



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6Z0F / pdb_00006z0f
Title : Crystal structure of the membrane pseudokinase YukC/EssB from *Bacillus subtilis* T7SS
Authors : Tassinari, M.; Bellinzoni, M.; Alzari, P.M.; Fronzes, R.; Gubellini, F.
Deposited on : 2020-05-08
Resolution : 2.55 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 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
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

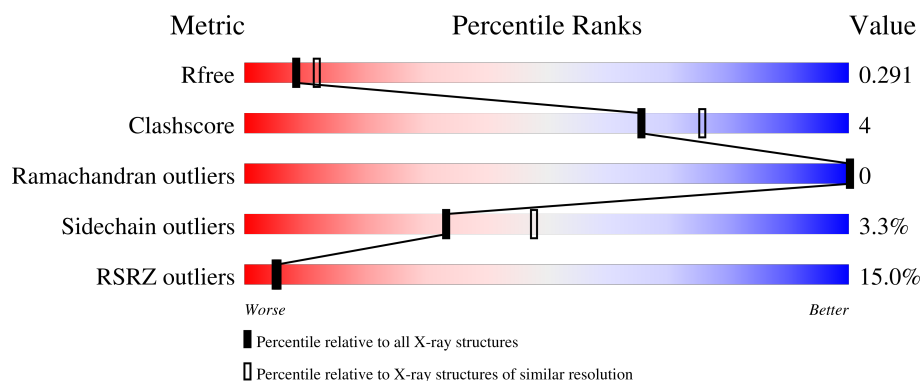
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	423	10% 82% 8% 9%
1	B	423	16% 77% 10% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5835 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 ESX secretion system protein YukC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2996	1932	480	582	2			
1	B	369	Total	C	N	O	S	0	0	0
			2831	1828	454	547	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	414	TRP	-	expression tag	UNP P71070
A	415	SER	-	expression tag	UNP P71070
A	416	HIS	-	expression tag	UNP P71070
A	417	PRO	-	expression tag	UNP P71070
A	418	GLN	-	expression tag	UNP P71070
A	419	PHE	-	expression tag	UNP P71070
A	420	GLU	-	expression tag	UNP P71070
A	421	LYS	-	expression tag	UNP P71070
A	422	ALA	-	expression tag	UNP P71070
A	423	ALA	-	expression tag	UNP P71070
B	414	TRP	-	expression tag	UNP P71070
B	415	SER	-	expression tag	UNP P71070
B	416	HIS	-	expression tag	UNP P71070
B	417	PRO	-	expression tag	UNP P71070
B	418	GLN	-	expression tag	UNP P71070
B	419	PHE	-	expression tag	UNP P71070
B	420	GLU	-	expression tag	UNP P71070
B	421	LYS	-	expression tag	UNP P71070
B	422	ALA	-	expression tag	UNP P71070
B	423	ALA	-	expression tag	UNP P71070

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total 6	O 6	0	0
2	B	2	Total 2	O 2	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.01Å 83.41Å 106.44Å 90.00° 108.16° 90.00°	Depositor
Resolution (Å)	29.42 – 2.55 29.42 – 2.55	Depositor EDS
% Data completeness (in resolution range)	65.0 (29.42-2.55) 64.9 (29.42-2.55)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.235 , 0.269 0.253 , 0.291	Depositor DCC
R_{free} test set	1333 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	73.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5835	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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	0.61	0/3063	0.97	6/4176 (0.1%)
1	B	0.61	0/2894	0.99	5/3949 (0.1%)
All	All	0.61	0/5957	0.98	11/8125 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	VAL	N-CA-CB	8.95	116.14	110.50
1	A	230	VAL	N-CA-CB	8.07	115.59	110.50
1	A	42	ASN	CA-CB-CG	7.37	119.97	112.60
1	B	42	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	346	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	102	LEU	CA-C-N	5.15	127.49	120.54
1	B	102	LEU	C-N-CA	5.15	127.49	120.54
1	B	51	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	51	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	102	LEU	CA-C-N	5.03	127.33	120.54
1	A	102	LEU	C-N-CA	5.03	127.33	120.54

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	2996	0	2797	25	0
1	B	2831	0	2623	31	0
2	A	6	0	0	0	0
2	B	2	0	0	0	0
All	All	5835	0	5420	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 4.

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:179:ALA:HB1	1:A:192:LEU:HD11	1.61	0.82
1:A:215:TRP:CD2	1:B:208:ILE:HD13	2.30	0.67
1:B:179:ALA:HB1	1:B:192:LEU:HD11	1.81	0.63
1:A:230:VAL:HG23	1:A:231:PRO:HD3	1.81	0.62
1:B:230:VAL:HG23	1:B:231:PRO:HD3	1.83	0.60
1:A:215:TRP:CG	1:B:208:ILE:HD11	2.37	0.59
1:A:215:TRP:CD1	1:B:208:ILE:HD11	2.38	0.58
1:B:215:TRP:HE1	1:B:219:ARG:NH2	2.02	0.58
1:A:228:LEU:HD23	1:B:229:LEU:HD21	1.86	0.56
1:A:209:HIS:ND1	1:B:209:HIS:ND1	2.41	0.54
1:A:229:LEU:HD21	1:B:228:LEU:HD23	1.89	0.54
1:A:250:ILE:HD12	1:B:247:HIS:CE1	2.45	0.51
1:B:141:GLU:HG2	1:B:145:GLN:HE21	1.77	0.50
1:B:140:GLU:H	1:B:140:GLU:CD	2.20	0.49
1:A:215:TRP:CE2	1:A:219:ARG:HD2	2.48	0.48
1:A:215:TRP:CE2	1:B:208:ILE:HD13	2.48	0.48
1:A:215:TRP:CG	1:B:208:ILE:CD1	2.96	0.48
1:A:230:VAL:CG2	1:A:231:PRO:HD3	2.44	0.48
1:A:39:LEU:HB3	1:A:42:ASN:HB3	1.96	0.48
1:B:208:ILE:HD12	1:B:210:ILE:HG12	1.96	0.47
1:A:215:TRP:CD2	1:B:208:ILE:CD1	2.97	0.47
1:A:247:HIS:CE1	1:B:250:ILE:HD12	2.49	0.46
1:A:247:HIS:ND1	1:B:247:HIS:ND1	2.61	0.46
1:B:230:VAL:CG2	1:B:231:PRO:HD3	2.46	0.45
1:A:239:ALA:HA	1:A:243:ALA:HB3	1.98	0.45
1:B:144:TRP:CE2	1:B:148:LYS:HD2	2.52	0.45
1:B:233:LEU:O	1:B:237:MET:HG2	2.17	0.45
1:B:239:ALA:HA	1:B:243:ALA:HB3	1.99	0.45
1:B:129:VAL:HB	1:B:132:SER:HB3	1.99	0.44
1:A:233:LEU:O	1:A:237:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HB	1:A:132:SER:HB3	2.00	0.43
1:B:215:TRP:HE1	1:B:219:ARG:CZ	2.31	0.43
1:A:291:GLU:OE2	1:A:304:GLU:OE2	2.36	0.42
1:A:153:LEU:HD22	1:A:161:PHE:HB2	2.01	0.42
1:B:153:LEU:HD22	1:B:161:PHE:HB2	2.01	0.42
1:B:253:SER:HB2	1:B:265:VAL:HG13	2.02	0.42
1:B:134:PRO:HA	1:B:135:PRO:C	2.44	0.42
1:A:250:ILE:HD12	1:B:247:HIS:HE1	1.84	0.41
1:B:128:GLY:HA3	1:B:135:PRO:HD2	2.02	0.41
1:A:33:ILE:HD12	1:A:133:ILE:HG12	2.02	0.41
1:B:97:VAL:HG21	1:B:147:LEU:HD13	2.02	0.41
1:A:134:PRO:HA	1:A:135:PRO:C	2.45	0.41
1:B:215:TRP:NE1	1:B:219:ARG:NH2	2.69	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	382/423 (90%)	366 (96%)	16 (4%)	0	100	100
1	B	365/423 (86%)	347 (95%)	18 (5%)	0	100	100
All	All	747/846 (88%)	713 (95%)	34 (5%)	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	299/374 (80%)	289 (97%)	10 (3%)	33	48
1	B	277/374 (74%)	268 (97%)	9 (3%)	34	49
All	All	576/748 (77%)	557 (97%)	19 (3%)	33	48

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	42	ASN
1	A	50	PHE
1	A	108	ILE
1	A	162	GLU
1	A	192	LEU
1	A	275	GLU
1	A	297	SER
1	A	305	ASN
1	A	365	ILE
1	B	44	ILE
1	B	50	PHE
1	B	108	ILE
1	B	112	GLU
1	B	162	GLU
1	B	192	LEU
1	B	275	GLU
1	B	305	ASN
1	B	356	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	254	ASN
1	A	259	ASN
1	B	48	ASN
1	B	145	GLN
1	B	254	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 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

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	384/423 (90%)	0.97	44 (11%) 9 9	54, 81, 136, 173	0
1	B	369/423 (87%)	1.10	69 (18%) 3 3	54, 88, 180, 212	0
All	All	753/846 (89%)	1.04	113 (15%) 5 5	54, 83, 145, 212	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	LEU	5.1
1	B	372	VAL	4.5
1	A	365	ILE	4.5
1	A	386	ASN	4.4
1	A	376	LEU	4.3
1	A	161	PHE	4.0
1	B	361	ASN	3.9
1	B	362	ASP	3.9
1	A	170	THR	3.7
1	A	341	ASN	3.6
1	A	345	TYR	3.6
1	A	168	ASN	3.6
1	B	365	ILE	3.5
1	A	247	HIS	3.5
1	A	176	GLU	3.4
1	B	17	ALA	3.3
1	A	241	PHE	3.3
1	B	346	PHE	3.3
1	B	140	GLU	3.3
1	B	50	PHE	3.2
1	B	200	LEU	3.2
1	A	275	GLU	3.2
1	B	317	PHE	3.2
1	A	91	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	283	TYR	3.1
1	A	169	GLU	3.1
1	A	173	PHE	3.1
1	A	9	LEU	3.1
1	B	168	ASN	3.1
1	B	373	ASN	3.1
1	B	287	THR	3.0
1	B	28	PHE	3.0
1	B	166	LYS	3.0
1	B	376	LEU	3.0
1	A	245	PRO	3.0
1	A	167	PHE	3.0
1	B	55	ILE	2.9
1	B	374	SER	2.9
1	B	215	TRP	2.9
1	B	241	PHE	2.9
1	B	307	LEU	2.8
1	A	165	LEU	2.8
1	B	42	ASN	2.7
1	A	8	TYR	2.7
1	B	377	GLU	2.7
1	B	84	LYS	2.7
1	B	165	LEU	2.7
1	A	112	GLU	2.7
1	B	375	GLU	2.7
1	B	220	TYR	2.6
1	B	41	ALA	2.6
1	B	343	TYR	2.6
1	B	169	GLU	2.6
1	B	369	LEU	2.6
1	A	383	ARG	2.6
1	A	343	TYR	2.6
1	A	47	ILE	2.5
1	B	44	ILE	2.5
1	A	13	LEU	2.5
1	A	373	ASN	2.5
1	A	4	GLU	2.5
1	A	372	VAL	2.5
1	A	80	ALA	2.5
1	A	370	ASP	2.5
1	B	340	TYR	2.4
1	B	348	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	366	GLN	2.4
1	B	303	ILE	2.4
1	B	8	TYR	2.4
1	B	210	ILE	2.3
1	B	167	PHE	2.3
1	B	48	ASN	2.3
1	A	210	ILE	2.3
1	A	254	ASN	2.3
1	A	346	PHE	2.3
1	B	57	VAL	2.3
1	B	308	VAL	2.3
1	A	369	LEU	2.3
1	B	302	ASN	2.2
1	B	205	LYS	2.2
1	B	338	LEU	2.2
1	B	53	LYS	2.2
1	B	112	GLU	2.2
1	B	138	ARG	2.2
1	B	135	PRO	2.2
1	B	237	MET	2.2
1	A	172	THR	2.2
1	A	287	THR	2.2
1	A	162	GLU	2.2
1	A	379	ALA	2.1
1	B	351	TYR	2.1
1	B	320	TRP	2.1
1	A	256	ALA	2.1
1	A	360	THR	2.1
1	B	207	TYR	2.1
1	B	108	ILE	2.1
1	B	265	VAL	2.1
1	B	101	ASN	2.1
1	B	360	THR	2.1
1	B	32	LYS	2.1
1	A	82	ASP	2.1
1	B	323	TYR	2.1
1	B	364	ASP	2.1
1	A	57	VAL	2.0
1	B	345	TYR	2.0
1	B	218	GLN	2.0
1	B	363	GLU	2.0
1	A	63	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	208	ILE	2.0
1	B	234	ILE	2.0
1	B	268	THR	2.0
1	B	332	ILE	2.0
1	B	342	ASP	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 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.