



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:01 am BST

PDB ID : 6N45
Title : Crystal structure of the cryptic polo box domain of human activated Plk4 variant 1
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Deposited on : 2018-11-17
Resolution : 2.64 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

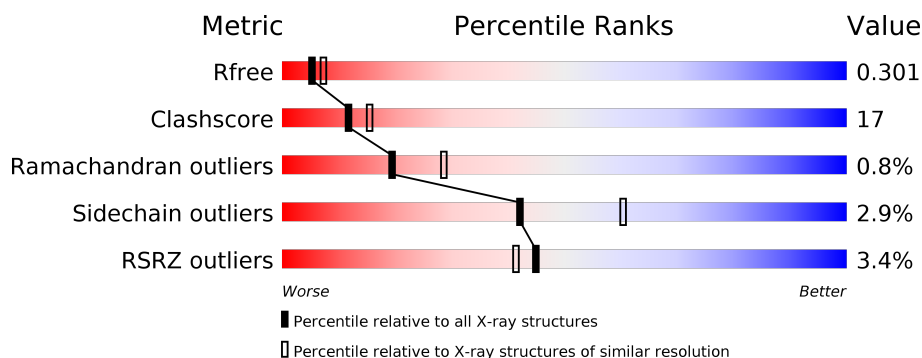
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 $\leq 5\%$. 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	266	<div> <div>3%</div> <div>58%</div> <div>18%</div> <div>22%</div> </div>
1	B	266	<div> <div>3%</div> <div>57%</div> <div>17%</div> <div>25%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2933 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 Chimera protein of Serine/threonine-protein kinase PLK4 and DDB1- and CUL4-associated factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1486	943	247	292	4			
1	B	200	Total	C	N	O	S	0	0	0
			1447	927	237	278	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	577	GLY	-	expression tag	UNP O00444
A	578	ALA	-	expression tag	UNP O00444
A	579	HIS	-	expression tag	UNP O00444
A	580	MET	-	expression tag	UNP O00444
A	698	GLU	SER	conflict	UNP O00444
A	700	GLU	SER	conflict	UNP O00444
A	704	GLU	THR	conflict	UNP O00444
A	707	ASP	THR	conflict	UNP O00444
A	809	VAL	-	linker	UNP O00444
B	577	GLY	-	expression tag	UNP O00444
B	578	ALA	-	expression tag	UNP O00444
B	579	HIS	-	expression tag	UNP O00444
B	580	MET	-	expression tag	UNP O00444
B	698	GLU	SER	conflict	UNP O00444
B	700	GLU	SER	conflict	UNP O00444
B	704	GLU	THR	conflict	UNP O00444
B	707	ASP	THR	conflict	UNP O00444
B	809	VAL	-	linker	UNP O00444

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	61.66 Å 61.66 Å 137.28 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.77 – 2.64 34.75 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.77-2.64) 99.9 (34.75-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.65 Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.234 , 0.314 0.240 , 0.301	Depositor DCC
R_{free} test set	838 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l 0.487 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2933	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

5 Model quality

5.1 Standard geometry

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	0.76	0/1519	0.97	0/2081
1	B	0.79	0/1479	0.93	0/2023
All	All	0.77	0/2998	0.95	0/4104

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

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	1486	0	1270	52	0
1	B	1447	0	1268	50	0
All	All	2933	0	2538	95	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 17.

All (95) 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:609:ALA:HB1	1:A:622:GLU:O	1.47	1.12
1:B:633:VAL:CG1	1:B:657:PHE:CB	2.46	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:GLU:HG2	1:A:734:HIS:HD2	1.35	0.91
1:B:633:VAL:HG12	1:B:657:PHE:CB	2.05	0.86
1:B:751:THR:HG22	1:B:751:THR:O	1.75	0.86
1:B:633:VAL:HG22	1:B:634:LYS:H	1.43	0.83
1:A:650:TYR:O	1:A:667:THR:HG21	1.80	0.81
1:B:633:VAL:HG12	1:B:657:PHE:O	1.87	0.75
1:A:596:ALA:HA	1:A:599:LEU:CD1	2.18	0.73
1:A:649:TYR:HB2	1:A:667:THR:HG22	1.72	0.72
1:B:588:ARG:HA	1:B:675:PHE:CE2	2.25	0.70
1:A:782:LEU:HD11	1:B:798:PHE:CE1	2.27	0.70
1:B:763:GLU:O	1:B:765:ILE:N	2.25	0.69
1:B:591:THR:HG22	1:B:592:SER:O	1.92	0.69
1:A:609:ALA:HB2	1:A:623:LEU:HA	1.73	0.69
1:A:782:LEU:HD11	1:B:798:PHE:CD1	2.27	0.69
1:A:598:ARG:NH2	1:A:716:GLU:OE2	2.25	0.69
1:A:597:HIS:HE1	1:A:642:ASP:HA	1.59	0.67
1:B:695:LEU:HD23	1:B:695:LEU:C	2.16	0.66
1:A:598:ARG:HH21	1:A:716:GLU:CD	1.99	0.66
1:A:667:THR:HG23	1:A:669:ASN:H	1.61	0.64
1:A:724:GLU:CG	1:A:734:HIS:HD2	2.10	0.61
1:B:708:ARG:O	1:B:728:TYR:CE2	2.53	0.61
1:A:596:ALA:HA	1:A:599:LEU:HD11	1.81	0.61
1:B:596:ALA:HA	1:B:599:LEU:HD22	1.83	0.61
1:A:640:SER:OG	1:A:645:THR:HB	2.00	0.61
1:B:650:TYR:O	1:B:667:THR:HG21	2.02	0.60
1:A:785:ILE:CG2	1:B:785:ILE:CG2	2.80	0.60
1:A:798:PHE:O	1:B:803:ILE:HG23	2.01	0.59
1:B:623:LEU:O	1:B:633:VAL:HG23	2.01	0.59
1:A:724:GLU:HG2	1:A:734:HIS:CD2	2.26	0.58
1:B:708:ARG:O	1:B:728:TYR:HE2	1.86	0.57
1:A:597:HIS:CE1	1:A:642:ASP:HA	2.40	0.57
1:B:588:ARG:HB2	1:B:675:PHE:CE2	2.40	0.57
1:A:596:ALA:HA	1:A:599:LEU:HD12	1.86	0.55
1:B:588:ARG:HA	1:B:675:PHE:CZ	2.41	0.55
1:B:709:TYR:HD2	1:B:771:HIS:CD2	2.25	0.55
1:B:667:THR:CG2	1:B:669:ASN:H	2.20	0.54
1:A:803:ILE:HG23	1:B:798:PHE:O	2.09	0.52
1:B:588:ARG:O	1:B:589:SER:C	2.49	0.51
1:B:751:THR:CG2	1:B:751:THR:O	2.44	0.51
1:B:706:PHE:CE1	1:B:711:LYS:HG3	2.46	0.51
1:B:790:GLU:HA	1:B:798:PHE:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:ALA:O	1:A:599:LEU:HG	2.12	0.50
1:B:754:SER:OG	1:B:754:SER:O	2.25	0.50
1:A:596:ALA:CA	1:A:599:LEU:HD12	2.41	0.50
1:B:633:VAL:HG22	1:B:634:LYS:N	2.21	0.49
1:B:695:LEU:HD23	1:B:695:LEU:O	2.12	0.49
1:B:588:ARG:HB2	1:B:675:PHE:HE2	1.76	0.48
1:A:645:THR:CG2	1:A:672:ARG:HD3	2.44	0.48
1:A:765:ILE:O	1:A:768:TYR:HB2	2.13	0.48
1:A:759:ASN:C	1:A:761:LEU:N	2.66	0.48
1:A:736:THR:HG22	1:A:739:PHE:H	1.79	0.47
1:B:588:ARG:CA	1:B:675:PHE:CE2	2.97	0.47
1:A:759:ASN:O	1:A:761:LEU:N	2.47	0.47
1:B:667:THR:HG23	1:B:669:ASN:H	1.79	0.47
1:B:798:PHE:O	1:B:801:ILE:CG2	2.63	0.47
1:A:793:THR:HG22	1:A:795:SER:OG	2.14	0.47
1:A:802:ILE:HD12	1:A:802:ILE:N	2.31	0.46
1:A:596:ALA:CB	1:A:599:LEU:HD12	2.45	0.46
1:B:602:ILE:O	1:B:612:SER:HA	2.15	0.46
1:A:649:TYR:CE2	1:A:666:PRO:HA	2.51	0.46
1:A:596:ALA:HB1	1:A:599:LEU:HD12	1.97	0.46
1:A:759:ASN:C	1:A:761:LEU:H	2.19	0.46
1:A:711:LYS:HE2	1:A:713:ILE:HD11	1.97	0.45
1:B:801:ILE:CD1	1:B:803:ILE:HD11	2.45	0.45
1:A:609:ALA:CB	1:A:623:LEU:HA	2.43	0.45
1:B:790:GLU:HA	1:B:798:PHE:CE2	2.52	0.45
1:B:731:VAL:HG12	1:B:732:LYS:N	2.31	0.45
1:A:588:ARG:C	1:A:590:ILE:N	2.71	0.44
1:B:667:THR:CG2	1:B:668:ASP:N	2.80	0.44
1:A:609:ALA:CB	1:A:622:GLU:O	2.39	0.44
1:B:736:THR:HB	1:B:739:PHE:O	2.18	0.43
1:B:788:GLU:HA	1:B:791:ARG:NH1	2.33	0.43
1:A:594:LEU:O	1:A:642:ASP:O	2.37	0.43
1:A:667:THR:HG23	1:A:669:ASN:N	2.29	0.43
1:A:760:SER:O	1:A:761:LEU:C	2.57	0.43
1:A:710:ALA:N	1:A:728:TYR:CE2	2.86	0.43
1:B:695:LEU:CD2	1:B:695:LEU:C	2.85	0.43
1:B:645:THR:CG2	1:B:672:ARG:HD3	2.48	0.42
1:A:801:ILE:HA	1:B:802:ILE:O	2.20	0.42
1:B:646:ILE:HD12	1:B:646:ILE:N	2.35	0.42
1:B:588:ARG:CB	1:B:675:PHE:HE2	2.33	0.42
1:A:603:ARG:CZ	1:A:661:ASP:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:PRO:O	1:A:680:GLU:C	2.59	0.42
1:A:680:GLU:HA	1:A:683:TRP:CD2	2.55	0.42
1:B:633:VAL:HG11	1:B:657:PHE:CB	2.41	0.42
1:A:588:ARG:O	1:A:590:ILE:N	2.52	0.41
1:A:788:GLU:HA	1:A:791:ARG:NH1	2.35	0.41
1:A:736:THR:HG22	1:A:738:ASP:N	2.36	0.41
1:A:796:ALA:HB3	1:B:705:TYR:OH	2.20	0.41
1:A:680:GLU:HA	1:A:683:TRP:CE2	2.55	0.41
1:B:798:PHE:O	1:B:801:ILE:HG22	2.21	0.41
1:B:633:VAL:HG22	1:B:635:GLU:H	1.86	0.40
1:A:586:THR:HG23	1:A:586:THR:O	2.21	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	199/266 (75%)	179 (90%)	20 (10%)	0	100	100
1	B	190/266 (71%)	175 (92%)	12 (6%)	3 (2%)	9	13
All	All	389/532 (73%)	354 (91%)	32 (8%)	3 (1%)	19	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	634	LYS
1	B	590	ILE
1	B	764	GLU

5.3.2 Protein sidechains ⓘ

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	138 / 241 (57%)	134 (97%)	4 (3%)	42	60
1	B	137 / 241 (57%)	133 (97%)	4 (3%)	42	60
All	All	275 / 482 (57%)	267 (97%)	8 (3%)	42	60

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	669	ASN
1	A	707	ASP
1	A	736	THR
1	A	801	ILE
1	B	661	ASP
1	B	667	THR
1	B	707	ASP
1	B	736	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	669	ASN
1	A	734	HIS
1	A	776	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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	207/266 (77%)	0.20	7 (3%) 45 41	60, 81, 116, 142	0
1	B	200/266 (75%)	0.16	7 (3%) 44 40	30, 78, 110, 139	0
All	All	407/532 (76%)	0.18	14 (3%) 45 41	30, 78, 113, 142	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	633	VAL	4.0
1	A	632	TYR	3.5
1	A	677	ASN	2.5
1	B	636	VAL	2.5
1	A	795	SER	2.5
1	B	733	ILE	2.5
1	B	647	THR	2.5
1	B	781	ALA	2.4
1	B	765	ILE	2.3
1	B	703	ILE	2.2
1	A	586	THR	2.2
1	A	624	VAL	2.1
1	A	595	VAL	2.1
1	A	647	THR	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 carbohydrates 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.