



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:00 am BST

PDB ID : 3BOQ  
Title : Crystal structure of MarR family transcriptional regulator from *Silicibacter pomeroyi*  
Authors : Chang, C.; Volkart, L.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2007-12-17  
Resolution : 2.39 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](mailto: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 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

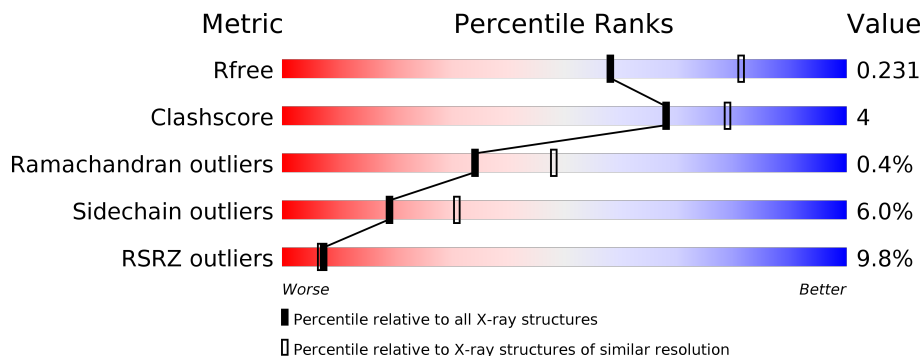
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	160	
1	B	160	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2144 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 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	136	1040	642	192	201	5	0	2	0
1	B	138	1056	655	195	201	5	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q5LLB8
A	-1	ASN	-	EXPRESSION TAG	UNP Q5LLB8
A	0	ALA	-	EXPRESSION TAG	UNP Q5LLB8
B	-2	SER	-	EXPRESSION TAG	UNP Q5LLB8
B	-1	ASN	-	EXPRESSION TAG	UNP Q5LLB8
B	0	ALA	-	EXPRESSION TAG	UNP Q5LLB8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total 26	O 26	0	0
2	B	22	Total 22	O 22	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.57Å 110.57Å 68.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.96 – 2.39 24.96 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.7 (24.96-2.39) 97.8 (24.96-2.39)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.76 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.203 , 0.233 0.201 , 0.231	Depositor DCC
$R_{free}$ test set	958 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtrriage
Anisotropy	0.593	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.105 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.68	0/1041	0.71	1/1390 (0.1%)
1	B	0.72	1/1058 (0.1%)	0.75	0/1413
All	All	0.70	1/2099 (0.0%)	0.73	1/2803 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	GLU	CB-CG	5.62	1.62	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH2	-5.66	117.47	120.30

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	1040	0	1060	10	0
1	B	1056	0	1072	9	0
2	A	26	0	0	0	0
2	B	22	0	0	0	0
All	All	2144	0	2132	16	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 4.

All (16) 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:A:8:SER:OG	1:A:11:GLN:HG3	1.70	0.92
1:A:50:MSE:HE2	1:A:113:PHE:HB2	1.90	0.53
1:B:36:LEU:O	1:B:40:THR:HB	2.09	0.51
1:A:14:GLN:HG2	1:B:136:MSE:SE	2.62	0.49
1:B:40:THR:HG22	1:B:42:LEU:HB2	1.95	0.48
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.80	0.47
1:B:35:GLN:O	1:B:39:GLU:HG3	2.15	0.46
1:A:88:MSE:HE1	1:A:112:THR:HG21	1.97	0.46
1:A:10:ARG:NH1	1:B:136:MSE:HE2	2.31	0.46
1:B:62:MSE:HE1	1:B:76:VAL:HG22	1.98	0.46
1:A:62:MSE:HE1	1:A:80:VAL:HG21	1.98	0.44
1:A:23:ARG:HG3	1:A:23:ARG:HH11	1.83	0.44
1:B:29:PHE:CE1	1:B:44:LEU:HD23	2.54	0.43
1:B:73:ASN:HB3	1:B:74:GLY:H	1.43	0.43
1:A:10:ARG:NH1	1:B:136:MSE:CE	2.82	0.42
1:A:88:MSE:CE	1:A:112:THR:HG21	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	134/160 (84%)	132 (98%)	2 (2%)	0	100	100
1	B	136/160 (85%)	132 (97%)	3 (2%)	1 (1%)	22	32
All	All	270/320 (84%)	264 (98%)	5 (2%)	1 (0%)	34	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	75	ASN

### 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	110/120 (92%)	104 (94%)	6 (6%)	21	35
1	B	110/120 (92%)	103 (94%)	7 (6%)	17	28
All	All	220/240 (92%)	207 (94%)	13 (6%)	19	32

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	72	THR
1	A	73	ASN
1	A	81	ASN
1	A	102	SER
1	A	134	GLN
1	B	19	LEU
1	B	42	LEU
1	B	43	SER
1	B	58	ASP
1	B	69	LEU
1	B	105	LEU
1	B	140	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	131/160 (81%)	1.01	10 (7%) 13 12	54, 71, 78, 89	0
1	B	133/160 (83%)	1.00	16 (12%) 4 3	47, 63, 73, 82	0
All	All	264/320 (82%)	1.01	26 (9%) 7 7	47, 68, 77, 89	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	ALA	3.9
1	B	148[A]	GLU	3.7
1	B	100	SER	3.4
1	A	74	GLY	3.2
1	B	55	ARG	2.9
1	A	148[A]	GLU	2.9
1	A	38[A]	ASP	2.8
1	B	74	GLY	2.7
1	A	60	LEU	2.6
1	A	111	THR	2.5
1	B	75	ASN	2.5
1	A	92	ALA	2.4
1	B	76	VAL	2.4
1	B	72	THR	2.3
1	A	91	LYS	2.3
1	A	79	LEU	2.2
1	B	63	GLY	2.2
1	B	65	LEU	2.2
1	B	144	ARG	2.1
1	A	28	VAL	2.1
1	B	131	VAL	2.1
1	B	101	PHE	2.1
1	A	34	ARG	2.1
1	B	58	ASP	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	141	ALA	2.0
1	B	64	LYS	2.0

## 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 carbohydrates 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.