



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:36 AM UTC

PDB ID : 7PP2 / pdb\_00007pp2  
Title : Complex of rice blast (*Magnaporthe oryzae*) effector protein AVR-Pii with the host target Exo70F2 from Rice (*Oryza sativa*)  
Authors : De la Concepcion, J.C.; Bentham, A.R.; Lawson, D.; Banfield, M.J.  
Deposited on : 2021-09-13  
Resolution : 2.69 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

<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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

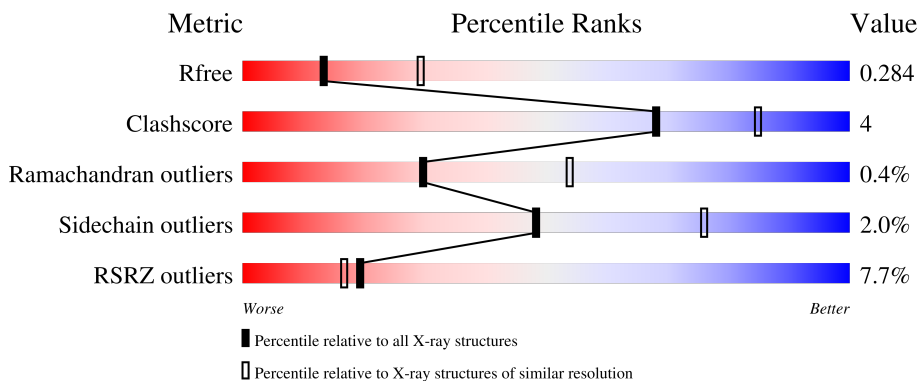
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	606	
2	B	51	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3740 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 Exocyst subunit Exo70 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3526	2241	604	663	18	0	0	0

- Molecule 2 is a protein called AVR-Pii protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	27	212	126	36	47	3	0	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	1	1	1	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.32Å 76.62Å 67.87Å 90.00° 107.76° 90.00°	Depositor
Resolution (Å)	66.56 – 2.69 66.56 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.7 (66.56-2.69) 99.6 (66.56-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.252 , 0.279 0.255 , 0.284	Depositor DCC
$R_{free}$ test set	977 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtrriage
Anisotropy	0.519	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3740	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% 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, 0.333 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:  
ZN

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	0.98	0/3581	1.59	0/4828
2	B	1.00	0/217	1.46	2/289 (0.7%)
All	All	0.98	0/3798	1.58	2/5117 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	56	TYR	CA-C-N	5.19	125.61	121.61
2	B	56	TYR	C-N-CA	5.19	125.61	121.61

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3526	0	3545	27	0
2	B	212	0	173	1	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
All	All	3740	0	3718	27	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 4.

All (27) 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:423:GLU:HG3	1:A:437:MET:HE1	1.57	0.85
1:A:519:MET:HE2	1:A:623:LEU:HD21	1.74	0.70
1:A:225:ASN:OD1	1:A:225:ASN:N	2.33	0.59
1:A:449:VAL:HG11	1:A:533:GLU:HB2	1.86	0.56
1:A:376:ALA:HA	1:A:402:LEU:HD11	1.87	0.55
1:A:636:ILE:HB	1:A:637:PRO:HD3	1.88	0.55
1:A:519:MET:HE1	1:A:627:LEU:HD11	1.92	0.51
1:A:435:HIS:CD2	1:A:436:PRO:HD2	2.49	0.48
1:A:288:VAL:HG21	1:A:354:ALA:HB1	1.96	0.47
1:A:166:ARG:O	1:A:170:VAL:HG23	2.15	0.46
1:A:220:GLY:O	1:A:224:VAL:HG23	2.15	0.46
1:A:641:ALA:O	1:A:645:ARG:HG2	2.17	0.46
1:A:419:VAL:HG11	2:B:65:PHE:HA	1.98	0.45
1:A:631:ILE:HG21	1:A:671:LEU:HD22	1.99	0.45
1:A:293:TRP:CZ3	1:A:364:LYS:HG2	2.52	0.45
1:A:435:HIS:CE1	1:A:504:LYS:HE3	2.52	0.44
1:A:170:VAL:HG13	1:A:266:ILE:HD11	2.00	0.43
1:A:170:VAL:HG13	1:A:266:ILE:CD1	2.49	0.43
1:A:296:LEU:HD11	1:A:300:MET:HE3	2.01	0.42
1:A:423:GLU:HG3	1:A:437:MET:CE	2.41	0.42
1:A:174:VAL:HG12	1:A:175:PRO:HD3	2.02	0.41
1:A:602:PHE:CD1	1:A:602:PHE:C	2.98	0.41
1:A:511:SER:O	1:A:514:GLU:HB3	2.20	0.41
1:A:559:ARG:O	1:A:563:MET:HB2	2.20	0.41
1:A:433:GLU:HG3	1:A:434:ILE:N	2.36	0.41
1:A:379:ILE:HB	1:A:380:PRO:HD3	2.03	0.40
1:A:174:VAL:CG1	1:A:175:PRO:HD3	2.52	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	426/606 (70%)	399 (94%)	25 (6%)	2 (0%)	24	48
2	B	25/51 (49%)	24 (96%)	1 (4%)	0	100	100
All	All	451/657 (69%)	423 (94%)	26 (6%)	2 (0%)	30	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	LEU
1	A	363	GLU

### 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	382/509 (75%)	375 (98%)	7 (2%)	51	78
2	B	24/44 (54%)	23 (96%)	1 (4%)	26	55
All	All	406/553 (73%)	398 (98%)	8 (2%)	48	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ARG
1	A	161	LEU
1	A	172	HIS
1	A	225	ASN
1	A	495	SER
1	A	538	LEU
1	A	602	PHE
2	B	50	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	435	HIS
1	A	601	ASN
1	A	613	GLN
1	A	634	ASN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	A	442/606 (72%)	0.68	36 (8%) 18 15	52, 81, 150, 169	0
2	B	27/51 (52%)	0.00	0 100 100	55, 66, 83, 100	0
All	All	469/657 (71%)	0.64	36 (7%) 19 17	52, 79, 149, 169	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	660	ILE	4.9
1	A	118	TYR	4.7
1	A	599	PHE	3.9
1	A	169	MET	3.3
1	A	332	LEU	3.2
1	A	121	ALA	3.2
1	A	87	ALA	3.1
1	A	217	THR	3.1
1	A	86	ALA	2.9
1	A	647	GLY	2.8
1	A	126	ILE	2.8
1	A	387	LEU	2.8
1	A	125	ALA	2.8
1	A	336	CYS	2.7
1	A	159	ALA	2.7
1	A	221	GLY	2.7
1	A	447	LEU	2.5
1	A	218	ALA	2.5
1	A	303	TRP	2.4
1	A	106	LEU	2.4
1	A	569	LEU	2.4
1	A	172	HIS	2.3
1	A	325	VAL	2.3
1	A	173	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	225	ASN	2.3
1	A	312	ARG	2.3
1	A	124	VAL	2.3
1	A	129	LEU	2.3
1	A	227	PHE	2.3
1	A	565	VAL	2.2
1	A	257	ARG	2.2
1	A	100	ASP	2.2
1	A	337	PHE	2.2
1	A	388	GLY	2.1
1	A	107	VAL	2.0
1	A	115	VAL	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](#)

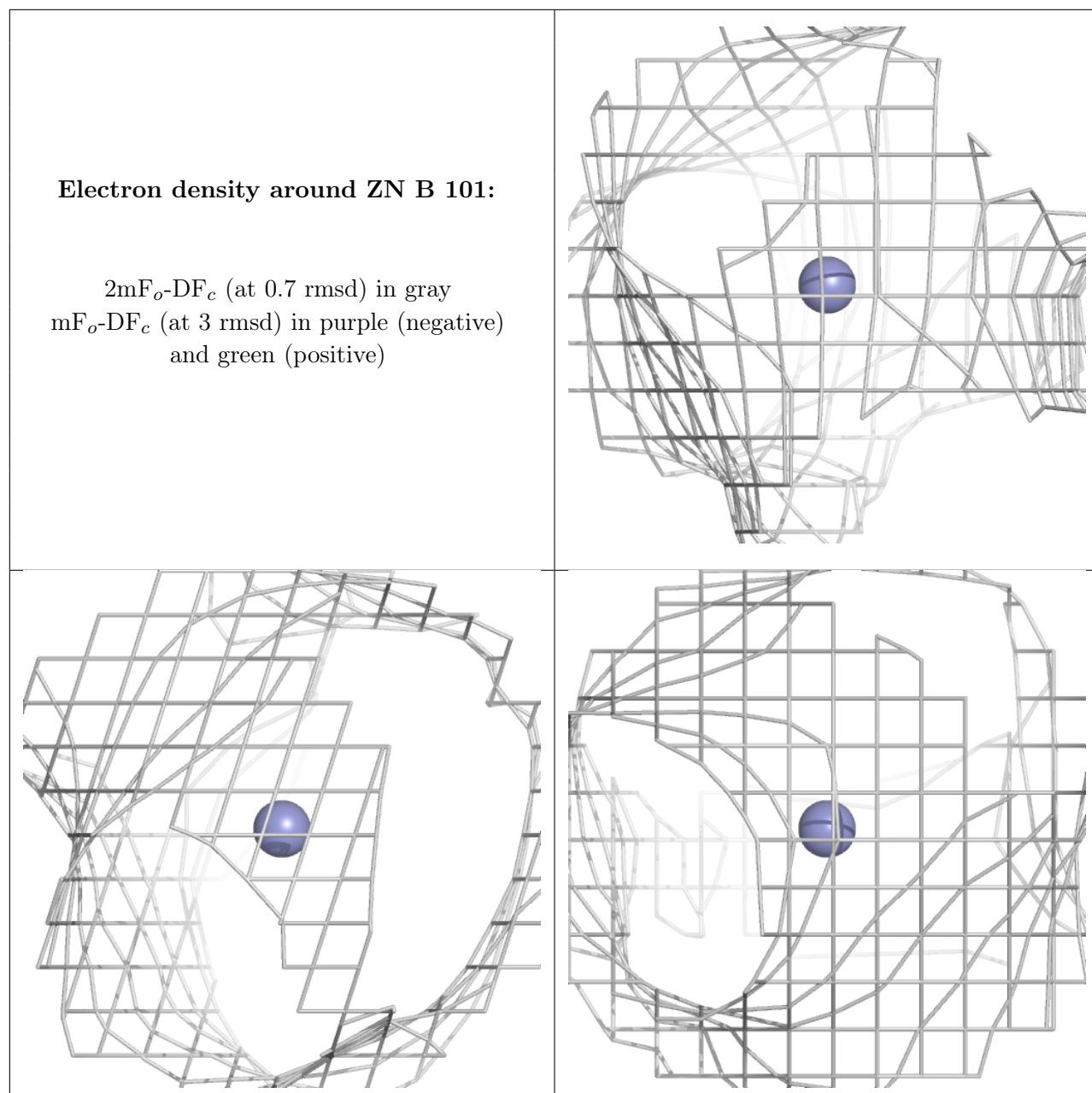
There are no oligosaccharides in this entry.

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	B	101	1/1	1.00	0.02	62,62,62,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.