



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2017 – 08:30 AM EDT

PDB ID : 2H27  
Title : Crystal Structure of Escherichia coli SigmaE Region 4 Bound to its-35 Element DNA  
Authors : Lane, W.J.; Darst, S.A.  
Deposited on : unknown  
Resolution : 2.30 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 : rb-20030345  
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) : rb-20030345

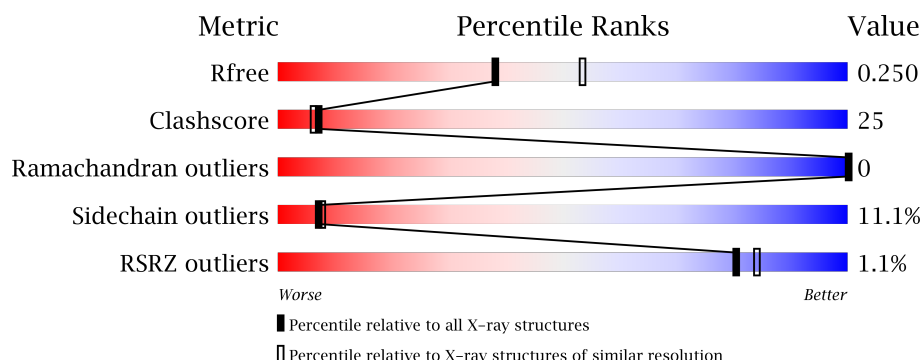
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	B	12	
1	E	12	
2	C	12	
2	F	12	
3	A	73	

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Mol	Chain	Length	Quality of chain
3	D	73	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	D	1	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2202 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 DNA chain called 5'-D(\*CP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			240	115	44	70	11			
1	E	12	Total	C	N	O	P	0	0	0
			240	115	44	70	11			

- Molecule 2 is a DNA chain called 5'-D(\*C\*CP\*GP\*AP\*AP\*GP\*TP\*TP\*CP\*CP\*GP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			224	107	43	64	10			
2	F	11	Total	C	N	O	P	0	0	0
			224	107	43	64	10			

- Molecule 3 is a protein called RNA polymerase Sigma E factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	71	Total	C	N	O	S	0	0	0
			573	358	104	107	4			
3	D	69	Total	C	N	O	S	0	0	0
			557	349	100	104	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	CLONING ARTIFACT	UNP P0AGB6
A	9	SER	-	CLONING ARTIFACT	UNP P0AGB6
A	10	HIS	-	CLONING ARTIFACT	UNP P0AGB6
D	8	GLY	-	CLONING ARTIFACT	UNP P0AGB6
D	9	SER	-	CLONING ARTIFACT	UNP P0AGB6
D	10	HIS	-	CLONING ARTIFACT	UNP P0AGB6

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

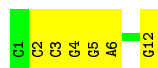
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	13	Total	O	0	0
			13	13		
5	C	10	Total	O	0	0
			10	10		
5	E	15	Total	O	0	0
			15	15		
5	F	10	Total	O	0	0
			10	10		
5	A	52	Total	O	0	0
			52	52		
5	D	36	Total	O	0	0
			36	36		

### 3 Residue-property plots

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.

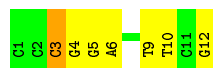
- Molecule 1: 5'-D(\*CP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*CP\*G)-3'

Chain B: 




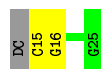
- Molecule 1: 5'-D(\*CP\*CP\*CP\*GP\*GP\*AP\*AP\*CP\*TP\*TP\*CP\*G)-3'

Chain E: 



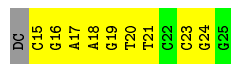
- Molecule 2: 5'-D(\*C\*CP\*GP\*AP\*AP\*GP\*TP\*TP\*CP\*CP\*GP\*G)-3'

Chain C: 



- Molecule 2: 5'-D(\*C\*CP\*GP\*AP\*AP\*GP\*TP\*TP\*CP\*CP\*GP\*G)-3'

Chain F: 



- Molecule 3: RNA polymerase Sigma E factor

Chain A: 



- Molecule 3: RNA polymerase Sigma E factor

Chain D: 

GLY	SER	HIS	M122	L123	E126	L127	R128	Q129	I130	V131	F132	R133	S137	E140	D141	L142	R143	M144	L148	R149	E150	L151	D152	G153	L154	S155	V156	E157	E158	R176	V185	Q186	P187	L188	I189	R190	ARG
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.01Å 68.71Å 61.13Å 90.00° 101.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.8 (20.00-2.30) 91.6 (19.99-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.253 0.237 , 0.250	Depositor DCC
$R_{free}$ test set	1801 reflections (9.84%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.81 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2531e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD

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	B	0.70	0/268	0.97	0/411
1	E	0.60	0/268	1.02	1/411 (0.2%)
2	C	0.37	0/251	0.69	0/386
2	F	0.86	1/251 (0.4%)	1.24	2/386 (0.5%)
3	A	0.47	0/579	0.79	1/779 (0.1%)
3	D	0.39	0/562	0.69	0/756
All	All	0.55	1/2179 (0.0%)	0.88	4/3129 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	23	DC	O3'-P	-5.61	1.54	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	133	ARG	NE-CZ-NH1	7.33	123.96	120.30
2	F	24	DG	O4'-C1'-N9	7.24	113.07	108.00
2	F	24	DG	C5'-C4'-C3'	-6.91	101.66	114.10
1	E	3	DC	OP1-P-OP2	-5.94	110.69	119.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts ⓘ

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	B	240	0	136	6	0
1	E	240	0	136	17	0
2	C	224	0	125	1	0
2	F	224	0	125	10	0
3	A	573	0	591	27	0
3	D	557	0	579	38	0
4	D	8	0	14	16	0
5	A	52	0	0	6	0
5	B	13	0	0	1	0
5	C	10	0	0	1	0
5	D	36	0	0	8	0
5	E	15	0	0	2	0
5	F	10	0	0	1	0
All	All	2202	0	1706	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 25.

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)
3:D:141:ASP:HB2	4:D:1:MPD:C1	1.69	1.21
3:A:157:GLU:OE2	5:A:232:HOH:O	1.61	1.17
3:A:150:GLU:OE2	5:A:227:HOH:O	1.63	1.16
3:D:141:ASP:HB2	4:D:1:MPD:H11	1.23	1.13
1:E:4:DG:P	4:D:1:MPD:CM	2.36	1.12

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	
3	A	69/73 (94%)	67 (97%)	2 (3%)	0	100	100
3	D	67/73 (92%)	67 (100%)	0	0	100	100
All	All	136/146 (93%)	134 (98%)	2 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
3	A	64/65 (98%)	56 (88%)	8 (12%)	5	5
3	D	62/65 (95%)	56 (90%)	6 (10%)	9	11
All	All	126/130 (97%)	112 (89%)	14 (11%)	7	8

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	189	ILE
3	A	190	ARG
3	D	133	ARG
3	A	188	LEU
3	D	130	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

1 ligand is 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	$\# Z  > 2$
4	MPD	D	1	1	7,7,7	0.42	0	9,10,10	0.56	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
4	MPD	D	1	1	-	0/5/5/5	0/0/0/0

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.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	MPD	16	0

## 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(Å²)	Q<0.9
1	B	12/12 (100%)	0.01	0	100100	33, 42, 54, 58	0
1	E	12/12 (100%)	-0.05	0	100100	33, 41, 52, 54	0
2	C	11/12 (91%)	0.06	0	100100	29, 38, 54, 63	0
2	F	11/12 (91%)	0.18	0	100100	29, 37, 53, 65	0
3	A	71/73 (97%)	0.18	2 (2%)	5361	22, 30, 58, 72	0
3	D	69/73 (94%)	0.13	0	100100	21, 32, 47, 54	0
All	All	186/194 (95%)	0.13	2 (1%)	8084	21, 34, 54, 72	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	9	SER	3.8
3	A	10	HIS	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 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
4	MPD	D	1	8/8	0.72	0.32	3.84	82,83,84,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.