WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2023 – 09:32 PM EDT

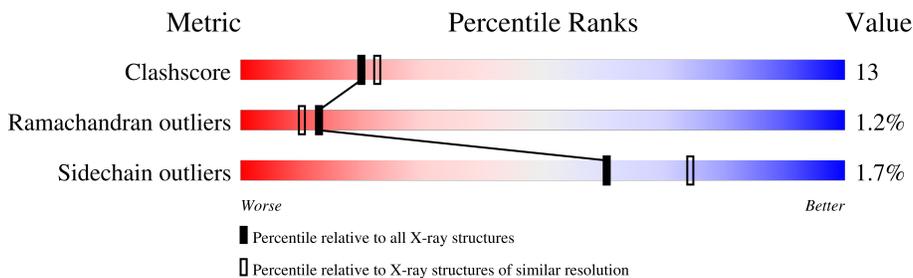|		
PDB ID	:	2P7L
Title	:	Crystal structure of monoclinic form of genomically encoded fosfomycin resistance protein, FosX, from Listeria monocytogenes at pH 5.75
Authors	:	Fillgrove, K.L.; Pakhomova, S.; Schaab, M.; Newcomer, M.E.; Armstrong, R.N.
Deposited on	:	2007-03-20
Resolution	:	2.20 Å(reported)

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 2.20 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	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		1.2%
Sidechain outliers		1.7%

Worse ———— Better

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 <=5%

Note EDS was not executed.

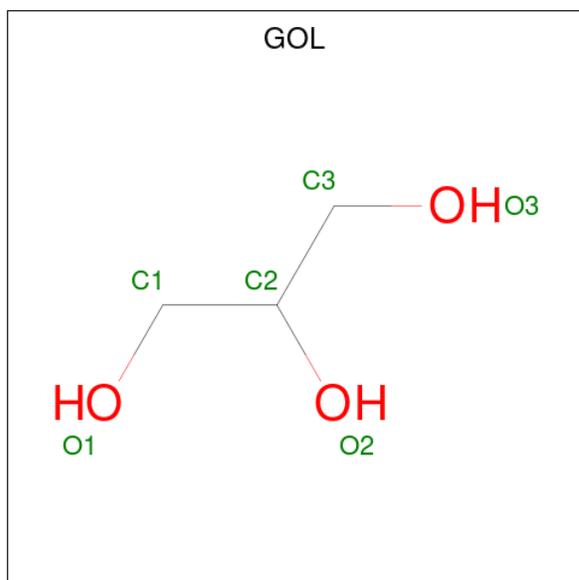| Mol	Chain	Length	Quality of chain
1	A	133	70% 24% 6%
1	B	133	68% 25% • 6%
1	C	133	72% 23% • •
1	D	133	65% 25% • 7%
1	E	133	71% 27% •
1	F	133	77% 19% • •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6306 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
1	A	125	Total	C	N	O	S	0	0	0
			1024	654	172	194	4			
1	B	125	Total	C	N	O	S	0	0	0
			1022	658	166	194	4			
1	C	129	Total	C	N	O	S	0	1	0
			1040	666	170	200	4			
1	D	124	Total	C	N	O	S	0	0	0
			1010	645	169	192	4			
1	E	130	Total	C	N	O	S	0	1	0
			1057	676	177	199	5			
1	F	130	Total	C	N	O	S	0	0	0
			1051	672	175	200	4			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 6	C 3	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	8	Total 8	O 8	0	0
3	C	11	Total 11	O 11	0	0
3	D	11	Total 11	O 11	0	0
3	E	39	Total 39	O 39	0	0
3	F	8	Total 8	O 8	0	0

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. 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
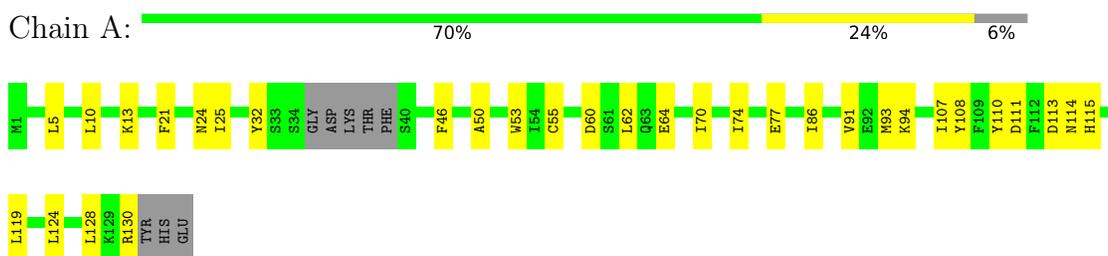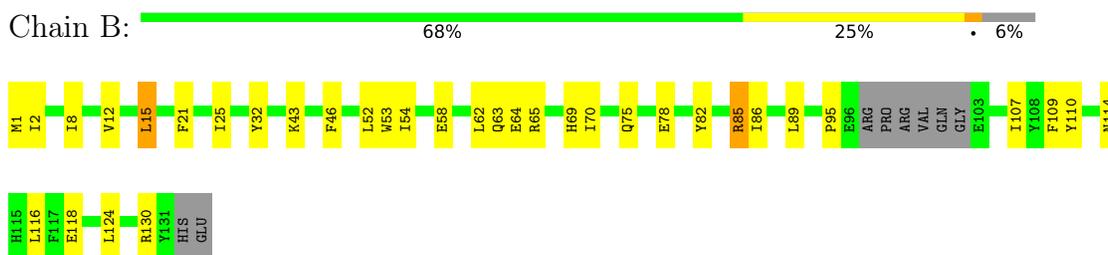
Chain A:

• Molecule 1: Glyoxalase family protein

Chain B:

• Molecule 1: Glyoxalase family protein

Chain C:

• Molecule 1: Glyoxalase family protein

Chain D:

F109 N114 T123 L124 E125 E126 K129 R130 Y131 HIS GLU
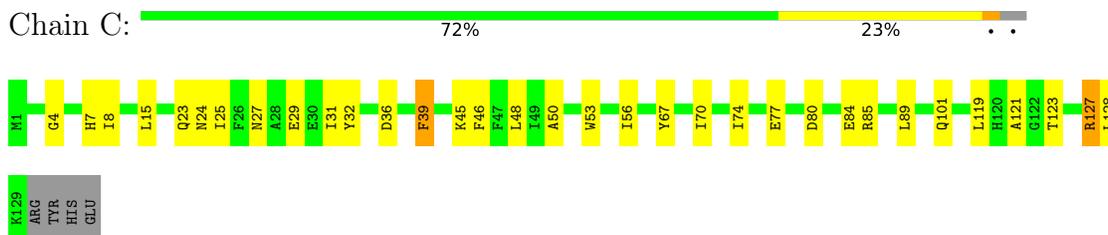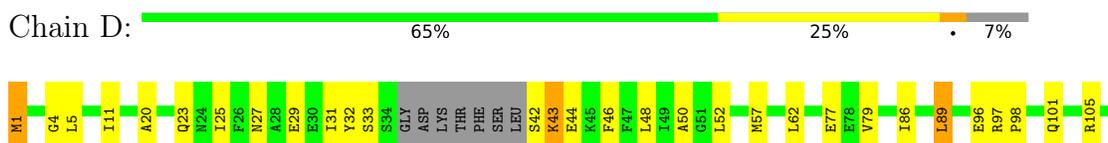
• Molecule 1: Glyoxalase family protein

Chain E:

71%   27%   ·

M1 I8 T9 L10 I11 L15 I25 Y32 F39 E44 K45 F46 F47 L48 I49 A50 G51 L52 C55 I70 A71 F72 Q75 S76 E77 E78 E81 Y82 T83 E84 R85 I86 K87 A88 L89 M93 R99 V100 Q101 G102 E103 G104 I107 H115 L119

T123 E126 K129 R130 TYR HIS GLU

• Molecule 1: Glyoxalase family protein

Chain F:

77%   19%   · ·

M1 G4 I8 T9 L10 I11 V12 L15 N27 Y32 K37 T38 F39 S42 F46 I56 M57 E58 I70 E77 E78 I86 V91 V100 Q101 G102 E103 G104 I107 E118 A121 K129 R130 TYR HIS GLU

4 Data and refinement statistics (i)

Xtriage (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	168.78Å 70.70Å 86.97Å 90.00° 113.98° 90.00°	Depositor
Resolution (Å)	27.70 – 2.20	Depositor
% Data completeness (in resolution range)	87.8 (27.70-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6306	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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: GOL

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	0.41	0/1043	0.59	0/1401
1	B	0.38	0/1042	0.59	0/1400
1	C	0.37	0/1065	0.56	0/1435
1	D	0.38	0/1029	0.60	0/1385
1	E	0.42	0/1082	0.62	0/1456
1	F	0.36	0/1072	0.57	0/1444
All	All	0.39	0/6333	0.59	0/8521

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	1024	0	1001	36	0
1	B	1022	0	997	34	0
1	C	1040	0	1000	24	0
1	D	1010	0	974	31	0
1	E	1057	0	1032	30	0
1	F	1051	0	1018	21	0
2	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	19	0	0	1	0
3	B	8	0	0	0	0
3	C	11	0	0	0	0
3	D	11	0	0	1	0
3	E	39	0	0	1	0
3	F	8	0	0	0	0
All	All	6306	0	6030	154	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 13.

The worst 5 of 154 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:87:LYS:HG2	1:E:93:MET:HE1	1.59	0.84
1:D:97:ARG:HB2	1:D:98:PRO:HD2	1.61	0.82
1:D:96:GLU:OE2	1:D:105:ARG:HD2	1.79	0.82
1:E:15:LEU:HD21	1:E:45:LYS:HG3	1.62	0.82
1:A:86:ILE:HG23	1:A:91:VAL:CG2	2.11	0.81

There are no symmetry-related clashes.

5.3   Torsion angles   ⓘ

5.3.1   Protein backbone   ⓘ

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	121/133 (91%)	118 (98%)	3 (2%)	0	100	100
1	B	121/133 (91%)	115 (95%)	4 (3%)	2 (2%)	9	6
1	C	128/133 (96%)	120 (94%)	6 (5%)	2 (2%)	9	7
1	D	120/133 (90%)	113 (94%)	5 (4%)	2 (2%)	9	6
1	E	129/133 (97%)	126 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	128/133 (96%)	119 (93%)	6 (5%)	3 (2%)	6	3
All	All	747/798 (94%)	711 (95%)	27 (4%)	9 (1%)	13	10

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	101	GLN
1	D	43	LYS
1	F	101	GLN
1	D	130	ARG
1	F	78	GLU

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	110/119 (92%)	109 (99%)	1 (1%)	78	88
1	B	110/119 (92%)	108 (98%)	2 (2%)	59	72
1	C	111/119 (93%)	109 (98%)	2 (2%)	59	72
1	D	107/119 (90%)	105 (98%)	2 (2%)	57	71
1	E	114/119 (96%)	113 (99%)	1 (1%)	78	88
1	F	112/119 (94%)	109 (97%)	3 (3%)	44	57
All	All	664/714 (93%)	653 (98%)	11 (2%)	60	74

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	39	PHE
1	F	15	LEU
1	F	39	PHE
1	F	27	ASN
1	C	127	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	D	101	GLN
1	E	16	ASN
1	F	63	GLN
1	E	23	GLN
1	C	23	GLN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	$\#|Z| > 2$
2	GOL	B	134	-	5,5,5	0.13	0	5,5,5	0.50	0

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.

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	134	-	-	0/4/4/4	-

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.