



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:36 PM GMT

PDB ID : 4TUU
Title : Isolated p110a subunit of PI3Ka provides a platform for structure-based drug design
Authors : Chen, P.; Deng, Y.-L.; Bergqvist, S.; Falk, M.; Liu, W.; Timofeevski, S.
Deposited on : 2014-06-24
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
<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 : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

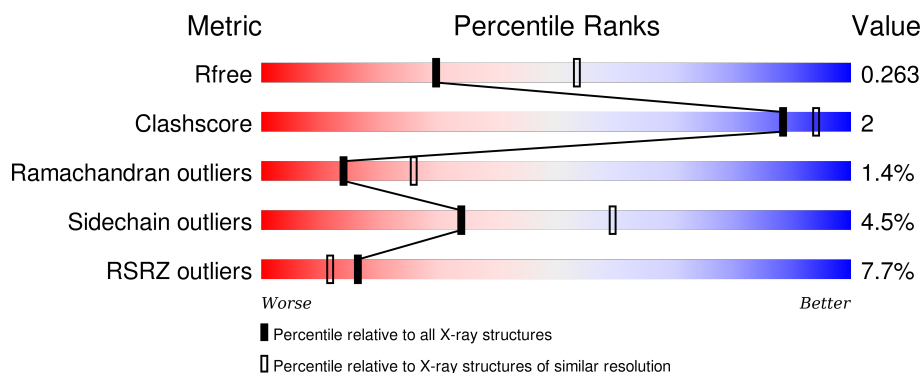
1 Overall quality at a glance

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}	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

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. 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	946	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6631 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 Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	879	Total	C	N	O	S	0	0	0
			6601	4231	1106	1206	58			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	expression tag	UNP P42336
A	104	SER	-	expression tag	UNP P42336

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.69Å 136.45Å 143.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.64 – 2.64 35.49 – 2.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.64-2.64) 100.0 (35.49-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.209 , 0.245 0.225 , 0.263	Depositor DCC
R_{free} test set	1720 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.2	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 33986 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6631	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.52	0/6751	0.70	1/9207 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	507	SER	C-N-CA	7.76	141.10	121.70

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	6601	0	5945	31	0
2	A	30	0	0	0	0
All	All	6631	0	5945	31	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 (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:A:633:ILE:CD1	1:A:633:ILE:CG1	1.78	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HG2	1:A:127:GLU:HG3	1.73	0.70
1:A:568:LEU:HG	1:A:583:MET:HE1	1.75	0.67
1:A:357:ARG:HE	1:A:372:ASN:HD21	1.45	0.65
1:A:395:ASP:HB3	1:A:575:ASN:O	1.98	0.63
1:A:776:LYS:HE2	1:A:804:GLY:HA3	1.82	0.61
1:A:807:LEU:HD12	1:A:846:GLY:HA3	1.83	0.60
1:A:568:LEU:HG	1:A:583:MET:CE	2.32	0.58
1:A:596:GLU:HG2	1:A:997:LEU:HD13	1.87	0.57
1:A:199:SER:HB2	1:A:200:PRO:HD2	1.88	0.55
1:A:357:ARG:NE	1:A:372:ASN:HD21	2.05	0.54
1:A:135:GLU:OE2	1:A:644:TYR:HB3	2.08	0.53
1:A:661:GLN:NE2	1:A:698:TYR:HB2	2.24	0.52
1:A:562:PRO:HG3	1:A:591:PRO:HG2	1.91	0.52
1:A:379:SER:O	1:A:381:PRO:HD3	2.10	0.51
1:A:766:LEU:HD12	1:A:766:LEU:H	1.76	0.49
1:A:341:ALA:HB3	1:A:381:PRO:HB2	1.96	0.47
1:A:346:VAL:HG22	1:A:347:ASN:H	1.80	0.47
1:A:514:SER:HB3	1:A:517:LEU:HD12	1.96	0.47
1:A:121:ILE:HD11	1:A:689:GLU:HA	1.98	0.46
1:A:251:ILE:HD13	1:A:293:LEU:HD22	1.99	0.45
1:A:336:ILE:HD13	1:A:402:LEU:HD22	1.98	0.44
1:A:354:ILE:HG12	1:A:378:CYS:HA	1.99	0.44
1:A:162:ARG:HH22	1:A:300:ASP:HB2	1.82	0.44
1:A:572:VAL:HG21	1:A:583:MET:HG2	2.00	0.43
1:A:121:ILE:HG12	1:A:688:LEU:HB3	2.00	0.43
1:A:776:LYS:HE2	1:A:804:GLY:CA	2.48	0.42
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.55	0.41
1:A:454:ASP:CG	1:A:455:LEU:H	2.23	0.41
1:A:199:SER:CB	1:A:200:PRO:HD2	2.51	0.41
1:A:1002:PHE:HB3	1:A:1019:ILE:HG12	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	863/946 (91%)	801 (93%)	50 (6%)	12 (1%)	14	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	LYS
1	A	508	TYR
1	A	199	SER
1	A	231	SER
1	A	511	ALA
1	A	830	ASP
1	A	862	CYS
1	A	915	ASP
1	A	933	ASP
1	A	453	GLU
1	A	381	PRO
1	A	510	HIS

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	624/860 (73%)	596 (96%)	28 (4%)	34	59

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	GLU
1	A	301	CYS
1	A	345	ASN
1	A	376	VAL
1	A	378	CYS
1	A	384	ASN
1	A	393	ILE

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Mol	Chain	Res	Type
1	A	410	LYS
1	A	461	VAL
1	A	462	THR
1	A	464	SER
1	A	554	HIS
1	A	612	ARG
1	A	626	ASP
1	A	661	GLN
1	A	679	THR
1	A	715	LEU
1	A	735	LEU
1	A	740	ARG
1	A	764	LEU
1	A	766	LEU
1	A	789	MET
1	A	805	ASP
1	A	811	MET
1	A	829	LEU
1	A	834	LEU
1	A	1017	ASP
1	A	1044	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	ASN
1	A	372	ASN
1	A	419	HIS
1	A	530	GLN
1	A	738	GLN
1	A	825	GLN

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 ⓘ

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, 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	879/946 (92%)	0.40	68 (7%) 16 12	35, 62, 106, 142	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	ASN	6.0
1	A	953	PRO	5.9
1	A	451	GLY	5.9
1	A	306	SER	5.8
1	A	873	ASN	5.3
1	A	299	MET	5.0
1	A	954	PHE	4.8
1	A	300	ASP	4.6
1	A	308	SER	4.5
1	A	502	ARG	4.4
1	A	936	HIS	4.0
1	A	307	TYR	4.0
1	A	520	ASP	3.8
1	A	1033	GLN	3.7
1	A	503	GLU	3.7
1	A	1039	PHE	3.6
1	A	501	SER	3.6
1	A	303	THR	3.4
1	A	775	ALA	3.3
1	A	182	TYR	3.3
1	A	891	ASP	3.3
1	A	518	ALA	3.3
1	A	864	GLY	2.9
1	A	302	PHE	2.9
1	A	963	VAL	2.9
1	A	1046	ALA	2.9
1	A	522	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	872	PHE	2.8
1	A	483	VAL	2.8
1	A	508	TYR	2.8
1	A	1035	ALA	2.8
1	A	482	SER	2.6
1	A	523	LEU	2.6
1	A	938	LEU	2.6
1	A	916	ARG	2.6
1	A	380	ASN	2.6
1	A	188	GLY	2.5
1	A	248	GLY	2.5
1	A	740	ARG	2.5
1	A	417	GLU	2.5
1	A	185	LEU	2.4
1	A	180	HIS	2.4
1	A	301	CYS	2.4
1	A	489	MET	2.4
1	A	131	VAL	2.4
1	A	488	ASP	2.3
1	A	141	ARG	2.3
1	A	550	PHE	2.3
1	A	278	MET	2.3
1	A	629	SER	2.2
1	A	972	THR	2.2
1	A	951	ARG	2.2
1	A	231	SER	2.2
1	A	978	GLU	2.2
1	A	305	PRO	2.2
1	A	1031	THR	2.2
1	A	214	ASP	2.2
1	A	246	TYR	2.1
1	A	490	SER	2.1
1	A	664	GLY	2.1
1	A	974	THR	2.1
1	A	157	ASN	2.1
1	A	937	PHE	2.1
1	A	960	PHE	2.1
1	A	450	HIS	2.1
1	A	557	TYR	2.1
1	A	212	ASN	2.0
1	A	537	ARG	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.