



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2023 – 10:44 PM EDT

PDB ID : 2P7Q
Title : Crystal structure of E126Q mutant of genomically encoded fosfomycin resistance protein, FosX, from *Listeria monocytogenes* complexed with MN(II) and 1S,2S-dihydroxypropylphosphonic acid
Authors : Fillgrove, K.L.; Pakhomova, S.; Schaab, M.; Newcomer, M.E.; Armstrong, R.N.
Deposited on : 2007-03-20
Resolution : 2.40 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

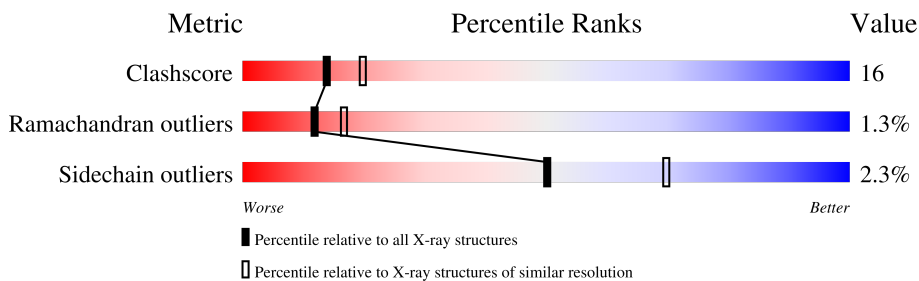
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	133	
1	B	133	
1	C	133	
1	D	133	
1	E	133	
1	F	133	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6355 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 Glyoxalase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	130	1046	666	175	201	4	0	0	0
1	B	122	986	635	159	188	4	0	0	0
1	C	126	1024	659	167	194	4	0	0	0
1	D	126	1024	656	170	194	4	0	0	0
1	E	131	1066	680	178	203	5	0	1	0
1	F	131	1058	677	175	202	4	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLN	GLU	engineered mutation	UNP Q71YW5
B	126	GLN	GLU	engineered mutation	UNP Q71YW5
C	126	GLN	GLU	engineered mutation	UNP Q71YW5
D	126	GLN	GLU	engineered mutation	UNP Q71YW5
E	126	GLN	GLU	engineered mutation	UNP Q71YW5
F	126	GLN	GLU	engineered mutation	UNP Q71YW5

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

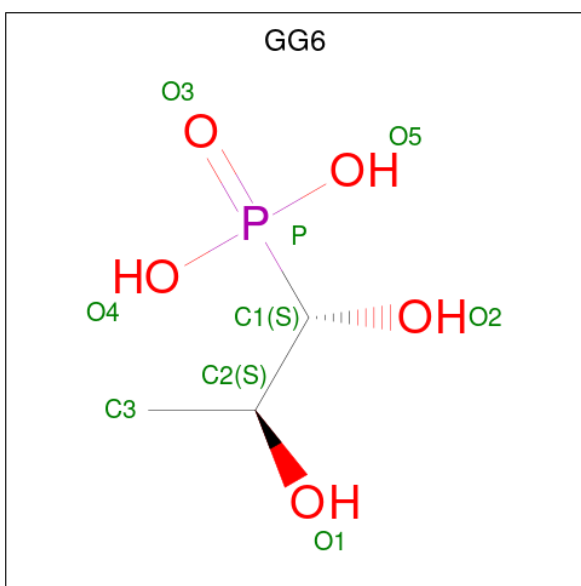
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is [(1S,2S)-1,2-DIHYDROXYPROPYL]PHOSPHONIC ACID (three-letter code: GG6) (formula: C₃H₉O₅P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			9	3	5	1		
3	B	1	Total	C	O	P	0	0
			9	3	5	1		
3	C	1	Total	C	O	P	0	0
			9	3	5	1		
3	D	1	Total	C	O	P	0	0
			9	3	5	1		
3	E	1	Total	C	O	P	0	0
			9	3	5	1		
3	F	1	Total	C	O	P	0	0
			9	3	5	1		

- Molecule 4 is water.

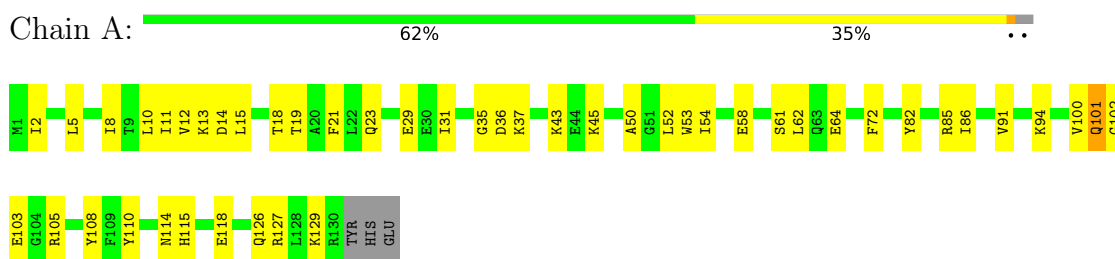
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	15	Total O 15 15	0	0
4	C	20	Total O 20 20	0	0
4	D	11	Total O 11 11	0	0
4	E	26	Total O 26 26	0	0
4	F	7	Total O 7 7	0	0

3 Residue-property plots [i](#)

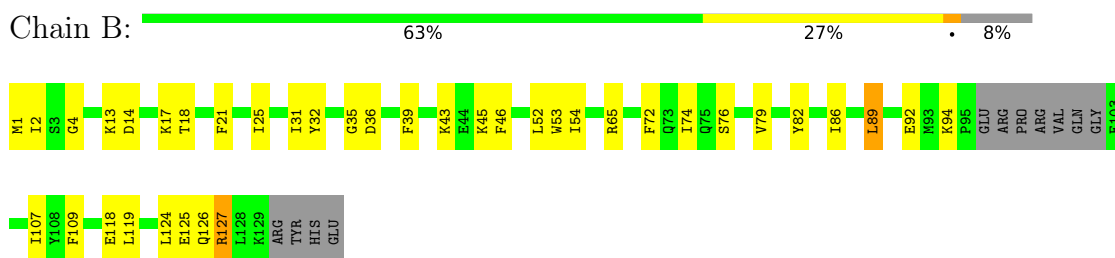
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

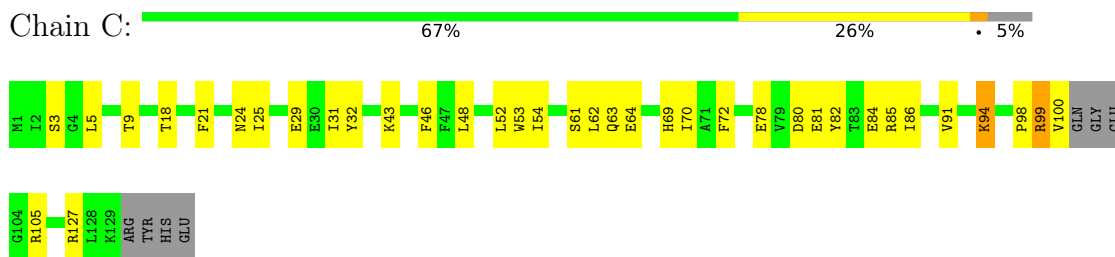
- Molecule 1: Glyoxalase family protein



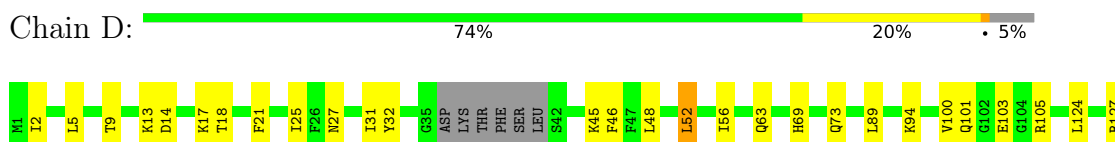
- Molecule 1: Glyoxalase family protein



- Molecule 1: Glyoxalase family protein



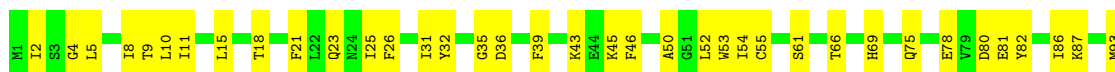
- Molecule 1: Glyoxalase family protein





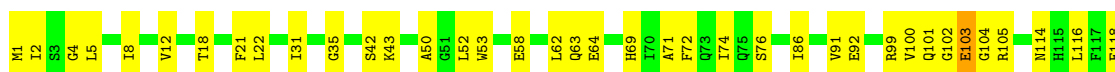
- Molecule 1: Glyoxalase family protein

Chain E: 59% 38%



- Molecule 1: Glyoxalase family protein

Chain F: 65% 32%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.01Å 69.45Å 83.97Å 90.00° 113.86° 90.00°	Depositor
Resolution (Å)	28.09 – 2.40	Depositor
% Data completeness (in resolution range)	80.6 (28.09-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6355	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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: MN, GG6

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	0.40	0/1066	0.63	0/1435
1	B	0.37	0/1005	0.57	0/1352
1	C	0.42	0/1044	0.61	0/1404
1	D	0.41	0/1044	0.63	0/1405
1	E	0.40	0/1091	0.62	0/1469
1	F	0.35	0/1079	0.59	0/1453
All	All	0.39	0/6329	0.61	0/8518

There are no bond length outliers.

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	1046	0	1009	45	0
1	B	986	0	958	32	0
1	C	1024	0	1004	36	0
1	D	1024	0	988	24	0
1	E	1066	0	1033	48	0
1	F	1058	0	1026	38	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	9	0	6	1	0
3	B	9	0	6	0	0
3	C	9	0	6	2	0
3	D	9	0	6	2	0
3	E	9	0	6	1	0
3	F	9	0	6	0	0
4	A	12	0	0	0	0
4	B	15	0	0	0	0
4	C	20	0	0	5	0
4	D	11	0	0	1	0
4	E	26	0	0	6	0
4	F	7	0	0	1	0
All	All	6355	0	6054	195	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 16.

The worst 5 of 195 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:5:LEU:HD23	1:E:52:LEU:HD11	1.50	0.94
1:E:52:LEU:HD23	1:E:54:ILE:HD11	1.54	0.88
1:C:32:TYR:HB3	1:C:46:PHE:HB2	1.66	0.76
1:F:1:MET:HG2	1:F:2:ILE:H	1.54	0.73
1:B:35:GLY:HA3	1:B:43:LYS:HA	1.71	0.72

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	128/133 (96%)	118 (92%)	7 (6%)	3 (2%)	6	7
1	B	118/133 (89%)	108 (92%)	9 (8%)	1 (1%)	19	29
1	C	122/133 (92%)	117 (96%)	3 (2%)	2 (2%)	9	13
1	D	122/133 (92%)	117 (96%)	5 (4%)	0	100	100
1	E	130/133 (98%)	121 (93%)	7 (5%)	2 (2%)	10	14
1	F	129/133 (97%)	120 (93%)	7 (5%)	2 (2%)	9	13
All	All	749/798 (94%)	701 (94%)	38 (5%)	10 (1%)	12	17

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	99	ARG
1	A	36	ASP
1	A	101	GLN
1	B	127	ARG
1	F	103	GLU

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	111/119 (93%)	110 (99%)	1 (1%)	78	90
1	B	106/119 (89%)	104 (98%)	2 (2%)	57	75
1	C	111/119 (93%)	108 (97%)	3 (3%)	44	65
1	D	108/119 (91%)	104 (96%)	4 (4%)	34	53
1	E	115/119 (97%)	112 (97%)	3 (3%)	46	66
1	F	113/119 (95%)	111 (98%)	2 (2%)	59	76
All	All	664/714 (93%)	649 (98%)	15 (2%)	50	70

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	52	LEU
1	F	42	SER
1	D	89	LEU
1	F	105	ARG
1	E	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	101	GLN
1	E	126	GLN
1	F	126	GLN
1	F	23	GLN
1	C	27	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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
3	GG6	C	4002	2	6,8,8	3.50	4 (66%)	6,12,12	1.17	0
3	GG6	F	5002	2	6,8,8	3.79	3 (50%)	6,12,12	1.19	0
3	GG6	B	1002	2	6,8,8	3.66	2 (33%)	6,12,12	1.26	1 (16%)
3	GG6	A	2002	2	6,8,8	3.51	3 (50%)	6,12,12	1.12	0
3	GG6	E	6002	2	6,8,8	3.48	2 (33%)	6,12,12	1.44	1 (16%)
3	GG6	D	3002	2	6,8,8	3.86	3 (50%)	6,12,12	1.34	1 (16%)

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
3	GG6	C	4002	2	-	0/7/10/10	-
3	GG6	F	5002	2	-	0/7/10/10	-
3	GG6	B	1002	2	-	0/7/10/10	-
3	GG6	A	2002	2	-	0/7/10/10	-
3	GG6	E	6002	2	-	0/7/10/10	-
3	GG6	D	3002	2	-	0/7/10/10	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5002	GG6	P-O4	-7.63	1.42	1.54
3	D	3002	GG6	P-O4	-7.29	1.43	1.54
3	E	6002	GG6	P-O4	-6.94	1.43	1.54
3	A	2002	GG6	P-O4	-6.86	1.44	1.54
3	B	1002	GG6	P-O4	-6.48	1.44	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	6002	GG6	O3-P-C1	-2.63	107.61	113.31
3	D	3002	GG6	O4-P-O3	-2.15	108.05	113.45
3	B	1002	GG6	O3-P-C1	-2.08	108.80	113.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4002	GG6	2	0
3	A	2002	GG6	1	0
3	E	6002	GG6	1	0
3	D	3002	GG6	2	0

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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.