



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 07:41 AM EDT

PDB ID : 5WBI
Title : Crystal structure of the Arabidopsis thaliana Raptor
Authors : Pavletich, N.P.; Jiang, X.
Deposited on : 2017-06-29
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

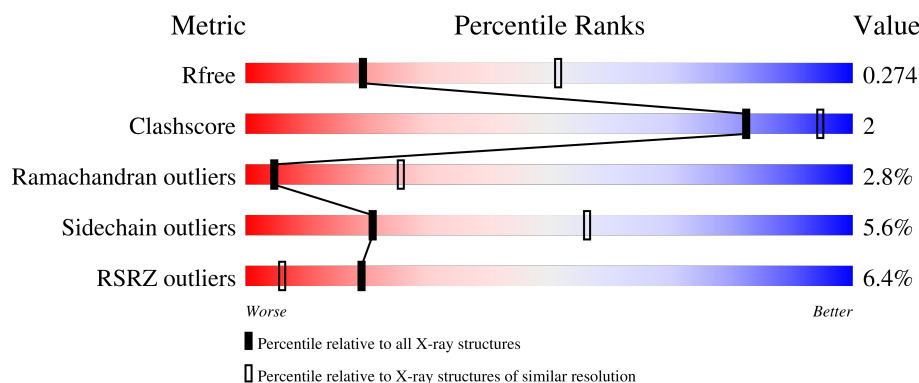
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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 $\leq 5\%$. 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	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8311 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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.12Å 112.55Å 134.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 48.38 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.2 (20.00-3.00) 91.2 (48.38-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.227 , 0.268 0.235 , 0.274	Depositor DCC
R_{free} test set	1079 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8311	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 3.67% 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	0.66	3/11552 (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	4

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	1065	PHE	CB-CA-C	-5.47	99.46	110.40
1	A	401	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	425	PRO	N-CA-CB	5.22	109.57	103.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1065	PHE	Peptide
1	A	1212	PRO	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	41	0
All	All	8311	0	8322	41	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 (41) 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:87:LEU:HG	1:A:707:LEU:HD12	1.86	0.58
1:A:655:ARG:NH2	1:A:1158:LYS:O	2.37	0.57
1:A:1211:ARG:N	1:A:1212:PRO:HD2	2.19	0.56
1:A:1068:HIS:HB3	1:A:1099:ARG:CZ	2.38	0.54
1:A:1232:LYS:HE3	1:A:1234:VAL:HG21	1.90	0.53
1:A:1240:GLY:HA2	1:A:1264:LEU:HB2	1.90	0.53
1:A:1223:SER:O	1:A:1234:VAL:HG23	2.09	0.53
1:A:1213:HIS:NE2	1:A:1235:SER:HB3	2.25	0.52
1:A:1195:LEU:HD21	1:A:1234:VAL:HG11	1.92	0.52
1:A:85:ALA:N	1:A:86:PRO:HD2	2.26	0.51
1:A:575:VAL:HG13	1:A:582:GLN:HG2	1.93	0.50
1:A:1263:SER:HB3	1:A:1281:ALA:HB3	1.93	0.50
1:A:1281:ALA:O	1:A:1310:GLY:HA2	2.11	0.50
1:A:237:THR:HB	1:A:238:PRO:HD3	1.93	0.49
1:A:1233:VAL:O	1:A:1234:VAL:O	2.30	0.49
1:A:408:HIS:O	1:A:409:MET:HB2	2.13	0.49
1:A:1179:SER:HB3	1:A:1185:GLN:HB3	1.96	0.48
1:A:684:ASP:O	1:A:686:LYS:N	2.48	0.47
1:A:308:LEU:HD11	1:A:343:LEU:HD21	1.97	0.47
1:A:1283:GLN:HE22	1:A:1302:PRO:HD3	1.79	0.46
1:A:351:THR:HG21	1:A:379:ARG:O	2.16	0.46
1:A:1257:ILE:HD12	1:A:1288:PHE:CD2	2.51	0.46
1:A:246:SER:O	1:A:279:CYS:SG	2.74	0.46
1:A:87:LEU:HG	1:A:707:LEU:CD1	2.47	0.45
1:A:87:LEU:HD13	1:A:965:THR:OG1	2.16	0.44
1:A:1225:GLN:HG3	1:A:1233:VAL:HG23	1.99	0.44
1:A:237:THR:HB	1:A:238:PRO:CD	2.48	0.44
1:A:1222:LEU:HB2	1:A:1234:VAL:HG22	2.00	0.44
1:A:1311:SER:HB3	1:A:1329:ALA:HB2	2.00	0.43
1:A:1063:ASN:HD21	1:A:1110:GLN:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:TYR:HB3	1:A:1309:ILE:HG21	2.00	0.43
1:A:1155:ASP:HB2	1:A:1162:VAL:HG21	1.99	0.43
1:A:408:HIS:O	1:A:408:HIS:CG	2.73	0.42
1:A:1195:LEU:HD11	1:A:1222:LEU:HD23	2.01	0.42
1:A:1315:LEU:HD22	1:A:1324:LEU:HD11	2.02	0.41
1:A:1054:TRP:CZ2	1:A:1059:ALA:HA	2.56	0.41
1:A:1048:ASN:HA	1:A:1073:LYS:HB3	2.02	0.41
1:A:137:ILE:HD11	1:A:154:ASN:HD22	1.85	0.40
1:A:1169:SER:O	1:A:1170:GLU:HB2	2.22	0.40
1:A:1155:ASP:O	1:A:1159:GLU:N	2.53	0.40
1:A:471:VAL:CG1	1:A:477:HIS:HB2	2.51	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	1044/1287 (81%)	929 (89%)	86 (8%)	29 (3%)	5	25

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	THR
1	A	409	MET
1	A	685	GLU
1	A	1212	PRO
1	A	1213	HIS
1	A	1234	VAL
1	A	87	LEU
1	A	125	ILE
1	A	130	CYS
1	A	246	SER

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Mol	Chain	Res	Type
1	A	556	SER
1	A	576	ASP
1	A	1254	TYR
1	A	1282	LYS
1	A	1331	SER
1	A	86	PRO
1	A	315	SER
1	A	401	LEU
1	A	503	GLY
1	A	516	THR
1	A	1119	ILE
1	A	263	SER
1	A	408	HIS
1	A	460	LYS
1	A	143	ALA
1	A	560	PHE
1	A	1068	HIS
1	A	1309	ILE
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%)	855 (94%)	51 (6%)	21 56

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	79	ASP
1	A	87	LEU
1	A	94	LEU
1	A	103	ARG
1	A	115	LEU
1	A	161	ARG

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Mol	Chain	Res	Type
1	A	175	THR
1	A	187	ARG
1	A	215	VAL
1	A	290	GLU
1	A	314	ARG
1	A	332	ARG
1	A	335	ASP
1	A	385	GLU
1	A	396	ILE
1	A	404	THR
1	A	408	HIS
1	A	415	MET
1	A	454	HIS
1	A	458	HIS
1	A	477	HIS
1	A	514	THR
1	A	515	THR
1	A	520	ARG
1	A	522	ILE
1	A	556	SER
1	A	580	ARG
1	A	586	LEU
1	A	589	ASN
1	A	705	SER
1	A	1025	ARG
1	A	1042	VAL
1	A	1087	SER
1	A	1110	GLN
1	A	1111	LYS
1	A	1117	SER
1	A	1180	GLN
1	A	1200	VAL
1	A	1206	LEU
1	A	1212	PRO
1	A	1220	VAL
1	A	1222	LEU
1	A	1223	SER
1	A	1246	ASP
1	A	1250	THR
1	A	1257	ILE
1	A	1283	GLN
1	A	1305	MET

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Mol	Chain	Res	Type
1	A	1314	CYS
1	A	1315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	357	ASN
1	A	370	GLN
1	A	578	HIS
1	A	1063	ASN
1	A	1110	GLN
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 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

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%)	0.15	68 (6%) 19 6	26, 67, 135, 214	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	SER	12.6
1	A	84	SER	12.4
1	A	266	SER	12.1
1	A	91	GLU	10.7
1	A	267	SER	10.1
1	A	89	THR	9.3
1	A	264	SER	8.8
1	A	88	GLY	7.5
1	A	1307	GLN	7.4
1	A	85	ALA	7.3
1	A	93	VAL	7.0
1	A	94	LEU	6.6
1	A	1309	ILE	5.8
1	A	83	ALA	5.5
1	A	263	SER	5.4
1	A	1310	GLY	4.8
1	A	265	GLY	4.8
1	A	87	LEU	4.6
1	A	269	SER	4.6
1	A	557	SER	4.5
1	A	128	SER	4.4
1	A	456	SER	4.3
1	A	81	SER	4.2
1	A	129	PRO	4.1
1	A	957	GLU	4.0
1	A	433	THR	4.0
1	A	130	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	126	LYS	3.8
1	A	146	LYS	3.8
1	A	118	THR	3.6
1	A	172	LEU	3.5
1	A	92	ILE	3.5
1	A	82	GLU	3.4
1	A	170	VAL	3.4
1	A	127	ILE	3.3
1	A	1021	ASN	3.3
1	A	1330	ASP	3.3
1	A	145	PRO	3.3
1	A	237	THR	3.2
1	A	268	GLY	3.1
1	A	62	THR	3.0
1	A	171	GLN	3.0
1	A	1306	ALA	3.0
1	A	86	PRO	3.0
1	A	132	ARG	2.8
1	A	960	LEU	2.8
1	A	1233	VAL	2.7
1	A	1283	GLN	2.6
1	A	558	GLY	2.6
1	A	177	ASP	2.5
1	A	958	ARG	2.5
1	A	80	ALA	2.5
1	A	261	TRP	2.5
1	A	148	LEU	2.4
1	A	319	GLU	2.4
1	A	262	GLY	2.4
1	A	1328	ALA	2.4
1	A	986	GLN	2.3
1	A	1308	LYS	2.3
1	A	210	ASN	2.2
1	A	317	LEU	2.1
1	A	150	THR	2.1
1	A	315	SER	2.1
1	A	1234	VAL	2.1
1	A	1311	SER	2.1
1	A	457	GLU	2.1
1	A	562	GLU	2.0
1	A	113	LEU	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 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.