



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:10 AM UTC

PDB ID : 3E6M / pdb_00003e6m
Title : The crystal structure of a MarR family transcriptional regulator from *Silicibacter pomeroyi* DSS.
Authors : Tan, K.; Volkart, L.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2008-08-15
Resolution : 2.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

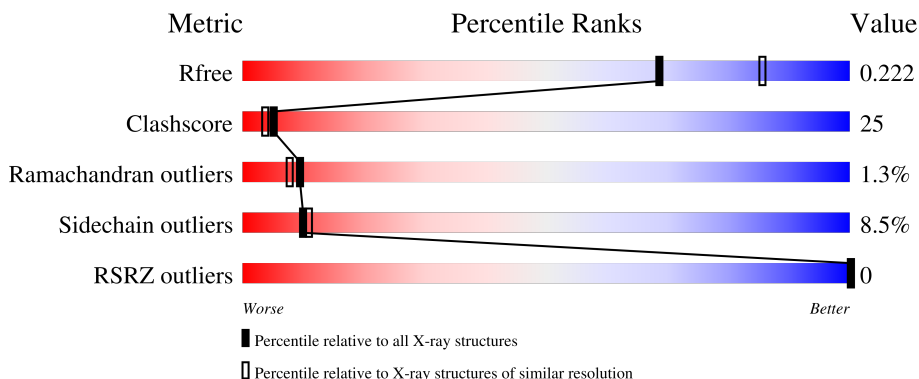
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	161	 52% 34% 5% 9%
1	B	161	 48% 37% 6% 9%
1	C	161	 47% 36% 7% 9%
1	D	161	 50% 39% . 7%
1	E	161	 50% 37% 5% 9%

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Mol	Chain	Length	Quality of chain
1	F	161	 54% 29% 7% • 9%
1	G	161	 46% 41% • • 8%
1	H	161	 57% 31% • 9%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9532 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 MarR family Transcriptional regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	146	1115	708	192	213	1	1	0	0	0
1	B	147	1132	717	192	221	1	1	0	0	0
1	C	146	1119	709	192	216	1	1	0	0	0
1	D	149	1142	723	194	223	1	1	0	0	0
1	E	147	1135	721	193	219	1	1	0	0	0
1	F	146	1128	715	192	219	1	1	0	0	0
1	G	148	1144	726	195	221	1	1	0	0	0
1	H	147	1132	717	192	221	1	1	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q5LLB9
A	-1	ASN	-	expression tag	UNP Q5LLB9
A	0	ALA	-	expression tag	UNP Q5LLB9
B	-2	SER	-	expression tag	UNP Q5LLB9
B	-1	ASN	-	expression tag	UNP Q5LLB9
B	0	ALA	-	expression tag	UNP Q5LLB9
C	-2	SER	-	expression tag	UNP Q5LLB9
C	-1	ASN	-	expression tag	UNP Q5LLB9
C	0	ALA	-	expression tag	UNP Q5LLB9
D	-2	SER	-	expression tag	UNP Q5LLB9
D	-1	ASN	-	expression tag	UNP Q5LLB9
D	0	ALA	-	expression tag	UNP Q5LLB9
E	-2	SER	-	expression tag	UNP Q5LLB9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	expression tag	UNP Q5LLB9
E	0	ALA	-	expression tag	UNP Q5LLB9
F	-2	SER	-	expression tag	UNP Q5LLB9
F	-1	ASN	-	expression tag	UNP Q5LLB9
F	0	ALA	-	expression tag	UNP Q5LLB9
G	-2	SER	-	expression tag	UNP Q5LLB9
G	-1	ASN	-	expression tag	UNP Q5LLB9
G	0	ALA	-	expression tag	UNP Q5LLB9
H	-2	SER	-	expression tag	UNP Q5LLB9
H	-1	ASN	-	expression tag	UNP Q5LLB9
H	0	ALA	-	expression tag	UNP Q5LLB9

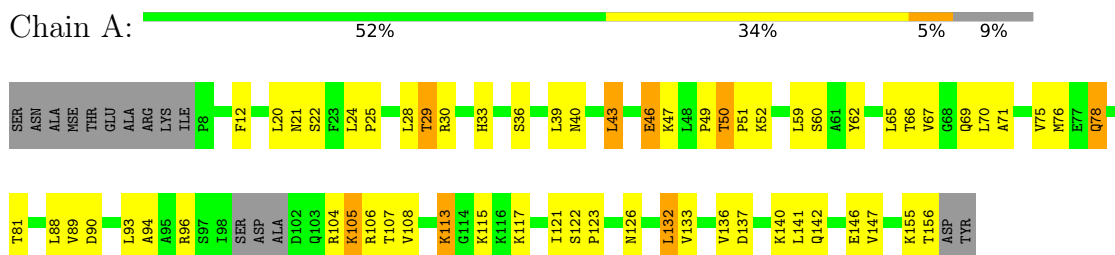
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	65	Total O 65 65	0	0
2	B	57	Total O 57 57	0	0
2	C	59	Total O 59 59	0	0
2	D	50	Total O 50 50	0	0
2	E	69	Total O 69 69	0	0
2	F	58	Total O 58 58	0	0
2	G	62	Total O 62 62	0	0
2	H	65	Total O 65 65	0	0

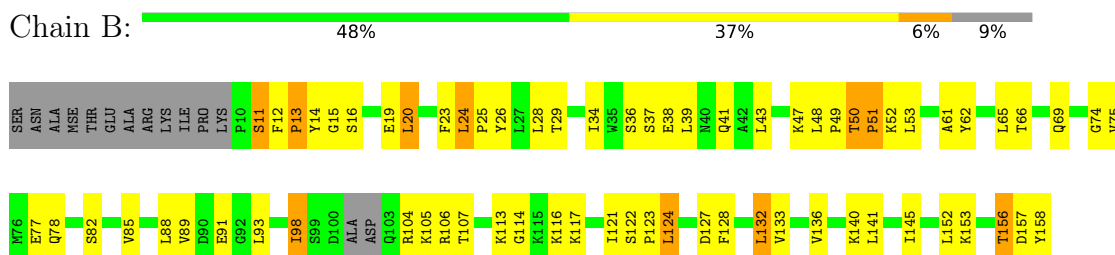
3 Residue-property plots [i](#)

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 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.

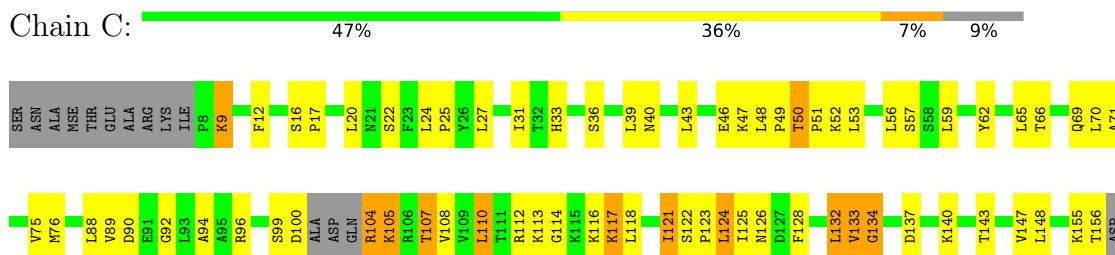
- Molecule 1: MarR family Transcriptional regulator



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- Molecule 1: MarR family Transcriptional regulator





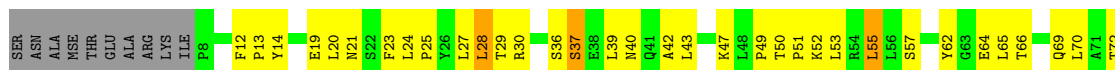
• Molecule 1: MarR family Transcriptional regulator



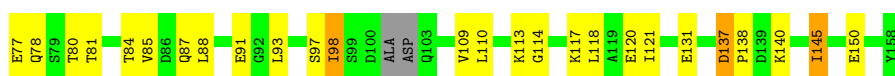
• Molecule 1: MarR family Transcriptional regulator



• Molecule 1: MarR family Transcriptional regulator



• Molecule 1: MarR family Transcriptional regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.43Å 93.20Å 101.56Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	39.60 – 2.20 39.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (39.60-2.20) 97.8 (39.60-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.185 , 0.230 0.185 , 0.222	Depositor DCC
R_{free} test set	3542 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtrriage
Anisotropy	0.756	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtrriage
Reported twinning fraction	0.486 for h,-k,-l	Depositor
Outliers	1 of 70328 reflections (0.001%)	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	9532	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3753e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [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	0.54	0/1131	0.91	0/1529
1	B	0.47	0/1148	0.95	1/1551 (0.1%)
1	C	0.56	0/1135	0.93	3/1534 (0.2%)
1	D	0.50	0/1159	0.95	2/1568 (0.1%)
1	E	0.52	0/1152	0.94	2/1556 (0.1%)
1	F	0.53	0/1144	0.94	4/1545 (0.3%)
1	G	0.54	0/1161	0.86	0/1568
1	H	0.50	0/1148	0.89	2/1551 (0.1%)
All	All	0.52	0/9178	0.92	14/12402 (0.1%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	122	SER	CA-C-N	-6.81	111.97	119.19
1	F	122	SER	C-N-CA	-6.81	111.97	119.19
1	F	11	SER	N-CA-C	6.35	124.33	110.80
1	F	12	PHE	N-CA-C	5.84	122.72	109.81
1	B	11	SER	N-CA-C	5.65	122.84	110.80

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	1115	0	1157	64	0
1	B	1132	0	1166	70	0
1	C	1119	0	1162	74	0
1	D	1142	0	1174	72	0
1	E	1135	0	1180	57	0
1	F	1128	0	1168	63	0
1	G	1144	0	1188	77	0
1	H	1132	0	1166	48	0
2	A	65	0	0	7	0
2	B	57	0	0	5	0
2	C	59	0	0	6	0
2	D	50	0	0	5	0
2	E	69	0	0	2	0
2	F	58	0	0	3	0
2	G	62	0	0	0	0
2	H	65	0	0	3	0
All	All	9532	0	9361	455	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 25.

The worst 5 of 455 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:G:156:THR:C	1:G:158:TYR:H	1.70	0.98
1:C:66:THR:HG21	1:C:105:LYS:HE3	1.45	0.97
1:F:40:ASN:HD21	1:F:50:THR:H	1.12	0.95
1:C:56:LEU:HB3	1:C:118:LEU:HD11	1.52	0.91
1:A:90:ASP:HB3	2:A:176:HOH:O	1.70	0.90

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	142/161 (88%)	131 (92%)	10 (7%)	1 (1%)	18	19
1	B	143/161 (89%)	124 (87%)	17 (12%)	2 (1%)	9	7
1	C	142/161 (88%)	126 (89%)	13 (9%)	3 (2%)	5	3
1	D	147/161 (91%)	122 (83%)	23 (16%)	2 (1%)	9	7
1	E	143/161 (89%)	134 (94%)	8 (6%)	1 (1%)	18	19
1	F	142/161 (88%)	134 (94%)	4 (3%)	4 (3%)	4	2
1	G	144/161 (89%)	132 (92%)	10 (7%)	2 (1%)	9	7
1	H	143/161 (89%)	134 (94%)	9 (6%)	0	100	100
All	All	1146/1288 (89%)	1037 (90%)	94 (8%)	15 (1%)	9	8

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	75	VAL
1	C	134	GLY
1	F	11	SER
1	F	134	GLY
1	G	157	ASP

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	125/138 (91%)	112 (90%)	13 (10%)	7	7
1	B	128/138 (93%)	117 (91%)	11 (9%)	10	10
1	C	127/138 (92%)	112 (88%)	15 (12%)	5	5
1	D	128/138 (93%)	119 (93%)	9 (7%)	14	16
1	E	129/138 (94%)	117 (91%)	12 (9%)	8	9
1	F	128/138 (93%)	119 (93%)	9 (7%)	14	16
1	G	130/138 (94%)	121 (93%)	9 (7%)	14	16
1	H	128/138 (93%)	119 (93%)	9 (7%)	14	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1023/1104 (93%)	936 (92%)	87 (8%)	10	11

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	121	ILE
1	G	55	LEU
1	E	152	LEU
1	F	67	VAL
1	G	121	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	129	HIS
1	G	69	GLN
1	G	40	ASN
1	G	129	HIS
1	C	78	GLN

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	145/161 (90%)	-1.20	0 100 100	42, 56, 90, 112	0
1	B	146/161 (90%)	-1.26	0 100 100	38, 62, 102, 129	0
1	C	145/161 (90%)	-1.22	0 100 100	27, 56, 89, 111	0
1	D	148/161 (91%)	-1.26	0 100 100	27, 59, 98, 120	0
1	E	146/161 (90%)	-1.24	0 100 100	37, 55, 90, 142	0
1	F	145/161 (90%)	-1.23	0 100 100	40, 60, 106, 154	0
1	G	147/161 (91%)	-1.28	0 100 100	34, 54, 98, 138	0
1	H	146/161 (90%)	-1.22	0 100 100	41, 58, 96, 146	0
All	All	1168/1288 (90%)	-1.24	0 100 100	27, 58, 98, 154	0

There are no RSRZ outliers to report.

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.