



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:28 am BST

PDB ID : 6OX7
Title : The complex of 1918 NS1-ED and the iSH2 domain of the human p85beta subunit of PI3K
Authors : Shen, Q.; Zhao, B.; Li, P.; Cho, J.H.
Deposited on : 2019-05-13
Resolution : 2.75 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

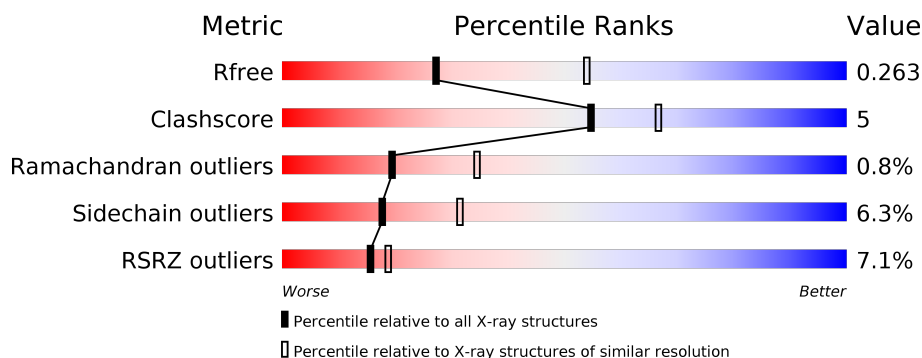
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	145	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>12%</div> </div> </div>
1	B	145	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>•</div> <div>18%</div> </div> </div>
2	C	165	<div> <div>11%</div> <div> <div></div> <div>63%</div> <div>13%</div> <div>•</div> <div>22%</div> </div> </div>
2	D	165	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>16%</div> <div>•</div> <div>13%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4262 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
1	A	127	Total	C	N	O	S	0	0	0
			1001	628	176	190	7			
1	B	119	Total	C	N	O	S	0	0	0
			942	596	163	176	7			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

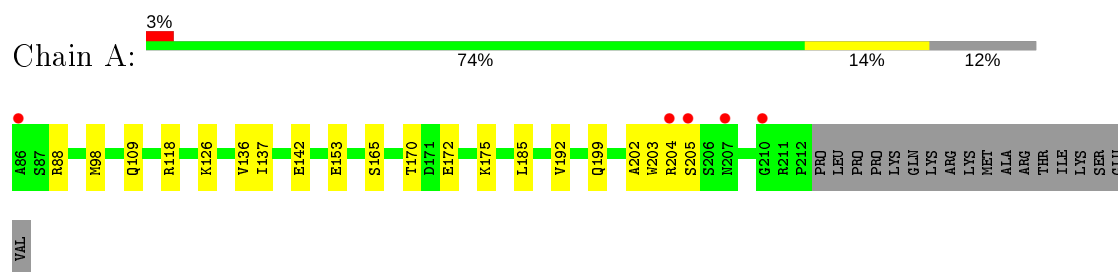
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	C	5	Total 5	O 5	0	0
3	B	11	Total 11	O 11	0	0
3	D	11	Total 11	O 11	0	0

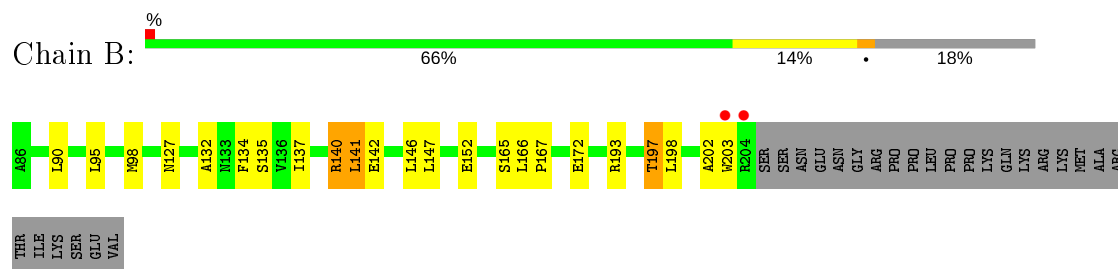
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

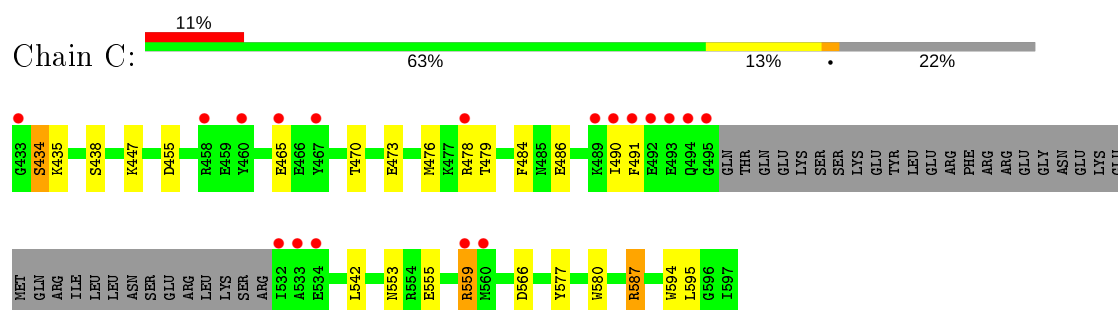
• Molecule 1: Non-structural protein 1



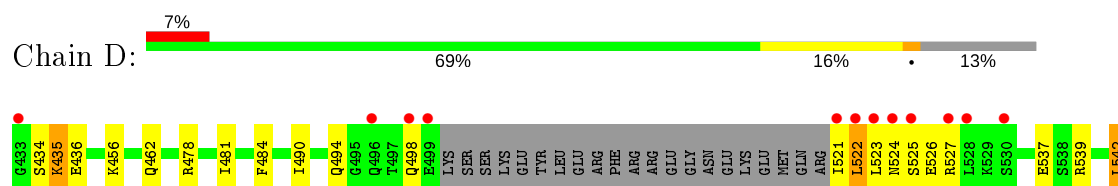
• Molecule 1: Non-structural protein 1



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit beta



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit beta



E543
R547
D557
N561
K572
W580
K584
Q588
I597

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.98Å 94.03Å 67.22Å 90.00° 105.31° 90.00°	Depositor
Resolution (Å)	44.65 – 2.75 44.65 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.65-2.75) 99.9 (44.65-2.75)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, R_{free}	0.228 , 0.263 0.229 , 0.263	Depositor DCC
R_{free} test set	901 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4262	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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 [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	0.23	0/1016	0.44	0/1371
1	B	0.23	0/956	0.44	0/1290
2	C	0.22	0/1094	0.35	0/1462
2	D	0.23	0/1220	0.36	0/1630
All	All	0.23	0/4286	0.40	0/5753

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	1001	0	1010	10	0
1	B	942	0	959	15	0
2	C	1081	0	1074	11	0
2	D	1207	0	1208	13	0
3	A	4	0	0	0	0
3	B	11	0	0	0	0
3	C	5	0	0	1	0
3	D	11	0	0	2	0
All	All	4262	0	4251	44	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 (44) 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	1.58	0.85
2:D:521:ILE:N	2:D:525:SER:HG	1.85	0.74
1:B:141:LEU:HD23	1:B:202:ALA:HB2	1.74	0.69
1:A:109:GLN:OE1	1:A:118:ARG:NH1	2.33	0.62
2:C:566:ASP:OD1	1:B:140:ARG:NH1	2.31	0.62
2:D:521:ILE:HG13	2:D:522:LEU:HD22	1.84	0.59
2:C:580:TRP:CG	1:B:167:PRO:HG3	2.37	0.59
2:C:555:GLU:OE2	2:C:559:ARG:NH1	2.36	0.58
1:B:127:ASN:HB2	1:B:152:GLU:HG3	1.90	0.54
1:B:137:ILE:HG12	1:B:142:GLU:HB2	1.91	0.53
1:B:98:MET:HG2	1:B:146:LEU:HD23	1.91	0.52
2:C:470:THR:OG1	2:C:553:ASN:OD1	2.26	0.52
2:C:490:ILE:HG23	2:C:491:PHE:HD1	1.75	0.51
2:D:588:GLN:NE2	3:D:601:HOH:O	2.44	0.51
1:A:137:ILE:HG22	1:A:142:GLU:HB2	1.92	0.51
2:C:577:TYR:CE2	1:B:167:PRO:HB2	2.46	0.50
2:D:481:ILE:HD11	2:D:542:LEU:HB3	1.94	0.50
1:A:185:LEU:HB3	1:A:192:VAL:HG21	1.95	0.48
2:D:557:ASP:OD1	2:D:561:ASN:ND2	2.46	0.48
1:B:134:PHE:CD1	1:B:141:LEU:HD22	2.50	0.47
1:A:170:THR:HG23	1:A:172:GLU:H	1.79	0.47
1:B:95:LEU:HA	1:B:98:MET:HE3	1.97	0.46
2:D:523:LEU:HD11	2:D:527:ARG:HE	1.80	0.45
1:A:175:LYS:HG2	1:A:202:ALA:HB1	1.98	0.44
2:C:473:GLU:HA	2:C:476:MET:HE2	1.99	0.44
2:D:484:PHE:HB3	2:D:539:ARG:HG3	2.00	0.44
1:B:90:LEU:HD13	1:B:197:THR:OG1	2.18	0.44
1:B:135:SER:HB3	2:D:572:LYS:HE2	1.99	0.44
1:B:132:ALA:HB2	1:B:147:LEU:HD12	1.99	0.44
1:A:170:THR:HG23	1:A:172:GLU:N	2.33	0.43
2:D:490:ILE:O	2:D:494:GLN:HG2	2.19	0.42
2:C:447:LYS:HG2	2:C:594:TRP:O	2.19	0.42
1:B:127:ASN:ND2	1:B:152:GLU:OE2	2.35	0.42
1:A:165:SER:HA	1:B:165:SER:HA	2.01	0.42
2:D:527:ARG:N	3:D:603:HOH:O	2.53	0.42
2:D:580:TRP:CZ3	2:D:584:LYS:HG3	2.55	0.42
1:B:198:LEU:O	1:B:203:TRP:N	2.51	0.41
1:A:88:ARG:HB2	1:A:136:VAL:HG22	2.02	0.41
2:C:455:ASP:OD1	3:C:601:HOH:O	2.22	0.41
2:C:587:ARG:HG2	2:C:587:ARG:H	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:435:LYS:HD3	2:D:436:GLU:N	2.36	0.41
2:D:543:GLU:O	2:D:547:ARG:HG3	2.20	0.41
2:C:434:SER:OG	2:C:435:LYS:N	2.54	0.40
1:A:98:MET:HE2	1:A:98:MET:HB3	1.95	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%)	116 (93%)	8 (6%)	1 (1%)	19	34
1	B	117/145 (81%)	112 (96%)	5 (4%)	0	100	100
2	C	125/165 (76%)	123 (98%)	1 (1%)	1 (1%)	19	34
2	D	140/165 (85%)	136 (97%)	2 (1%)	2 (1%)	11	19
All	All	507/620 (82%)	487 (96%)	16 (3%)	4 (1%)	19	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	SER
2	D	434	SER
2	C	434	SER
2	D	498	GLN

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	111/128 (87%)	108 (97%)	3 (3%)	44	65
1	B	104/128 (81%)	98 (94%)	6 (6%)	20	35
2	C	116/151 (77%)	106 (91%)	10 (9%)	10	18
2	D	131/151 (87%)	121 (92%)	10 (8%)	13	23
All	All	462/558 (83%)	433 (94%)	29 (6%)	18	31

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	A	153	GLU
1	A	204	ARG
2	C	438	SER
2	C	465	GLU
2	C	478	ARG
2	C	479	THR
2	C	484	PHE
2	C	486	GLU
2	C	542	LEU
2	C	559	ARG
2	C	587	ARG
2	C	595	LEU
1	B	140	ARG
1	B	141	LEU
1	B	166	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	522	LEU
2	D	524	ASN
2	D	526	GLU
2	D	537	GLU
2	D	542	LEU
2	D	597	ILE

Some 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 carbohydrates 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, 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%)	0.33	5 (3%) 39 46	30, 47, 107, 151	0
1	B	119/145 (82%)	0.01	2 (1%) 70 78	27, 44, 65, 103	0
2	C	129/165 (78%)	0.77	18 (13%) 2 3	32, 66, 128, 155	0
2	D	144/165 (87%)	0.55	12 (8%) 11 13	31, 59, 124, 148	0
All	All	519/620 (83%)	0.42	37 (7%) 16 19	27, 55, 114, 155	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	521	ILE	13.6
2	C	490	ILE	9.2
2	C	491	PHE	7.7
2	C	494	GLN	6.4
1	A	205	SER	6.2
2	D	522	LEU	5.8
2	D	523	LEU	5.5
2	C	493	GLU	5.5
2	C	433	GLY	5.3
2	D	525	SER	5.1
2	C	495	GLY	4.9
2	C	532	ILE	4.6
2	C	533	ALA	4.4
2	C	492	GLU	3.8
2	D	524	ASN	3.4
1	B	204	ARG	3.4
2	C	489	LYS	3.3
1	A	207	ASN	3.2
2	D	528	LEU	3.0
2	C	534	GLU	2.9
2	D	499	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	559	ARG	2.8
2	D	527	ARG	2.8
2	D	433	GLY	2.8
1	A	204	ARG	2.6
2	D	530	SER	2.6
1	B	203	TRP	2.6
2	D	496	GLN	2.5
2	C	478	ARG	2.5
2	C	467	TYR	2.4
1	A	210	GLY	2.3
2	D	498	GLN	2.3
1	A	86	ALA	2.2
2	C	458	ARG	2.1
2	C	560	MET	2.1
2	C	465	GLU	2.0
2	C	460	TYR	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.