



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:56 am GMT

PDB ID : 2J9P  
Title : CRYSTAL STRUCTURE OF THE BACILLUS SUBTILIS PBP4A, AND ITS COMPLEX WITH A PEPTIDOGLYCAN MIMETIC PEPTIDE.  
Authors : Sauvage, E.; Herman, R.; Kerff, F.; Duez, C.; Charlier, P.  
Deposited on : 2006-11-15  
Resolution : 2.80 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

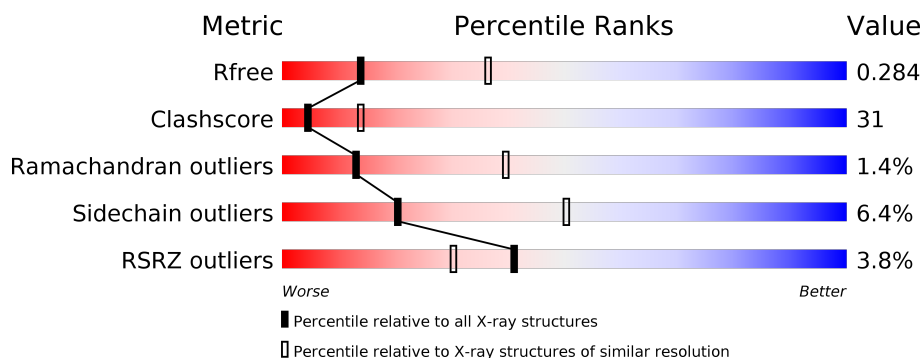
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 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	A	462	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>41%</div> <div>5% •</div> </div> </div>
1	B	462	<div> <div>5%</div> <div> <div></div> <div>46%</div> <div>49%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

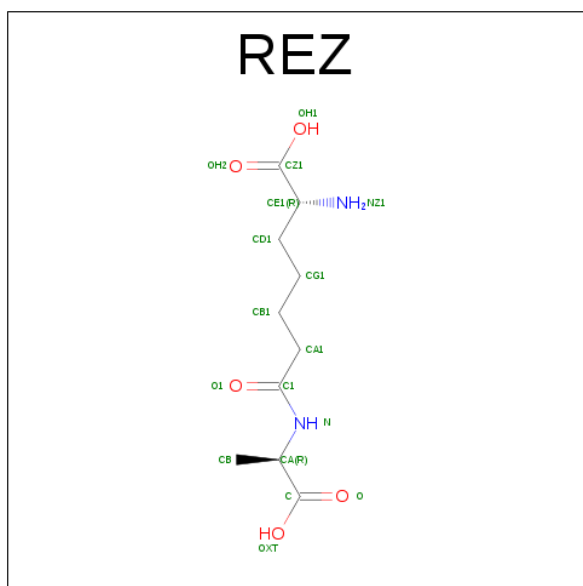
There are 3 unique types of molecules in this entry. The entry contains 6966 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PENICILLIN-BINDING PROTEIN.

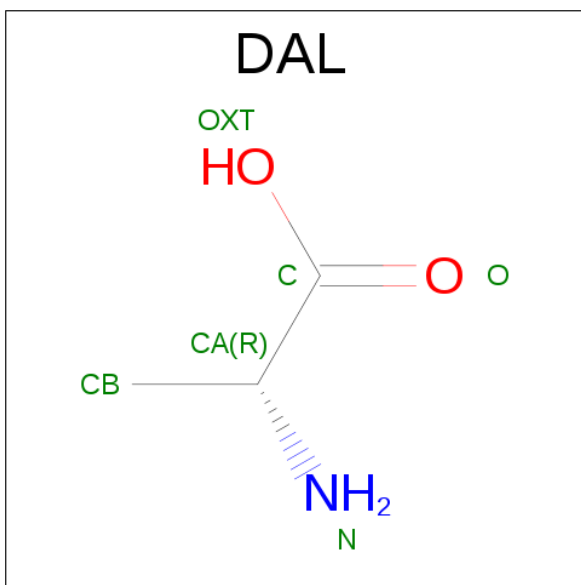
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3461	2169	582	700	10			
1	B	458	Total	C	N	O	S	0	0	0
			3461	2169	582	700	10			

- Molecule 2 is (2R)-2-AMINO-7-{[(1R)-1-CARBOXYETHYL]AMINO}-7-OXOHEPTANOIC ACID (three-letter code: REZ) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	10	2	4		
2	B	1	Total	C	N	O	0	0
			16	10	2	4		

- Molecule 3 is D-ALANINE (three-letter code: DAL) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	3	1	2		
3	B	1	Total	C	N	O	0	0
			6	3	1	2		



Q454	Q455	A456	Y457	L458	L459	A460	N461	Q462	W373	F374	Y377	L378	N379	S380	L381	P382	N386	P387	D388	R389	R396	M399	K400	G401	T402	P403	A404	Q405	G406	K407	V408	R409	A410	K411	T412	G413	S414	L415	T417	V418	S422	G423	T427	K428	S429	V434	F435	S436	N440	G441	L442	I443	D444	E445	D450	I451	E452	D453	P294	F295	W296	K297	N301	G302	H303	A304	E305	V306	L307	V308	K309	E310	M311	K315	E318	G319	S320	W321	E322	K323	E326	V327	L328	N329	S330	T331	L332	P333	E334	V337	L342	V343	L344	R345	G349	H352	I353	D354	A355	S358	S362	Q363	L364	L365	T368	Q369	E226	G227	S228	V229	P230	V231	D232	A233	N234	K235	T236	K237	E238	W239	I240	S241	V242	W243	E244	P245	Y248	A249	L250	D251	L252	F253	K254	Q255	S256	L257	K258	K259	Q260	G261	I262	T263	W264	K265	I268	A273	P274	S275	S276	V279	L280	L281	R284	S285	M286	P287	L288	L291	F292	V293
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.86Å 77.59Å 164.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.80 24.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.7 (19.90-2.80) 89.8 (24.59-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.208 , 0.290 0.208 , 0.284	Depositor DCC
$R_{free}$ test set	1049 reflections (4.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: REZ, DAL

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	0.41	0/3520	0.69	0/4765
1	B	0.34	0/3520	0.61	0/4765
All	All	0.38	0/7040	0.65	0/9530

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	3461	0	3463	199	1
1	B	3461	0	3463	234	1
2	A	16	0	16	5	0
2	B	16	0	16	2	0
3	A	6	0	6	2	0
3	B	6	0	6	0	0
All	All	6966	0	6970	435	1

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 31.

The worst 5 of 435 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:B:111:GLU:HA	1:B:260:GLN:HE21	1.03	1.05
1:B:57:LEU:HD23	1:B:364:LEU:HD22	1.39	1.00
1:B:407:LYS:HZ3	1:B:428:LYS:HD3	1.26	0.99
1:A:415:LEU:O	1:A:445:GLU:HG2	1.66	0.96
1:A:86:LYS:HB3	1:A:120:VAL:HG13	1.47	0.94

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:OE1	1:B:146:GLU:OE1[4_555]	2.05	0.15

## 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	456/462 (99%)	413 (91%)	37 (8%)	6 (1%)	14	41
1	B	456/462 (99%)	397 (87%)	52 (11%)	7 (2%)	12	37
All	All	912/924 (99%)	810 (89%)	89 (10%)	13 (1%)	13	39

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	429	SER
1	A	80	GLY
1	A	118	VAL
1	B	16	ALA
1	B	133	ASP

### 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	382/385 (99%)	352 (92%)	30 (8%)	14	38
1	B	382/385 (99%)	363 (95%)	19 (5%)	28	62
All	All	764/770 (99%)	715 (94%)	49 (6%)	20	50

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	PHE
1	A	371	GLN
1	B	379	ASN
1	A	321	TRP
1	A	386	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	90	ASN
1	B	178	GLN
1	B	386	ASN
1	A	405	GLN
1	B	18	HIS

### 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

4 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	REZ	A	500	1	10,15,16	0.82	0	9,18,20	1.00	1 (11%)
3	DAL	A	501	-	2,5,5	0.60	0	2,6,6	0.32	0
2	REZ	B	500	1	10,15,16	0.71	0	9,18,20	0.69	0
3	DAL	B	501	-	2,5,5	0.34	0	2,6,6	0.52	0

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	REZ	A	500	1	-	0/11/17/19	0/0/0/0
3	DAL	A	501	-	-	0/0/4/4	0/0/0/0
2	REZ	B	500	1	-	0/11/17/19	0/0/0/0
3	DAL	B	501	-	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	REZ	CA-N-C1	-2.04	119.95	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	REZ	5	0
3	A	501	DAL	2	0
2	B	500	REZ	2	0

## 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	458/462 (99%)	-0.26	10 (2%) 62 52	14, 29, 57, 71	0
1	B	458/462 (99%)	0.19	25 (5%) 26 17	22, 52, 82, 102	0
All	All	916/924 (99%)	-0.03	35 (3%) 41 30	14, 42, 76, 102	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	GLY	7.9
1	B	83	LYS	4.7
1	B	180	GLU	3.8
1	B	263	THR	3.7
1	B	436	SER	3.6

### 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	REZ	A	500	16/17	0.93	0.21	1.66	41,49,54,54	0
2	REZ	B	500	16/17	0.95	0.20	1.16	47,51,55,56	0
3	DAL	B	501	6/6	0.96	0.25	0.94	46,46,46,47	0
3	DAL	A	501	6/6	0.91	0.21	0.91	37,39,39,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.