



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2024 – 12:32 PM JST

PDB ID : 8YLI  
Title : Crystal structure of Pectobacterium atrosepticum PecS in complex with operator DNA  
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Deposited on : 2024-03-06  
Resolution : 2.90 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

<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>.

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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  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

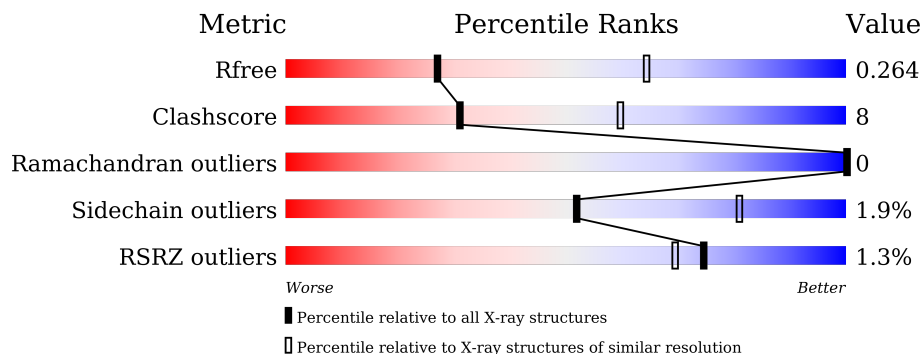
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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 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	170	 2% (poor fit), 82% (0 outliers), 12% (1 outlier), 5% (2 outliers), 5% (3+ outliers)
1	B	170	 80% (0 outliers), 14% (1 outlier), 5% (2 outliers), 5% (3+ outliers)
2	C	28	 4% (poor fit), 50% (0 outliers), 50% (1 outlier)
3	D	28	 54% (0 outliers), 46% (1 outlier)

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3472 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	161	1146	721	210	207	8	0	0	0
1	B	162	1184	745	211	220	8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	SER	-	expression tag	UNP Q6D5K4
A	11	ALA	-	expression tag	UNP Q6D5K4
A	12	LYS	-	expression tag	UNP Q6D5K4
A	13	ASP	-	expression tag	UNP Q6D5K4
A	14	LEU	-	expression tag	UNP Q6D5K4
B	10	SER	-	expression tag	UNP Q6D5K4
B	11	ALA	-	expression tag	UNP Q6D5K4
B	12	LYS	-	expression tag	UNP Q6D5K4
B	13	ASP	-	expression tag	UNP Q6D5K4
B	14	LEU	-	expression tag	UNP Q6D5K4

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	28	568	276	96	169	27	0	0	0


- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	28	574	277	107	163	27	0	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 ( $RSRZ > 2$ ). 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.

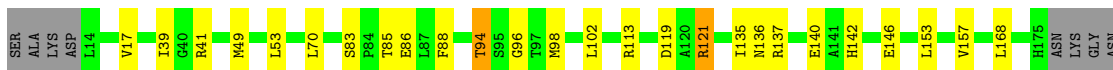
- Molecule 1: Regulatory protein

Chain A: 



- Molecule 1: Regulatory protein

Chain B: 



- Molecule 2: DNA (28-MER)

Chain C: 



- Molecule 3: DNA (28-MER)

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.17Å 80.50Å 75.23Å 90.00° 93.48° 90.00°	Depositor
Resolution (Å)	27.46 – 2.90 27.46 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (27.46-2.90) 98.9 (27.46-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.89Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.225 , 0.274 0.218 , 0.264	Depositor DCC
$R_{free}$ test set	1100 reflections (5.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtrriage
Anisotropy	0.408	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 84.1	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	0.95	EDS
Total number of atoms	3472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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](#)

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	0.31	0/1164	0.55	0/1585
1	B	0.35	0/1202	0.54	0/1636
2	C	0.73	0/635	0.98	0/978
3	D	0.73	0/645	0.94	0/994
All	All	0.51	0/3646	0.73	0/5193

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 [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	1146	0	1054	16	0
1	B	1184	0	1118	20	0
2	C	568	0	322	13	0
3	D	574	0	319	11	0
All	All	3472	0	2813	50	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 8.

The worst 5 of 50 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:94:THR:HG21	3:D:17:DC:H2'	1.62	0.81
1:B:94:THR:HG21	2:C:17:DC:H2'	1.64	0.78
3:D:25:DA:H2''	3:D:26:DT:H5''	1.81	0.63
3:D:1:DT:H2''	3:D:2:DT:H5'	1.81	0.62
2:C:17:DC:H2''	2:C:18:DA:C8	2.35	0.62

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	159/170 (94%)	157 (99%)	2 (1%)	0	100	100
1	B	160/170 (94%)	157 (98%)	3 (2%)	0	100	100
All	All	319/340 (94%)	314 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	101/146 (69%)	99 (98%)	2 (2%)	50	79
1	B	112/146 (77%)	110 (98%)	2 (2%)	54	82
All	All	213/292 (73%)	209 (98%)	4 (2%)	52	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	THR
1	A	121	ARG
1	B	94	THR
1	B	121	ARG

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	164	ASN
1	A	175	HIS
1	B	142	HIS
1	B	164	ASN
1	B	175	HIS

### 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](#)

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 [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	161/170 (94%)	0.03	4 (2%) 58 52	56, 70, 93, 114	0
1	B	162/170 (95%)	-0.17	0 100 100	51, 70, 87, 97	0
2	C	28/28 (100%)	0.26	1 (3%) 46 40	75, 105, 134, 142	0
3	D	28/28 (100%)	-0.00	0 100 100	69, 98, 132, 133	0
All	All	379/396 (95%)	-0.04	5 (1%) 74 69	51, 72, 112, 142	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	ASP	3.6
1	A	115	GLN	2.5
1	A	152	VAL	2.4
1	A	118	LEU	2.0
2	C	3	DA	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.