



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 06:56 am BST

PDB ID : 5WBK  
Title : Crystal structure of the arabidopsis thaliana Raptor in complex with the TOS peptide of human S6K1  
Authors : Pavletich, N.P.; Jiang, X.  
Deposited on : 2017-06-29  
Resolution : 3.11 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](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

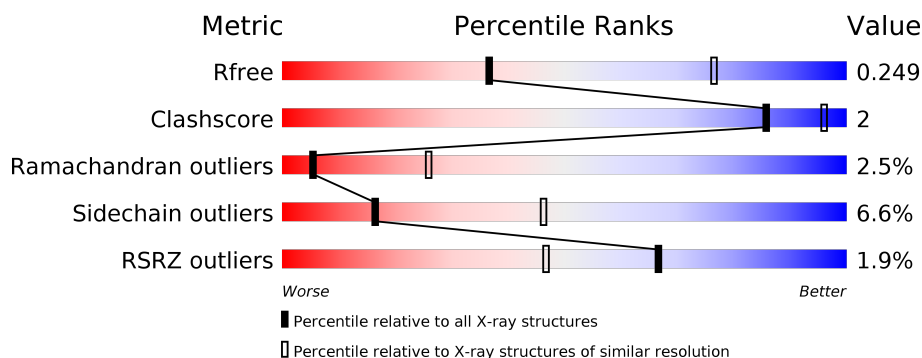
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	1287	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>9%</div> <div>18%</div> </div> </div>
2	T	14	<div> <div>57%</div> <div>43%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8332 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 Regulatory-associated protein of TOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1053	Total	C	N	O	S	0	0	0
			8273	5296	1420	1515	42			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q93YQ1
A	-1	VAL	-	expression tag	UNP Q93YQ1
A	0	ASP	-	expression tag	UNP Q93YQ1

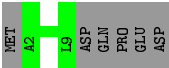
- Molecule 2 is a protein called Ribosomal protein S6 kinase beta-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	T	8	Total	C	N	O	0	0	0
			59	39	8	12			

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 ( $\text{RSRZ} > 2$ ). 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.

- [illegible]

- Chain T:  57% 43%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.10Å 113.10Å 152.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.11 76.98 – 3.11	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-3.11) 92.5 (76.98-3.11)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.209 , 0.255 0.216 , 0.249	Depositor DCC
$R_{free}$ test set	1129 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.5	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8332	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<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	0.40	0/8463	0.66	3/11496 (0.0%)
2	T	0.53	0/59	0.44	0/79
All	All	0.40	0/8522	0.66	3/11575 (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	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	425	PRO	N-CA-CB	5.33	109.70	103.30
1	A	401	LEU	CA-CB-CG	5.03	126.88	115.30
1	A	1163	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1212	PRO	Peptide
1	A	1235	SER	Peptide

### 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	8273	0	8274	37	0
2	T	59	0	55	0	0
All	All	8332	0	8329	37	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 (37) 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:1063:ASN:ND2	1:A:1106:THR:O	2.28	0.67
1:A:237:THR:HB	1:A:238:PRO:HD3	1.89	0.55
1:A:408:HIS:CG	1:A:408:HIS:O	2.59	0.54
1:A:158:GLN:HB3	1:A:301:THR:CG2	2.38	0.54
1:A:357:ASN:HD21	1:A:463:GLU:HA	1.74	0.53
1:A:158:GLN:HB3	1:A:301:THR:HG23	1.92	0.52
1:A:1051:ILE:HB	1:A:1065:PHE:HB2	1.93	0.50
1:A:1077:LYS:HB2	1:A:1092:ALA:HB3	1.96	0.47
1:A:134:GLU:HA	1:A:294:ASP:HB2	1.97	0.47
1:A:290:GLU:O	1:A:313:ARG:NH1	2.48	0.47
1:A:469:LEU:HD13	1:A:502:VAL:HG12	1.96	0.46
1:A:1048:ASN:HA	1:A:1073:LYS:HB3	1.97	0.46
1:A:228:ILE:HG22	1:A:258:LEU:HD11	1.98	0.46
1:A:1063:ASN:HD21	1:A:1110:GLN:HG2	1.81	0.46
1:A:1032:THR:HA	1:A:1314:CYS:HB3	1.98	0.45
1:A:1058:GLU:HB2	1:A:1060:THR:HG22	1.99	0.45
1:A:684:ASP:O	1:A:686:LYS:N	2.50	0.45
1:A:1233:VAL:O	1:A:1243:GLN:O	2.36	0.44
1:A:655:ARG:NH2	1:A:1158:LYS:O	2.43	0.43
1:A:1063:ASN:ND2	1:A:1110:GLN:HG2	2.33	0.43
1:A:382:LEU:HD22	1:A:404:THR:HG21	1.98	0.43
1:A:286:PRO:HB3	1:A:391:ALA:HB1	2.00	0.43
1:A:1211:ARG:O	1:A:1212:PRO:O	2.37	0.43
1:A:1222:LEU:HB2	1:A:1234:VAL:HG22	2.00	0.43
1:A:659:VAL:HG13	1:A:697:LEU:HD22	2.01	0.42
1:A:1211:ARG:N	1:A:1212:PRO:HD2	2.33	0.42
1:A:1225:GLN:HG3	1:A:1233:VAL:HG23	2.01	0.42
1:A:291:PHE:CZ	1:A:391:ALA:HB2	2.55	0.42
1:A:1223:SER:O	1:A:1234:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1034:LEU:HD21	1:A:1080:LEU:HG	2.03	0.41
1:A:1046:ASP:OD1	1:A:1047:GLU:N	2.54	0.41
1:A:1234:VAL:CG1	1:A:1235:SER:N	2.85	0.40
1:A:1022:TRP:CZ3	1:A:1024:THR:HG22	2.56	0.40
1:A:1225:GLN:CG	1:A:1233:VAL:HG23	2.52	0.40
1:A:275:LEU:O	1:A:397:SER:HA	2.21	0.40
1:A:116:ASN:HB3	1:A:119:VAL:HB	2.02	0.40
1:A:1232:LYS:HG2	1:A:1234:VAL:HG21	2.03	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	1037/1287 (81%)	928 (90%)	83 (8%)	26 (2%)	5	26
2	T	6/14 (43%)	6 (100%)	0	0	100	100
All	All	1043/1301 (80%)	934 (90%)	83 (8%)	26 (2%)	5	26

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	THR
1	A	318	LYS
1	A	685	GLU
1	A	1212	PRO
1	A	1213	HIS
1	A	1234	VAL
1	A	409	MET
1	A	440	PHE
1	A	576	ASP
1	A	86	PRO

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Mol	Chain	Res	Type
1	A	270	SER
1	A	317	LEU
1	A	401	LEU
1	A	1254	TYR
1	A	191	LYS
1	A	560	PHE
1	A	1068	HIS
1	A	520	ARG
1	A	1119	ILE
1	A	1233	VAL
1	A	1312	VAL
1	A	1330	ASP
1	A	460	LYS
1	A	1037	PRO
1	A	1211	ARG
1	A	143	ALA

### 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	901/1097 (82%)	841 (93%)	60 (7%)	16	45
2	T	6/12 (50%)	6 (100%)	0	100	100
All	All	907/1109 (82%)	847 (93%)	60 (7%)	16	46

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LEU
1	A	94	LEU
1	A	99	ARG
1	A	100	LEU
1	A	115	LEU
1	A	161	ARG
1	A	165	ARG

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Mol	Chain	Res	Type
1	A	175	THR
1	A	182	LEU
1	A	192	THR
1	A	213	ILE
1	A	215	VAL
1	A	252	LEU
1	A	273	CYS
1	A	280	ASP
1	A	301	THR
1	A	320	ILE
1	A	321	ILE
1	A	332	ARG
1	A	344	ASN
1	A	396	ILE
1	A	404	THR
1	A	408	HIS
1	A	415	MET
1	A	435	PHE
1	A	465	LEU
1	A	480	ARG
1	A	487	ARG
1	A	504	ILE
1	A	522	ILE
1	A	555	ASP
1	A	560	PHE
1	A	580	ARG
1	A	586	LEU
1	A	589	ASN
1	A	624	TRP
1	A	662	LEU
1	A	667	ASP
1	A	716	LEU
1	A	843	LEU
1	A	865	GLU
1	A	1014	LEU
1	A	1016	ASN
1	A	1018	PRO
1	A	1025	ARG
1	A	1030	THR
1	A	1110	GLN
1	A	1111	LYS
1	A	1117	SER

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Mol	Chain	Res	Type
1	A	1145	SER
1	A	1148	THR
1	A	1163	ARG
1	A	1180	GLN
1	A	1200	VAL
1	A	1212	PRO
1	A	1222	LEU
1	A	1229	ASP
1	A	1245	LEU
1	A	1254	TYR
1	A	1300	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	ASN
1	A	614	GLN
1	A	1110	GLN
1	A	1180	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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<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	1053/1287 (81%)	0.03	20 (1%) 66 47	50, 99, 159, 252	0
2	T	8/14 (57%)	0.55	0 100 100	124, 133, 139, 142	0
All	All	1061/1301 (81%)	0.03	20 (1%) 66 47	50, 99, 158, 252	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	ASP	13.6
1	A	1311	SER	6.6
1	A	680	GLU	6.1
1	A	681	PHE	6.1
1	A	1310	GLY	5.8
1	A	683	ASP	4.5
1	A	319	GLU	4.3
1	A	264	SER	3.9
1	A	101	LYS	3.7
1	A	1233	VAL	3.3
1	A	320	ILE	3.1
1	A	62	THR	2.8
1	A	81	SER	2.7
1	A	82	GLU	2.5
1	A	80	ALA	2.4
1	A	318	LYS	2.4
1	A	433	THR	2.4
1	A	102	GLU	2.3
1	A	1259	ALA	2.2
1	A	1232	LYS	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 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.