Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 01:52 PM EDT

PDB ID	:	2FA5
Title	:	The crystal structure of an unliganded multiple antibiotic-resistance repressor (MarR) from Xanthomonas campestris
Authors	:	Chin, K.H.; Tu, Z.L.; Li, J.N.; Chou, C.C.; Wang, A.H.J.; Chou, S.H.
Deposited on	:	2005-12-06
Resolution	:	1.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

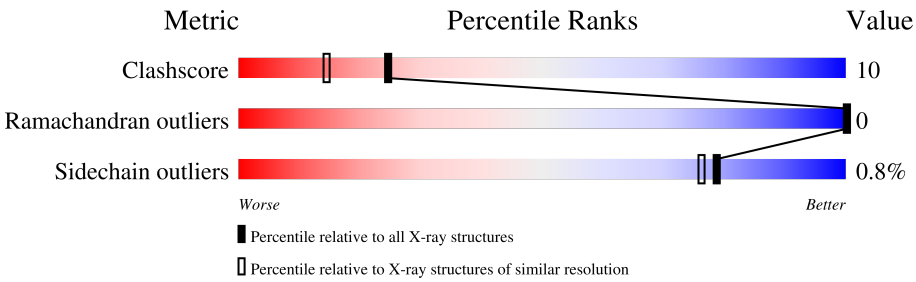
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)

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 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	162	64% 22% 14%
1	B	162	70% 17% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2538 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 transcriptional regulator marR/emrR family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	139	1095	691	199	199	6	0	0	0
1	B	142	1128	710	206	206	6	0	1	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8PDA5
A	47	MSE	MET	modified residue	UNP Q8PDA5
A	75	MSE	MET	modified residue	UNP Q8PDA5
A	106	MSE	MET	modified residue	UNP Q8PDA5
A	127	MSE	MET	modified residue	UNP Q8PDA5
A	132	MSE	MET	modified residue	UNP Q8PDA5
A	158	MSE	MET	modified residue	UNP Q8PDA5
B	1	MSE	MET	modified residue	UNP Q8PDA5
B	47	MSE	MET	modified residue	UNP Q8PDA5
B	75	MSE	MET	modified residue	UNP Q8PDA5
B	106	MSE	MET	modified residue	UNP Q8PDA5
B	127	MSE	MET	modified residue	UNP Q8PDA5
B	132	MSE	MET	modified residue	UNP Q8PDA5
B	158	MSE	MET	modified residue	UNP Q8PDA5

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	137	137	137	0	0
			Total	O		
3	B	176	176	176	0	0

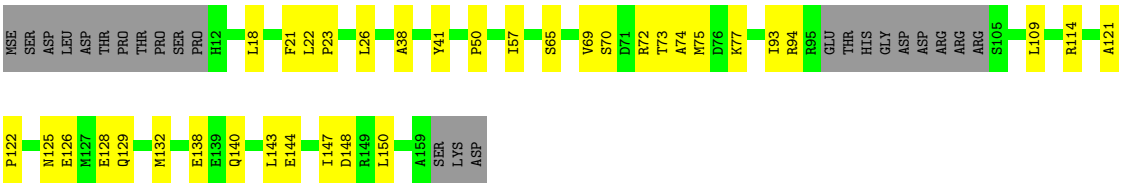
3 Residue-property plots (i)

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.

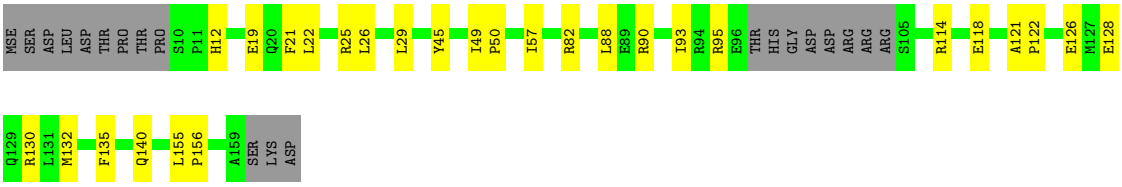
• Molecule 1: transcriptional regulator marR/emrR family

Chain A:



• Molecule 1: transcriptional regulator marR/emrR family

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	71.42Å 71.42Å 110.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.78 – 1.80	Depositor
% Data completeness (in resolution range)	90.6 (29.78-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2538	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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: 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	0.28	0/1105	0.52	0/1482
1	B	0.29	0/1139	0.51	0/1528
All	All	0.29	0/2244	0.52	0/3010

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	1095	0	1130	29	0
1	B	1128	0	1160	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	137	0	0	1	0
3	B	176	0	0	0	0
All	All	2538	0	2290	44	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 10.

All (44) 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:126:GLU:HG2	1:B:130:ARG:NH1	2.12	0.65
1:A:26:LEU:HD11	1:B:26:LEU:HD22	1.81	0.61
1:A:150:LEU:HD13	1:B:135:PHE:HE2	1.67	0.60
1:A:140:GLN:O	1:A:144:GLU:HG3	2.02	0.58
1:A:22:LEU:HB3	1:A:23:PRO:HD3	1.87	0.57
1:B:132:MSE:HE2	1:B:140:GLN:NE2	2.20	0.56
1:B:19:GLU:O	1:B:25[A]:ARG:HD3	2.05	0.55
1:A:114:ARG:NH1	1:B:12:HIS:HB3	2.21	0.55
1:B:114:ARG:O	1:B:118:GLU:HG3	2.07	0.54
1:B:121:ALA:HB3	1:B:122:PRO:HD3	1.88	0.54
1:B:88:LEU:HD11	1:B:95:ARG:HH11	1.72	0.54
1:B:126:GLU:HG2	1:B:130:ARG:HH12	1.73	0.53
1:A:70:SER:CB	1:A:77:LYS:HD3	2.38	0.53
1:A:94:ARG:HG3	1:A:94:ARG:HH21	1.74	0.52
1:B:25[A]:ARG:HH21	1:B:25[A]:ARG:HG3	1.76	0.51
1:A:150:LEU:HD23	1:B:29:LEU:HD21	1.93	0.51
1:A:21:PHE:CE1	1:B:128:GLU:HG3	2.45	0.51
1:A:22:LEU:C	1:A:22:LEU:HD13	2.34	0.47
1:A:121:ALA:HB3	1:A:122:PRO:HD3	1.96	0.47
1:A:57:ILE:HD12	1:A:72:ARG:HD2	1.95	0.47
1:A:150:LEU:HD13	1:B:135:PHE:CE2	2.48	0.47
1:A:122:PRO:O	1:A:126:GLU:HG3	2.16	0.46
1:B:155:LEU:N	1:B:156:PRO:HD2	2.31	0.46
1:B:82:ARG:HH11	1:B:82:ARG:HG3	1.81	0.45
1:A:93:ILE:HG22	1:A:109:LEU:HD23	1.99	0.45
1:A:73:THR:O	1:A:74:ALA:HB3	2.17	0.45
1:A:143:LEU:O	1:A:147:ILE:HG12	2.17	0.45
1:B:45:TYR:O	1:B:90:ARG:NH1	2.48	0.44
1:A:18:LEU:CD1	1:B:57:ILE:HD13	2.47	0.44
1:A:50:PRO:HA	1:A:75:MSE:HE1	1.99	0.44
1:B:88:LEU:HD23	1:B:93:ILE:HG13	2.00	0.43
1:A:38:ALA:HA	1:A:41:TYR:CZ	2.53	0.43
1:A:65:SER:O	1:A:69:VAL:HG23	2.19	0.43
1:B:25[A]:ARG:HG3	1:B:25[A]:ARG:NH2	2.34	0.43
1:A:125:ASN:O	1:A:129:GLN:HG3	2.19	0.43
1:A:128:GLU:HG3	1:B:21:PHE:CE1	2.54	0.42
1:B:49:ILE:N	1:B:50:PRO:HD2	2.33	0.42
1:A:73:THR:OG1	1:A:75:MSE:HG3	2.20	0.42
1:B:88:LEU:CD1	1:B:95:ARG:HH11	2.33	0.42
1:A:114:ARG:NH1	3:A:423:HOH:O	2.53	0.41
1:A:94:ARG:HG3	1:A:94:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASP:OD2	1:B:25[B]:ARG:NH2	2.52	0.41
1:A:114:ARG:CZ	1:B:12:HIS:HB3	2.51	0.41
1:A:132:MSE:CE	1:A:140:GLN:HG3	2.50	0.41

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	135/162 (83%)	135 (100%)	0	0	100	100
1	B	139/162 (86%)	138 (99%)	1 (1%)	0	100	100
All	All	274/324 (85%)	273 (100%)	1 (0%)	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	118/133 (89%)	117 (99%)	1 (1%)	79	76
1	B	122/133 (92%)	121 (99%)	1 (1%)	79	76
All	All	240/266 (90%)	238 (99%)	2 (1%)	79	76

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	B	22	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	141	GLN
1	B	20	GLN
1	B	31	ASN
1	B	36	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)

Of 2 ligands modelled in this entry, 2 are 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 (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.