



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 09:45 am BST

PDB ID : 3MWG
Title : Crystal structure of Staphylococcus aureus SirA
Authors : Grigg, J.C.; Murphy, M.E.P.
Deposited on : 2010-05-05
Resolution : 2.10 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 ⓘ 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

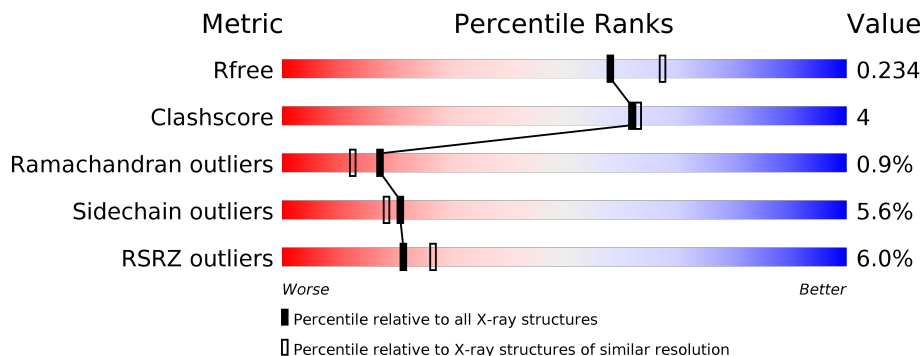
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 ≥ 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	279	
1	B	279	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4597 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 Iron-regulated ABC transporter siderophore-binding protein SirA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	276	2183	1389	366	426	2	0	0	0
1	B	274	2168	1381	363	422	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLY	-	EXPRESSION TAG	UNP Q7A869
A	53	SER	-	EXPRESSION TAG	UNP Q7A869
B	52	GLY	-	EXPRESSION TAG	UNP Q7A869
B	53	SER	-	EXPRESSION TAG	UNP Q7A869

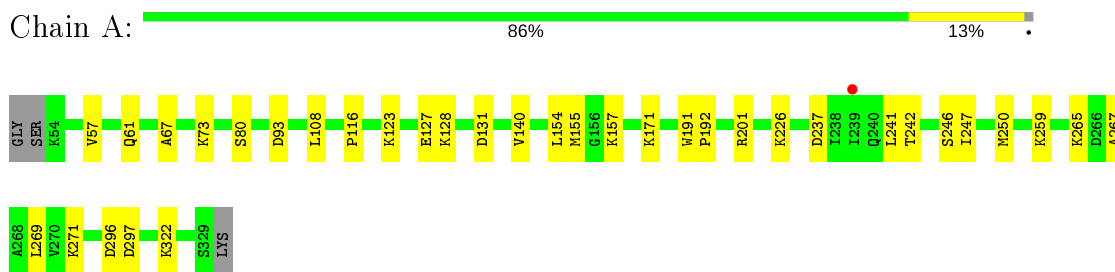
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total 177	O 177	0	0
2	B	69	Total 69	O 69	0	0

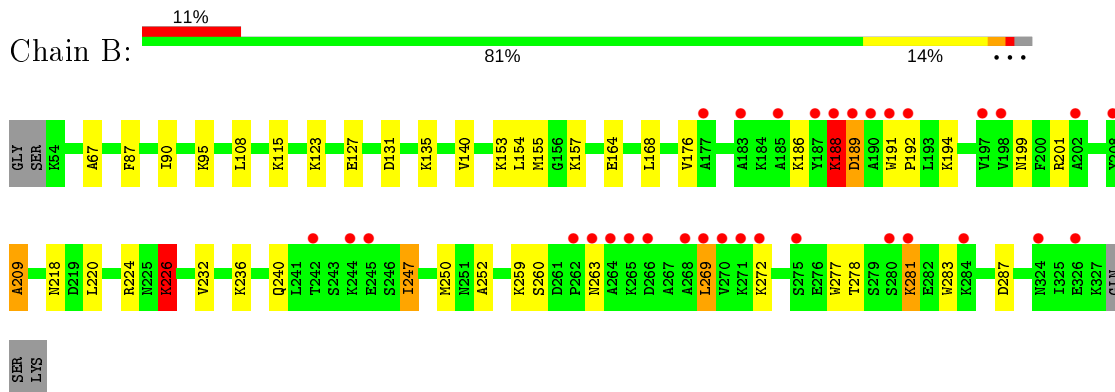
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Iron-regulated ABC transporter siderophore-binding protein SirA



- Molecule 1: Iron-regulated ABC transporter siderophore-binding protein SirA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.14Å 61.51Å 114.65Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	31.65 – 2.10 31.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.6 (31.65-2.10) 99.1 (31.65-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.08Å)	Xtrriage
Refinement program	REFMAC refmac_5.5.0109	Depositor
R, R_{free}	0.192 , 0.236 0.191 , 0.234	Depositor DCC
R_{free} test set	1724 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4597	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.64	0/2217	0.65	0/2985
1	B	0.52	0/2202	0.59	0/2965
All	All	0.58	0/4419	0.62	0/5950

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	2183	0	2233	13	0
1	B	2168	0	2220	27	0
2	A	177	0	0	2	0
2	B	69	0	0	0	0
All	All	4597	0	4453	39	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 (39) 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:73:LYS:HD2	1:A:93:ASP:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LYS:H	1:B:281:LYS:HD2	1.45	0.82
1:B:188:LYS:O	1:B:189:ASP:HB2	1.85	0.75
1:A:267:ALA:O	1:A:271:LYS:HG2	1.97	0.64
1:B:191:TRP:CD2	1:B:192:PRO:HA	2.34	0.62
1:A:247:ILE:O	1:A:250:MSE:HG2	2.01	0.61
1:A:67:ALA:HB2	1:A:155:MSE:HE1	1.83	0.61
1:B:153:LYS:O	1:B:157:LYS:HG2	2.00	0.60
1:B:131:ASP:O	1:B:135:LYS:HG3	2.05	0.57
1:B:218:ASN:ND2	1:B:224:ARG:HH22	2.03	0.55
1:B:269:LEU:H	1:B:269:LEU:HD22	1.74	0.52
1:B:247:ILE:O	1:B:250:MSE:HG2	2.09	0.52
1:B:218:ASN:HD22	1:B:224:ARG:HH22	1.59	0.51
1:B:67:ALA:HB2	1:B:155:MSE:HE1	1.92	0.51
1:B:188:LYS:HE2	1:B:191:TRP:HB3	1.93	0.50
1:B:194:LYS:O	1:B:252:ALA:HB1	2.11	0.50
1:A:123:LYS:O	1:A:127:GLU:HB2	2.11	0.49
1:A:322:LYS:HE3	2:A:378:HOH:O	2.14	0.48
1:B:281:LYS:HD2	1:B:281:LYS:N	2.23	0.47
1:B:123:LYS:O	1:B:127:GLU:HB2	2.14	0.47
1:B:278:THR:HA	1:B:283:TRP:CD1	2.51	0.46
1:A:237:ASP:OD2	2:A:433:HOH:O	2.21	0.46
1:B:278:THR:HG22	1:B:283:TRP:CE2	2.52	0.45
1:B:87:PHE:HB2	1:B:90:ILE:HG22	1.99	0.45
1:B:281:LYS:H	1:B:281:LYS:CD	2.25	0.44
1:A:191:TRP:CD2	1:A:192:PRO:HA	2.53	0.43
1:B:188:LYS:HA	1:B:188:LYS:HE2	2.00	0.43
1:B:226:LYS:HD2	1:B:226:LYS:N	2.34	0.43
1:A:241:LEU:HD22	1:A:246:SER:HB3	2.01	0.42
1:B:140:VAL:HB	1:B:154:LEU:HD21	2.01	0.42
1:B:176:VAL:HG13	1:B:220:LEU:HD23	2.01	0.42
1:A:57:VAL:HG23	1:A:116:PRO:HB3	2.02	0.42
1:B:209:ALA:HB1	1:B:232:VAL:HG22	2.03	0.41
1:A:61:GLN:OE1	1:A:80:SER:HA	2.21	0.41
1:B:199:ASN:OD1	1:B:201:ARG:NE	2.51	0.41
1:A:140:VAL:HB	1:A:154:LEU:HD21	2.02	0.41
1:A:131:ASP:OD2	1:B:123:LYS:HE2	2.21	0.40
1:B:247:ILE:HD11	1:B:277:TRP:CE3	2.55	0.40
1:B:164:GLU:O	1:B:168:LEU:HG	2.21	0.40

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	274/279 (98%)	268 (98%)	6 (2%)	0	100	100
1	B	272/279 (98%)	260 (96%)	7 (3%)	5 (2%)	8	4
All	All	546/558 (98%)	528 (97%)	13 (2%)	5 (1%)	17	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	189	ASP
1	B	209	ALA
1	B	188	LYS
1	B	226	LYS
1	B	260	SER

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	240/240 (100%)	228 (95%)	12 (5%)	24	23
1	B	238/240 (99%)	223 (94%)	15 (6%)	18	15
All	All	478/480 (100%)	451 (94%)	27 (6%)	21	18

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU

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Mol	Chain	Res	Type
1	A	128	LYS
1	A	157	LYS
1	A	171	LYS
1	A	201	ARG
1	A	226	LYS
1	A	242	THR
1	A	259	LYS
1	A	265	LYS
1	A	269	LEU
1	A	296	ASP
1	A	297	ASP
1	B	95	LYS
1	B	108	LEU
1	B	115	LYS
1	B	186	LYS
1	B	188	LYS
1	B	226	LYS
1	B	236	LYS
1	B	240	GLN
1	B	247	ILE
1	B	259	LYS
1	B	263	ASN
1	B	269	LEU
1	B	272	LYS
1	B	281	LYS
1	B	287	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	263	ASN
1	A	328	GLN
1	B	102	GLN
1	B	218	ASN
1	B	285	ASN
1	B	293	GLN

5.3.3 RNA

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

6.1 Protein, DNA and RNA chains

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	274/279 (98%)	-0.29	1 (0%) 92 93	17, 27, 46, 54	0
1	B	272/279 (97%)	0.60	32 (11%) 4 5	20, 49, 85, 90	0
All	All	546/558 (97%)	0.15	33 (6%) 21 27	17, 34, 78, 90	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	ASP	6.6
1	B	190	ALA	5.6
1	B	281	LYS	5.5
1	B	202	ALA	4.2
1	B	245	GLU	4.1
1	B	268	ALA	4.0
1	B	189	ASP	3.9
1	B	265	LYS	3.8
1	B	188	LYS	3.6
1	B	185	ALA	3.6
1	B	262	PRO	3.5
1	B	272	LYS	3.3
1	B	197	VAL	3.2
1	B	244	LYS	3.1
1	B	326	GLU	3.0
1	B	208	TYR	2.7
1	B	198	VAL	2.7
1	B	187	TYR	2.7
1	B	275	SER	2.6
1	B	264	ALA	2.6
1	B	263	ASN	2.6
1	B	242	THR	2.5
1	B	284	LYS	2.5
1	B	324	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	269	LEU	2.4
1	B	280	SER	2.4
1	B	191	TRP	2.4
1	B	192	PRO	2.3
1	B	177	ALA	2.2
1	A	239	ILE	2.1
1	B	183	ALA	2.1
1	B	270	VAL	2.1
1	B	271	LYS	2.1

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.