Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 12:47 PM EDT

PDB ID	:	6U28
Title	:	Crystal structure of 1918 NS1-ED W187A in complex with the p85-beta-iSH2 domain of human PI3K
Authors	:	Cho, J.H.; Zhao, B.; Savage, N.; Li, P.
Deposited on	:	2019-08-19
Resolution	:	2.95 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:

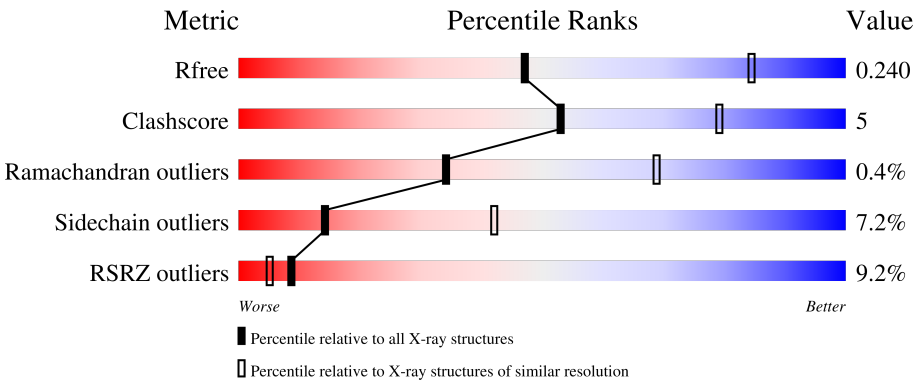
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	145	6%, 74%, 12%, •, 12%
1	B	145	%, 62%, 17%, •, 18%
2	C	165	13%, 62%, 13%, •, 22%
2	D	165	10%, 73%, 12%, •, 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4219 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	995	625	173	190	7	0	0	0
1	B	119	936	593	160	176	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	ALA	TRP	engineered mutation	UNP Q99AU3
B	187	ALA	TRP	engineered mutation	UNP Q99AU3

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	129	1081	671	196	211	3	0	0	0
2	D	144	1207	747	221	236	3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

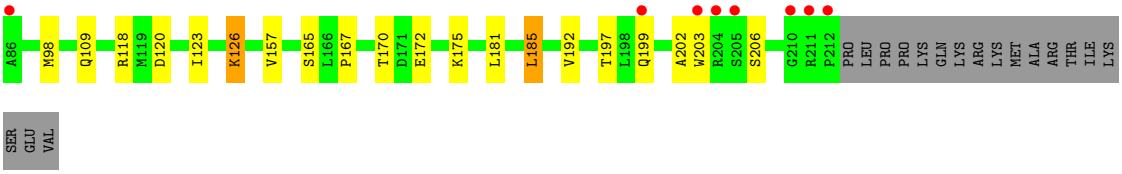
Chain	Residue	Modelled	Actual	Comment	Reference
C	433	GLY	-	expression tag	UNP O00459
C	434	SER	-	expression tag	UNP O00459
C	501	SER	CYS	engineered mutation	UNP O00459
D	433	GLY	-	expression tag	UNP O00459
D	434	SER	-	expression tag	UNP O00459
D	501	SER	CYS	engineered mutation	UNP O00459

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.

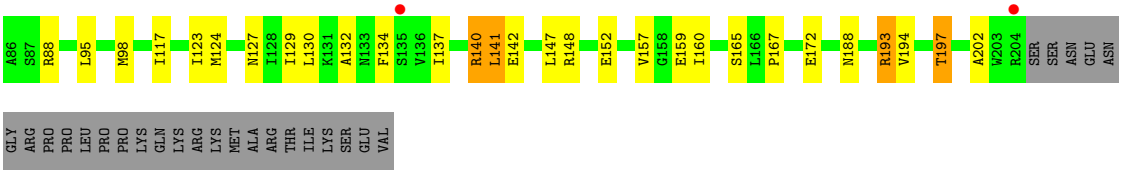
• Molecule 1: Non-structural protein 1

Chain A:



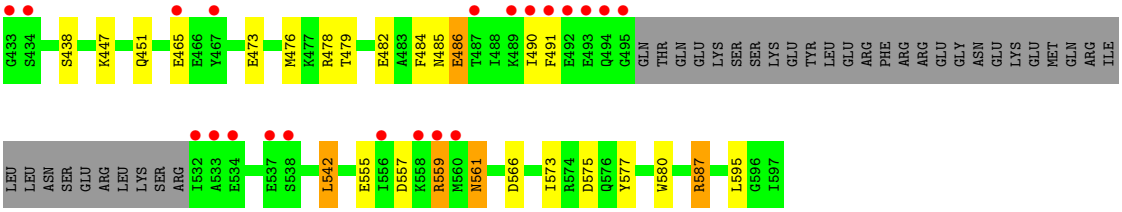
• Molecule 1: Non-structural protein 1

Chain B:



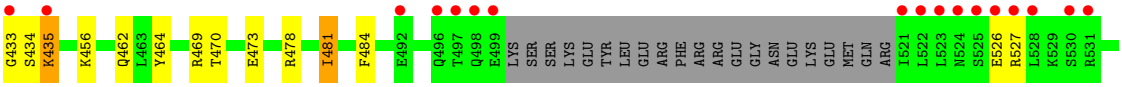
• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit beta

Chain C:



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit beta

Chain D:



E537
S538
R539
L542
E543
Q549
N553
M560
L567
W580
I597

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.19Å 92.39Å 66.94Å 90.00° 105.17° 90.00°	Depositor
Resolution (Å)	34.15 – 2.95 34.14 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.15-2.95) 99.8 (34.14-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.223 , 0.239 0.223 , 0.240	Depositor DCC
R_{free} test set	701 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	67.9	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4219	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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	0.24	0/1010	0.46	0/1364
1	B	0.24	0/950	0.45	0/1283
2	C	0.22	0/1094	0.35	0/1462
2	D	0.23	0/1220	0.37	0/1630
All	All	0.23	0/4274	0.40	0/5739

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	995	0	1002	12	0
1	B	936	0	951	17	0
2	C	1081	0	1074	12	0
2	D	1207	0	1208	11	0
All	All	4219	0	4235	46	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 5.

All (46) 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:199:GLN:HA	1:A:203:TRP:HB3	1.61	0.82
1:B:148:ARG:HG2	1:B:159:GLU:HG3	1.82	0.60
2:C:580:TRP:CG	1:B:167:PRO:HG3	2.37	0.60
2:D:469:ARG:NH1	2:D:473:GLU:OE2	2.39	0.56
2:C:566:ASP:OD1	1:B:140:ARG:NH1	2.39	0.55
1:B:141:LEU:HD23	1:B:202:ALA:HB2	1.87	0.54
2:D:470:THR:OG1	2:D:553:ASN:OD1	2.23	0.54
1:A:98:MET:HE1	2:C:575:ASP:HB3	1.92	0.52
1:A:109:GLN:OE1	1:A:118:ARG:NH1	2.43	0.52
1:A:185:LEU:HB3	1:A:192:VAL:HG21	1.92	0.52
2:D:481:ILE:HG12	2:D:542:LEU:HD13	1.92	0.51
1:B:137:ILE:HG12	1:B:142:GLU:HB2	1.93	0.51
2:C:490:ILE:HG23	2:C:491:PHE:HD1	1.77	0.49
1:B:127:ASN:HB2	1:B:152:GLU:HG3	1.95	0.49
1:B:95:LEU:HA	1:B:98:MET:HE3	1.94	0.49
2:C:577:TYR:CE2	1:B:167:PRO:HB2	2.48	0.49
2:D:464:TYR:HD2	2:D:560:MET:HE1	1.79	0.47
1:A:181:LEU:O	1:A:185:LEU:HB2	2.15	0.47
2:C:473:GLU:HA	2:C:476:MET:HE2	1.96	0.47
2:D:484:PHE:HB3	2:D:539:ARG:HG3	1.98	0.46
1:B:134:PHE:CD1	1:B:141:LEU:HD22	2.51	0.46
1:A:170:THR:HG23	1:A:172:GLU:H	1.80	0.45
2:C:542:LEU:HD23	2:C:542:LEU:HA	1.81	0.45
2:C:447:LYS:O	2:C:451:GLN:HG2	2.18	0.44
1:A:165:SER:HA	1:B:165:SER:HA	2.00	0.44
1:B:123:ILE:HG13	1:B:157:VAL:HB	2.00	0.44
2:D:433:GLY:O	2:D:435:LYS:N	2.51	0.44
2:D:473:GLU:OE1	2:D:549:GLN:NE2	2.51	0.44
2:C:587:ARG:H	2:C:587:ARG:HG2	1.55	0.44
2:D:481:ILE:HD13	2:D:481:ILE:HA	1.88	0.43
1:B:134:PHE:CZ	1:B:197:THR:HG23	2.54	0.43
1:A:175:LYS:HG2	1:A:202:ALA:HB1	2.00	0.42
2:C:557:ASP:O	2:C:561:ASN:HB2	2.18	0.42
1:B:129:ILE:HA	1:B:193:ARG:O	2.20	0.42
2:C:482:GLU:O	2:C:486:GLU:HB2	2.18	0.42
1:A:167:PRO:HD3	2:D:580:TRP:CD1	2.55	0.42
1:B:124:MET:HG2	1:B:188:ASN:HB3	2.02	0.42
2:C:555:GLU:OE2	2:C:559:ARG:NH1	2.53	0.41
1:A:123:ILE:HG13	1:A:157:VAL:HB	2.03	0.41
1:A:126:LYS:HB3	1:A:126:LYS:HE3	1.71	0.41
2:D:527:ARG:HA	2:D:527:ARG:HD3	1.81	0.41
1:A:120:ASP:HB3	1:A:123:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:567:LEU:HD12	2:D:567:LEU:HA	1.88	0.41
1:B:117:ILE:HG23	1:B:160:ILE:HG12	2.02	0.40
1:B:130:LEU:HD12	1:B:194:VAL:HG12	2.03	0.40
1:B:132:ALA:HB2	1:B:147:LEU:HD12	2.04	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	125/145 (86%)	114 (91%)	10 (8%)	1 (1%)	19	53
1	B	117/145 (81%)	113 (97%)	4 (3%)	0	100	100
2	C	125/165 (76%)	122 (98%)	3 (2%)	0	100	100
2	D	140/165 (85%)	136 (97%)	3 (2%)	1 (1%)	22	56
All	All	507/620 (82%)	485 (96%)	20 (4%)	2 (0%)	34	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	SER
2	D	434	SER

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	110/127 (87%)	107 (97%)	3 (3%)	44	74
1	B	103/127 (81%)	97 (94%)	6 (6%)	20	51
2	C	116/151 (77%)	103 (89%)	13 (11%)	6	22
2	D	131/151 (87%)	120 (92%)	11 (8%)	11	35
All	All	460/556 (83%)	427 (93%)	33 (7%)	14	42

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	A	185	LEU
1	A	197	THR
2	C	438	SER
2	C	465	GLU
2	C	478	ARG
2	C	479	THR
2	C	484	PHE
2	C	485	ASN
2	C	486	GLU
2	C	542	LEU
2	C	559	ARG
2	C	561	ASN
2	C	573	ILE
2	C	587	ARG
2	C	595	LEU
1	B	88	ARG
1	B	140	ARG
1	B	141	LEU
1	B	172	GLU
1	B	193	ARG
1	B	197	THR
2	D	435	LYS
2	D	456	LYS
2	D	462	GLN
2	D	478	ARG
2	D	481	ILE
2	D	526	GLU
2	D	537	GLU
2	D	539	ARG
2	D	542	LEU
2	D	543	GLU
2	D	597	ILE

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

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	127/145 (87%)	0.27	8 (6%)	20	11	41, 61, 110, 134	0
1	B	119/145 (82%)	0.04	2 (1%)	70	53	42, 58, 78, 114	0
2	C	129/165 (78%)	0.82	21 (16%)	1	1	43, 83, 138, 163	0
2	D	144/165 (87%)	0.72	17 (11%)	4	2	40, 73, 140, 173	0
All	All	519/620 (83%)	0.48	48 (9%)	9	5	40, 68, 131, 173	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	521	ILE	13.5
2	D	525	SER	8.2
2	C	533	ALA	6.2
2	C	490	ILE	6.2
2	D	523	LEU	6.1
2	C	491	PHE	5.8
2	C	433	GLY	5.6
2	D	522	LEU	5.5
2	C	495	GLY	5.0
2	C	494	GLN	4.8
2	D	528	LEU	4.8
2	D	524	ASN	4.7
2	C	534	GLU	4.5
2	C	532	ILE	4.4
1	A	210	GLY	4.4
1	A	205	SER	4.3
2	D	496	GLN	4.0
2	D	531	ARG	3.9
2	C	493	GLU	3.5
2	D	530	SER	3.4
2	D	527	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	465	GLU	3.4
1	A	212	PRO	3.4
2	D	499	GLU	3.3
1	A	203	TRP	3.0
2	D	526	GLU	2.9
2	C	538	SER	2.9
2	C	492	GLU	2.8
1	A	204	ARG	2.8
2	D	433	GLY	2.7
2	C	489	LYS	2.7
2	C	487	THR	2.7
2	D	497	THR	2.5
1	B	204	ARG	2.4
2	D	498	GLN	2.4
2	D	492	GLU	2.4
1	A	211	ARG	2.4
2	C	559	ARG	2.4
2	C	434	SER	2.4
2	C	556	ILE	2.4
2	C	560	MET	2.3
1	B	135	SER	2.3
1	A	86	ALA	2.3
2	C	537	GLU	2.2
1	A	199	GLN	2.2
2	C	558	LYS	2.2
2	D	435	LYS	2.1
2	C	467	TYR	2.1

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.