



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:31 AM UTC

PDB ID : 3BF0 / pdb\_00003bf0  
Title : Crystal structure of Escherichia coli Signal peptide peptidase (SppA), Native crystals  
Authors : Paetzel, M.  
Deposited on : 2007-11-20  
Resolution : 2.55 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 : 4-5-2 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

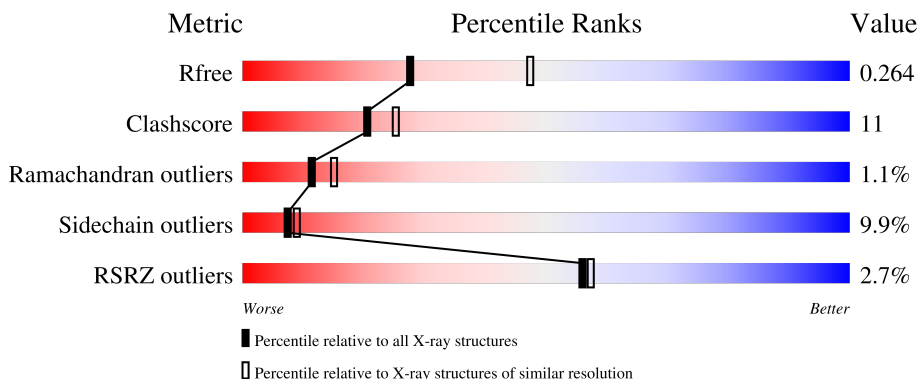
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	593	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 20%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      59%      17%      •      20%</p>
1	B	593	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 20%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      60%      16%      • •      20%</p>
1	C	593	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 19%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">3%      60%      17%      •      19%</p>
1	D	593	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 20%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      59%      18%      • •      20%</p>

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 14865 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 Protease 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	474	3587	2263	614	702	8	0	0	0
1	B	474	3583	2260	613	702	8	0	0	0
1	C	478	3606	2273	617	708	8	0	0	0
1	D	476	3601	2270	616	707	8	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	expression tag	UNP P08395
A	27	GLY	-	expression tag	UNP P08395
A	28	SER	-	expression tag	UNP P08395
A	29	SER	-	expression tag	UNP P08395
A	30	HIS	-	expression tag	UNP P08395
A	31	HIS	-	expression tag	UNP P08395
A	32	HIS	-	expression tag	UNP P08395
A	33	HIS	-	expression tag	UNP P08395
A	34	HIS	-	expression tag	UNP P08395
A	35	HIS	-	expression tag	UNP P08395
A	36	SER	-	expression tag	UNP P08395
A	37	SER	-	expression tag	UNP P08395
A	38	GLY	-	expression tag	UNP P08395
A	39	LEU	-	expression tag	UNP P08395
A	40	VAL	-	expression tag	UNP P08395
A	41	PRO	-	expression tag	UNP P08395
A	42	ARG	-	expression tag	UNP P08395
A	43	GLY	-	expression tag	UNP P08395
A	44	SER	-	expression tag	UNP P08395
A	45	HIS	-	expression tag	UNP P08395
A	46	MET	-	expression tag	UNP P08395

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	MET	-	expression tag	UNP P08395
B	27	GLY	-	expression tag	UNP P08395
B	28	SER	-	expression tag	UNP P08395
B	29	SER	-	expression tag	UNP P08395
B	30	HIS	-	expression tag	UNP P08395
B	31	HIS	-	expression tag	UNP P08395
B	32	HIS	-	expression tag	UNP P08395
B	33	HIS	-	expression tag	UNP P08395
B	34	HIS	-	expression tag	UNP P08395
B	35	HIS	-	expression tag	UNP P08395
B	36	SER	-	expression tag	UNP P08395
B	37	SER	-	expression tag	UNP P08395
B	38	GLY	-	expression tag	UNP P08395
B	39	LEU	-	expression tag	UNP P08395
B	40	VAL	-	expression tag	UNP P08395
B	41	PRO	-	expression tag	UNP P08395
B	42	ARG	-	expression tag	UNP P08395
B	43	GLY	-	expression tag	UNP P08395
B	44	SER	-	expression tag	UNP P08395
B	45	HIS	-	expression tag	UNP P08395
B	46	MET	-	expression tag	UNP P08395
C	26	MET	-	expression tag	UNP P08395
C	27	GLY	-	expression tag	UNP P08395
C	28	SER	-	expression tag	UNP P08395
C	29	SER	-	expression tag	UNP P08395
C	30	HIS	-	expression tag	UNP P08395
C	31	HIS	-	expression tag	UNP P08395
C	32	HIS	-	expression tag	UNP P08395
C	33	HIS	-	expression tag	UNP P08395
C	34	HIS	-	expression tag	UNP P08395
C	35	HIS	-	expression tag	UNP P08395
C	36	SER	-	expression tag	UNP P08395
C	37	SER	-	expression tag	UNP P08395
C	38	GLY	-	expression tag	UNP P08395
C	39	LEU	-	expression tag	UNP P08395
C	40	VAL	-	expression tag	UNP P08395
C	41	PRO	-	expression tag	UNP P08395
C	42	ARG	-	expression tag	UNP P08395
C	43	GLY	-	expression tag	UNP P08395
C	44	SER	-	expression tag	UNP P08395
C	45	HIS	-	expression tag	UNP P08395
C	46	MET	-	expression tag	UNP P08395

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Chain	Residue	Modelled	Actual	Comment	Reference
D	26	MET	-	expression tag	UNP P08395
D	27	GLY	-	expression tag	UNP P08395
D	28	SER	-	expression tag	UNP P08395
D	29	SER	-	expression tag	UNP P08395
D	30	HIS	-	expression tag	UNP P08395
D	31	HIS	-	expression tag	UNP P08395
D	32	HIS	-	expression tag	UNP P08395
D	33	HIS	-	expression tag	UNP P08395
D	34	HIS	-	expression tag	UNP P08395
D	35	HIS	-	expression tag	UNP P08395
D	36	SER	-	expression tag	UNP P08395
D	37	SER	-	expression tag	UNP P08395
D	38	GLY	-	expression tag	UNP P08395
D	39	LEU	-	expression tag	UNP P08395
D	40	VAL	-	expression tag	UNP P08395
D	41	PRO	-	expression tag	UNP P08395
D	42	ARG	-	expression tag	UNP P08395
D	43	GLY	-	expression tag	UNP P08395
D	44	SER	-	expression tag	UNP P08395
D	45	HIS	-	expression tag	UNP P08395
D	46	MET	-	expression tag	UNP P08395

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	116	Total O 116 116	0	0
2	B	127	Total O 127 127	0	0
2	C	144	Total O 144 144	0	0
2	D	101	Total O 101 101	0	0





R496	R540	R541	R542	Q544	W545	H546	L547	E548	Y549	TYR	VAL	ASP	GLU	PRO	THR	PHE	PHE	ASP	LYS	VAL	MET	ASP	ASN	ASN	MET	SER	GLY	SER	VAL	ARG	ALA	MET	LEU	PRO	ASP	ALA	ALA	PHE	GLN	ALA	MET	LEU	PRO	ALA	PRO	LEU	ALA	SER
VAL	ALA	SER	THR	VAL	LYS	SER	GLU	SER	ASP	LYS	LEU	ALA	ALA	PHE	ASN	ASP	PRO	GLN	ASN	ARG	TYR	ALA	PHE	CYS	LEU	THR	CYS	ALA	ASN	MET	ARG																	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.17Å 153.49Å 100.66Å 90.00° 104.25° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 50.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.55) 96.1 (50.00-2.55)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.07 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.214 , 0.252 0.208 , 0.264	Depositor DCC
$R_{free}$ test set	4338 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtrriage
Anisotropy	0.551	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 31.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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	0.93	1/3654 (0.0%)	1.04	8/4960 (0.2%)
1	B	0.93	1/3650 (0.0%)	1.10	11/4956 (0.2%)
1	C	0.96	5/3673 (0.1%)	1.09	10/4988 (0.2%)
1	D	0.90	1/3668 (0.0%)	1.05	7/4979 (0.1%)
All	All	0.93	8/14645 (0.1%)	1.07	36/19883 (0.2%)

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	1
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	540	ALA	CA-C	10.19	1.57	1.52
1	D	542	VAL	CA-CB	6.82	1.63	1.54
1	C	411	GLY	C-O	-6.08	1.17	1.24
1	C	410	GLY	C-O	-5.79	1.16	1.23
1	C	438	ILE	CA-CB	5.35	1.60	1.54

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	VAL	N-CA-C	9.47	124.87	113.22
1	C	541	LYS	N-CA-C	7.94	118.74	108.34
1	D	541	LYS	N-CA-C	7.69	119.83	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	GLY	N-CA-C	6.97	119.15	112.04
1	A	57	GLY	N-CA-C	6.81	118.42	111.95

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	541	LYS	Peptide
1	B	541	LYS	Peptide
1	C	541	LYS	Peptide
1	D	340	GLY	Peptide
1	D	541	LYS	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	3587	0	3550	82	0
1	B	3583	0	3539	92	0
1	C	3606	0	3549	72	0
1	D	3601	0	3559	94	0
2	A	116	0	0	4	0
2	B	127	0	0	3	0
2	C	144	0	0	6	0
2	D	101	0	0	4	0
All	All	14865	0	14197	320	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 11.

The worst 5 of 320 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:542:VAL:HG12	1:B:543:LYS:N	1.40	1.18
1:D:403:MET:CE	1:D:423:ALA:HB2	1.72	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:VAL:CG1	1:B:543:LYS:N	2.08	1.12
1:B:542:VAL:CG1	1:B:543:LYS:H	1.54	1.10
1:D:403:MET:HE2	1:D:423:ALA:HB2	1.07	1.07

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	470/593 (79%)	440 (94%)	28 (6%)	2 (0%)	30 39
1	B	470/593 (79%)	442 (94%)	22 (5%)	6 (1%)	9 12
1	C	474/593 (80%)	447 (94%)	22 (5%)	5 (1%)	11 15
1	D	472/593 (80%)	442 (94%)	22 (5%)	8 (2%)	7 8
All	All	1886/2372 (80%)	1771 (94%)	94 (5%)	21 (1%)	11 15

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	GLN
1	B	541	LYS
1	B	542	VAL
1	C	324	THR
1	C	540	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	374/475 (79%)	335 (90%)	39 (10%)	7	8
1	B	373/475 (78%)	335 (90%)	38 (10%)	7	8
1	C	374/475 (79%)	338 (90%)	36 (10%)	8	9
1	D	376/475 (79%)	341 (91%)	35 (9%)	8	10
All	All	1497/1900 (79%)	1349 (90%)	148 (10%)	7	9

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	114	THR
1	D	520	ASN
1	D	179	LEU
1	D	282	VAL
1	B	197	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	508	GLN
1	D	419	ASN
1	C	185	ASN
1	D	346	ASN
1	D	520	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](#)

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	474/593 (79%)	0.08	14 (2%) 52 54	14, 28, 51, 65	0
1	B	474/593 (79%)	-0.01	12 (2%) 58 59	14, 25, 48, 59	0
1	C	478/593 (80%)	-0.05	16 (3%) 49 50	14, 25, 49, 62	0
1	D	476/593 (80%)	-0.01	9 (1%) 66 66	14, 27, 49, 60	0
All	All	1902/2372 (80%)	0.00	51 (2%) 56 57	14, 26, 49, 65	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	TRP	5.6
1	A	324	THR	5.5
1	D	343	THR	5.4
1	D	545	TRP	5.2
1	B	545	TRP	4.8

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.