



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:11 PM UTC

PDB ID : 3ZZT / pdb_00003zzt
Title : Crystal structure of Staphylococcus aureus elongation factor G with a fusidic
-acid-resistant mutation F88L
Authors : Koripella, R.K.; Chen, Y.; Selmer, M.; Sanyal, S.
Deposited on : 2011-09-05
Resolution : 2.95 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

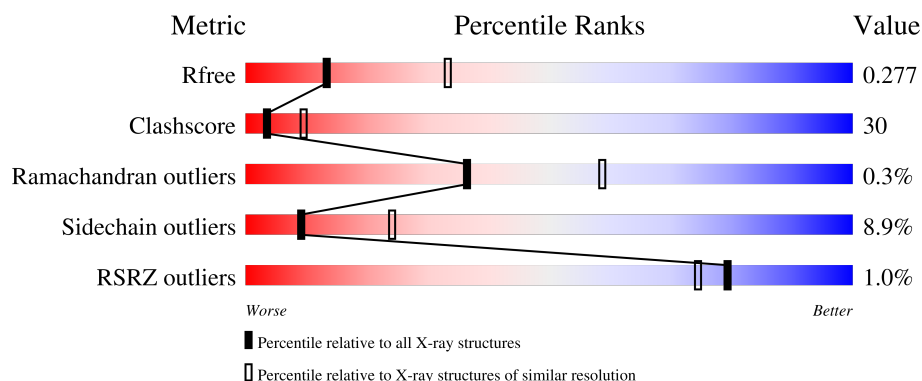
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

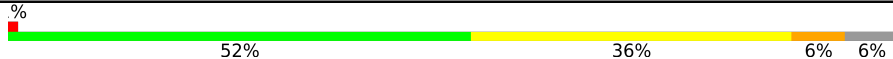
The reported resolution of this entry is 2.95 Å.

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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	693	
1	B	693	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10059 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
			5018	3150	841	1000	27			
1	B	649	Total	C	N	O	S	0	0	1
			5018	3150	841	1000	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	LEU	PHE	engineered mutation	UNP P68790
B	88	LEU	PHE	engineered mutation	UNP P68790

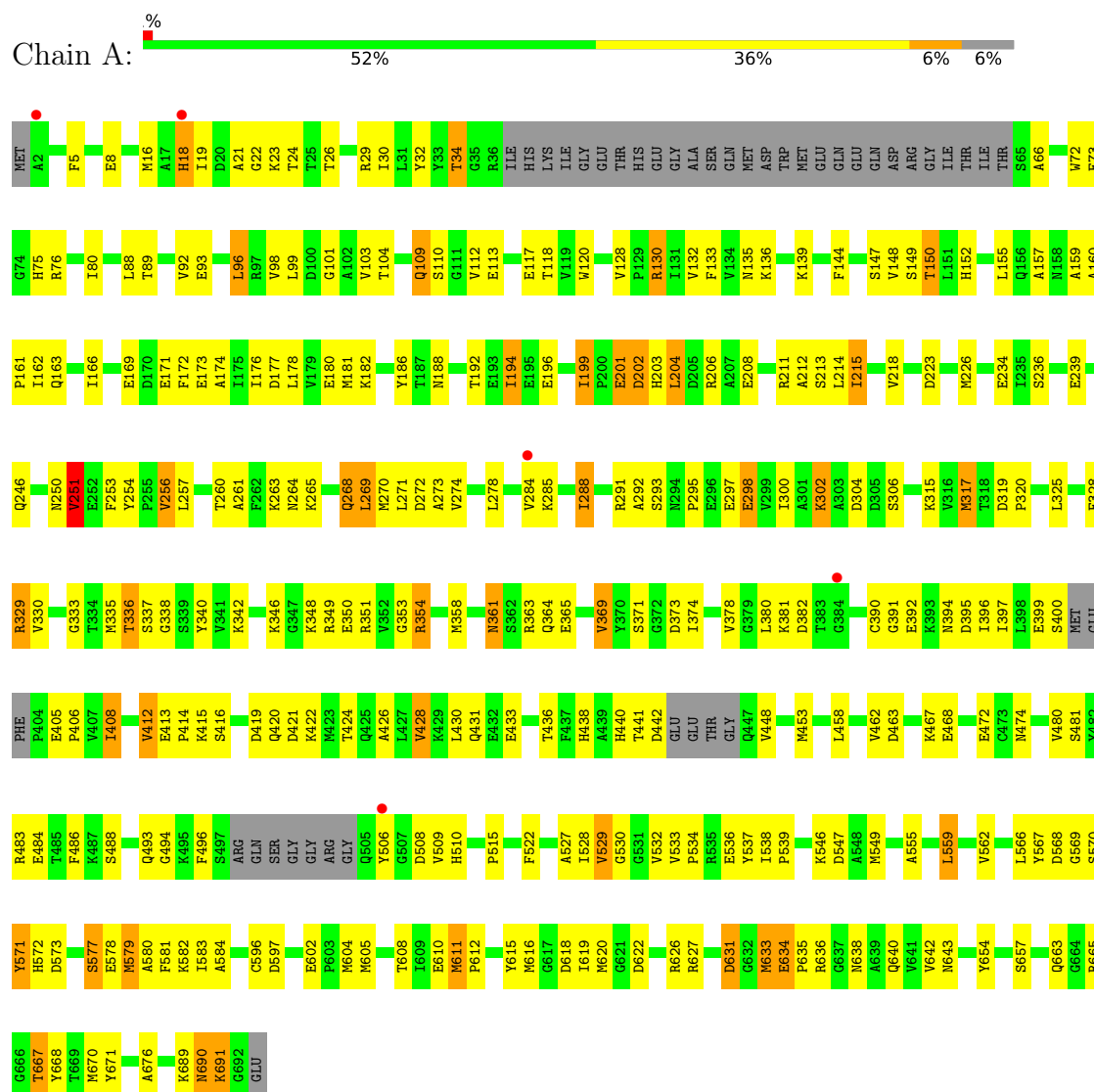
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	6	Total	O	0	0
			6	6		

3 Residue-property plots

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



• Molecule 1: ELONGATION FACTOR G



Met	A2	R3	L7	E8	K9	T15	M16	A17	H18	I19	D20	K23	T24	T25	E28	R29	I30	L31	T34	G35	R36	ILE	HIS	LYS	ILE	GLY	THR	HIS	GLU	GLY	ALA	SER	GLN	MET	ASP	TRP	MET	GLU	GLN	GLU	GLN	ASP	ARG	GLY	ILE	THR	ILE	THR	S65	T68	T69	A70						
	H75	R76		P83	G84	H85	V86	D87	L88	T89	V90	E91	V92	E93	R94	S95	A100	G101	A102	V103	T104	V105	L106	D107	A108		V112	K185	E113	P114	Q115	T116	E117	T118	V119	V120	R121	Q122		Y126	G127	V128	P129	R130	I131	V132	F133	V134	N135	R211	K136	A137	D138	K139	A142	N143	F144	
	E145	Y146	S149	R154	A159	A160	P161	T162	Q163	L164	P165	E169	D170	E171	F172	E173	A174	I175	I176	D177	L178	V179	E180	M181		F184	K185	V251	S332	T187		T192	E193	I194	E195	E196	I197		P200	E201	D202	H203	L204	D205	R206	A207	E208	E209	V274	A210	R211	A212	S213	L214	T215	E216	A217	V218
	A219	E220	T221	S222	E223	E224	L225	M226	E227	K228	Y229	L230	E233	E234	I235	S236	V237	E238	E239	L240	K241	E242	A243	R245	Q246	A247	T248	T249	R250	V251	E252	F253	Y254	E255	V256	L257		T260		K265	G266	V267	Q268	L269	M270	L271	D272	A273	V274	L275	D276	Y277		S280	P281	K285	V286	
	T287	L288	G289	H290	R291	A292	S293	N294	V299	D304	D305	S306	A307	E308	F309	A310	A311	L312	V316	N394	D395	I396	L397	L398	E399	S400	MET	GLU	PHE	P404	L410	S411	V412	E413	P414	K415	N343	K342	K343	S344	T345	K346	G347	K348	R349	E350	R351	V352	A353	R354	L355	L356		N361	S362	R363	S364	T365
	T441	D442	GLU	THR	GLY	Q447	V448	I449	I450	M453	L456	H457	L458	D459	I460	L461	V462	D463	R464	M465	K466	F469	M470	V471	E472	C473	M474	V475	G476	A477	P478	M479	V480	S481	Y482	R483	E484	T485	F486	K487	Q491	V492	Q493	S497	ARG	GLN	SER	GLY	GLY	ARG	GLY	Q505	H510					
I511	E512	I528	V533	P534	Y537	I538	P539	S540	V541	G544	L545	K546	D547	A548	M549	L554	Y557	P558	L559	K565	L566	V574	D575	M579	K582	G585	G586	T587	Y668	D597	I600	L601	M605	I609	E610	M611	P612	Y615	M616	G617	D618	I619	M620	G621	D622													
V623	T624	S625	R626	V630	D631	S632	M633	E634	P635	R636	Q640	V641	M642	M643	A644	V645	P646	P647	L648	S649	E650	M651	Y654	A655	T656	S657	L658	R659	T662	Q663	G664	R665	G666	T667	C596	G668	T669	M670	V671	F672	E677	V678	P679	K680	S681	E684	D685	T686	K689	N690	R691	G692	GLU					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.97Å 127.93Å 107.44Å 90.00° 107.86° 90.00°	Depositor
Resolution (Å)	47.40 – 2.95 47.40 – 2.95	Depositor EDS
% Data completeness (in resolution range)	90.3 (47.40-2.95) 90.3 (47.40-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.96Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.241 , 0.294 (Not available) , 0.277	Depositor DCC
R_{free} test set	1524 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10059	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.33	1/5103 (0.0%)	0.81	10/6900 (0.1%)
1	B	0.38	1/5103 (0.0%)	0.82	5/6900 (0.1%)
All	All	0.36	2/10206 (0.0%)	0.81	15/13800 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	691	LYS	C-N	-7.13	1.23	1.33
1	B	691	LYS	C-N	-7.05	1.23	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	571	TYR	N-CA-C	6.65	117.02	108.24
1	B	396	ILE	N-CA-C	6.39	117.82	109.58
1	B	294	ASN	CA-C-N	6.33	125.75	118.85
1	B	294	ASN	C-N-CA	6.33	125.75	118.85
1	B	395	ASP	N-CA-C	6.16	120.93	113.17

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	A	5018	0	4934	254	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5018	0	4934	337	0
2	A	17	0	0	4	0
2	B	6	0	0	1	0
All	All	10059	0	9868	590	1

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 30.

The worst 5 of 590 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:363:ARG:HG3	1:B:363:ARG:HH11	1.01	1.17
1:B:268:GLN:N	1:B:268:GLN:OE1	1.86	1.09
1:B:186:TYR:OH	1:B:268:GLN:NE2	1.86	1.07
1:B:242:GLU:N	1:B:242:GLU:OE1	1.91	1.03
1:B:128:VAL:O	1:B:130:ARG:NH1	1.92	1.02

All (1) 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:169:GLU:OE2	1:A:340:TYR:OH[1_455]	2.18	0.02

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%)	592 (93%)	46 (7%)	1 (0%)	43	66
1	B	639/693 (92%)	583 (91%)	53 (8%)	3 (0%)	24	49
All	All	1278/1386 (92%)	1175 (92%)	99 (8%)	4 (0%)	36	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	691	LYS
1	B	394	ASN
1	B	251	VAL
1	A	251	VAL

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	543/579 (94%)	498 (92%)	45 (8%)	10	27
1	B	543/579 (94%)	491 (90%)	52 (10%)	8	22
All	All	1086/1158 (94%)	989 (91%)	97 (9%)	9	24

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	192	THR
1	B	294	ASN
1	B	203	HIS
1	B	235	ILE
1	B	332	SER

Sometimes 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	75	HIS
1	B	78	ASN
1	B	425	GLN
1	B	357	GLN
1	A	661	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 oligosaccharides 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%)	-0.11	5 (0%) 82 78	41, 81, 128, 172	0
1	B	649/693 (93%)	0.10	8 (1%) 76 71	43, 97, 157, 227	0
All	All	1298/1386 (93%)	-0.00	13 (1%) 79 74	41, 89, 145, 227	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	641	VAL	4.2
1	B	18	HIS	2.8
1	A	284	VAL	2.7
1	B	142	ALA	2.6
1	A	2	ALA	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 oligosaccharides 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.