Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 03:28 PM EDT

PDB ID	:	5KSS
Title	:	Stationary phase survival protein E (SurE) from Xylella fastidiosa - XFSurE-Ds (Dimer Smaller)
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Deposited on	:	2016-07-09
Resolution	:	2.82 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 (1)) were used in the production of this report:

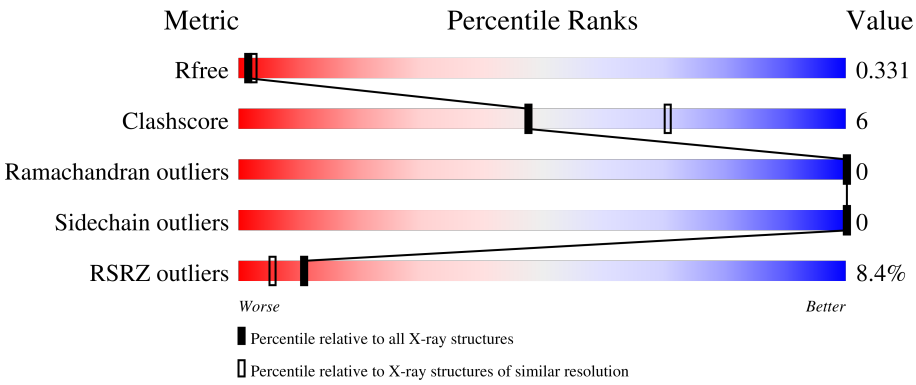
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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% 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	270	7% 81% 12% 7%
1	B	270	9% 78% 14% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	505	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3825 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 5'-nucleotidase SurE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	252	1913	1193	341	372	7	97	0	0
1	B	249	1887	1176	338	366	7	96	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	-	expression tag	UNP Q9PF20
A	264	GLU	-	expression tag	UNP Q9PF20
A	265	HIS	-	expression tag	UNP Q9PF20
A	266	HIS	-	expression tag	UNP Q9PF20
A	267	HIS	-	expression tag	UNP Q9PF20
A	268	HIS	-	expression tag	UNP Q9PF20
A	269	HIS	-	expression tag	UNP Q9PF20
A	270	HIS	-	expression tag	UNP Q9PF20
B	263	LEU	-	expression tag	UNP Q9PF20
B	264	GLU	-	expression tag	UNP Q9PF20
B	265	HIS	-	expression tag	UNP Q9PF20
B	266	HIS	-	expression tag	UNP Q9PF20
B	267	HIS	-	expression tag	UNP Q9PF20
B	268	HIS	-	expression tag	UNP Q9PF20
B	269	HIS	-	expression tag	UNP Q9PF20
B	270	HIS	-	expression tag	UNP Q9PF20

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total I 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is water.

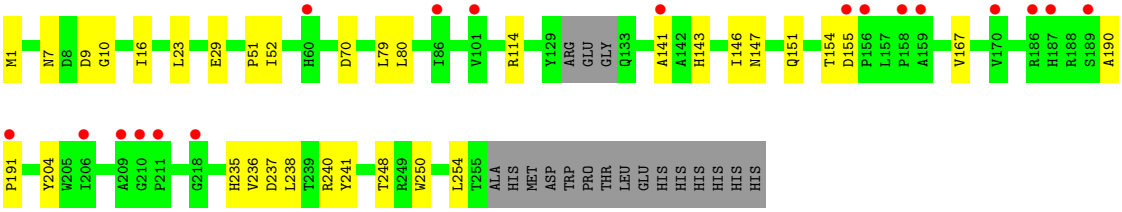
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	11	Total O 11 11	0	0
5	B	7	Total O 7 7	0	0

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.

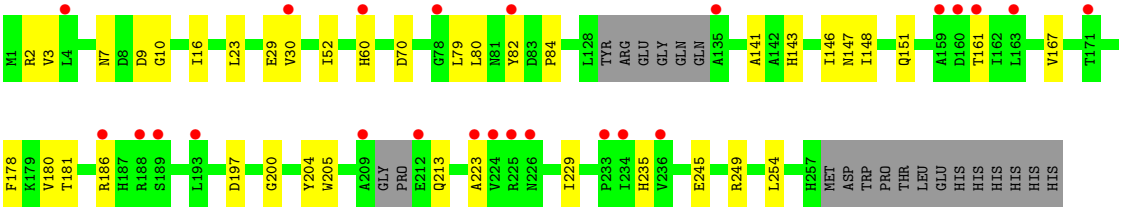
- Molecule 1: 5'-nucleotidase SurE

Chain A:



- Molecule 1: 5'-nucleotidase SurE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.94Å 80.12Å 71.51Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	43.94 – 2.82 58.79 – 2.82	Depositor EDS
% Data completeness (in resolution range)	82.4 (43.94-2.82) 82.4 (58.79-2.82)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.272 , 0.329 0.274 , 0.331	Depositor DCC
R_{free} test set	489 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	3825	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, CL, MN

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	0.20	0/1951	0.39	0/2672
1	B	0.20	0/1923	0.39	0/2632
All	All	0.20	0/3874	0.39	0/5304

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	1913	0	1888	25	0
1	B	1887	0	1864	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	11	0	0	0	0
5	B	7	0	0	0	0
All	All	3825	0	3752	43	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 6.

All (43) 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:235:HIS:NE2	3:A:505:IOD:I	2.95	0.69
1:A:235:HIS:CE1	3:A:505:IOD:I	3.17	0.67
1:B:181:THR:HG21	1:B:223:ALA:HB2	1.86	0.58
1:B:143:HIS:O	1:B:147:ASN:ND2	2.38	0.56
1:B:178:PHE:HE1	1:B:229:ILE:HD12	1.71	0.56
1:A:114:ARG:HG2	1:A:236:VAL:HG11	1.87	0.56
1:A:143:HIS:O	1:A:147:ASN:ND2	2.38	0.56
1:A:79:LEU:HD13	1:B:204:TYR:HE2	1.72	0.55
1:B:7:ASN:HD22	1:B:16:ILE:HD12	1.75	0.52
1:B:30:VAL:O	1:B:60:HIS:ND1	2.40	0.51
1:A:240:ARG:HD3	1:B:161:THR:HB	1.91	0.51
1:A:23:LEU:HD23	1:A:146:ILE:HG22	1.94	0.50
1:A:52:ILE:HD13	1:A:70:ASP:HB3	1.94	0.50
1:A:7:ASN:HD22	1:A:16:ILE:HD12	1.76	0.49
1:A:79:LEU:HG	1:A:80:LEU:HG	1.95	0.49
1:B:2:ARG:HB2	1:B:84:PRO:HA	1.95	0.48
1:B:23:LEU:HD23	1:B:146:ILE:HG22	1.94	0.48
1:B:52:ILE:HD13	1:B:70:ASP:HB3	1.94	0.48
1:B:79:LEU:HG	1:B:80:LEU:HG	1.96	0.48
1:B:29:GLU:O	1:B:82:TYR:OH	2.32	0.48
1:B:178:PHE:CE1	1:B:229:ILE:HD12	2.49	0.47
1:A:1:MET:O	1:A:29:GLU:N	2.43	0.47
1:B:245:GLU:HG2	1:B:249:ARG:HH12	1.80	0.47
1:A:79:LEU:HD13	1:B:204:TYR:CE2	2.49	0.47
1:A:237:ASP:OD2	1:A:241:TYR:OH	2.26	0.46
1:A:254:LEU:HD13	1:B:151:GLN:HB2	1.97	0.46
1:B:3:VAL:HG11	1:B:23:LEU:HD13	1.97	0.46
1:A:141:ALA:HA	1:A:167:VAL:HG21	1.98	0.45
1:B:197:ASP:OD1	1:B:200:GLY:N	2.49	0.45
1:B:141:ALA:HA	1:B:167:VAL:HG21	1.98	0.45
1:A:7:ASN:OD1	1:A:9:ASP:N	2.50	0.45
1:A:238:LEU:O	1:B:235:HIS:N	2.35	0.44
1:A:204:TYR:HE2	1:B:79:LEU:HD13	1.82	0.43
1:B:7:ASN:OD1	1:B:9:ASP:N	2.50	0.43
1:A:248:THR:HA	1:B:180:VAL:HG21	2.01	0.43
1:A:7:ASN:OD1	1:A:10:GLY:N	2.51	0.43
1:A:250:TRP:HH2	1:B:148:ILE:HG23	1.83	0.43
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ASN:OD1	1:B:10:GLY:N	2.52	0.42
1:A:151:GLN:HB2	1:B:254:LEU:HD13	2.02	0.41
1:A:154:THR:OG1	1:A:155:ASP:N	2.54	0.41
1:A:51:PRO:HD3	1:B:205:TRP:CZ2	2.56	0.40
1:B:186:ARG:HA	1:B:213:GLN:HB2	2.03	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	248/270 (92%)	229 (92%)	19 (8%)	0	100	100
1	B	243/270 (90%)	223 (92%)	20 (8%)	0	100	100
All	All	491/540 (91%)	452 (92%)	39 (8%)	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	208/224 (93%)	208 (100%)	0	100	100
1	B	205/224 (92%)	205 (100%)	0	100	100
All	All	413/448 (92%)	413 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	143	HIS
1	B	143	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 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)

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	252/270 (93%)	0.60	18 (7%)	16	9	49, 73, 127, 152	25 (9%)
1	B	249/270 (92%)	0.77	24 (9%)	8	4	51, 83, 124, 165	23 (9%)
All	All	501/540 (92%)	0.69	42 (8%)	11	5	49, 79, 125, 165	48 (9%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	SER	5.3
1	B	135	ALA	4.9
1	A	159	ALA	4.6
1	A	209	ALA	4.3
1	A	155	ASP	4.2
1	B	186	ARG	4.0
1	B	225	ARG	4.0
1	B	161	THR	3.9
1	B	224	VAL	3.8
1	A	141	ALA	3.6
1	A	156	PRO	3.5
1	B	189	SER	3.4
1	B	60	HIS	3.3
1	B	226	ASN	3.2
1	B	163	LEU	3.1
1	B	78	GLY	3.0
1	A	218	GLY	3.0
1	B	160	ASP	2.9
1	B	30	VAL	2.8
1	B	193	LEU	2.8
1	A	158	PRO	2.7
1	A	191	PRO	2.6
1	B	212	GLU	2.5
1	A	186	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	206	ILE	2.4
1	A	60	HIS	2.3
1	B	82	TYR	2.3
1	B	233	PRO	2.2
1	B	223	ALA	2.2
1	A	187	HIS	2.2
1	B	209	ALA	2.1
1	B	188	ARG	2.1
1	B	4	LEU	2.1
1	A	86	ILE	2.1
1	B	234	ILE	2.1
1	B	171	THR	2.1
1	B	236	VAL	2.1
1	A	210	GLY	2.1
1	A	101	VAL	2.1
1	B	159	ALA	2.0
1	A	170	VAL	2.0
1	A	211	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	B	502	1/1	0.90	0.12	77,77,77,77	0
3	IOD	A	502	1/1	0.92	0.19	102,102,102,102	1
4	CL	A	504	1/1	0.93	0.21	60,60,60,60	0
3	IOD	A	503	1/1	0.95	0.14	75,75,75,75	1
2	MN	A	501	1/1	0.97	0.18	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	B	501	1/1	0.98	0.14	66,66,66,66	0
3	IOD	A	505	1/1	0.98	0.05	71,71,71,71	1

6.5 Other polymers (i)

There are no such residues in this entry.