Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2021 – 09:01 am BST

PDB ID	:	7APJ
Title	:	Structure of autoinhibited Akt1 reveals mechanism of PIP3-mediated activation
Authors	:	Truebestein, L.; Hornegger, H.; Leonard, T.A.
Deposited on	:	2020-10-16
Resolution	:	2.05 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:

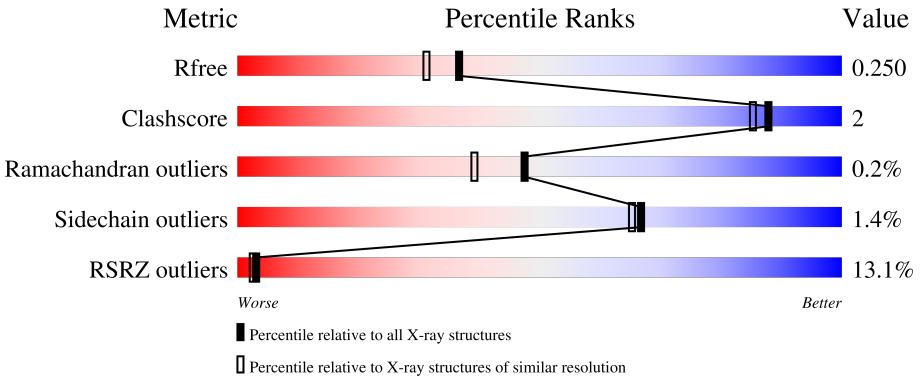
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	440	13% 80% 7% 12%
2	B	126	7% 90% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4259 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 RAC-alpha serine/threonine-protein kinase,Non-specific serine/threonine protein kinase,RAC-alpha serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3197	2048	544	589	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P31749
A	0	ARG	-	expression tag	UNP P31749
A	2	ASN	SER	engineered mutation	UNP P31749

- Molecule 2 is a protein called NB41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			899	559	168	168	4			

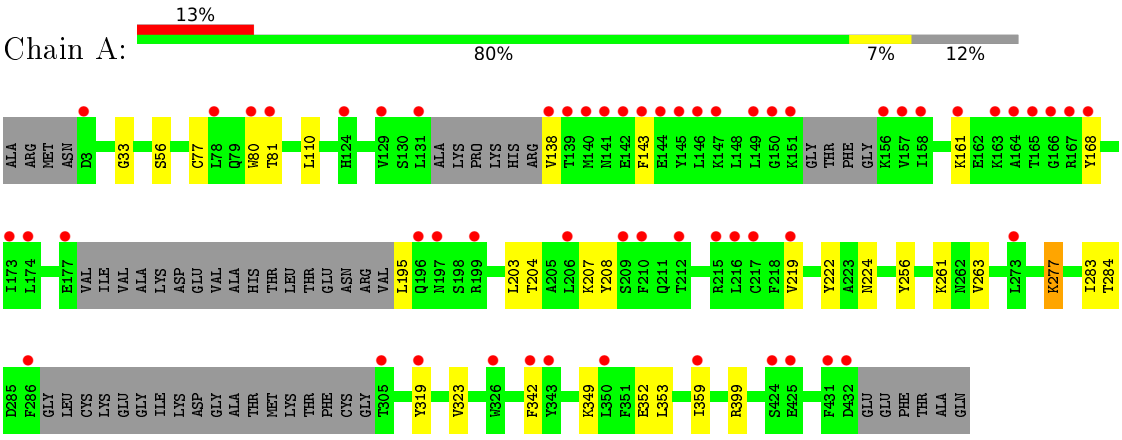
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total	O	0	0
			138	138		
3	B	25	Total	O	0	0
			25	25		

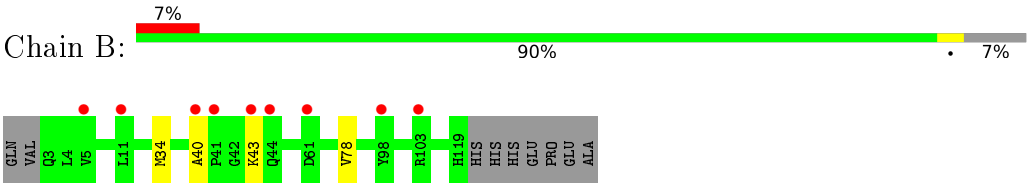
3 Residue-property plots (i)

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: RAC-alpha serine/threonine-protein kinase,Non-specific serine/threonine protein kinase,RAC-alpha serine/threonine-protein kinase



• Molecule 2: NB41



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.01Å 72.20Å 120.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.55 – 2.05 45.60 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.55-2.05) 99.8 (45.60-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.211 , 0.252 0.211 , 0.250	Depositor DCC
R_{free} test set	1952 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4259	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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

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	0.25	0/3271	0.42	0/4405
2	B	0.25	0/916	0.46	0/1241
All	All	0.25	0/4187	0.43	0/5646

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	3197	0	3145	14	0
2	B	899	0	893	2	0
3	A	138	0	0	2	0
3	B	25	0	0	0	0
All	All	4259	0	4038	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 2.

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:A:208:TYR:HB2	1:A:219:VAL:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD23	1:A:283:ILE:HB	1.86	0.58
1:A:319:TYR:HD2	1:A:323:VAL:HG21	1.71	0.55
1:A:195:LEU:N	3:A:505:HOH:O	2.37	0.55
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.88	0.55
1:A:342:PHE:CZ	1:A:359:ILE:HG12	2.45	0.52
1:A:80:TRP:CD1	1:A:81:THR:HG23	2.48	0.48
1:A:161:LYS:HE2	1:A:168:TYR:CE1	2.49	0.48
1:A:256:TYR:OH	1:A:261:LYS:HE3	2.17	0.45
1:A:56:SER:O	1:A:77:CYS:HB2	2.17	0.45
2:B:34:MET:HG3	2:B:78:VAL:HG21	2.00	0.44
1:A:204:THR:OG1	1:A:284:THR:HG22	2.18	0.43
1:A:277:LYS:HD3	3:A:543:HOH:O	2.18	0.42
1:A:222:TYR:CE2	1:A:224:ASN:HB3	2.54	0.42
1:A:349:LYS:O	1:A:353:LEU:HG	2.20	0.41
1:A:33:GLY:HA3	1:A:110:LEU:HD11	2.02	0.41

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	375/440 (85%)	359 (96%)	15 (4%)	1 (0%)	41	31
2	B	115/126 (91%)	115 (100%)	0	0	100	100
All	All	490/566 (87%)	474 (97%)	15 (3%)	1 (0%)	47	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	143	PHE

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	345/388 (89%)	339 (98%)	6 (2%)	60 57
2	B	96/104 (92%)	96 (100%)	0	100 100
All	All	441/492 (90%)	435 (99%)	6 (1%)	67 65

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	VAL
1	A	207	LYS
1	A	263	VAL
1	A	277	LYS
1	A	352	GLU
1	A	399	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 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, 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	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	385/440 (87%)	1.00	57 (14%) 2 1	28, 50, 104, 125	0
2	B	117/126 (92%)	0.62	9 (7%) 13 14	33, 57, 82, 102	0
All	All	502/566 (88%)	0.91	66 (13%) 3 2	28, 53, 102, 125	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	ASN	7.8
1	A	165	THR	6.8
1	A	149	LEU	5.9
1	A	145	TYR	5.4
1	A	166	GLY	5.1
1	A	150	GLY	4.6
1	A	217	CYS	4.5
1	A	80	TRP	4.5
2	B	40	ALA	4.4
2	B	103	ARG	4.4
1	A	196	GLN	4.3
1	A	174	LEU	4.1
1	A	209	SER	4.1
1	A	319	TYR	4.1
1	A	146	LEU	4.0
1	A	216	LEU	4.0
1	A	432	ASP	4.0
1	A	424	SER	3.9
1	A	78	LEU	3.9
1	A	131	LEU	3.8
1	A	138	VAL	3.8
1	A	161	LYS	3.7
1	A	3	ASP	3.7
1	A	129	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	210	PHE	3.5
1	A	173	ILE	3.5
2	B	44	GLN	3.4
1	A	431	PHE	3.4
1	A	199	ARG	3.4
1	A	147	LYS	3.4
1	A	167	ARG	3.4
2	B	43	LYS	3.4
1	A	157	VAL	3.4
1	A	212	THR	3.2
1	A	81	THR	3.1
1	A	286	PHE	3.1
1	A	151	LYS	3.1
1	A	143	PHE	3.0
1	A	305	THR	3.0
1	A	144	GLU	2.9
1	A	158	ILE	2.9
1	A	163	LYS	2.7
1	A	215	ARG	2.7
2	B	11	LEU	2.7
2	B	41	PRO	2.6
1	A	156	LYS	2.6
1	A	343	TYR	2.5
1	A	425	GLU	2.5
1	A	140	MET	2.4
1	A	139	THR	2.4
1	A	219	VAL	2.3
1	A	124	HIS	2.3
1	A	359	ILE	2.3
1	A	168	TYR	2.3
1	A	206	LEU	2.2
1	A	177	GLU	2.2
1	A	273	LEU	2.2
1	A	342	PHE	2.2
1	A	164	ALA	2.1
1	A	142	GLU	2.1
2	B	5	VAL	2.1
1	A	326	TRP	2.1
1	A	197	ASN	2.1
1	A	350	LEU	2.1
2	B	98	TYR	2.1
2	B	61	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.