



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 01:54 AM EDT

PDB ID : 6B8D  
Title : 1.78 Angstrom Resolution Crystal Structure of N-terminal Fragment (residues 1-405) of Elongation Factor G from Haemophilus influenzae  
Authors : Minasov, G.; Shuvalova, L.; Dubrovskaya, I.; Kiryukhina, O.; Grimshaw, S.; Kwon, K.; Anderson, W.F.; Satchell, K.J.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : unknown  
Resolution : 1.78 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

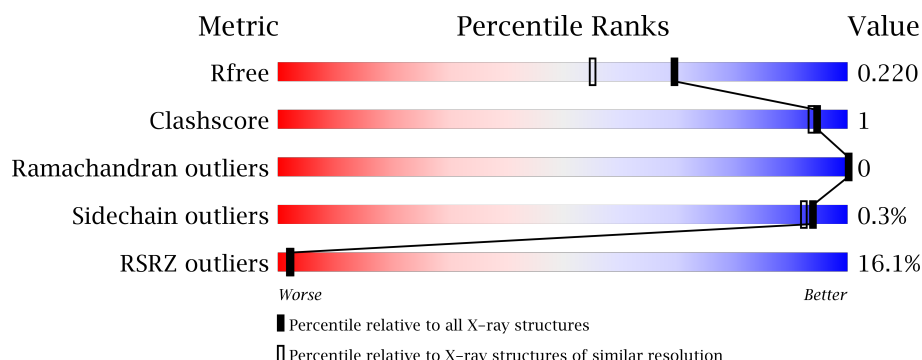
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	408	<div> <div>15%</div> <div>89%</div> <div>7%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3330 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 Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	10	0
			3021	1892	524	589	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P43925
A	-1	ASN	-	expression tag	UNP P43925
A	0	ALA	-	expression tag	UNP P43925

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

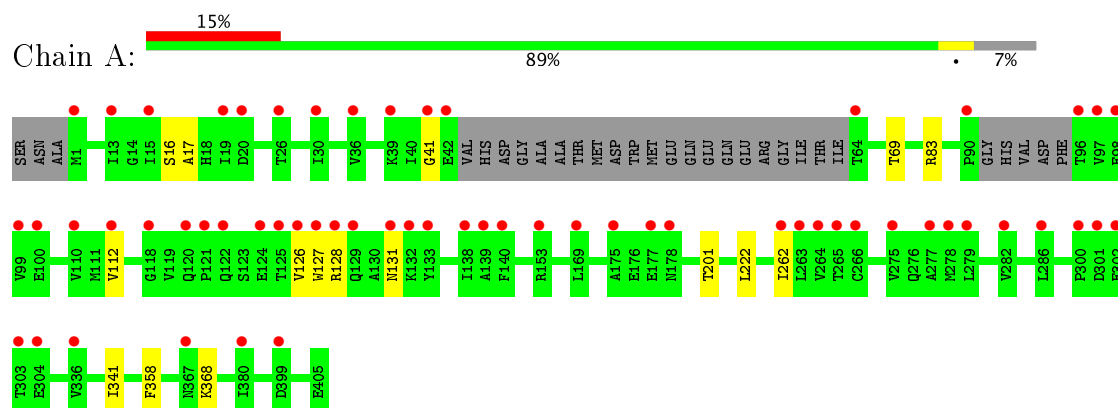
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	290	Total	O	0	21
			308	308		

### 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: Elongation factor G



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.82Å 88.49Å 130.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.80 – 1.78 29.80 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.80-1.78) 99.9 (29.80-1.78)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.173 , 0.214 0.182 , 0.220	Depositor DCC
$R_{free}$ test set	2357 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.030 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: CL

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	0.43	0/3068	0.67	1/4152 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	222	LEU	CA-CB-CG	5.17	127.19	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	3021	0	2996	9	0
2	A	1	0	0	0	0
3	A	308	0	0	0	0
All	All	3330	0	2996	9	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 1.

All (9) 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:A:262[B]:ILE:O	1:A:262[B]:ILE:HG13	1.78	0.81
1:A:341:ILE:HD11	1:A:358:PHE:CD1	2.43	0.53
1:A:262[B]:ILE:O	1:A:262[B]:ILE:CG1	2.56	0.52
1:A:128:ARG:NH2	1:A:131:ASN:HD22	2.10	0.49
1:A:16[B]:SER:OG	1:A:126:VAL:HG11	2.14	0.48
1:A:17:ALA:HB2	1:A:112:VAL:HB	1.99	0.45
1:A:127:TRP:HH2	1:A:262[B]:ILE:HG21	1.85	0.41
1:A:41:GLY:O	1:A:201:THR:HA	2.21	0.40
1:A:69:THR:HG23	1:A:83:ARG:HD2	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	A	383/408 (94%)	378 (99%)	5 (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	324/337 (96%)	323 (100%)	1 (0%)	94	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	LYS

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

### 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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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 ⓘ

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	379/408 (92%)	0.81	61 (16%) 2 2	22, 41, 70, 99	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	VAL	8.4
1	A	96	THR	7.0
1	A	99	VAL	6.9
1	A	1	MET	6.9
1	A	121	PRO	6.3
1	A	19[A]	ILE	5.8
1	A	128	ARG	5.4
1	A	122	GLN	5.2
1	A	125	THR	5.0
1	A	98	GLU	4.5
1	A	133	TYR	4.5
1	A	42	GLU	4.5
1	A	124	GLU	4.2
1	A	126	VAL	4.2
1	A	264	VAL	4.2
1	A	367	ASN	3.9
1	A	127	TRP	3.9
1	A	301	ASP	3.7
1	A	140	PHE	3.5
1	A	169	LEU	3.5
1	A	129	GLN	3.5
1	A	275	VAL	3.5
1	A	263	LEU	3.4
1	A	303	THR	3.4
1	A	20	ASP	3.4
1	A	279	LEU	3.3
1	A	118	GLY	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	112	VAL	3.2
1	A	178	ASN	3.2
1	A	265	THR	3.2
1	A	131	ASN	3.1
1	A	399	ASP	3.1
1	A	15	ILE	3.0
1	A	138	ILE	3.0
1	A	132	LYS	3.0
1	A	139	ALA	3.0
1	A	177	GLU	3.0
1	A	277	ALA	2.9
1	A	100	GLU	2.9
1	A	90	PRO	2.9
1	A	300	PRO	2.9
1	A	64	THR	2.8
1	A	336	VAL	2.7
1	A	110	VAL	2.7
1	A	278	MET	2.7
1	A	26	THR	2.5
1	A	39	LYS	2.5
1	A	304	GLU	2.3
1	A	266	CYS	2.3
1	A	13	ILE	2.3
1	A	175	ALA	2.2
1	A	41	GLY	2.2
1	A	153	ARG	2.2
1	A	262[A]	ILE	2.2
1	A	302	GLU	2.2
1	A	30	ILE	2.1
1	A	36	VAL	2.1
1	A	380	ILE	2.1
1	A	286	LEU	2.1
1	A	282	VAL	2.0
1	A	120	GLN	2.0

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

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	CL	A	501	1/1	0.87	0.07	-	72,72,72,72	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.