-	expression tag	UNP O00444
A	-6	HIS	-	expression tag	UNP O00444
A	-5	MET	-	expression tag	UNP O00444
A	113	GLU	SER	conflict	UNP O00444
A	115	GLU	SER	conflict	UNP O00444
A	119	GLU	THR	conflict	UNP O00444
A	122	ASP	THR	conflict	UNP O00444
B	-25	MET	-	initiating methionine	UNP O00444
B	-24	GLY	-	expression tag	UNP O00444
B	-23	SER	-	expression tag	UNP O00444
B	-22	SER	-	expression tag	UNP O00444
B	-21	HIS	-	expression tag	UNP O00444
B	-20	HIS	-	expression tag	UNP O00444
B	-19	HIS	-	expression tag	UNP O00444
B	-18	HIS	-	expression tag	UNP O00444
B	-17	HIS	-	expression tag	UNP O00444
B	-16	HIS	-	expression tag	UNP O00444
B	-15	SER	-	expression tag	UNP O00444
B	-14	SER	-	expression tag	UNP O00444
B	-13	GLY	-	expression tag	UNP O00444
B	-12	LEU	-	expression tag	UNP O00444
B	-11	VAL	-	expression tag	UNP O00444
B	-10	PRO	-	expression tag	UNP O00444
B	-9	ARG	-	expression tag	UNP O00444
B	-8	GLY	-	expression tag	UNP O00444
B	-7	SER	-	expression tag	UNP O00444
B	-6	HIS	-	expression tag	UNP O00444
B	-5	MET	-	expression tag	UNP O00444
B	113	GLU	SER	conflict	UNP O00444
B	115	GLU	SER	conflict	UNP O00444
B	119	GLU	THR	conflict	UNP O00444
B	122	ASP	THR	conflict	UNP O00444
C	-25	MET	-	initiating methionine	UNP O00444
C	-24	GLY	-	expression tag	UNP O00444
C	-23	SER	-	expression tag	UNP O00444
C	-22	SER	-	expression tag	UNP O00444
C	-21	HIS	-	expression tag	UNP O00444

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-20	HIS	-	expression tag	UNP O00444
C	-19	HIS	-	expression tag	UNP O00444
C	-18	HIS	-	expression tag	UNP O00444
C	-17	HIS	-	expression tag	UNP O00444
C	-16	HIS	-	expression tag	UNP O00444
C	-15	SER	-	expression tag	UNP O00444
C	-14	SER	-	expression tag	UNP O00444
C	-13	GLY	-	expression tag	UNP O00444
C	-12	LEU	-	expression tag	UNP O00444
C	-11	VAL	-	expression tag	UNP O00444
C	-10	PRO	-	expression tag	UNP O00444
C	-9	ARG	-	expression tag	UNP O00444
C	-8	GLY	-	expression tag	UNP O00444
C	-7	SER	-	expression tag	UNP O00444
C	-6	HIS	-	expression tag	UNP O00444
C	-5	MET	-	expression tag	UNP O00444
C	113	GLU	SER	conflict	UNP O00444
C	115	GLU	SER	conflict	UNP O00444
C	119	GLU	THR	conflict	UNP O00444
C	122	ASP	THR	conflict	UNP O00444
D	-25	MET	-	initiating methionine	UNP O00444
D	-24	GLY	-	expression tag	UNP O00444
D	-23	SER	-	expression tag	UNP O00444
D	-22	SER	-	expression tag	UNP O00444
D	-21	HIS	-	expression tag	UNP O00444
D	-20	HIS	-	expression tag	UNP O00444
D	-19	HIS	-	expression tag	UNP O00444
D	-18	HIS	-	expression tag	UNP O00444
D	-17	HIS	-	expression tag	UNP O00444
D	-16	HIS	-	expression tag	UNP O00444
D	-15	SER	-	expression tag	UNP O00444
D	-14	SER	-	expression tag	UNP O00444
D	-13	GLY	-	expression tag	UNP O00444
D	-12	LEU	-	expression tag	UNP O00444
D	-11	VAL	-	expression tag	UNP O00444
D	-10	PRO	-	expression tag	UNP O00444
D	-9	ARG	-	expression tag	UNP O00444
D	-8	GLY	-	expression tag	UNP O00444
D	-7	SER	-	expression tag	UNP O00444
D	-6	HIS	-	expression tag	UNP O00444
D	-5	MET	-	expression tag	UNP O00444
D	113	GLU	SER	conflict	UNP O00444

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Chain	Residue	Modelled	Actual	Comment	Reference
D	115	GLU	SER	conflict	UNP O00444
D	119	GLU	THR	conflict	UNP O00444
D	122	ASP	THR	conflict	UNP O00444
E	-25	MET	-	initiating methionine	UNP O00444
E	-24	GLY	-	expression tag	UNP O00444
E	-23	SER	-	expression tag	UNP O00444
E	-22	SER	-	expression tag	UNP O00444
E	-21	HIS	-	expression tag	UNP O00444
E	-20	HIS	-	expression tag	UNP O00444
E	-19	HIS	-	expression tag	UNP O00444
E	-18	HIS	-	expression tag	UNP O00444
E	-17	HIS	-	expression tag	UNP O00444
E	-16	HIS	-	expression tag	UNP O00444
E	-15	SER	-	expression tag	UNP O00444
E	-14	SER	-	expression tag	UNP O00444
E	-13	GLY	-	expression tag	UNP O00444
E	-12	LEU	-	expression tag	UNP O00444
E	-11	VAL	-	expression tag	UNP O00444
E	-10	PRO	-	expression tag	UNP O00444
E	-9	ARG	-	expression tag	UNP O00444
E	-8	GLY	-	expression tag	UNP O00444
E	-7	SER	-	expression tag	UNP O00444
E	-6	HIS	-	expression tag	UNP O00444
E	-5	MET	-	expression tag	UNP O00444
E	113	GLU	SER	conflict	UNP O00444
E	115	GLU	SER	conflict	UNP O00444
E	119	GLU	THR	conflict	UNP O00444
E	122	ASP	THR	conflict	UNP O00444
F	-25	MET	-	initiating methionine	UNP O00444
F	-24	GLY	-	expression tag	UNP O00444
F	-23	SER	-	expression tag	UNP O00444
F	-22	SER	-	expression tag	UNP O00444
F	-21	HIS	-	expression tag	UNP O00444
F	-20	HIS	-	expression tag	UNP O00444
F	-19	HIS	-	expression tag	UNP O00444
F	-18	HIS	-	expression tag	UNP O00444
F	-17	HIS	-	expression tag	UNP O00444
F	-16	HIS	-	expression tag	UNP O00444
F	-15	SER	-	expression tag	UNP O00444
F	-14	SER	-	expression tag	UNP O00444
F	-13	GLY	-	expression tag	UNP O00444
F	-12	LEU	-	expression tag	UNP O00444

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	VAL	-	expression tag	UNP O00444
F	-10	PRO	-	expression tag	UNP O00444
F	-9	ARG	-	expression tag	UNP O00444
F	-8	GLY	-	expression tag	UNP O00444
F	-7	SER	-	expression tag	UNP O00444
F	-6	HIS	-	expression tag	UNP O00444
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F	119	GLU	THR	conflict	UNP O00444
F	122	ASP	THR	conflict	UNP O00444
G	-25	MET	-	initiating methionine	UNP O00444
G	-24	GLY	-	expression tag	UNP O00444
G	-23	SER	-	expression tag	UNP O00444
G	-22	SER	-	expression tag	UNP O00444
G	-21	HIS	-	expression tag	UNP O00444
G	-20	HIS	-	expression tag	UNP O00444
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H	-22	SER	-	expression tag	UNP O00444
H	-21	HIS	-	expression tag	UNP O00444
H	-20	HIS	-	expression tag	UNP O00444

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H	-16	HIS	-	expression tag	UNP O00444
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H	-14	SER	-	expression tag	UNP O00444
H	-13	GLY	-	expression tag	UNP O00444
H	-12	LEU	-	expression tag	UNP O00444
H	-11	VAL	-	expression tag	UNP O00444
H	-10	PRO	-	expression tag	UNP O00444
H	-9	ARG	-	expression tag	UNP O00444
H	-8	GLY	-	expression tag	UNP O00444
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H	-5	MET	-	expression tag	UNP O00444
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H	115	GLU	SER	conflict	UNP O00444
H	119	GLU	THR	conflict	UNP O00444
H	122	ASP	THR	conflict	UNP O00444

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	110.83Å　110.83Å　205.68Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	37.81　–　3.71	Depositor
% Data completeness (in resolution range)	99.3 (37.81-3.71)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.66Å)	Xtriage
Refinement program	PHENIX 1.14_3235	Depositor
R, R_{free}	0.271　,　0.309	Depositor
Wilson B-factor (Å^2)	146.0	Xtriage
Anisotropy	0.231	Xtriage
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l 0.448 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
Total number of atoms	14000	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]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.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

There are no ligands in this entry.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

5.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.