



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:56 AM GMT

PDB ID : 2O7P  
Title : The crystal structure of RibD from Escherichia coli in complex with the oxidised NADP<sup>+</sup> cofactor in the active site of the reductase domain  
Authors : Moche, M.; Stenmark, P.; Gurmu, D.; Nordlund, P.; Structural Proteomics in Europe (SPINE)  
Deposited on : 2006-12-11  
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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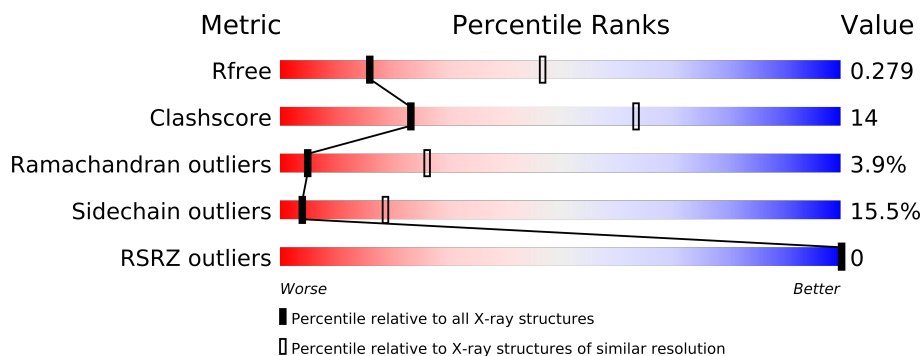
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	380	
1	B	380	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5523 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Riboflavin biosynthesis protein ribD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	Se	0	0	0
			2733	1720	495	503	6	9			
1	B	353	Total	C	N	O	S	Se	0	0	0
			2694	1698	489	496	3	8			

There are 46 discrepancies between the modelled and reference sequences:

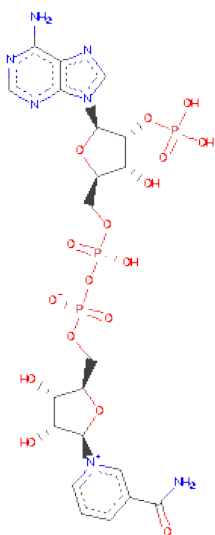
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	THR	-	CLONING ARTIFACT	UNP P25539
A	-3	LEU	-	CLONING ARTIFACT	UNP P25539
A	-2	TYR	-	CLONING ARTIFACT	UNP P25539
A	-1	ILE	-	CLONING ARTIFACT	UNP P25539
A	0	GLN	-	CLONING ARTIFACT	UNP P25539
A	1	GLY	-	CLONING ARTIFACT	UNP P25539
A	7	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	58	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	100	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	127	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	128	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	142	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	163	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	285	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	286	MSE	MET	MODIFIED RESIDUE	UNP P25539
A	368	SER	-	CLONING ARTIFACT	UNP P25539
A	369	THR	-	CLONING ARTIFACT	UNP P25539
A	370	HIS	-	EXPRESSION TAG	UNP P25539
A	371	HIS	-	EXPRESSION TAG	UNP P25539
A	372	HIS	-	EXPRESSION TAG	UNP P25539
A	373	HIS	-	EXPRESSION TAG	UNP P25539
A	374	HIS	-	EXPRESSION TAG	UNP P25539
A	375	HIS	-	EXPRESSION TAG	UNP P25539
B	-4	THR	-	CLONING ARTIFACT	UNP P25539
B	-3	LEU	-	CLONING ARTIFACT	UNP P25539

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	TYR	-	CLONING ARTIFACT	UNP P25539
B	-1	ILE	-	CLONING ARTIFACT	UNP P25539
B	0	GLN	-	CLONING ARTIFACT	UNP P25539
B	1	GLY	-	CLONING ARTIFACT	UNP P25539
B	7	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	58	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	100	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	127	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	128	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	142	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	163	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	285	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	286	MSE	MET	MODIFIED RESIDUE	UNP P25539
B	368	SER	-	CLONING ARTIFACT	UNP P25539
B	369	THR	-	CLONING ARTIFACT	UNP P25539
B	370	HIS	-	EXPRESSION TAG	UNP P25539
B	371	HIS	-	EXPRESSION TAG	UNP P25539
B	372	HIS	-	EXPRESSION TAG	UNP P25539
B	373	HIS	-	EXPRESSION TAG	UNP P25539
B	374	HIS	-	EXPRESSION TAG	UNP P25539
B	375	HIS	-	EXPRESSION TAG	UNP P25539

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.00Å 173.00Å 77.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.93 – 3.00 28.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.93-3.00) 99.9 (28.92-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.212 , 0.267 0.234 , 0.279	Depositor DCC
$R_{free}$ test set	1359 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	93.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.1	EDS
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 27038 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.82	4/2776 (0.1%)	0.87	3/3753 (0.1%)
1	B	0.82	7/2736 (0.3%)	0.83	4/3703 (0.1%)
All	All	0.82	11/5512 (0.2%)	0.85	7/7456 (0.1%)

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
1	B	0	3
All	All	0	5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	GLN	CD-OE1	8.29	1.42	1.24
1	B	116	GLN	CD-NE2	8.20	1.53	1.32
1	B	62	LYS	CD-CE	7.45	1.69	1.51
1	A	297	TRP	CD2-CE3	6.82	1.50	1.40
1	A	297	TRP	CD1-NE1	6.46	1.49	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	GLN	CG-CD-OE1	-7.85	105.90	121.60
1	A	67	THR	N-CA-C	7.03	129.99	111.00
1	B	116	GLN	OE1-CD-NE2	5.72	135.05	121.90
1	A	143	ARG	NE-CZ-NH1	5.53	123.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	LEU	CA-CB-CG	5.19	127.23	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	GLY	Peptide
1	A	217	ALA	Peptide
1	B	116	GLN	Sidechain
1	B	217	ALA	Peptide
1	B	366	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2733	0	2727	83	0
1	B	2694	0	2686	78	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
All	All	5523	0	5463	158	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 158 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:212:ASP:OD1	1:A:214:GLN:HG2	1.54	1.07
1:B:213:GLU:OE1	1:B:213:GLU:HA	1.59	1.03
1:A:194:SER:HB3	1:A:233:ASP:HB3	1.46	0.97
1:B:206:VAL:H	1:B:226:GLN:NE2	1.63	0.96
1:A:170:TRP:HH2	1:A:200:ASP:OD1	1.47	0.96

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	350/380 (92%)	309 (88%)	29 (8%)	12 (3%)	6	31
1	B	345/380 (91%)	295 (86%)	35 (10%)	15 (4%)	4	23
All	All	695/760 (91%)	604 (87%)	64 (9%)	27 (4%)	5	26

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	95	ARG
1	A	217	ALA
1	A	328	SER
1	B	95	ARG

### 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	284/302 (94%)	238 (84%)	46 (16%)	3	17
1	B	277/302 (92%)	236 (85%)	41 (15%)	4	21
All	All	561/604 (93%)	474 (84%)	87 (16%)	4	19

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	HIS
1	B	20	THR
1	B	260	SER
1	A	291	GLN

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Mol	Chain	Res	Type
1	A	349	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	B	104	ASN
1	B	226	GLN
1	A	226	GLN
1	A	247	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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
2	NAP	A	402	-	52,52,52	1.42	4 (7%)	80,80,80	1.68	7 (8%)
2	NAP	B	1402	-	52,52,52	1.40	4 (7%)	80,80,80	1.59	7 (8%)

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	NAP	A	402	-	-	0/35/67/67	0/3/5/5
2	NAP	B	1402	-	-	1/35/67/67	0/3/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1402	NAP	O7N-C7N	7.76	1.42	1.24
2	A	402	NAP	O7N-C7N	7.40	1.41	1.24
2	A	402	NAP	C2A-N3A	3.34	1.38	1.32
2	B	1402	NAP	C2A-N3A	2.80	1.37	1.32
2	B	1402	NAP	C2A-N1A	2.67	1.39	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1402	NAP	N3A-C2A-N1A	-9.43	120.83	128.71
2	A	402	NAP	N3A-C2A-N1A	-8.78	121.37	128.71
2	B	1402	NAP	O4D-C1D-N1N	5.19	113.26	107.95
2	A	402	NAP	O4D-C1D-N1N	4.82	112.89	107.95
2	A	402	NAP	N3A-C4A-N9A	4.16	132.95	125.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1402	NAP	C2D-C1D-N1N-C2N

There are no ring outliers.

## 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	358/380 (94%)	-0.18	0 100 100	68, 82, 108, 122	0
1	B	353/380 (92%)	-0.16	0 100 100	63, 81, 110, 118	0
All	All	711/760 (93%)	-0.17	0 100 100	63, 81, 109, 122	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAP	A	402	48/48	0.16	-0.72	71,81,89,93	0
2	NAP	B	1402	48/48	0.14	-1.02	95,107,141,143	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.