



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:30 PM GMT

PDB ID : 1B44  
Title : CRYSTAL STRUCTURE OF THE B SUBUNIT OF HEAT-LABILE ENTEROTOXIN FROM E. COLI CARRYING A PEPTIDE WITH ANTI-HSV ACTIVITY  
Authors : Matkovic-Calogovic, D.; Loregian, A.; D'Acunto, M.R.; Battistutta, R.; Tossi, A.; Palu, G.; Zanotti, G.  
Deposited on : 1999-01-04  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

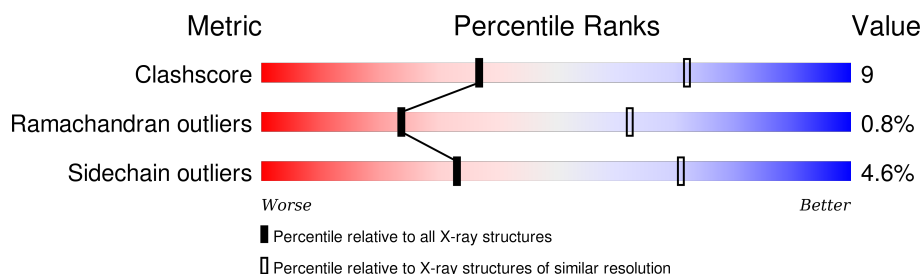
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	129	
1	E	129	
1	F	129	
1	G	129	
1	H	129	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4186 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 PROTEIN (B-POL SUBUNIT OF HEAT-LABILE ENTEROTOXIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	106	Total	C	N	O	S	0	0	0
			835	525	140	164	6			
1	E	107	Total	C	N	O	S	0	0	0
			846	534	141	165	6			
1	F	106	Total	C	N	O	S	0	0	0
			835	525	140	164	6			
1	G	106	Total	C	N	O	S	0	0	0
			835	525	140	164	6			
1	H	106	Total	C	N	O	S	0	0	0
			835	525	140	164	6			

There are 5 discrepancies between the modelled and reference sequences:

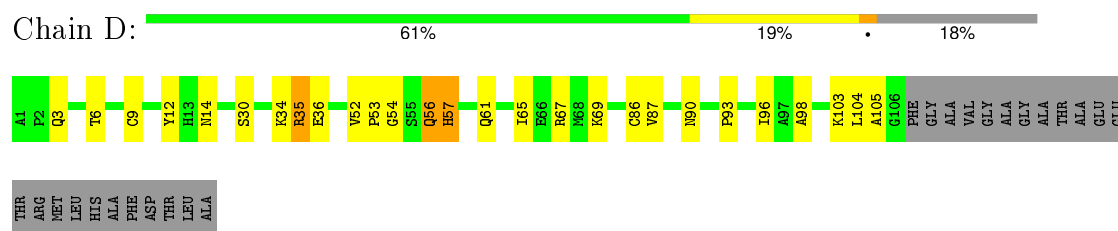
Chain	Residue	Modelled	Actual	Comment	Reference
D	103	LYS	ASN	CONFLICT	UNP P13811
E	103	LYS	ASN	CONFLICT	UNP P13811
F	103	LYS	ASN	CONFLICT	UNP P13811
G	103	LYS	ASN	CONFLICT	UNP P13811
H	103	LYS	ASN	CONFLICT	UNP P13811

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

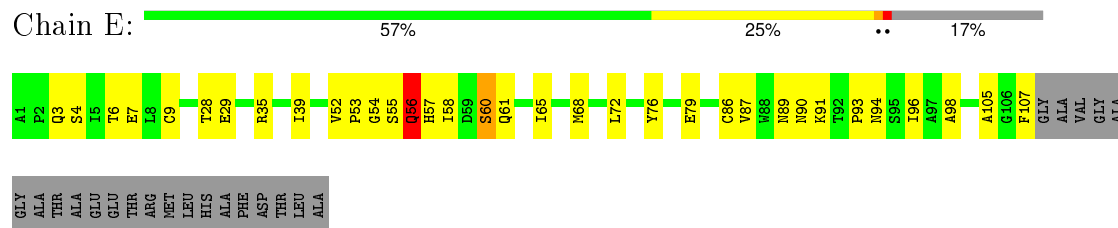
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

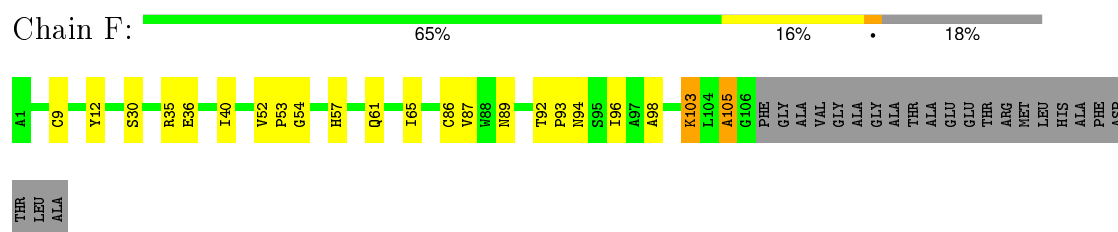
- Molecule 1: PROTEIN (B-POL SUBUNIT OF HEAT-LABILE ENTEROTOXIN)



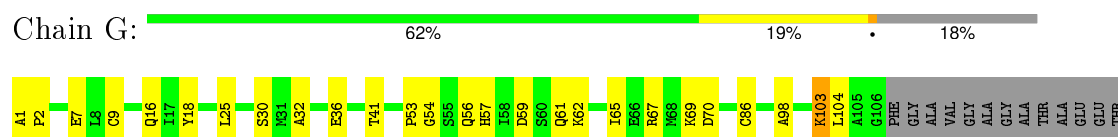
- Molecule 1: PROTEIN (B-POL SUBUNIT OF HEAT-LABILE ENTEROTOXIN)



- Molecule 1: PROTEIN (B-POL SUBUNIT OF HEAT-LABILE ENTEROTOXIN)



- Molecule 1: PROTEIN (B-POL SUBUNIT OF HEAT-LABILE ENTEROTOXIN)



ARG
MET
LEU
HIS
ALA
PHE
ASP
THR
LEU
ALA

- Molecule 1: PROTEIN (B-POL SUBUNIT OF HEAT-LABILE ENTEROTOXIN)

Chain H: 

67%

15%

•

18%

A1	P2	Q3	T6	C9	S10	E11	T28	K34	R35	I39	Q56	H57	Y76	L77	C86	V87	T92	P93	I96	A97	A98	E102	G106	PHE	GLY	ALA	VAL	GLY	ALA	GLY	ALA	THR	ALA	GLU	GLU	THR	ARG	MET	LEU	HIS	ALA	PHE	ASP	THR	LEU	ALA
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.10Å 127.10Å 176.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	65.0 (10.00-3.30)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
Refinement program	X-PLOR 3.84	Depositor
R, $R_{free}$	0.212 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

## 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	D	0.41	0/847	0.65	0/1142
1	E	0.46	0/859	0.67	1/1158 (0.1%)
1	F	0.40	0/847	0.66	0/1142
1	G	0.41	0/847	0.63	0/1142
1	H	0.41	0/847	0.61	0/1142
All	All	0.42	0/4247	0.65	1/5726 (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	E	56	GLN	N-CA-C	5.40	125.58	111.00

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	D	835	0	851	27	0
1	E	846	0	860	23	0
1	F	835	0	851	13	0
1	G	835	0	851	20	0
1	H	835	0	851	19	0
All	All	4186	0	4264	79	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.

All (79) 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:E:53:PRO:HA	1:E:57:HIS:HD2	1.42	0.84
1:F:54:GLY:H	1:F:57:HIS:HD2	1.38	0.71
1:D:103:LYS:NZ	1:E:79:GLU:HG2	2.06	0.70
1:D:30:SER:O	1:D:36:GLU:HA	1.92	0.69
1:D:103:LYS:HZ2	1:E:79:GLU:HG2	1.57	0.68
1:G:53:PRO:HA	1:G:57:HIS:CD2	2.33	0.64
1:F:89:ASN:HA	1:F:94:ASN:ND2	2.14	0.62
1:D:54:GLY:H	1:D:57:HIS:CD2	2.18	0.62
1:G:54:GLY:H	1:G:57:HIS:HD2	1.46	0.61
1:D:35:ARG:HH12	1:H:2:PRO:HD3	1.65	0.61
1:H:86:CYS:HB3	1:H:98:ALA:HB3	1.83	0.60
1:F:86:CYS:HB3	1:F:98:ALA:HB3	1.84	0.59
1:G:2:PRO:HD3	1:H:35:ARG:HH11	1.68	0.59
1:D:61:GLN:O	1:D:65:ILE:HG13	2.02	0.59
1:D:35:ARG:HH22	1:H:2:PRO:HD3	1.69	0.58
1:D:86:CYS:HB3	1:D:98:ALA:HB3	1.86	0.57
1:D:35:ARG:NH1	1:H:2:PRO:HD3	2.20	0.57
1:E:53:PRO:HA	1:E:57:HIS:CD2	2.31	0.56
1:G:2:PRO:HD3	1:H:35:ARG:NH1	2.21	0.55
1:D:65:ILE:HG22	1:D:69:LYS:HE2	1.88	0.55
1:D:3:GLN:HG2	1:E:93:PRO:HD3	1.89	0.55
1:D:35:ARG:NH2	1:H:2:PRO:HD3	2.23	0.54
1:G:86:CYS:HB3	1:G:98:ALA:HB3	1.90	0.54
1:G:54:GLY:H	1:G:57:HIS:CD2	2.26	0.54
1:D:93:PRO:HD3	1:H:3:GLN:HG2	1.90	0.53
1:E:86:CYS:HB3	1:E:98:ALA:HB3	1.90	0.53
1:D:14:ASN:ND2	1:D:90:ASN:ND2	2.57	0.53
1:H:87:VAL:HG12	1:H:96:ILE:HA	1.90	0.53
1:H:56:GLN:HG2	1:H:57:HIS:CD2	2.44	0.52
1:G:103:LYS:NZ	1:H:77:LEU:HA	2.24	0.52
1:F:53:PRO:HA	1:F:57:HIS:CD2	2.45	0.52
1:G:2:PRO:CD	1:H:35:ARG:HH11	2.22	0.52
1:D:87:VAL:HG12	1:D:96:ILE:HA	1.92	0.51
1:D:103:LYS:HG2	1:E:76:TYR:OH	2.12	0.50
1:G:16:GLN:NE2	1:G:18:TYR:CE1	2.79	0.50
1:E:4:SER:HB3	1:E:7:GLU:HB2	1.94	0.50
1:G:65:ILE:HG22	1:G:69:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:PRO:HA	1:G:57:HIS:HD2	1.77	0.49
1:E:87:VAL:HG12	1:E:96:ILE:HA	1.94	0.49
1:D:35:ARG:HA	1:D:52:VAL:HG21	1.95	0.49
1:D:34:LYS:O	1:D:35:ARG:HG3	2.13	0.48
1:D:103:LYS:HZ1	1:E:79:GLU:CD	2.17	0.48
1:F:40:ILE:HD11	1:F:96:ILE:HD11	1.96	0.47
1:D:103:LYS:NZ	1:E:79:GLU:CG	2.78	0.47
1:E:52:VAL:O	1:E:54:GLY:N	2.48	0.47
1:D:57:HIS:N	1:D:57:HIS:CD2	2.82	0.47
1:F:61:GLN:O	1:F:65:ILE:HG13	2.15	0.46
1:E:89:ASN:HA	1:E:94:ASN:ND2	2.31	0.46
1:G:1:ALA:HA	1:H:35:ARG:NH1	2.31	0.46
1:G:57:HIS:HA	1:G:61:GLN:OE1	2.16	0.46
1:F:52:VAL:HA	1:F:53:PRO:HD3	1.86	0.45
1:D:56:GLN:HG2	1:D:57:HIS:CD2	2.51	0.45
1:D:67:ARG:HG2	1:E:29:GLU:OE2	2.17	0.45
1:E:55:SER:O	1:E:56:GLN:CB	2.65	0.44
1:E:55:SER:O	1:E:56:GLN:HB2	2.17	0.44
1:H:34:LYS:CE	1:H:34:LYS:HA	2.48	0.44
1:G:59:ASP:O	1:G:62:LYS:HB2	2.18	0.44
1:H:102:GLU:O	1:H:102:GLU:HG3	2.18	0.43
1:F:103:LYS:C	1:F:105:ALA:H	2.20	0.43
1:D:35:ARG:NH2	1:H:11:GLU:CD	2.73	0.42
1:E:61:GLN:O	1:E:65:ILE:HG13	2.19	0.42
1:D:53:PRO:HG3	1:D:65:ILE:HD13	2.02	0.42
1:D:103:LYS:HZ1	1:E:79:GLU:CG	2.32	0.42
1:G:103:LYS:HD2	1:H:76:TYR:CZ	2.54	0.42
1:G:67:ARG:O	1:G:70:ASP:HB2	2.19	0.42
1:G:30:SER:O	1:G:36:GLU:HA	2.19	0.42
1:F:87:VAL:HG12	1:F:96:ILE:HA	2.01	0.42
1:D:12:TYR:OH	1:E:35:ARG:HB2	2.20	0.41
1:F:12:TYR:CZ	1:G:32:ALA:HB1	2.56	0.41
1:F:92:THR:HA	1:F:93:PRO:HA	1.93	0.41
1:E:68:MET:O	1:E:72:LEU:HG	2.21	0.41
1:H:28:THR:HB	1:H:39:ILE:HB	2.03	0.41
1:G:2:PRO:HA	1:G:7:GLU:OE2	2.21	0.41
1:F:30:SER:O	1:F:36:GLU:HA	2.20	0.41
1:G:25:LEU:HB3	1:G:41:THR:O	2.20	0.41
1:E:60:SER:HB3	1:F:36:GLU:OE2	2.21	0.41
1:H:92:THR:HA	1:H:93:PRO:HA	1.91	0.41
1:E:90:ASN:OD1	1:E:91:LYS:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:THR:HB	1:E:39:ILE:HB	2.03	0.40

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	D	104/129 (81%)	96 (92%)	7 (7%)	1 (1%)	19	58
1	E	105/129 (81%)	94 (90%)	9 (9%)	2 (2%)	10	45
1	F	104/129 (81%)	97 (93%)	6 (6%)	1 (1%)	19	58
1	G	104/129 (81%)	101 (97%)	3 (3%)	0	100	100
1	H	104/129 (81%)	96 (92%)	8 (8%)	0	100	100
All	All	521/645 (81%)	484 (93%)	33 (6%)	4 (1%)	24	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	56	GLN
1	D	105	ALA
1	F	105	ALA
1	E	105	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	D	95/109 (87%)	89 (94%)	6 (6%)	22	60
1	E	96/109 (88%)	90 (94%)	6 (6%)	22	60
1	F	95/109 (87%)	92 (97%)	3 (3%)	46	79
1	G	95/109 (87%)	91 (96%)	4 (4%)	36	73
1	H	95/109 (87%)	92 (97%)	3 (3%)	46	79
All	All	476/545 (87%)	454 (95%)	22 (5%)	33	71

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	6	THR
1	D	9	CYS
1	D	35	ARG
1	D	56	GLN
1	D	57	HIS
1	D	104	LEU
1	E	3	GLN
1	E	6	THR
1	E	9	CYS
1	E	58	ILE
1	E	60	SER
1	E	107	PHE
1	F	9	CYS
1	F	35	ARG
1	F	103	LYS
1	G	9	CYS
1	G	56	GLN
1	G	103	LYS
1	G	104	LEU
1	H	6	THR
1	H	9	CYS
1	H	34	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	14	ASN
1	D	57	HIS
1	D	90	ASN
1	D	94	ASN

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Mol	Chain	Res	Type
1	E	57	HIS
1	E	94	ASN
1	F	57	HIS
1	F	94	ASN
1	G	56	GLN
1	G	57	HIS
1	G	94	ASN
1	H	90	ASN
1	H	94	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 [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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.