Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 08:27 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)

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:

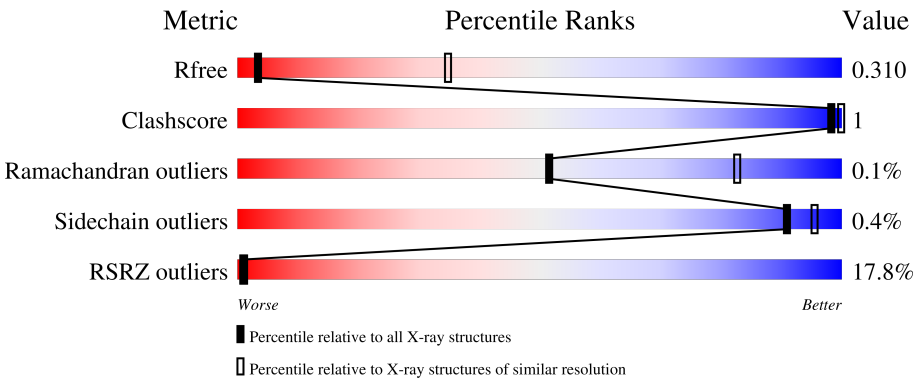
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.71 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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	249	16% 85% 15%
1	B	249	22% 84% • 15%
1	C	249	13% 82% • 15%
1	D	249	21% 82% • 15%
1	E	249	12% 83% • 15%

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Mol	Chain	Length	Quality of chain
1	F	249	10% 84% • 15%
1	G	249	14% 83% • 15%
1	H	249	13% 85% 15%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	212	1750	1118	294	332	6	0	0	0
1	B	212	1750	1118	294	332	6	0	0	0
1	C	212	1750	1118	294	332	6	0	0	0
1	D	212	1750	1118	294	332	6	0	0	0
1	E	212	1750	1118	294	332	6	0	0	0
1	F	212	1750	1118	294	332	6	0	0	0
1	G	212	1750	1118	294	332	6	0	0	0
1	H	212	1750	1118	294	332	6	0	0	0

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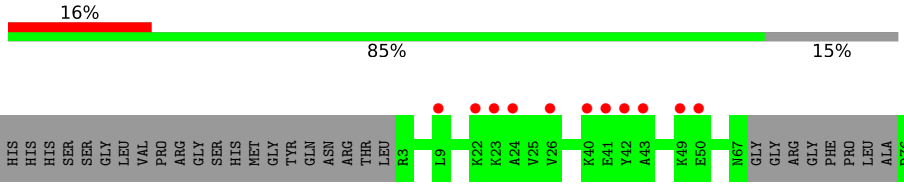
Chain	Residue	Modelled	Actual	Comment	Reference
H	-19	HIS	-	expression tag	UNP O00444
H	-18	HIS	-	expression tag	UNP O00444
H	-17	HIS	-	expression tag	UNP O00444
H	-16	HIS	-	expression tag	UNP O00444
H	-15	SER	-	expression tag	UNP O00444
H	-14	SER	-	expression tag	UNP O00444
H	-13	GLY	-	expression tag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

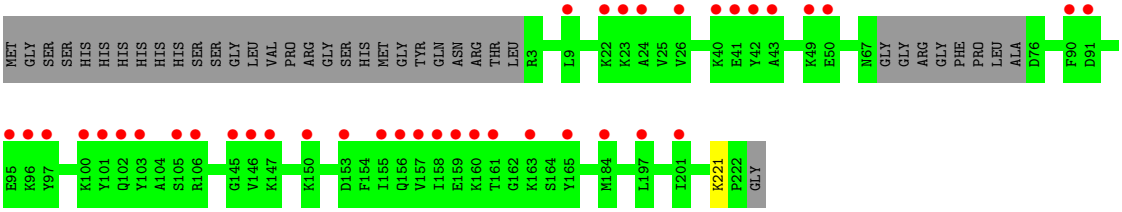
3 Residue-property plots (i)

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 PLK4

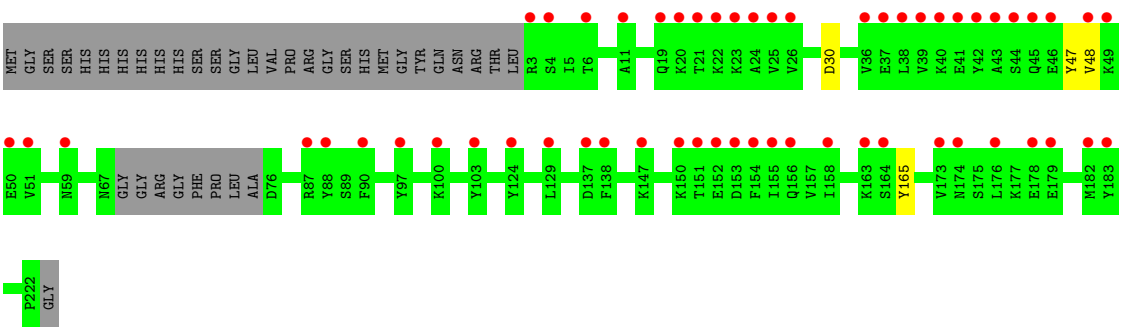
Chain A:





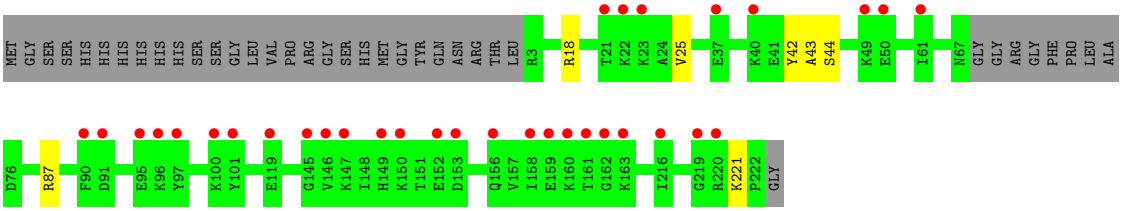
• Molecule 1: Serine/threonine-protein kinase PLK4

Chain B:



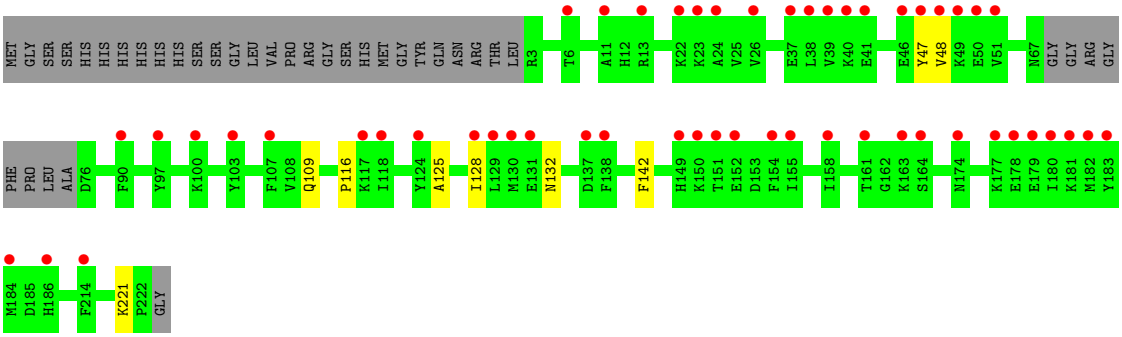
• Molecule 1: Serine/threonine-protein kinase PLK4

Chain C:



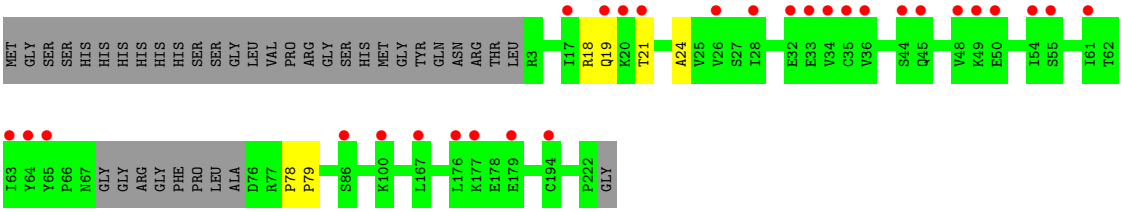
• Molecule 1: Serine/threonine-protein kinase PLK4

Chain D:



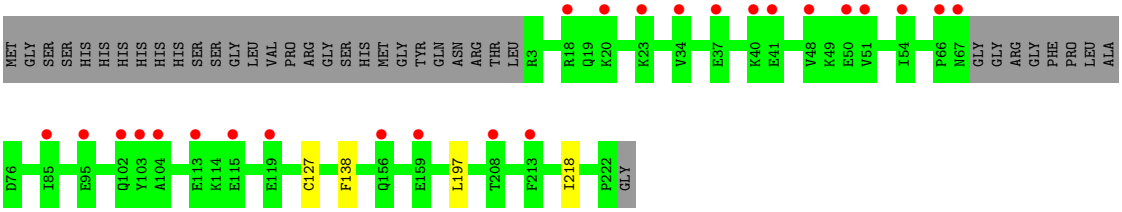
- Molecule 1: Serine/threonine-protein kinase PLK4

Chain E:



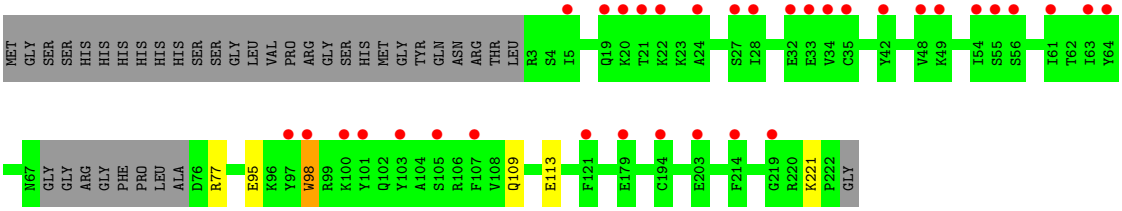
- Molecule 1: Serine/threonine-protein kinase PLK4

Chain F:



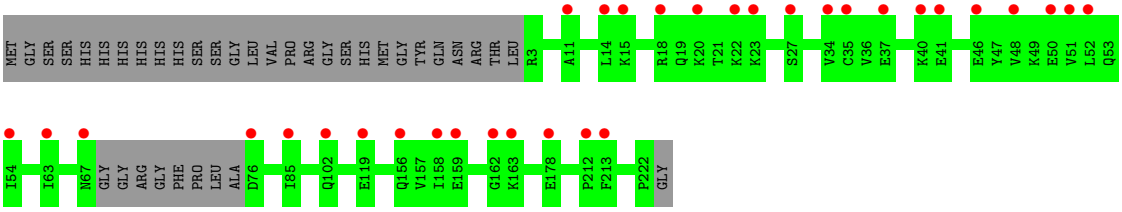
- Molecule 1: Serine/threonine-protein kinase PLK4

Chain G:



- Molecule 1: Serine/threonine-protein kinase PLK4

Chain H:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET GLY TYR GLN ASN ARG THR LEU R3
A11
L14 K15
R18 Q19 K20 T21 K22 K23
S27
V34 C35 V36 E37
K40 E41
E46 Y47 V48 K49 E50 V51 L52 Q53
I54
I63
N67 GLY GLY ARG GLY PHE PRO LEU ALA
D76
I85
Q102
E119
Q156 V157 I158 E159
G162 K163
E178
P212 F213
P222 GLY

4 Data and refinement statistics (i)

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 45.33 – 3.71	Depositor EDS
% Data completeness (in resolution range)	99.3 (37.81-3.71) 99.8 (45.33-3.71)	Depositor EDS
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 0.271 , 0.310	Depositor DCC
R_{free} test set	2002 reflections (6.70%)	wwPDB-VP
Wilson B-factor (Å^2)	146.0	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 140.3	EDS
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
F_o,F_c correlation	0.90	EDS
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.*

[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.

5 Model quality (i)

5.1 Standard geometry (i)

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	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.31	0/1789	0.52	0/2413
1	B	0.31	0/1789	0.54	0/2413
1	C	0.31	0/1789	0.52	0/2413
1	D	0.30	0/1789	0.54	0/2413
1	E	0.31	0/1789	0.54	0/2413
1	F	0.32	0/1789	0.53	0/2413
1	G	0.32	0/1789	0.53	0/2413
1	H	0.30	0/1789	0.52	0/2413
All	All	0.31	0/14312	0.53	0/19304

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	A	1750	0	1746	0	0
1	B	1750	0	1746	4	0
1	C	1750	0	1746	2	0
1	D	1750	0	1746	4	0
1	E	1750	0	1746	4	0
1	F	1750	0	1746	2	0
1	G	1750	0	1746	2	0
1	H	1750	0	1746	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14000	0	13968	16	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 1.

All (16) 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:165:TYR:HA	1:E:18:ARG:O	2.05	0.56
1:B:47:TYR:CG	1:B:48:VAL:N	2.81	0.48
1:D:47:TYR:CG	1:D:48:VAL:N	2.82	0.48
1:B:165:TYR:HB3	1:E:19:GLN:HA	1.97	0.47
1:F:127:CYS:HB3	1:F:138:PHE:CZ	2.53	0.43
1:D:109:GLN:NE2	1:D:132:ASN:OD1	2.50	0.43
1:B:30:ASP:OD1	1:B:30:ASP:N	2.52	0.43
1:C:42:TYR:O	1:C:44:SER:N	2.51	0.43
1:E:21:THR:OG1	1:E:24:ALA:O	2.28	0.42
1:G:95:GLU:O	1:G:98:TRP:HB3	2.20	0.41
1:C:18:ARG:CZ	1:C:25:VAL:HG11	2.50	0.41
1:D:125:ALA:HB2	1:D:142:PHE:CD2	2.56	0.41
1:D:116:PRO:HB3	1:D:128:ILE:HG23	2.03	0.41
1:E:78:PRO:HA	1:E:79:PRO:HD3	1.96	0.41
1:G:109:GLN:O	1:G:113:GLU:HG3	2.20	0.41
1:F:197:LEU:HD13	1:F:218:ILE:HD13	2.02	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	Percentiles
1	A	208/249 (84%)	204 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	208/249 (84%)	203 (98%)	5 (2%)	0	100	100
1	C	208/249 (84%)	204 (98%)	3 (1%)	1 (0%)	29	66
1	D	208/249 (84%)	201 (97%)	7 (3%)	0	100	100
1	E	208/249 (84%)	204 (98%)	4 (2%)	0	100	100
1	F	208/249 (84%)	205 (99%)	3 (1%)	0	100	100
1	G	208/249 (84%)	203 (98%)	5 (2%)	0	100	100
1	H	208/249 (84%)	204 (98%)	4 (2%)	0	100	100
All	All	1664/1992 (84%)	1628 (98%)	35 (2%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	ALA

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	A	197/225 (88%)	196 (100%)	1 (0%)	88	94
1	B	197/225 (88%)	197 (100%)	0	100	100
1	C	197/225 (88%)	195 (99%)	2 (1%)	76	86
1	D	197/225 (88%)	196 (100%)	1 (0%)	88	94
1	E	197/225 (88%)	197 (100%)	0	100	100
1	F	197/225 (88%)	197 (100%)	0	100	100
1	G	197/225 (88%)	194 (98%)	3 (2%)	65	81
1	H	197/225 (88%)	197 (100%)	0	100	100
All	All	1576/1800 (88%)	1569 (100%)	7 (0%)	91	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LYS
1	C	87	ARG
1	C	221	LYS
1	D	221	LYS
1	G	77	ARG
1	G	98	TRP
1	G	221	LYS

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

Mol	Chain	Res	Type
1	G	53	GLN
1	H	53	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)

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, 95th 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	A	212/249 (85%)	0.99	39 (18%)	1	1	92, 167, 255, 286	0
1	B	212/249 (85%)	1.41	56 (26%)	0	0	96, 171, 248, 282	0
1	C	212/249 (85%)	0.86	33 (15%)	2	1	90, 166, 256, 283	0
1	D	212/249 (85%)	1.25	53 (25%)	0	0	95, 168, 256, 278	0
1	E	212/249 (85%)	0.82	29 (13%)	3	3	100, 148, 216, 240	0
1	F	212/249 (85%)	0.71	25 (11%)	4	4	90, 154, 217, 248	0
1	G	212/249 (85%)	0.85	34 (16%)	1	1	99, 153, 224, 263	0
1	H	212/249 (85%)	0.82	33 (15%)	2	1	89, 153, 229, 275	0
All	All	1696/1992 (85%)	0.96	302 (17%)	1	1	89, 159, 246, 286	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	TYR	10.3
1	B	50	GLU	10.3
1	B	40	LYS	9.9
1	D	50	GLU	9.7
1	C	97	TYR	9.6
1	A	41	GLU	9.4
1	D	40	LYS	9.1
1	E	49	LYS	8.7
1	D	179	GLU	8.4
1	A	159	GLU	8.1
1	C	23	LYS	7.8
1	B	90	PHE	7.6
1	C	91	ASP	7.5
1	B	178	GLU	6.8
1	H	41	GLU	6.8
1	G	34	VAL	6.7

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Mol	Chain	Res	Type	RSRZ
1	B	41	GLU	6.7
1	D	174	ASN	6.6
1	D	22	LYS	6.6
1	B	49	LYS	6.4
1	D	49	LYS	6.4
1	D	137	ASP	6.3
1	D	39	VAL	6.3
1	C	22	LYS	6.3
1	C	160	LYS	6.3
1	B	179	GLU	6.2
1	B	24	ALA	6.2
1	D	150	LYS	6.2
1	B	155	ILE	6.0
1	F	41	GLU	6.0
1	E	34	VAL	5.9
1	F	67	ASN	5.8
1	A	95	GLU	5.8
1	B	22	LYS	5.7
1	D	178	GLU	5.7
1	B	154	PHE	5.6
1	F	40	LYS	5.6
1	G	21	THR	5.6
1	E	21	THR	5.5
1	G	54	ILE	5.4
1	D	38	LEU	5.3
1	B	150	LYS	5.3
1	C	161	THR	5.2
1	C	163	LYS	5.1
1	A	42	TYR	5.1
1	D	48	VAL	5.1
1	C	159	GLU	5.0
1	G	64	TYR	5.0
1	H	18	ARG	5.0
1	D	151	THR	4.9
1	B	37	GLU	4.8
1	B	21	THR	4.8
1	A	101	TYR	4.8
1	A	102	GLN	4.8
1	E	54	ILE	4.8
1	B	43	ALA	4.7
1	A	160	LYS	4.7
1	D	129	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	50	GLU	4.7
1	G	20	LYS	4.7
1	B	39	VAL	4.7
1	A	40	LYS	4.6
1	B	173	VAL	4.6
1	A	163	LYS	4.6
1	D	37	GLU	4.6
1	D	24	ALA	4.6
1	A	23	LYS	4.6
1	F	50	GLU	4.6
1	D	184	MET	4.6
1	E	48	VAL	4.6
1	B	45	GLN	4.5
1	B	103	TYR	4.5
1	D	152	GLU	4.5
1	C	95	GLU	4.5
1	G	55	SER	4.5
1	B	4	SER	4.5
1	B	88	TYR	4.4
1	B	23	LYS	4.4
1	H	159	GLU	4.4
1	E	45	GLN	4.4
1	B	38	LEU	4.4
1	E	100	LYS	4.4
1	D	182	MET	4.4
1	D	41	GLU	4.4
1	B	59	ASN	4.2
1	F	85	ILE	4.2
1	B	152	GLU	4.1
1	B	164	SER	4.1
1	A	165	TYR	4.1
1	H	40	LYS	4.1
1	D	164	SER	4.0
1	H	213	PHE	4.0
1	D	118	ILE	4.0
1	E	35	CYS	4.0
1	A	161	THR	4.0
1	B	42	TYR	4.0
1	G	63	ILE	4.0
1	G	35	CYS	4.0
1	A	158	ILE	3.9
1	H	102	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	55	SER	3.9
1	G	33	GLU	3.9
1	H	51	VAL	3.9
1	F	51	VAL	3.8
1	B	20	LYS	3.8
1	F	102	GLN	3.8
1	A	43	ALA	3.8
1	H	76	ASP	3.8
1	B	129	LEU	3.8
1	D	161	THR	3.8
1	H	85	ILE	3.7
1	H	178	GLU	3.7
1	E	20	LYS	3.7
1	G	100	LYS	3.6
1	A	24	ALA	3.6
1	C	96	LYS	3.6
1	B	138	PHE	3.5
1	F	119	GLU	3.5
1	E	63	ILE	3.5
1	A	96	LYS	3.5
1	E	19	GLN	3.5
1	D	23	LYS	3.5
1	G	27	SER	3.5
1	A	50	GLU	3.4
1	A	90	PHE	3.4
1	D	26	VAL	3.4
1	C	150	LYS	3.4
1	E	50	GLU	3.4
1	F	66	PRO	3.4
1	G	179	GLU	3.4
1	A	145	GLY	3.4
1	D	103	TYR	3.4
1	H	52	LEU	3.4
1	A	147	LYS	3.3
1	H	22	LYS	3.3
1	H	35	CYS	3.3
1	E	64	TYR	3.3
1	B	151	THR	3.3
1	A	156	GLN	3.3
1	F	48	VAL	3.3
1	B	153	ASP	3.3
1	D	90	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	6	THR	3.3
1	G	48	VAL	3.3
1	C	149	HIS	3.2
1	E	176	LEU	3.2
1	H	27	SER	3.2
1	F	104	ALA	3.2
1	B	174	ASN	3.2
1	G	219	GLY	3.2
1	C	158	ILE	3.2
1	G	32	GLU	3.2
1	G	28	ILE	3.1
1	B	183	TYR	3.1
1	B	147	LYS	3.1
1	B	3	ARG	3.1
1	D	117	LYS	3.1
1	D	183	TYR	3.1
1	D	177	LYS	3.1
1	E	28	ILE	3.1
1	B	176	LEU	3.1
1	B	158	ILE	3.0
1	B	182	MET	3.0
1	G	49	LYS	3.0
1	G	121	PHE	3.0
1	B	6	THR	3.0
1	C	156	GLN	3.0
1	A	155	ILE	2.9
1	D	154	PHE	2.9
1	A	184	MET	2.9
1	E	194	CYS	2.9
1	D	155	ILE	2.9
1	C	101	TYR	2.9
1	H	163	LYS	2.9
1	D	13	ARG	2.8
1	E	65	TYR	2.8
1	A	146	VAL	2.8
1	H	48	VAL	2.8
1	F	18	ARG	2.8
1	A	150	LYS	2.8
1	H	20	LYS	2.8
1	H	11	ALA	2.8
1	D	158	ILE	2.8
1	F	115	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	25	VAL	2.8
1	G	5	ILE	2.8
1	H	23	LYS	2.8
1	D	186	HIS	2.7
1	A	22	LYS	2.7
1	G	103	TYR	2.7
1	C	40	LYS	2.7
1	G	98	TRP	2.7
1	B	97	TYR	2.7
1	B	19	GLN	2.7
1	A	9	LEU	2.7
1	D	47	TYR	2.6
1	H	14	LEU	2.6
1	D	51	VAL	2.6
1	C	37	GLU	2.6
1	D	138	PHE	2.6
1	C	146	VAL	2.6
1	G	19	GLN	2.6
1	H	34	VAL	2.5
1	B	87	ARG	2.5
1	D	11	ALA	2.5
1	F	34	VAL	2.5
1	F	156	GLN	2.5
1	G	61	ILE	2.5
1	H	212	PRO	2.5
1	F	213	PHE	2.5
1	F	95	GLU	2.5
1	G	105	SER	2.5
1	C	153	ASP	2.5
1	E	179	GLU	2.5
1	H	37	GLU	2.5
1	G	24	ALA	2.5
1	E	86	SER	2.5
1	E	26	VAL	2.5
1	B	163	LYS	2.5
1	F	37	GLU	2.5
1	H	67	ASN	2.4
1	A	106	ARG	2.4
1	C	90	PHE	2.4
1	F	103	TYR	2.4
1	A	105	SER	2.4
1	E	167	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	177	LYS	2.4
1	C	100	LYS	2.4
1	G	22	LYS	2.4
1	H	162	GLY	2.4
1	E	44	SER	2.4
1	D	163	LYS	2.4
1	H	158	ILE	2.4
1	D	97	TYR	2.4
1	C	162	GLY	2.4
1	D	130	MET	2.4
1	B	124	TYR	2.4
1	A	197	LEU	2.4
1	B	11	ALA	2.4
1	A	100	LYS	2.4
1	D	107	PHE	2.4
1	A	153	ASP	2.4
1	A	26	VAL	2.3
1	B	44	SER	2.3
1	A	49	LYS	2.3
1	G	42	TYR	2.3
1	C	145	GLY	2.3
1	C	220	ARG	2.3
1	D	128	ILE	2.3
1	D	100	LYS	2.3
1	C	152	GLU	2.3
1	C	147	LYS	2.3
1	E	17	ILE	2.3
1	C	21	THR	2.2
1	F	20	LYS	2.2
1	H	63	ILE	2.2
1	D	149	HIS	2.2
1	B	51	VAL	2.2
1	H	119	GLU	2.2
1	B	156	GLN	2.2
1	H	156	GLN	2.2
1	F	23	LYS	2.2
1	F	54	ILE	2.2
1	D	46	GLU	2.2
1	E	33	GLU	2.2
1	H	54	ILE	2.2
1	D	214	PHE	2.2
1	H	15	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	119	GLU	2.2
1	E	32	GLU	2.2
1	G	194	CYS	2.2
1	D	180	ILE	2.2
1	A	91	ASP	2.2
1	G	107	PHE	2.2
1	H	46	GLU	2.2
1	F	159	GLU	2.2
1	G	56	SER	2.2
1	G	101	TYR	2.2
1	E	61	ILE	2.2
1	F	113	GLU	2.1
1	B	36	VAL	2.1
1	F	208	THR	2.1
1	D	124	TYR	2.1
1	H	50	GLU	2.1
1	A	157	VAL	2.1
1	B	46	GLU	2.1
1	A	103	TYR	2.1
1	B	48	VAL	2.1
1	D	181	LYS	2.1
1	C	49	LYS	2.1
1	G	97	TYR	2.1
1	B	137	ASP	2.1
1	A	201	ILE	2.1
1	G	203	GLU	2.1
1	D	131	GLU	2.0
1	C	61	ILE	2.0
1	B	100	LYS	2.0
1	C	219	GLY	2.0
1	E	36	VAL	2.0
1	G	214	PHE	2.0
1	C	216	ILE	2.0
1	B	26	VAL	2.0

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 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.