



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:50 AM GMT

PDB ID : 3NBX  
Title : Crystal structure of E. coli RavA (Regulatory ATPase variant A) in complex with ADP  
Authors : El Bakkouri, M.  
Deposited on : 2010-06-04  
Resolution : 2.91 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  
<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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

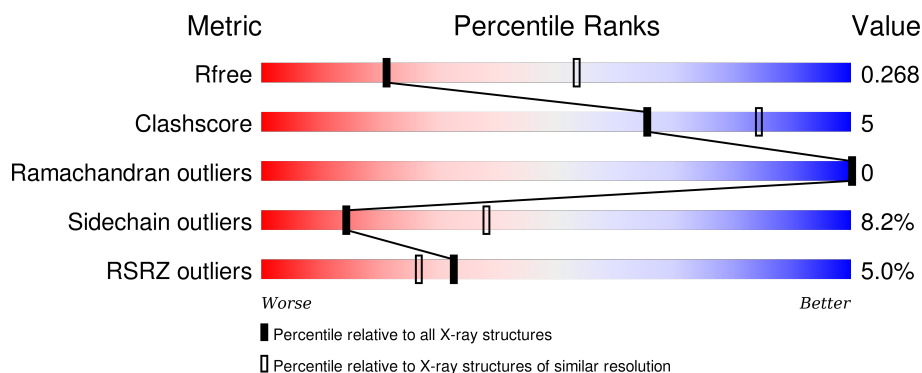
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	91344	1643 (2.94-2.90)
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	X	500	<div> <div>5%</div> <div>78%</div> <div>18%</div> <div>••</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3923 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 ATPase ravA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	X	481	3847	2446	682	708	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-1	GLY	-	EXPRESSION TAG	UNP P31473
X	0	MET	-	EXPRESSION TAG	UNP P31473

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	X	1	27	10	5	10	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	X	44	Total	O	0	0
			44	44		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Chain X:

5% 78% 18%

GLY MET MET ALA H3 P4 H5 E9 R10 R13 E19 S26 L31 S41 V42 F43 L44 A51 I55 A56 R57 K60 F63 A66 F69 E70 M73 S77 L86 S87 ILE GLN ALA LEU LYS ASP GLU ARG TYR E98 R99 L100 T101 S102 I110 V111 F112 E115 I116 W117 I123 L124 H125 T126 T129 N132 Q135 F136 R137 N138 G139 A140 H141 V142 K144 I145 L150 V151 P158 E159 D161 S162 S163 R170 W176 M189 N199 P200 V201 V207 E211 L224 M234 L242 D243 D244 P274 L277 I278 K281 Q289 K302 Q330 K333 T334 K336 K339 K340 L341 T348 Y351 Q352 L353 F354 K356 V357 T358 T363 L366 Q367 K368 L372 R373 D374 E376 V377 N378 R379 T380 S381 K398 Q408 K409 Q428 L429

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.23 Å   162.23 Å   55.32 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	29.70 – 2.91 29.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.70-2.91) 97.9 (29.65-2.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.223 , 0.269 0.226 , 0.268	Depositor DCC
$R_{free}$ test set	939 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.5	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.8	EDS
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 20352 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ADP

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	X	0.34	0/3919	0.51	0/5300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	X	3847	0	3896	39	0
2	X	27	0	12	0	0
3	X	5	0	0	0	0
4	X	44	0	0	0	0
All	All	3923	0	3908	39	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 5.

All (39) 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:X:159:GLU:HB2	1:X:162:SER:HB2	1.54	0.87
1:X:63:PHE:HB2	1:X:66:ALA:HB2	1.80	0.63
1:X:3:HIS:HB2	1:X:4:PRO:HD3	1.81	0.62
1:X:9:GLU:OE1	1:X:13:ARG:NH1	2.34	0.59
1:X:372:LEU:HD12	1:X:377:VAL:HG11	1.87	0.56
1:X:10:ARG:HH12	1:X:211:GLU:CD	2.09	0.56
1:X:73:MET:HB2	1:X:115:GLU:O	2.08	0.53
1:X:132:ASN:OD1	1:X:170:ARG:HD3	2.10	0.52
1:X:10:ARG:NH2	1:X:207:VAL:HA	2.26	0.51
1:X:69:PHE:HB3	1:X:111:VAL:HG12	1.94	0.50
1:X:378:VAL:HG23	1:X:379:HIS:HD2	1.77	0.50
1:X:86:LEU:HA	1:X:99:ARG:HA	1.94	0.50
1:X:10:ARG:HH22	1:X:207:VAL:HA	1.80	0.47
1:X:132:ASN:HD21	1:X:170:ARG:HH11	1.60	0.47
1:X:70:GLU:HG3	1:X:112:PHE:HD2	1.80	0.47
1:X:117:TRP:CE2	1:X:158:PRO:HD3	2.50	0.46
1:X:51:ALA:O	1:X:55:ILE:HG23	2.16	0.46
1:X:302:MET:HB3	1:X:481:ILE:CD1	2.46	0.46
1:X:353:LEU:HB2	1:X:357:VAL:HG22	1.98	0.45
1:X:302:MET:HB3	1:X:481:ILE:HD11	1.98	0.45
1:X:19:GLU:OE2	1:X:26:SER:HB3	2.17	0.45
1:X:129:THR:HG21	1:X:137:ARG:HH21	1.82	0.45
1:X:60:LYS:HA	1:X:110:ILE:HD13	1.98	0.45
1:X:352:GLN:H	1:X:352:GLN:CD	2.20	0.45
1:X:363:THR:HA	1:X:381:SER:HA	1.99	0.44
1:X:111:VAL:HG23	1:X:150:LEU:HD12	1.98	0.44
1:X:339:ILE:HG13	1:X:351:TYR:HB3	2.00	0.43
1:X:77:SER:O	1:X:123:ILE:HD11	2.18	0.43
1:X:278:ILE:O	1:X:281:LYS:HG2	2.18	0.43
1:X:63:PHE:CD1	1:X:207:VAL:HG22	2.54	0.43
1:X:242:LEU:HA	1:X:243:PRO:HD3	1.87	0.43
1:X:398:ARG:NH1	1:X:409:LYS:HE2	2.34	0.43
1:X:274:PRO:O	1:X:277:LEU:HB2	2.19	0.42
1:X:450:LEU:HD23	1:X:496:GLN:HB3	2.01	0.42
1:X:57:ARG:O	1:X:60:LYS:HG2	2.20	0.42
1:X:145:ILE:HG13	1:X:145:ILE:H	1.74	0.41
1:X:199:ASN:ND2	1:X:201:VAL:H	2.19	0.40
1:X:278:ILE:HB	1:X:473:ILE:HD12	2.03	0.40
1:X:482:GLU:O	1:X:486:GLN:HG2	2.22	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	X	475/500 (95%)	453 (95%)	22 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	X	416/429 (97%)	382 (92%)	34 (8%)	14	38

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	26	SER
1	X	31	LEU
1	X	42	VAL
1	X	44	LEU
1	X	86	LEU
1	X	124	LEU
1	X	126	THR
1	X	144	LYS
1	X	151	VAL
1	X	163	SER
1	X	170	ARG
1	X	189	MET
1	X	224	LEU

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Mol	Chain	Res	Type
1	X	234	MET
1	X	244	ASP
1	X	289	GLN
1	X	330	GLN
1	X	334	THR
1	X	336	LEU
1	X	341	LEU
1	X	352	GLN
1	X	358	THR
1	X	363	THR
1	X	366	LEU
1	X	367	GLN
1	X	368	LYS
1	X	374	ASP
1	X	376	GLU
1	X	408	GLN
1	X	434	LEU
1	X	468	GLN
1	X	469	LYS
1	X	478	LEU
1	X	494	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	64	GLN
1	X	199	ASN
1	X	227	HIS
1	X	237	GLN
1	X	325	GLN
1	X	330	GLN
1	X	367	GLN
1	X	379	HIS
1	X	408	GLN
1	X	449	GLN
1	X	491	GLN
1	X	494	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	$\# Z  > 2$
3	SO4	X	499	-	4,4,4	0.20	0	6,6,6	0.11	0
2	ADP	X	800	-	22,29,29	1.06	1 (4%)	27,45,45	1.86	3 (11%)

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
3	SO4	X	499	-	-	0/0/0/0	0/0/0/0
2	ADP	X	800	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	800	ADP	C5-C4	3.21	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	800	ADP	N3-C2-N1	-7.44	123.19	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	800	ADP	C4-C5-N7	-2.96	106.75	109.48
2	X	800	ADP	PA-O3A-PB	-2.88	123.00	132.67

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 ⓘ

### 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	X	481/500 (96%)	0.20	24 (4%)	32 27	22, 73, 108, 133	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	141	HIS	4.6
1	X	100	LEU	4.3
1	X	3	HIS	4.1
1	X	355	VAL	4.1
1	X	160	ALA	4.0
1	X	143	GLU	4.0
1	X	87	SER	4.0
1	X	138	ASN	3.6
1	X	4	PRO	3.3
1	X	86	LEU	3.2
1	X	98	GLU	2.9
1	X	144	LYS	2.8
1	X	333	LYS	2.8
1	X	354	PRO	2.7
1	X	135	GLN	2.7
1	X	351	TYR	2.7
1	X	176	TRP	2.4
1	X	41	SER	2.4
1	X	102	SER	2.4
1	X	5	HIS	2.3
1	X	101	THR	2.2
1	X	139	GLY	2.1
1	X	348	ARG	2.1
1	X	428	GLN	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](#)

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	ADP	X	800	27/27	0.96	0.17	-0.63	51,56,60,62	0
3	SO4	X	499	5/5	0.88	0.36	-	109,113,117,135	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.