



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 01:34 PM EDT

PDB ID : 2OU7
Title : Structure of the Catalytic Domain of Human Polo-like Kinase 1
Authors : Ding, Y.-H.; Kothe, M.; Kohls, D.; Low, S.
Deposited on : unknown
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/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 : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

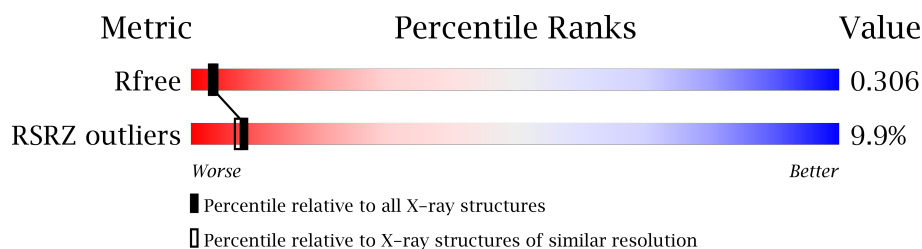
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	501	-	-	-	X
3	ACT	A	502	-	-	-	X
3	ACT	A	503	-	-	-	X
5	ANP	A	500[A]	-	-	-	X
5	ANP	A	500[B]	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2522 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 PLK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	1	0
			2370	1524	421	414	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	CLONING ARTIFACT	UNP P53350
A	12	PRO	-	CLONING ARTIFACT	UNP P53350
A	210	VAL	THR	ENGINEERED	UNP P53350

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

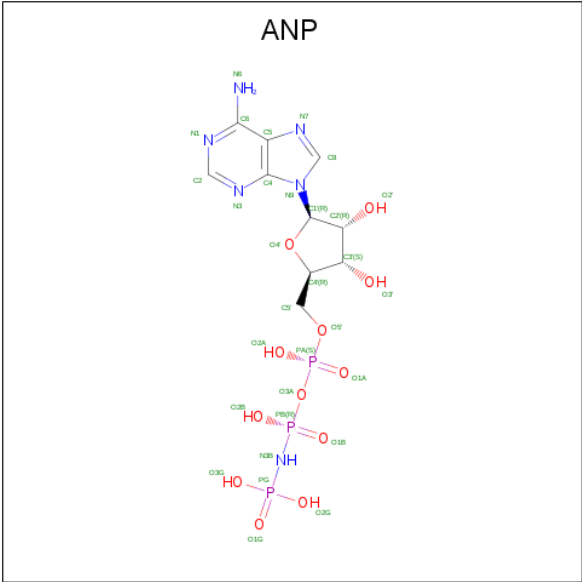


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			44	10	7	21	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	97	Total	O	0	0
			97	97		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	65.96Å 65.96Å 154.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.90 – 2.40 45.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (45.90-2.40) 93.9 (45.88-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.235 0.290 , 0.306	Depositor DCC
R_{free} test set	755 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.773	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2522	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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4.5 Carbohydrates [i](#)

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4.6 Ligand geometry [i](#)

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4.7 Other polymers [i](#)

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4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

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	292/335 (87%)	0.70	29 (9%) 8 7	7, 16, 56, 69	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ALA	8.2
1	A	39	GLU	4.9
1	A	83	ILE	4.4
1	A	64	PHE	3.6
1	A	38	LYS	3.5
1	A	60	GLY	3.5
1	A	57	ARG	3.3
1	A	73	ALA	3.3
1	A	49	SER	3.1
1	A	40	ILE	3.0
1	A	58	PHE	3.0
1	A	139	LEU	3.0
1	A	50	ARG	2.8
1	A	138	LEU	2.8
1	A	66	LYS	2.6
1	A	68	PHE	2.6
1	A	42	GLU	2.6
1	A	113	VAL	2.5
1	A	67	CYS	2.4
1	A	148	LEU	2.4
1	A	137	SER	2.3
1	A	74	ASP	2.2
1	A	80	ALA	2.2
1	A	292	ALA	2.2
1	A	78	VAL	2.2
1	A	41	PRO	2.1
1	A	47	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	272	LYS	2.1
1	A	114	VAL	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
3	ACT	A	502	4/4	0.96	0.32	4.64	51,52,52,53	0
5	ANP	A	500[A]	31/31	0.68	0.31	4.52	80,84,86,86	13
2	ZN	A	501	1/1	0.93	0.31	4.37	44,44,44,44	0
3	ACT	A	503	4/4	0.91	0.36	2.19	37,38,40,41	0
5	ANP	A	500[B]	31/31	0.68	0.31	2.10	77,83,85,86	13
4	MG	A	505	1/1	0.29	0.92	-	28,28,28,28	1
4	MG	A	504	1/1	0.37	0.57	-	55,55,55,55	1

5.5 Other polymers [i](#)

There are no such residues in this entry.