



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 06:18 pm BST

PDB ID : 5NNV  
Title : Structure of a Bacillus subtilis Smc coiled coil middle fragment  
Authors : Diebold-Durand, M.-L.; Basquin, J.; Gruber, S.  
Deposited on : 2017-04-10  
Resolution : 3.29 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

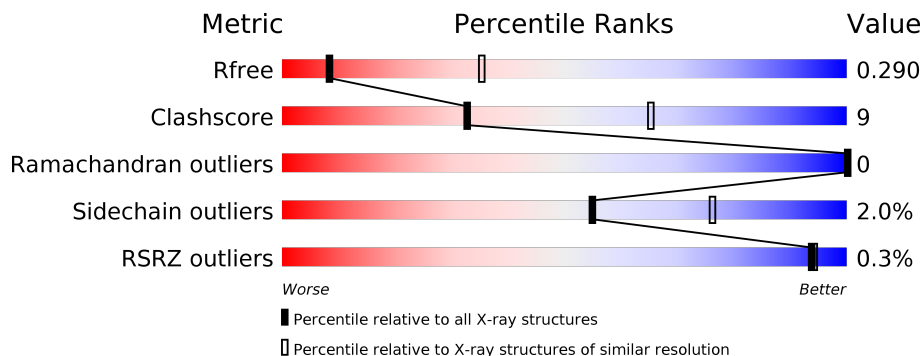
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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	282	
1	B	282	
1	C	282	
1	D	282	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6042 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 Chromosome partition protein Smc,Chromosome partition protein Smc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	233	Total	C	N	O	S	Se	0	0	0
			1493	907	274	309	1	2			
1	B	231	Total	C	N	O	S	Se	0	0	0
			1490	903	275	309	1	2			
1	C	237	Total	C	N	O	S	Se	0	0	0
			1470	886	264	316	1	3			
1	D	252	Total	C	N	O	Se		0	0	0
			1589	956	287	343	3				

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLY	-	expression tag	UNP P51834
A	243	SER	-	expression tag	UNP P51834
A	244	GLY	-	expression tag	UNP P51834
A	245	MSE	-	expression tag	UNP P51834
A	786	SER	-	linker	UNP P51834
A	787	GLY	-	linker	UNP P51834
A	788	GLY	-	linker	UNP P51834
A	789	SER	-	linker	UNP P51834
A	790	GLY	-	linker	UNP P51834
A	791	GLY	-	linker	UNP P51834
A	792	SER	-	linker	UNP P51834
B	242	GLY	-	expression tag	UNP P51834
B	243	SER	-	expression tag	UNP P51834
B	244	GLY	-	expression tag	UNP P51834
B	245	MSE	-	expression tag	UNP P51834
B	786	SER	-	linker	UNP P51834
B	787	GLY	-	linker	UNP P51834
B	788	GLY	-	linker	UNP P51834
B	789	SER	-	linker	UNP P51834
B	790	GLY	-	linker	UNP P51834

*Continued on next page...*

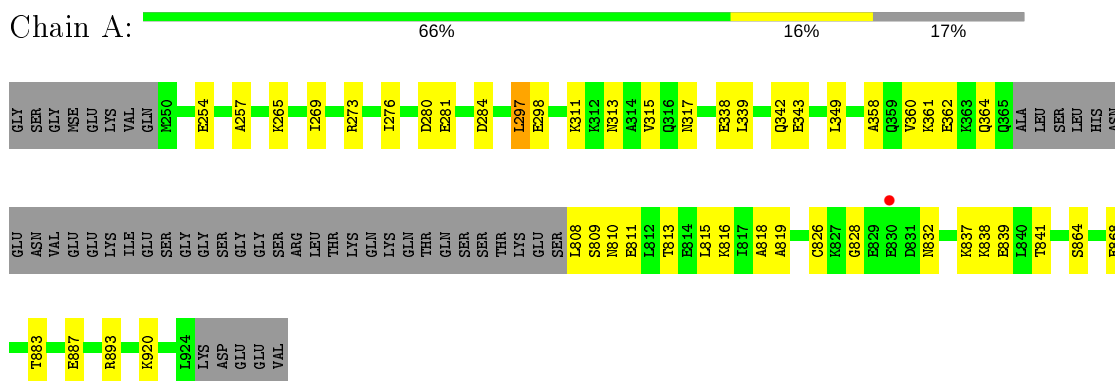
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	791	GLY	-	linker	UNP P51834
B	792	SER	-	linker	UNP P51834
C	242	GLY	-	expression tag	UNP P51834
C	243	SER	-	expression tag	UNP P51834
C	244	GLY	-	expression tag	UNP P51834
C	245	MSE	-	expression tag	UNP P51834
C	786	SER	-	linker	UNP P51834
C	787	GLY	-	linker	UNP P51834
C	788	GLY	-	linker	UNP P51834
C	789	SER	-	linker	UNP P51834
C	790	GLY	-	linker	UNP P51834
C	791	GLY	-	linker	UNP P51834
C	792	SER	-	linker	UNP P51834
D	242	GLY	-	expression tag	UNP P51834
D	243	SER	-	expression tag	UNP P51834
D	244	GLY	-	expression tag	UNP P51834
D	245	MSE	-	expression tag	UNP P51834
D	786	SER	-	linker	UNP P51834
D	787	GLY	-	linker	UNP P51834
D	788	GLY	-	linker	UNP P51834
D	789	SER	-	linker	UNP P51834
D	790	GLY	-	linker	UNP P51834
D	791	GLY	-	linker	UNP P51834
D	792	SER	-	linker	UNP P51834

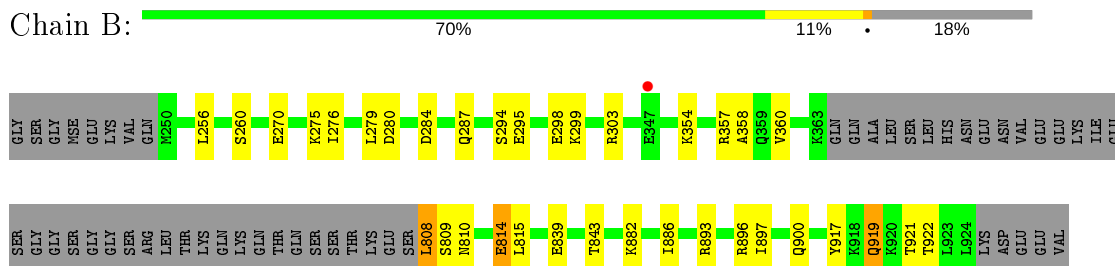
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

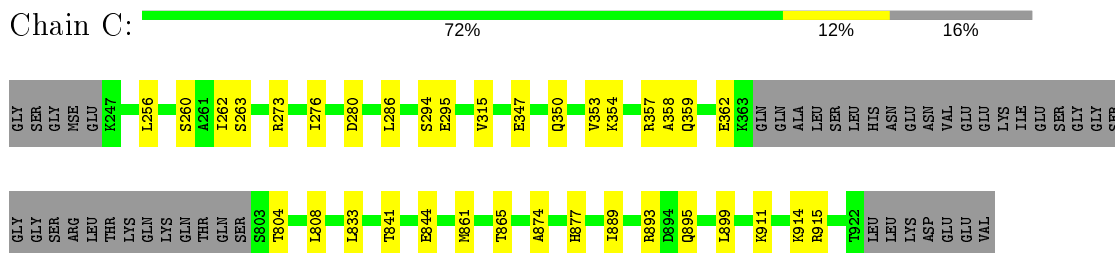
- Molecule 1: Chromosome partition protein Smc,Chromosome partition protein Smc



- Molecule 1: Chromosome partition protein Smc,Chromosome partition protein Smc



- Molecule 1: Chromosome partition protein Smc,Chromosome partition protein Smc



- Molecule 1: Chromosome partition protein Smc,Chromosome partition protein Smc



GLY	GLY	GLY	GLY	K247	Y248	Q249	E253	E254	E255	L256	A257	S260	S263	R273	V283	D284	E285	L286	Q287	Q288	V289	S294	E295	L300	K304	A314	V315	Q316	A366	H370	H371	E372	ASN	VAL	GLU	GLU	GLY	LYS	ILE	GLU	SER	GLY	GLY	SER	GLY	GLY	SER	GLY	SER	ARG
-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LEU	THR	LYS	GLN	LYS	GLN	THR	GLN	S802	S803	T804	S807	L808	S809	L812	T813	G828	M832	F856	L857	E860	M861	N880	D881	K882	F883	K884	T885	I886	D894	K898	F915	L916	Y917	T921	T922	L923	D926	E927	VAL
-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.31Å 42.74Å 174.60Å 89.97° 93.64° 89.97°	Depositor
Resolution (Å)	50.00 – 3.29 87.12 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-3.29) 96.7 (87.12-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.262 , 0.298 0.258 , 0.290	Depositor DCC
$R_{free}$ test set	863 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.8	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 88.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.397 for -h,k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.02% 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	0.22	0/1492	0.47	0/2032
1	B	0.23	0/1491	0.49	1/2031 (0.0%)
1	C	0.23	0/1469	0.44	0/2006
1	D	0.22	0/1588	0.45	0/2168
All	All	0.23	0/6040	0.46	1/8237 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	808	LEU	CA-CB-CG	5.86	128.77	115.30

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	1493	0	1191	29	0
1	B	1490	0	1171	24	0
1	C	1470	0	1078	22	0
1	D	1589	0	1199	28	0
All	All	6042	0	4639	93	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 9.



The worst 5 of 93 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:D:294:SER:OG	1:D:882:LYS:NZ	2.09	0.85
1:C:295:GLU:OE2	1:D:294:SER:OG	1.94	0.85
1:A:361:LYS:NZ	1:A:364:GLN:OE1	2.12	0.83
1:A:313:ASN:O	1:A:317:ASN:ND2	2.14	0.79
1:B:294:SER:OG	1:B:882:LYS:NZ	2.19	0.73

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	229/282 (81%)	226 (99%)	3 (1%)	0	100	100
1	B	227/282 (80%)	225 (99%)	2 (1%)	0	100	100
1	C	233/282 (83%)	232 (100%)	1 (0%)	0	100	100
1	D	248/282 (88%)	244 (98%)	4 (2%)	0	100	100
All	All	937/1128 (83%)	927 (99%)	10 (1%)	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	101/246 (41%)	99 (98%)	2 (2%)	55	76
1	B	101/246 (41%)	98 (97%)	3 (3%)	41	68
1	C	91/246 (37%)	90 (99%)	1 (1%)	73	85
1	D	106/246 (43%)	104 (98%)	2 (2%)	57	77
All	All	399/984 (40%)	391 (98%)	8 (2%)	55	76

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	814	GLU
1	D	316	GLN
1	C	833	LEU
1	B	270	GLU
1	B	919	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	230/282 (81%)	-0.54	1 (0%) 92   93	67, 104, 227, 273	0
1	B	228/282 (80%)	-0.72	1 (0%) 92   93	46, 104, 190, 210	0
1	C	234/282 (82%)	-0.73	0 100   100	48, 96, 171, 190	0
1	D	249/282 (88%)	-0.75	1 (0%) 92   93	41, 93, 166, 178	0
All	All	941/1128 (83%)	-0.68	3 (0%) 94   94	41, 99, 184, 273	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	802	SER	3.0
1	A	830	GLU	2.9
1	B	347	GLU	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 carbohydrates 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.