



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2017 – 12:57 PM EST

PDB ID : 5WBJ
Title : Crystal structure of the arabidopsis thaliana Raptor in complex with the TOS peptide of human 4EBP1
Authors : Pavletich, N.P.; Jiang, X.
Deposited on : unknown
Resolution : 3.00 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

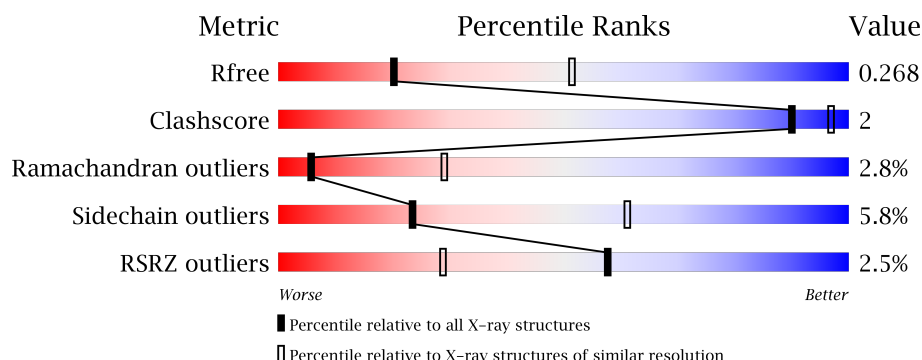
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	1287	<div> <div>2%</div> <div>73%</div> <div>8%</div> <div>18%</div> </div>
2	T	20	<div> <div>5%</div> <div>40%</div> <div>60%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8379 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	1058	Total	C	N	O	S	0	0	0
			8311	5322	1426	1521	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

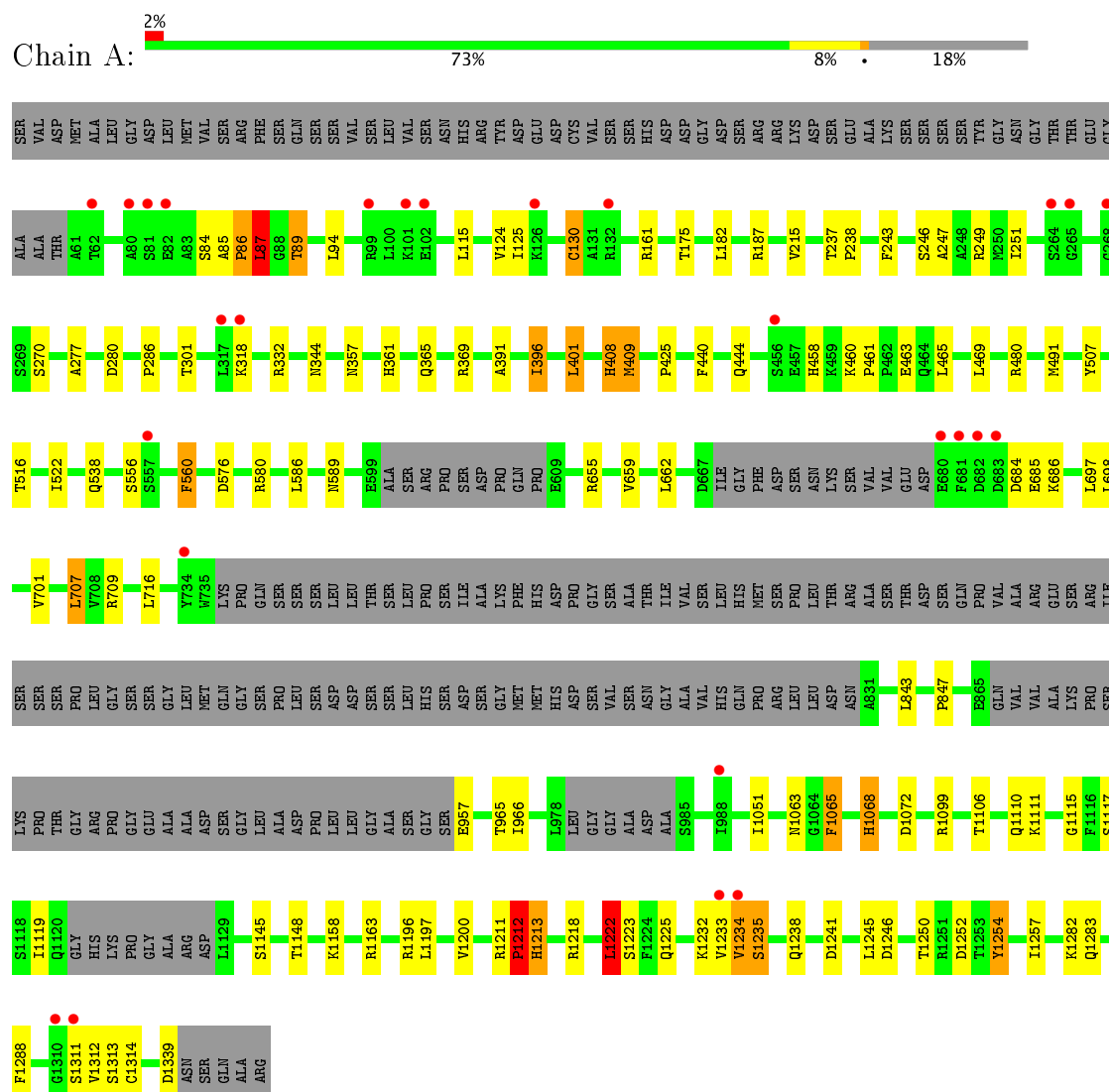
- Molecule 2 is a protein called Eukaryotic translation initiation factor 4E-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	8	Total	C	N	O	S	0	0	0
			68	42	9	16	1			

3 Residue-property plots

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: Regulatory-associated protein of TOR 1



ARG	
ASN	
SER	
PRO	
GLU	
ASP	
LYS	
ARG	
ALA	
GLY	
GLU	
E111	
I118	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.10Å 113.10Å 153.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 76.75 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-3.00) 91.6 (76.75-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.215 , 0.270 0.220 , 0.268	Depositor DCC
R_{free} test set	1403 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8379	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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

5.1 Standard geometry

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	0/8503	0.67	3/11552 (0.0%)
2	T	0.46	0/68	0.58	0/89
All	All	0.40	0/8571	0.67	3/11641 (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

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	401	LEU	CA-CB-CG	5.62	128.22	115.30
1	A	425	PRO	N-CA-CB	5.52	109.93	103.30
1	A	1222	LEU	CA-CB-CG	5.36	127.63	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1065	PHE	Peptide
1	A	1235	SER	Peptide
1	A	1283	GLN	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	8311	0	8322	35	0
2	T	68	0	57	0	0
All	All	8379	0	8379	35	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 (35) 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:1233:VAL:O	1:A:1234:VAL:O	2.08	0.70
1:A:408:HIS:O	1:A:409:MET:HB2	2.01	0.60
1:A:85:ALA:O	1:A:87:LEU:N	2.34	0.58
1:A:655:ARG:NH2	1:A:1158:LYS:O	2.36	0.58
1:A:249:ARG:HG2	1:A:396:ILE:HD11	1.86	0.58
1:A:1063:ASN:ND2	1:A:1106:THR:O	2.40	0.54
1:A:1222:LEU:HB2	1:A:1234:VAL:HG22	1.91	0.51
1:A:1212:PRO:O	1:A:1213:HIS:ND1	2.43	0.51
1:A:87:LEU:HD21	1:A:966:ILE:HA	1.93	0.50
1:A:1068:HIS:HB3	1:A:1099:ARG:CZ	2.41	0.50
1:A:357:ASN:HD21	1:A:463:GLU:HA	1.76	0.50
1:A:1225:GLN:HG3	1:A:1233:VAL:HG23	1.95	0.48
1:A:1223:SER:O	1:A:1234:VAL:HG23	2.13	0.48
1:A:1218:ARG:NH1	1:A:1238:GLN:OE1	2.46	0.48
1:A:1311:SER:O	1:A:1313:SER:N	2.47	0.48
1:A:1257:ILE:HD12	1:A:1288:PHE:CD2	2.49	0.47
1:A:1211:ARG:N	1:A:1212:PRO:HD2	2.30	0.47
1:A:1051:ILE:HB	1:A:1065:PHE:HB2	1.96	0.47
1:A:1213:HIS:NE2	1:A:1235:SER:HB3	2.30	0.47
1:A:684:ASP:O	1:A:686:LYS:N	2.47	0.47
1:A:277:ALA:HB3	1:A:396:ILE:HD12	1.97	0.46
1:A:659:VAL:HG13	1:A:697:LEU:HD22	1.97	0.46
1:A:698:LEU:HA	1:A:701:VAL:HG23	1.97	0.46
1:A:709:ARG:NH2	1:A:1115:GLY:O	2.48	0.45
1:A:87:LEU:HG	1:A:707:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:HD11	1:A:507:TYR:CD1	2.53	0.44
1:A:237:THR:HB	1:A:238:PRO:HD3	2.01	0.42
1:A:85:ALA:HA	1:A:89:THR:HG22	2.00	0.42
1:A:847:PRO:O	1:A:1099:ARG:NH1	2.52	0.42
1:A:1213:HIS:HB3	1:A:1241:ASP:OD2	2.20	0.42
1:A:243:PHE:CE1	1:A:251:ILE:HG21	2.56	0.41
1:A:243:PHE:CZ	1:A:251:ILE:HG21	2.55	0.41
1:A:286:PRO:HB3	1:A:391:ALA:HB1	2.02	0.41
1:A:1197:LEU:HD11	1:A:1232:LYS:HD3	2.03	0.40
1:A:85:ALA:N	1:A:86:PRO:HD2	2.37	0.40

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	1044/1287 (81%)	932 (89%)	83 (8%)	29 (3%)	6	29
2	T	6/20 (30%)	5 (83%)	1 (17%)	0	100	100
All	All	1050/1307 (80%)	937 (89%)	84 (8%)	29 (3%)	6	29

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	685	GLU
1	A	1068	HIS
1	A	1212	PRO
1	A	1213	HIS
1	A	1234	VAL
1	A	125	ILE
1	A	130	CYS

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Mol	Chain	Res	Type
1	A	246	SER
1	A	409	MET
1	A	440	PHE
1	A	538	GLN
1	A	1282	LYS
1	A	87	LEU
1	A	270	SER
1	A	361	HIS
1	A	401	LEU
1	A	576	ASP
1	A	1254	TYR
1	A	247	ALA
1	A	460	LYS
1	A	516	THR
1	A	556	SER
1	A	318	LYS
1	A	560	PHE
1	A	1119	ILE
1	A	1312	VAL
1	A	461	PRO
1	A	124	VAL

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	906/1097 (83%)	853 (94%)	53 (6%)	23	61
2	T	8/17 (47%)	8 (100%)	0	100	100
All	All	914/1114 (82%)	861 (94%)	53 (6%)	23	61

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	87	LEU

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Mol	Chain	Res	Type
1	A	89	THR
1	A	94	LEU
1	A	115	LEU
1	A	130	CYS
1	A	161	ARG
1	A	175	THR
1	A	182	LEU
1	A	187	ARG
1	A	215	VAL
1	A	280	ASP
1	A	301	THR
1	A	332	ARG
1	A	344	ASN
1	A	365	GLN
1	A	369	ARG
1	A	396	ILE
1	A	408	HIS
1	A	444	GLN
1	A	458	HIS
1	A	465	LEU
1	A	480	ARG
1	A	491	MET
1	A	522	ILE
1	A	560	PHE
1	A	580	ARG
1	A	586	LEU
1	A	589	ASN
1	A	662	LEU
1	A	707	LEU
1	A	716	LEU
1	A	843	LEU
1	A	957	GLU
1	A	965	THR
1	A	1072	ASP
1	A	1110	GLN
1	A	1111	LYS
1	A	1117	SER
1	A	1145	SER
1	A	1148	THR
1	A	1163	ARG
1	A	1196	ARG
1	A	1200	VAL

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Mol	Chain	Res	Type
1	A	1212	PRO
1	A	1222	LEU
1	A	1245	LEU
1	A	1246	ASP
1	A	1250	THR
1	A	1252	ASP
1	A	1254	TYR
1	A	1314	CYS
1	A	1339	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	ASN
1	A	1283	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 [i](#)

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	1058/1287 (82%)	0.03	26 (2%) 58 29	56, 97, 157, 217	0
2	T	8/20 (40%)	0.03	1 (12%) 4 2	93, 114, 126, 143	0
All	All	1066/1307 (81%)	0.03	27 (2%) 58 29	56, 97, 157, 217	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	ASP	9.0
1	A	1310	GLY	9.0
1	A	557	SER	6.6
1	A	683	ASP	5.1
1	A	1311	SER	5.0
1	A	318	LYS	3.7
2	T	118	ILE	3.5
1	A	126	LYS	3.4
1	A	680	GLU	3.3
1	A	264	SER	3.3
1	A	80	ALA	3.3
1	A	101	LYS	3.3
1	A	102	GLU	3.2
1	A	1233	VAL	3.0
1	A	734	TYR	2.9
1	A	82	GLU	2.8
1	A	988	ILE	2.8
1	A	99	ARG	2.5
1	A	81	SER	2.5
1	A	1234	VAL	2.4
1	A	132	ARG	2.3
1	A	317	LEU	2.3
1	A	265	GLY	2.2
1	A	456	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	681	PHE	2.2
1	A	268	GLY	2.1
1	A	62	THR	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.