wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:31 PM GMT

PDB ID	:	1FZP
Title	:	CRYSTAL STRUCTURES OF SARA: A PLEIOTROPIC REGULATOR OF VIRULENCE GENES IN S. AUREUS
Authors	:	Schumacher, M.A.; Hurlburt, B.; Brennan, R.G.
Deposited on	:	2000-10-03
Resolution	:	2.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

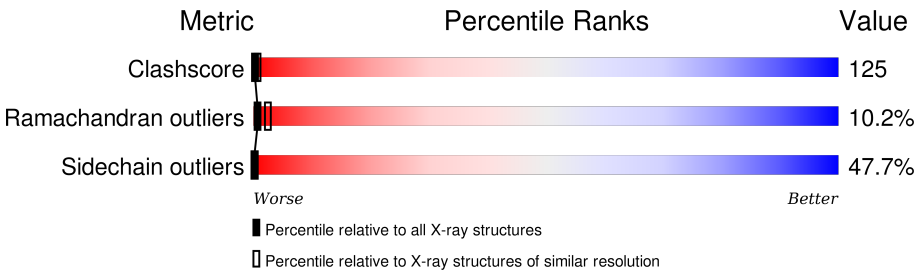
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.95 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	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)

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. 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% 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	K	7	100%
1	W	7	100%
2	B	123	7% 33% 34% 11% 15%
2	D	123	9% 32% 31% 10% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1997 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 DNA chain called 5'-D(P*AP*TP*AP*TP*AP*TP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	W	7	144	70	26	41	7	0	0	0
1	K	7	144	70	26	41	7	0	0	0

- Molecule 2 is a protein called STAPHYLOCOCCAL ACCESSORY REGULATOR A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	100	832	537	135	158	2	0	0	0
2	B	105	875	563	145	165	2	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	B	1	1	1	0	0
3	D	1	1	1	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 errors 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.

Note EDS was not executed.

- Molecule 1: 5'-D(P*AP*TP*AP*TP*AP*TP*A)-3'

Chain W:

A3 T4 A5 T6 A7 T8 A9

- Molecule 1: 5'-D(P*AP*TP*AP*TP*AP*TP*A)-3'

Chain K:

A3 T4 A5 T6 A7 T8 A9

- Molecule 2: STAPHYLOCOCCAL ACCESSORY REGULATOR A

Chain D:

A2 I3 T4 K5 I6 N7 D8 C9 F10 E11 L12 L13 S14 M15 V16 T17 Y18 A19 D20 K21 L22 K23 S24 L25 I26 K27 K28 E29 F30 S31 I32 S33 F34 E35 E36 F37 A38 V39 L40 T41 Y42 I43 S44 E45 N46 K47 E48 K49 E50 Y51 Y52 L53 K54 D55 I56 ILE ASN HIS LEU ASN

TYR LYS GLN PRO GLN V67 V68 K69 A70 V71 K72 I73 L74 S75 Q76 E77 D78 Y79 F80 K83 R84 N85 E86 H87 D88 E89 R90 T91 V92 L93 I94 L95 V96 N97 A98 Q99 Q100 R101 K102 K103 I104 E105 S106 L107 L108 S109 R110 V111 ASN LYS ARG ILE THR GLU ALA ASN ASN GLU ILE

GLU LEU

- Molecule 2: STAPHYLOCOCCAL ACCESSORY REGULATOR A

Chain B:

A2 I3 T4 K5 I6 N7 D8 C9 F10 E11 L12 L13 S14 M15 V16 T17 Y18 A19 D20 K21 L22 K23 S24 L25 I26 K27 K28 E29 F30 S31 I32 S33 F34 E35 E36 F37 A38 V39 L40 T41 Y42 I43 S44 E45 N46 K47 E48 K49 E50 Y51 Y52 L53 K54 D55 I56 ILE ASN HIS LEU ASN

TYR LYS GLN PRO GLN V67 V68 K69 I73 L74 S75 Q76 E77 D78 Y79 F80 D81 K82 K83 R84 N85 E86 H87 D88 E89 R90 T91 V92 L93 I94 L95 V96 N97 A98 Q99 Q100 R101 K102 K103 I104 E105 S106 L107 L108 S109 R110 V111 N112 K113 R114 I115 T116 GLU ALA ASN ASN GLU ILE GLU

LEU

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.50Å 65.20Å 57.80Å 90.00° 118.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.95	Depositor
% Data completeness (in resolution range)	89.0 (10.00-2.95)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.220 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1997	wwPDB-VP
Average B, all atoms (Å^2)	43.0	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: CA

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	K	1.85	4/161 (2.5%)	2.87	17/246 (6.9%)
1	W	1.93	5/161 (3.1%)	2.82	18/246 (7.3%)
2	B	0.87	1/884 (0.1%)	1.51	16/1181 (1.4%)
2	D	0.99	1/841 (0.1%)	1.51	19/1124 (1.7%)
All	All	1.14	11/2047 (0.5%)	1.82	70/2797 (2.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	1	0
2	D	1	0
All	All	2	0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	9	CYS	CB-SG	8.80	1.97	1.82
1	W	8	DT	C5'-C4'	7.80	1.59	1.51
1	W	4	DT	C5-C7	7.73	1.54	1.50
1	K	4	DT	C5-C7	7.56	1.54	1.50
1	K	8	DT	C5-C7	6.30	1.53	1.50

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	8	DT	O4'-C4'-C3'	-18.45	94.93	106.00
1	K	3	DA	O5'-P-OP2	-18.20	88.86	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	3	DA	OP1-P-OP2	16.08	143.72	119.60
1	K	8	DT	O4'-C4'-C3'	-11.99	98.81	106.00
1	W	7	DA	O4'-C4'-C3'	-11.91	98.86	106.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	43	ILE	CA
2	B	13	LEU	CA

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	K	144	0	81	43	0
1	W	144	0	81	46	0
2	B	875	0	916	210	0
2	D	832	0	866	235	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
All	All	1997	0	1944	489	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 125.

The worst 5 of 489 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)
2:D:8:ASP:HB2	2:D:13:LEU:CD2	1.24	1.59
1:W:5:DA:H61	1:K:5:DA:N6	1.17	1.41
1:W:5:DA:N6	1:K:5:DA:H61	1.17	1.34
1:W:3:DA:N1	1:K:7:DA:N6	1.83	1.27
2:D:8:ASP:CB	2:D:13:LEU:CD2	2.20	1.18

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
2	B	101/123 (82%)	73 (72%)	19 (19%)	9 (9%)	1 4
2	D	96/123 (78%)	72 (75%)	13 (14%)	11 (12%)	0 2
All	All	197/246 (80%)	145 (74%)	32 (16%)	20 (10%)	1 2

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	3	ILE
2	D	30	PHE
2	D	31	SER
2	D	100	GLN
2	B	3	ILE

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
2	B	100/117 (86%)	50 (50%)	50 (50%)	0 0
2	D	95/117 (81%)	52 (55%)	43 (45%)	0 0
All	All	195/234 (83%)	102 (52%)	93 (48%)	0 0

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	111	VAL
2	B	28	LYS
2	B	107	LEU
2	B	3	ILE
2	B	11	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	7	ASN
2	B	99	GLN
2	B	76	GLN
2	D	99	GLN
2	B	85	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 carbohydrates 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.