

# wwPDB X-ray Structure Validation Summary Report (i)

#### Oct 6, 2024 – 09:31 am BST

PDB ID : 2YJL

Title: Structural characterization of a secretin pilot protein from the type III secre-

tion system (T3SS) of Pseudomonas aeruginosa

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Deposited on : 2011-05-20

Resolution : 1.81 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{-}467$ 

Mogul : 1.8.4, CSD as541be (2020)

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)

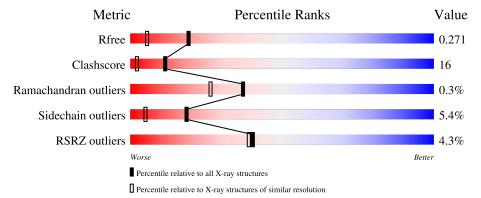
Validation Pipeline (wwPDB-VP) : 2.39

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
$R_{free}$	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

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 >=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 <=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	٨	125	2%				
1	A	120	67%	18% • 14%			
1	В	125	72%	15% • 10%			
1	С	125	64%	20% • 15%			



## 2 Entry composition (i)

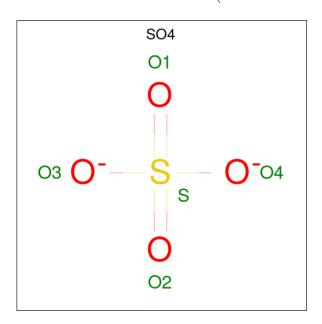
There are 4 unique types of molecules in this entry. The entry contains 2879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EXOENZYME S SYNTHESIS PROTEIN B.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace				
1	Λ	108	Total	С	N	О	S	0	0	0	6	0
1	A	100	882	552	173	154	3	0	O	0		
1	D	113	Total	С	N	О	S	0 10	) 10	0		
1	Б	110	937	591	180	163	3			0		
1	С	106	Total	С	N	О	S	0	Q	0		
1		100	884	557	173	151	3		0	U		

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	С	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms		eroOcc	AltConf
2	С	1	Total O S 5 4 1		0	0

• Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	59	Total O 59 59	0	0
4	В	60	Total O 60 60	0	0
4	С	36	Total O 36 36	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: EXOENZYME S SYNTHESIS PROTEIN B

Chain A:

67%

18%

18%

18%

14%

• Molecule 1: EXOENZYME S SYNTHESIS PROTEIN B

Chain B:

72%

15%

• Molecule 1: EXOENZYME S SYNTHESIS PROTEIN B

Chain C:

64%

20%

15%

15%



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	124.16Å 48.36Å 71.60Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $96.92^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	35.54 - 1.81	Depositor
Resolution (A)	35.54 - 1.81	EDS
% Data completeness	90.1 (35.54-1.81)	Depositor
(in resolution range)	90.1 (35.54-1.81)	EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.46 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
D D	0.217 , 0.262	Depositor
$R, R_{free}$	0.222 , $0.271$	DCC
$R_{free}$ test set	3463 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.40 , 47.1	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.09% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 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: NI, SO4

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	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.46	0/909	0.62	0/1228
1	В	0.50	0/980	0.64	0/1327
1	С	0.39	0/917	0.59	0/1238
All	All	0.45	0/2806	0.62	0/3793

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	В	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Group
1	В	40	ALA	Peptide

### 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	882	0	916	32	0
1	В	937	0	990	34	0
1	С	884	0	931	24	0
2	A	10	0	0	0	0
2	С	10	0	0	0	0
3	A	1	0	0	0	0
4	A	59	0	0	16	0
4	В	60	0	0	6	0
4	С	36	0	0	9	0
All	All	2879	0	2837	88	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 16.

The worst 5 of 88 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$	
1:A:131:ALA:C	4:A:2059:HOH:O	1.67	1.25	
1:C:54:GLN:HG2	4:C:2012:HOH:O	1.29	1.25	
1:A:42[B]:GLN:HG3	4:A:2017:HOH:O	1.35	1.22	
1:A:58:GLN:HG3	4:A:2024:HOH:O	1.42	1.20	
1:B:119[B]:ARG:HH11	1:B:119[B]:ARG:HG3	1.10	1.13	

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	Percentile	$\mathbf{s}$
1	A	112/125 (90%)	111 (99%)	1 (1%)	0	100 100	
1	В	121/125 (97%)	116 (96%)	4 (3%)	1 (1%)	16 6	
1	С	112/125~(90%)	110 (98%)	2 (2%)	0	100 100	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	345/375~(92%)	337 (98%)	7 (2%)	1 (0%)	37 26	

#### All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	40	ALA

#### 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	92/100~(92%)	90 (98%)	2 (2%)	47 31		
1	В	100/100 (100%)	92 (92%)	8 (8%)	10 1		
1	С	93/100 (93%)	86 (92%)	7 (8%)	11 1		
All	All	285/300 (95%)	268 (94%)	17 (6%)	18 3		

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

Mol	Chain	Res	Type
1	С	73[B]	ARG
1	С	119	ARG
1	В	73	ARG
1	В	82	ARG
1	В	117	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	58	GLN
1	С	108	GLN
1	С	109	GLN
1	В	108	GLN
1	A	44	GLN



#### 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 5 ligands modelled in this entry, 1 is 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	Tuno	Chain	Res Link		Bond lengths			Bond angles		
MIOI	Type	pe Chain Res	nes	ites   Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	SO4	С	152	-	4,4,4	0.37	0	6,6,6	0.30	0
2	SO4	A	151	-	4,4,4	0.41	0	6,6,6	0.18	0
2	SO4	С	151	-	4,4,4	0.37	0	6,6,6	0.24	0
2	SO4	A	150	-	4,4,4	0.35	0	6,6,6	0.30	0

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 (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,  $95^{th}$  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	$OWAB(A^2)$	Q<0.9
1	A	108/125~(86%)	0.09	3 (2%) 55 54	11, 26, 42, 62	6 (5%)
1	В	113/125 (90%)	0.21	5 (4%) 39 38	13, 24, 50, 77	10 (8%)
1	С	106/125 (84%)	0.48	6 (5%) 30 29	18, 32, 49, 58	8 (7%)
All	All	327/375 (87%)	0.26	14 (4%) 40 39	11, 28, 48, 77	24 (7%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	40	ALA	4.5
1	В	24	SER	4.1
1	A	131	ALA	3.5
1	В	39	GLN	3.4
1	С	41[A]	ARG	3.1

## 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)

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,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	SO4	A	151	5/5	0.83	0.13	42,63,63,71	0
2	SO4	С	151	5/5	0.86	0.13	63,65,76,82	0
2	SO4	С	152	5/5	0.91	0.09	47,55,57,58	0
3	NI	A	160	1/1	0.96	0.06	64,64,64,64	0
2	SO4	A	150	5/5	0.99	0.04	22,24,25,26	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

