



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 08:39 am BST

PDB ID : 5WBU  
Title : Crystal structure of mTOR(deltaN)-mLST8-PRAS40(alpha-helix & beta-strand) complex  
Authors : Pavletich, N.P.; Yang, H.  
Deposited on : 2017-06-29  
Resolution : 3.42 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

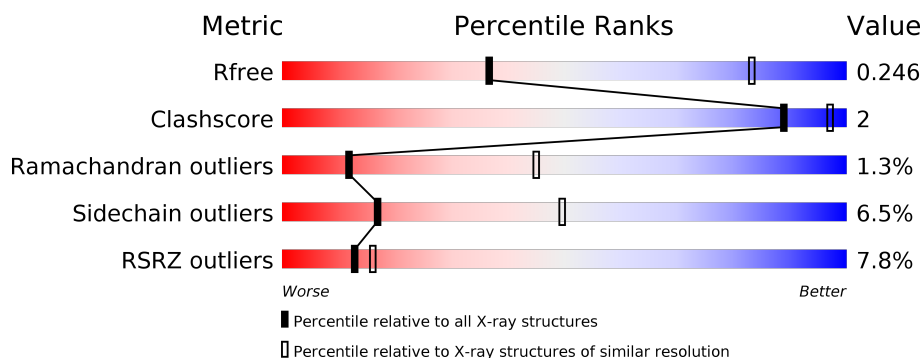
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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  $\geq 3$ , 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	1177	<div> <div>9%</div> <div>79%</div> <div>9%</div> <div>11%</div> </div>
1	B	1177	<div> <div>6%</div> <div>80%</div> <div>9%</div> <div>10%</div> </div>
2	C	328	<div> <div>5%</div> <div>85%</div> <div>10%</div> <div>•</div> </div>
2	D	328	<div> <div>3%</div> <div>85%</div> <div>10%</div> <div>•</div> </div>
3	O	88	<div> <div>3%</div> <div>9%</div> <div>90%</div> </div>
3	P	88	<div> <div>3%</div> <div>9%</div> <div>90%</div> </div>

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Mol	Chain	Length	Quality of chain
3	Q	88	<div><div><div></div><div></div><div></div></div><div>10%23%76%</div></div>
3	R	88	<div><div><div></div><div></div><div></div></div><div>3%23%76%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22553 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 mTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1058	Total	C	N	O	S	0	0	0
			8608	5472	1521	1552	63			
1	A	1052	Total	C	N	O	S	0	0	0
			8557	5439	1511	1544	63			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1373	GLY	-	expression tag	UNP P42345
B	1374	THR	-	expression tag	UNP P42345
B	1375	GLY	-	expression tag	UNP P42345
A	1373	GLY	-	expression tag	UNP P42345
A	1374	THR	-	expression tag	UNP P42345
A	1375	GLY	-	expression tag	UNP P42345

- Molecule 2 is a protein called Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			
2	C	317	Total	C	N	O	S	0	0	0
			2456	1526	436	476	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q9BVC4
D	0	SER	-	expression tag	UNP Q9BVC4
C	-1	GLY	-	expression tag	UNP Q9BVC4
C	0	SER	-	expression tag	UNP Q9BVC4

- Molecule 3 is a protein called Proline-rich AKT1 substrate 1.

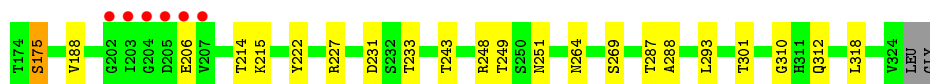
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	0	0	0
			77	54	12	11			
3	R	21	Total	C	N	O	0	0	0
			161	97	30	33			
3	O	9	Total	C	N	O	0	0	0
			77	54	12	11			
3	Q	21	Total	C	N	O	0	0	0
			161	97	30	33			

There are 16 discrepancies between the modelled and reference sequences:

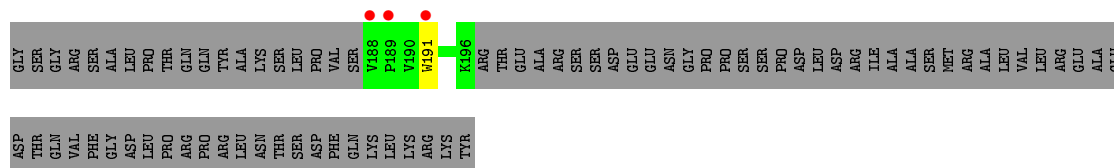
Chain	Residue	Modelled	Actual	Comment	Reference
P	169	GLY	-	expression tag	UNP Q96B36
P	170	SER	-	expression tag	UNP Q96B36
P	171	GLY	-	expression tag	UNP Q96B36
P	172	ARG	-	expression tag	UNP Q96B36
R	169	GLY	-	expression tag	UNP Q96B36
R	170	SER	-	expression tag	UNP Q96B36
R	171	GLY	-	expression tag	UNP Q96B36
R	172	ARG	-	expression tag	UNP Q96B36
O	169	GLY	-	expression tag	UNP Q96B36
O	170	SER	-	expression tag	UNP Q96B36
O	171	GLY	-	expression tag	UNP Q96B36
O	172	ARG	-	expression tag	UNP Q96B36
Q	169	GLY	-	expression tag	UNP Q96B36
Q	170	SER	-	expression tag	UNP Q96B36
Q	171	GLY	-	expression tag	UNP Q96B36
Q	172	ARG	-	expression tag	UNP Q96B36



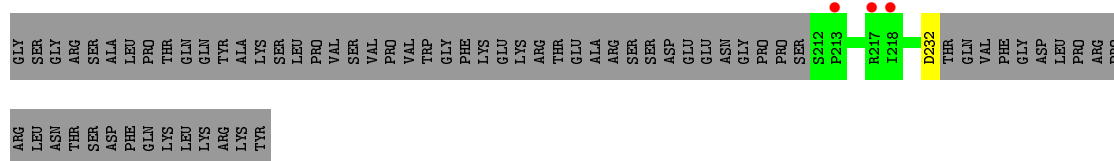




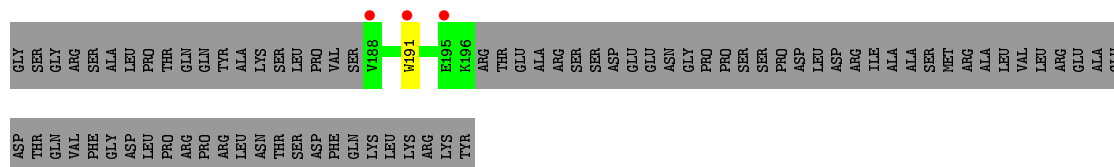
• Molecule 3: Proline-rich AKT1 substrate 1



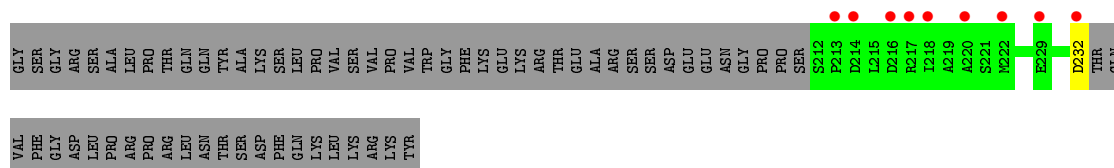
• Molecule 3: Proline-rich AKT1 substrate 1



• Molecule 3: Proline-rich AKT1 substrate 1



• Molecule 3: Proline-rich AKT1 substrate 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.40 Å   163.20 Å   207.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.01 – 3.42 75.95 – 3.22	Depositor EDS
% Data completeness (in resolution range)	81.5 (50.01-3.42) 78.7 (75.95-3.22)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.235   ,   0.266 0.236   ,   0.246	Depositor DCC
$R_{free}$ test set	1812 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22553	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.21 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5768e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	0.45	0/8752	0.66	1/11847 (0.0%)
1	B	0.46	0/8805	0.67	1/11920 (0.0%)
2	C	0.42	0/2514	0.73	0/3426
2	D	0.45	0/2514	0.74	1/3426 (0.0%)
3	O	0.51	0/80	0.56	0/107
3	P	0.48	0/80	0.56	0/107
3	Q	0.50	0/161	0.67	0/216
3	R	0.51	0/161	0.67	0/216
All	All	0.45	0/23067	0.68	3/31265 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
2	C	0	1
2	D	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2254	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	2254	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	D	248	ARG	NE-CZ-NH1	5.38	122.99	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1444	GLU	Peptide
1	B	1444	GLU	Peptide
1	B	1680	ASP	Peptide
1	B	1732	ILE	Peptide
2	D	76	ASN	Peptide

## 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	8557	0	8533	36	0
1	B	8608	0	8593	35	0
2	C	2456	0	2341	9	0
2	D	2456	0	2341	10	0
3	O	77	0	78	0	0
3	P	77	0	78	0	0
3	Q	161	0	161	0	0
3	R	161	0	161	0	0
All	All	22553	0	22286	83	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.

The worst 5 of 83 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:2421:PHE:HA	1:A:2424:ASP:HB2	1.76	0.66
1:B:2421:PHE:HA	1:B:2424:ASP:HB2	1.77	0.66
1:A:1930:ILE:HD11	1:A:1934:THR:HG21	1.79	0.65
1:B:1930:ILE:HD11	1:B:1934:THR:HG21	1.79	0.64
1:B:1681:PRO:O	1:B:1683:ARG:N	2.31	0.64

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	1044/1177 (89%)	982 (94%)	53 (5%)	9 (1%)	17	53
1	B	1052/1177 (89%)	984 (94%)	56 (5%)	12 (1%)	14	49
2	C	315/328 (96%)	285 (90%)	23 (7%)	7 (2%)	6	35
2	D	315/328 (96%)	284 (90%)	24 (8%)	7 (2%)	6	35
3	O	7/88 (8%)	6 (86%)	1 (14%)	0	100	100
3	P	7/88 (8%)	6 (86%)	1 (14%)	0	100	100
3	Q	19/88 (22%)	18 (95%)	1 (5%)	0	100	100
3	R	19/88 (22%)	18 (95%)	1 (5%)	0	100	100
All	All	2778/3362 (83%)	2583 (93%)	160 (6%)	35 (1%)	12	45

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1630	VAL
1	B	1682	SER
1	B	1692	VAL
1	B	1709	ARG
2	D	74	ASN

### 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	925/1025 (90%)	868 (94%)	57 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	931/1025 (91%)	872 (94%)	59 (6%)	18	51
2	C	269/277 (97%)	249 (93%)	20 (7%)	13	44
2	D	269/277 (97%)	249 (93%)	20 (7%)	13	44
3	O	8/76 (10%)	7 (88%)	1 (12%)	4	21
3	P	8/76 (10%)	7 (88%)	1 (12%)	4	21
3	Q	17/76 (22%)	16 (94%)	1 (6%)	19	52
3	R	17/76 (22%)	16 (94%)	1 (6%)	19	52
All	All	2444/2908 (84%)	2284 (94%)	160 (6%)	17	49

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	243	THR
1	A	1590	MET
2	C	188	VAL
2	D	249	THR
1	A	1417	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	209	GLN
1	A	1492	GLN
1	A	2189	HIS
1	B	2148	GLN
1	A	2148	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1052/1177 (89%)	0.50	105 (9%) 7 9	55, 112, 215, 261	0
1	B	1058/1177 (89%)	0.36	68 (6%) 19 21	46, 97, 204, 227	0
2	C	317/328 (96%)	0.36	18 (5%) 23 25	60, 107, 177, 221	0
2	D	317/328 (96%)	0.16	11 (3%) 44 44	41, 77, 143, 228	0
3	O	9/88 (10%)	1.63	3 (33%) 0 0	128, 166, 178, 184	0
3	P	9/88 (10%)	1.26	3 (33%) 0 0	102, 151, 168, 171	0
3	Q	21/88 (23%)	1.91	9 (42%) 0 0	175, 203, 244, 261	0
3	R	21/88 (23%)	0.81	3 (14%) 2 4	160, 174, 191, 196	0
All	All	2804/3362 (83%)	0.41	220 (7%) 13 16	41, 101, 207, 261	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1503	LEU	8.0
1	B	1500	LYS	7.7
1	B	1607	LEU	7.1
1	B	1579	ALA	7.1
2	C	205	ASP	6.9

### 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 carbohydrates 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.