Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID	:	8SUU / pdb_00008suu
Title	:	Crystal structure of YisK from Bacillus subtilis in apo form
Authors	:	Krieger, I.V.; Chemelewski, V.; Guo, T.; Sperber, A.; Herman, J.; Sacchettini, J.C.
Deposited on	:	2023-05-13
Resolution	:	2.26 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:

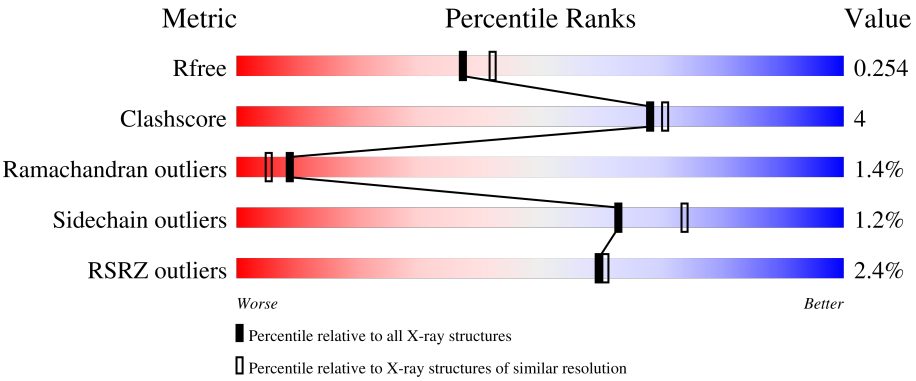
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	312	2% 85% 8% • 6%
1	B	312	3% 82% 9% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4552 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 Fumarylacetoacetate hydrolase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2269	1440	382	436	11			
1	B	288	Total	C	N	O	S	0	0	0
			2231	1420	374	426	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A0A0D6X359
A	-1	ALA	-	expression tag	UNP A0A0D6X359
A	0	SER	-	expression tag	UNP A0A0D6X359
A	302	LEU	-	expression tag	UNP A0A0D6X359
A	303	GLU	-	expression tag	UNP A0A0D6X359
A	304	HIS	-	expression tag	UNP A0A0D6X359
A	305	HIS	-	expression tag	UNP A0A0D6X359
A	306	HIS	-	expression tag	UNP A0A0D6X359
A	307	HIS	-	expression tag	UNP A0A0D6X359
A	308	HIS	-	expression tag	UNP A0A0D6X359
A	309	HIS	-	expression tag	UNP A0A0D6X359
B	-2	MET	-	initiating methionine	UNP A0A0D6X359
B	-1	ALA	-	expression tag	UNP A0A0D6X359
B	0	SER	-	expression tag	UNP A0A0D6X359
B	302	LEU	-	expression tag	UNP A0A0D6X359
B	303	GLU	-	expression tag	UNP A0A0D6X359
B	304	HIS	-	expression tag	UNP A0A0D6X359
B	305	HIS	-	expression tag	UNP A0A0D6X359
B	306	HIS	-	expression tag	UNP A0A0D6X359
B	307	HIS	-	expression tag	UNP A0A0D6X359
B	308	HIS	-	expression tag	UNP A0A0D6X359
B	309	HIS	-	expression tag	UNP A0A0D6X359

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is water.

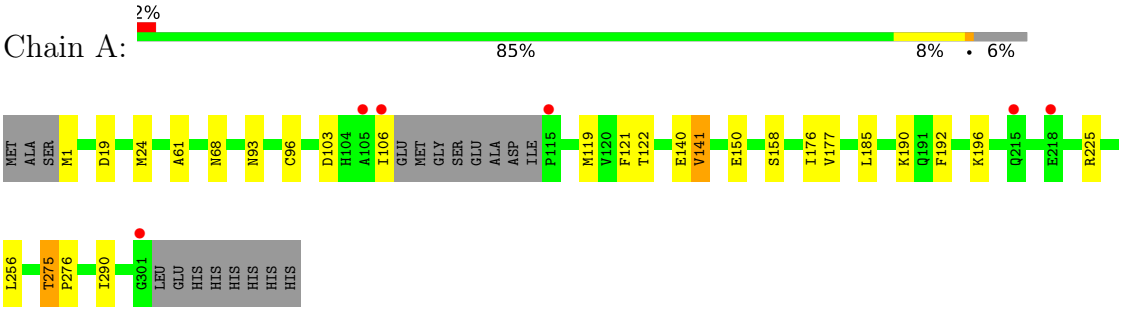
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	30	Total O 30 30	0	0
3	B	20	Total O 20 20	0	0

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.

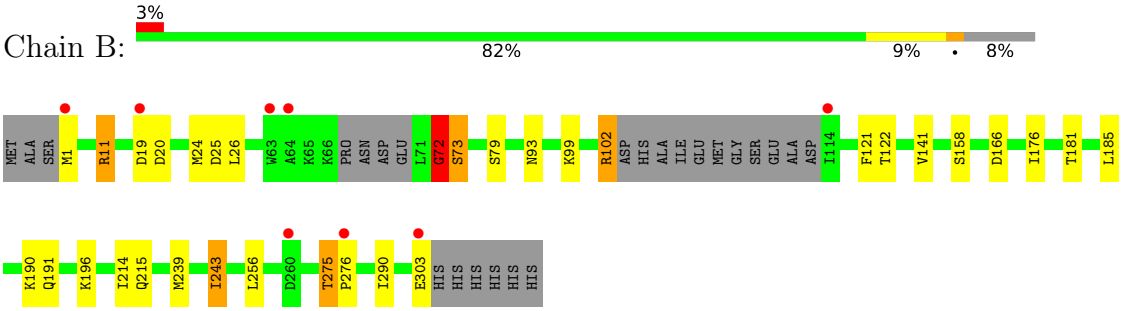
• Molecule 1: Fumarylacetoacetate hydrolase family protein

Chain A:



• Molecule 1: Fumarylacetoacetate hydrolase family protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	53.94Å 93.77Å 125.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.93 – 2.26 46.93 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.93-2.26) 99.9 (46.93-2.26)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 2.27Å)	Xtriage
Refinement program	REFMAC 2000	Depositor
R, R_{free}	0.211 , 0.255 (Not available) , 0.254	Depositor DCC
R_{free} test set	1995 reflections (6.53%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 26.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4552	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/2312	0.85	3/3117 (0.1%)
1	B	0.57	1/2271 (0.0%)	0.86	2/3059 (0.1%)
All	All	0.57	1/4583 (0.0%)	0.86	5/6176 (0.1%)

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
1	A	0	2
1	B	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	243	ILE	CA-CB	6.75	1.57	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	19	ASP	N-CA-C	-7.05	99.50	110.42
1	B	275	THR	CB-CA-C	6.73	118.55	108.86
1	A	275	THR	CB-CA-C	6.51	118.23	108.86
1	A	275	THR	N-CA-C	-5.58	102.58	110.29
1	B	275	THR	N-CA-C	-5.29	102.99	110.29

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	ARG	Sidechain
1	A	275	THR	Peptide
1	B	102	ARG	Sidechain
1	B	11	ARG	Sidechain
1	B	275	THR	Peptide
1	B	72	GLY	Peptide

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	2269	0	2298	14	0
1	B	2231	0	2274	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	0	0	0
3	B	20	0	0	0	0
All	All	4552	0	4572	33	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 (33) 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:B:239:MET:HE1	1:B:243:ILE:CD1	2.12	0.80
1:B:72:GLY:HA3	1:B:73:SER:HB2	1.67	0.76
1:B:72:GLY:HA3	1:B:73:SER:CB	2.18	0.74
1:B:239:MET:HE1	1:B:243:ILE:HD12	1.76	0.67
1:B:24:MET:HE3	1:B:26:LEU:HD23	1.77	0.66
1:B:11:ARG:NH2	1:B:25:ASP:OD2	2.27	0.65
1:A:24:MET:HE1	1:A:61:ALA:HA	1.85	0.59
1:B:181:THR:HG23	1:B:196:LYS:HD3	1.86	0.58
1:B:176:ILE:HG12	1:B:290:ILE:HD12	1.88	0.55
1:B:72:GLY:CA	1:B:73:SER:CB	2.86	0.54
1:A:119:MET:HE2	1:B:191:GLN:HG2	1.91	0.53
1:A:140:GLU:O	1:A:141:VAL:HB	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLU:O	1:A:141:VAL:CB	2.59	0.51
1:B:141:VAL:CG1	1:B:185:LEU:HD11	2.40	0.51
1:B:1:MET:HA	1:B:1:MET:HE2	1.92	0.51
1:A:150:GLU:HB2	1:A:177:VAL:HG23	1.94	0.49
1:A:141:VAL:CG1	1:A:185:LEU:HD11	2.42	0.49
1:B:121:PHE:CE1	1:B:196:LYS:HE3	2.48	0.48
1:A:176:ILE:HG12	1:A:290:ILE:HD12	1.97	0.47
1:B:93:ASN:HB3	1:B:122:THR:HB	1.97	0.46
1:A:140:GLU:O	1:A:141:VAL:HG23	2.16	0.45
1:A:93:ASN:HB3	1:A:122:THR:HB	1.98	0.45
1:A:158:SER:HA	1:A:256:LEU:O	2.17	0.45
1:A:103:ASP:OD1	1:A:106:ILE:HD12	2.17	0.44
1:A:141:VAL:HG12	1:A:185:LEU:HD11	2.00	0.44
1:B:102:ARG:HD3	1:B:102:ARG:C	2.42	0.44
1:B:214:ILE:C	1:B:215:GLN:HG2	2.43	0.43
1:B:214:ILE:O	1:B:215:GLN:CG	2.66	0.43
1:A:192:PHE:O	1:A:196:LYS:HB2	2.19	0.42
1:A:96:CYS:HB2	1:A:121:PHE:CE1	2.54	0.42
1:B:141:VAL:HG12	1:B:185:LEU:HD11	2.02	0.41
1:B:303:GLU:OE1	1:B:303:GLU:N	2.52	0.41
1:B:158:SER:HA	1:B:256:LEU:O	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	289/312 (93%)	281 (97%)	5 (2%)	3 (1%)	12 10
1	B	282/312 (90%)	267 (95%)	10 (4%)	5 (2%)	6 3
All	All	571/624 (92%)	548 (96%)	15 (3%)	8 (1%)	9 5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	VAL
1	A	276	PRO
1	B	73	SER
1	B	276	PRO
1	B	19	ASP
1	A	190	LYS
1	B	190	LYS
1	B	72	GLY

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	253/269 (94%)	251 (99%)	2 (1%)	73 80
1	B	249/269 (93%)	245 (98%)	4 (2%)	55 66
All	All	502/538 (93%)	496 (99%)	6 (1%)	63 74

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	68	ASN
1	B	20	ASP
1	B	79	SER
1	B	99	LYS
1	B	166	ASP

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	68	ASN
1	A	84	HIS
1	A	117	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	293/312 (93%)	0.24	6 (2%)	65	65	43, 58, 84, 112	0
1	B	288/312 (92%)	0.30	8 (2%)	55	55	46, 64, 92, 110	0
All	All	581/624 (93%)	0.27	14 (2%)	59	61	43, 61, 88, 112	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ALA	4.0
1	A	106	ILE	4.0
1	A	301	GLY	3.9
1	B	114	ILE	3.8
1	A	115	PRO	3.6
1	B	64	ALA	3.6
1	B	63	TRP	3.3
1	B	276	PRO	3.0
1	A	215	GLN	2.9
1	A	218	GLU	2.5
1	B	1	MET	2.1
1	B	19	ASP	2.1
1	B	303	GLU	2.0
1	B	260	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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
2	MN	A	401	1/1	0.95	0.06	89,89,89,89	0
2	MN	B	401	1/1	0.98	0.07	113,113,113,113	0

6.5 Other polymers

There are no such residues in this entry.