



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:35 PM GMT

PDB ID : 3ZZ0
Title : Crystal structure of ribosomal elongation factor (EF)-G from *Staphylococcus aureus* with a fusidic acid hyper-sensitivity mutation M16I
Authors : Koripella, R.K.; Chen, Y.; Selmer, M.; Sanyal, S.
Deposited on : 2011-08-30
Resolution : 2.80 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
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

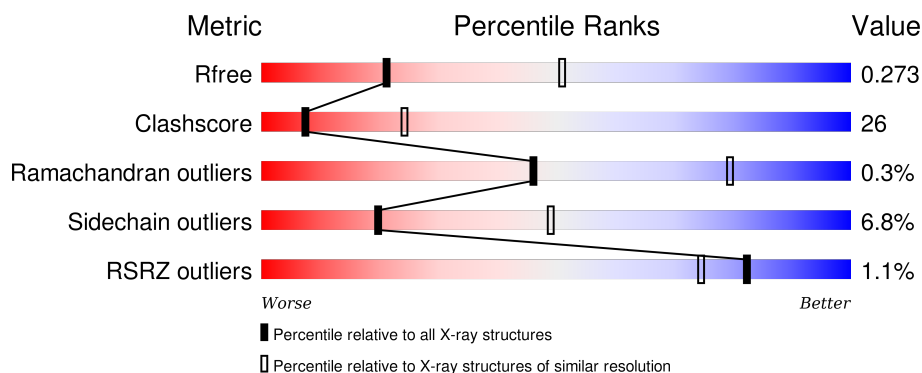
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 ≥ 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	693	
1	B	693	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10068 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	649	Total	C	N	O	S	0	0	1
			5021	3154	841	1000	26			
1	B	649	Total	C	N	O	S	0	0	1
			5021	3154	841	1000	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ILE	MET	ENGINEERED MUTATION	UNP P68790
B	16	ILE	MET	ENGINEERED MUTATION	UNP P68790

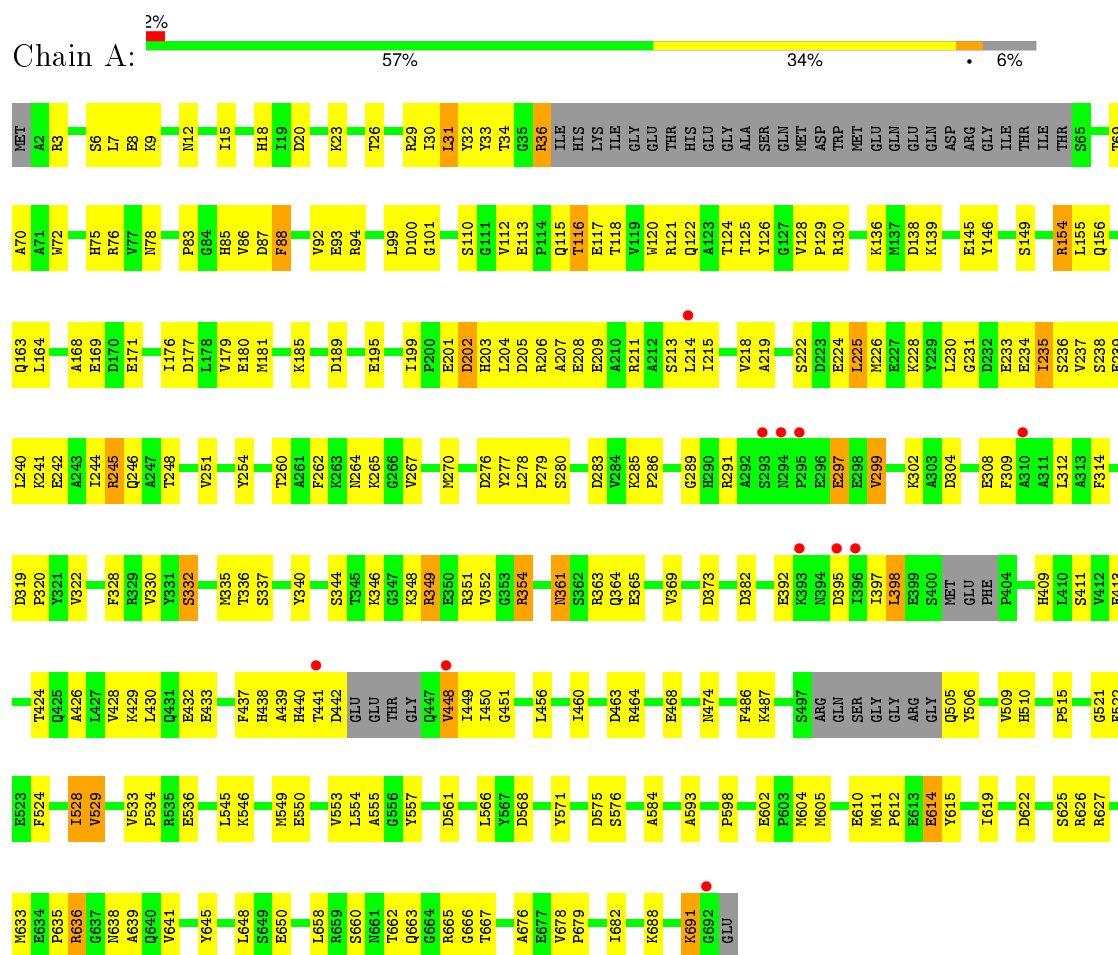
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	O	0	0
			11	11		
2	B	15	Total	O	0	0
			15	15		

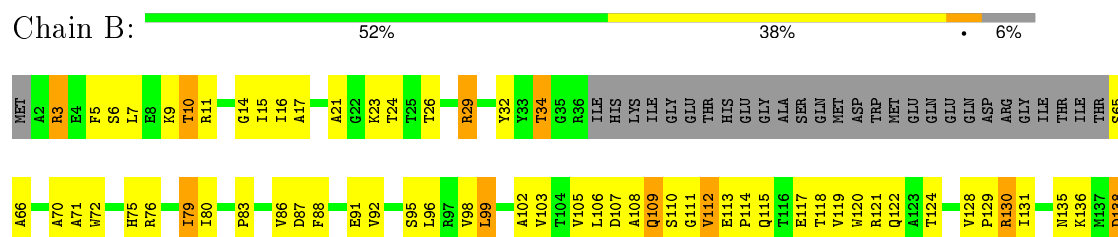
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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



• Molecule 1: ELONGATION FACTOR G



K139	I215	D804	G384	G451	E550	V668
L140	V218	K385	T385	G454	N551	T669
G141	A219	S306	G386	E455	A555	H670
	E220	A307	D387	L456	G556	F672
F144	T221	E225	E220	H457	Y557	
V148	S222	D223	C390	L458	P558	A683
S149	D223	K315	G391	D459	L559	B684
T150	E224	E225	E392	I460		
L151	L225	K317	K393	D463	K563	T687
	M226	T318	N394	R464	A564	K688
R154	E227	D319	D395	M465	K565	K691
L155	K228	P320	K396		L566	G692
	Y229	Y321	I397	A477	Y667	GLU
A159	L230	V322	L398	P478	D568	
E160			E399	F478		
P161	I235	L325	S400	M479	H572	
I162	K241	T326	MET	Y482	D575	
Q163	GLU	F327	GLU			
L164			PHE	T485	A592	
P165	R345	R329	P404	S489	P598	
I166	Q246	V330	E405	V492	E602	
	A247		P406			
E169	T248	G333	Y407	K495	I609	
			I408		E610	
A174	V251	K335	H409	K496	M611	
I175		T336	L410	S497	P612	
I176	Y254	S337	V412	F496		
D177	P255		E413	A597		
L178	V256	V341	ARG	GLN	Y615	
V179	L257	K342	P414	SER		
E180		R343	P414	GLY	D618	
M181	T260	S344	K417	GLY	I619	
K182		T345		GLY		
C183	K263	K346	D421	ARG	G632	
F184		G347	K422	GLY	M633	
K185	M270	R348	M423	O505	E634	
Y186		K349	T424		R635	
K185	A273	E350	Q425	H510	R636	
T187	V274		A426	I511	N643	
I188	I275	G353			L648	
D189	D276	R354	K429	T514	Y654	
	Y277	L355	L430	P515		
E193	L278	L366	K439	T518	E523	
I194	P279		E433		N526	
E195		H359	D434			
E196	L282		P435	E523		
			T436	N526		
	I287		H437			
H203		R363	F437			
L204	E290	E365		R536		
D205	K291	I366	D442			
R206	A292	T367	GLU	I538		
A207	S293	T368	THR	V541	S657	
E208	N294	V369	GLY		L658	
E209	P295	V370	THR		R659	
E209	E296	S371	GLY	K546		
A210	E297		Q447	D547		
R211	E297		Y448		Q663	
	E298		I449	A548		
L214	V299	K381	I460	N549		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.94Å 125.46Å 106.27Å 90.00° 107.52° 90.00°	Depositor
Resolution (Å)	46.71 – 2.80 46.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (46.71-2.80) 91.2 (46.71-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.249 , 0.276 0.243 , 0.273	Depositor DCC
R_{free} test set	1737 reflections (4.76%)	DCC
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.8	EDS
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36516 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10068	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.28	1/5107 (0.0%)	0.49	0/6906
1	B	0.28	1/5107 (0.0%)	0.52	0/6906
All	All	0.28	2/10214 (0.0%)	0.50	0/13812

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	691	LYS	C-N	-5.21	1.23	1.33
1	B	691	LYS	C-N	-5.16	1.23	1.33

There are no bond angle outliers.

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	5021	0	4934	235	1
1	B	5021	0	4934	275	2
2	A	11	0	0	2	0
2	B	15	0	0	1	0
All	All	10068	0	9868	509	2

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 26.

The worst 5 of 509 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:109:GLN:OE1	1:B:109:GLN:N	1.80	1.12
1:A:615:TYR:OH	1:A:663:GLN:NE2	1.84	1.11
1:B:526:ASN:HD21	1:B:538:ILE:HD13	1.23	1.04
1:B:211:ARG:HH12	1:B:235:ILE:HD11	1.22	1.03
1:A:354:ARG:HH11	1:A:354:ARG:HG2	1.23	1.02

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:NZ	1:B:205:ASP:OD1[2_555]	1.95	0.25
1:B:535:ARG:NH2	1:B:618:ASP:OD1[1_455]	2.13	0.07

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	639/693 (92%)	600 (94%)	38 (6%)	1 (0%)	52 84
1	B	639/693 (92%)	588 (92%)	48 (8%)	3 (0%)	34 69
All	All	1278/1386 (92%)	1188 (93%)	86 (7%)	4 (0%)	46 79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	VAL
1	B	435	PRO
1	B	381	LYS
1	A	251	VAL

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	
1	A	543/579 (94%)	507 (93%)	36 (7%)	21	51
1	B	543/579 (94%)	505 (93%)	38 (7%)	19	47
All	All	1086/1158 (94%)	1012 (93%)	74 (7%)	20	49

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	636	ARG
1	B	86	VAL
1	B	514	THR
1	A	660	SER
1	B	10	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	290	HIS
1	B	572	HIS
1	B	438	HIS
1	A	663	GLN
1	B	510	HIS

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 [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 [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, 95th 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 ²)	Q<0.9
1	A	649/693 (93%)	0.05	11 (1%) 73 63	41, 82, 141, 252	0
1	B	649/693 (93%)	-0.02	3 (0%) 91 88	47, 87, 137, 274	0
All	All	1298/1386 (93%)	0.02	14 (1%) 82 74	41, 85, 139, 274	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	ALA	3.9
1	A	295	PRO	3.8
1	A	395	ASP	3.0
1	A	293	SER	2.7
1	B	559	LEU	2.6

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.