



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:29 am GMT

PDB ID : 2J0V  
Title : THE CRYSTAL STRUCTURE OF ARABIDOPSIS THALIANA RAC7-  
ROP9: THE FIRST RAS SUPERFAMILY GTPASE FROM THE PLANT  
KINGDOM  
Authors : Sormo, C.G.; Leiros, I.; Brembu, T.; Winge, P.; Os, V.; Bones, A.M.  
Deposited on : 2006-08-07  
Resolution : 1.78 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

<http://wwpdb.org/validation/2016/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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

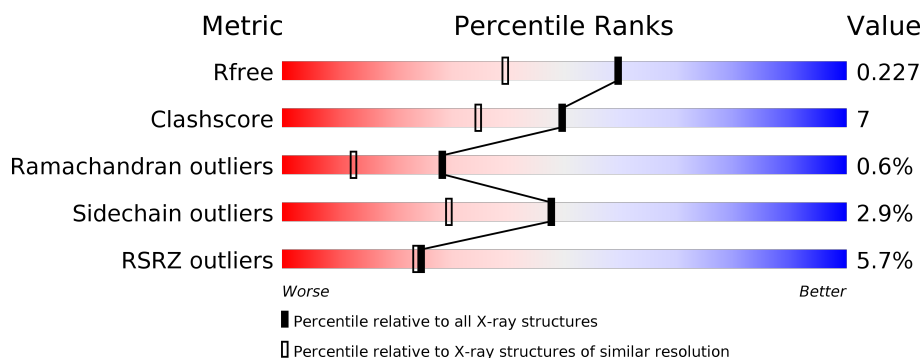
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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. 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	212	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>16%</div> <div>16%</div> </div> </div>
1	B	212	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>11%</div> <div>13%</div> </div> </div>
1	C	212	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>11%</div> <div>25%</div> </div> </div>
1	D	212	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>10%</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5787 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 RAC-LIKE GTP-BINDING PROTEIN ARAC7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1369	875	228	259	7			
1	B	184	Total	C	N	O	S	0	0	0
			1423	908	244	264	7			
1	C	159	Total	C	N	O	S	0	0	0
			1214	783	197	228	6			
1	D	178	Total	C	N	O	S	0	0	0
			1369	875	229	258	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	VAL	ALA	ENGINEERED MUTATION	UNP O82480
B	3	VAL	ALA	ENGINEERED MUTATION	UNP O82480
D	3	VAL	ALA	ENGINEERED MUTATION	UNP O82480

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	C	1	Total 28	C 10	N 5	O 11	P 2	0	0
2	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	74	Total O 74 74	0	0

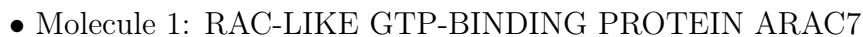
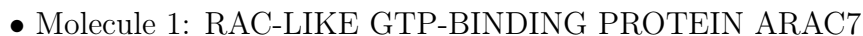
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	97	Total 97	O 97	0	0
4	C	59	Total 59	O 59	0	0
4	D	66	Total 66	O 66	0	0



● Molecule 1: RAC-LIKE GTP-BINDING PROTEIN ARAC7



ARG	ARG	LYS	GLU	VAL	PRO	ARG	ARG	ARG	LYS	ASN	HIS	ARG	ARG	SER	GLY	CYS	SER	ILE	ALA	SER	ILE	VAL	CYS	GLY	GLY	CYS	THR	ALA	ALA
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.76Å 30.20Å 139.36Å 90.00° 100.06° 90.00°	Depositor
Resolution (Å)	37.80 – 1.78 37.79 – 1.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.80-1.78) 100.0 (37.79-1.78)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.187 , 0.227 0.186 , 0.227	Depositor DCC
$R_{free}$ test set	3106 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5787	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	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 37.62 % 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 4.1740e-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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG

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	0.78	0/1395	0.78	0/1893
1	B	0.85	0/1451	0.83	2/1967 (0.1%)
1	C	0.73	0/1235	0.75	0/1674
1	D	0.74	0/1396	0.75	1/1895 (0.1%)
All	All	0.78	0/5477	0.78	3/7429 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	145	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	66	ASP	C-N-CA	5.02	134.24	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	ASP	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	1369	0	1368	20	0
1	B	1423	0	1441	21	0
1	C	1214	0	1218	19	0
1	D	1369	0	1368	21	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	74	0	0	2	0
4	B	97	0	0	2	0
4	C	59	0	0	1	0
4	D	66	0	0	5	0
All	All	5787	0	5443	73	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 7.

The worst 5 of 73 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:160:THR:OG1	1:A:162:GLN:HG3	1.53	1.07
1:D:160:THR:OG1	1:D:162:GLN:HG3	1.60	0.99
1:B:71:ARG:NH2	1:B:76:ARG:HH21	1.62	0.97
1:B:71:ARG:NH2	1:B:76:ARG:NH2	2.24	0.86
1:D:105:ARG:HH11	1:D:105:ARG:HG2	1.44	0.82

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	174/212 (82%)	167 (96%)	7 (4%)	0	100	100
1	B	182/212 (86%)	173 (95%)	6 (3%)	3 (2%)	11	2
1	C	153/212 (72%)	150 (98%)	3 (2%)	0	100	100
1	D	174/212 (82%)	168 (97%)	5 (3%)	1 (1%)	28	12
All	All	683/848 (80%)	658 (96%)	21 (3%)	4 (1%)	28	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	ASN
1	B	50	ASP
1	B	132	HIS
1	D	66	ASP

### 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	150/180 (83%)	144 (96%)	6 (4%)	36	17
1	B	156/180 (87%)	150 (96%)	6 (4%)	38	19
1	C	131/180 (73%)	130 (99%)	1 (1%)	85	80
1	D	150/180 (83%)	146 (97%)	4 (3%)	50	32
All	All	587/720 (82%)	570 (97%)	17 (3%)	48	29

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	LEU
1	B	106	ARG
1	D	67	TYR
1	B	50	ASP
1	D	90	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	55	ASN
1	D	95	ASN
1	D	147	GLN
1	C	46	ASN
1	D	134	ASN

### 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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GDP	A	1179	3	25,30,30	1.49	3 (12%)	26,47,47	1.92	6 (23%)
2	GDP	B	1182	3	25,30,30	1.65	5 (20%)	26,47,47	2.54	10 (38%)
2	GDP	C	1178	3	25,30,30	1.22	2 (8%)	26,47,47	1.95	6 (23%)
2	GDP	D	1180	3	25,30,30	1.20	2 (8%)	26,47,47	1.99	7 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	1179	3	-	0/12/32/32	0/3/3/3
2	GDP	B	1182	3	-	0/12/32/32	0/3/3/3
2	GDP	C	1178	3	-	0/12/32/32	0/3/3/3
2	GDP	D	1180	3	-	0/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1179	GDP	PB-O3B	-2.35	1.45	1.54
2	B	1182	GDP	PB-O3A	2.16	1.63	1.60
2	B	1182	GDP	C6-N1	2.24	1.37	1.33
2	B	1182	GDP	C5-C4	2.59	1.46	1.40
2	D	1180	GDP	C5-C4	3.17	1.47	1.40

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1178	GDP	C5-C6-N1	-4.96	116.43	123.48
2	B	1182	GDP	C5-C6-N1	-4.48	117.11	123.48
2	B	1182	GDP	N3-C2-N1	-4.38	121.06	127.46
2	B	1182	GDP	C4-C5-N7	-4.29	105.26	109.41
2	D	1180	GDP	C6-C5-C4	-4.13	116.74	120.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	178/212 (83%)	0.16	8 (4%) 34 33	7, 16, 34, 53	0
1	B	184/212 (86%)	0.00	6 (3%) 47 46	7, 14, 31, 39	0
1	C	159/212 (75%)	0.17	11 (6%) 18 17	11, 19, 38, 44	0
1	D	178/212 (83%)	0.23	15 (8%) 12 11	9, 18, 40, 53	0
All	All	699/848 (82%)	0.14	40 (5%) 24 24	7, 17, 38, 53	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	TYR	7.8
1	A	51	GLY	7.4
1	B	133	THR	5.2
1	D	1	MET	5.2
1	D	67	TYR	4.8

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GDP	B	1182	28/28	0.99	0.07	-0.49	5,9,11,12	0
2	GDP	D	1180	28/28	0.99	0.07	-0.56	8,11,13,16	0
3	MG	B	1183	1/1	0.99	0.07	-0.68	9,9,9,9	0
2	GDP	C	1178	28/28	0.98	0.07	-0.80	10,13,17,17	0
2	GDP	A	1179	28/28	0.99	0.07	-0.81	7,10,12,13	0
3	MG	D	1181	1/1	1.00	0.06	-1.53	11,11,11,11	0
3	MG	A	1180	1/1	1.00	0.04	-4.13	10,10,10,10	0
3	MG	C	1179	1/1	0.99	0.03	-5.55	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.