

# wwPDB X-ray Structure Validation Summary Report (i)

#### May 26, 2020 – 12:19 pm BST

PDB ID : 2IKK

Title : Structural Genomics, the crystal structure of the C-terminal domain of Yurk

from Bacillus subtilis subsp. subtilis str. 168

Authors: Tan, K.; Hatzos, C.; Abdullah, J.; Joachimiak, A.; Midwest Center for Struc-

tural Genomics (MCSG)

Deposited on : 2006-10-02

Resolution : 1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

Mol Probity : 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)

al geometry (DNA, RNA) : Parkinson et al. (1996)

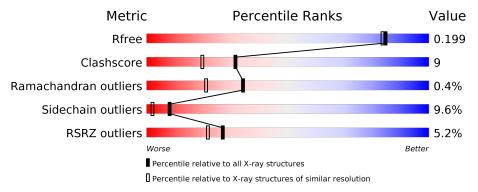
Ideal geometry (DNA, RNA) : Parki Validation Pipeline (wwPDB-VP) : 2.11

## 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 1.80 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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 <=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	173	5% 64%	16%	5%	16%		
1	В	173	68%	13%		16%		



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2548 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 Hypothetical transcriptional regulator yurK.

$\mathbf{Mol}$	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace		
1	Λ	146	Total	С	N	О	S	Se	0	0 0	0	
1	Λ	140	1183	762	190	227	2	2	0		0	
1	D	145	Total	С	N	О	S	Se	0	0	0	
T	D	140	1176	758	188	226	2	2				

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	MSE	-	EXPRESSION TAG	UNP O32152
A	71	HIS	_	EXPRESSION TAG	UNP O32152
A	72	HIS	-	EXPRESSION TAG	UNP O32152
A	73	HIS	-	EXPRESSION TAG	UNP O32152
A	74	HIS	_	EXPRESSION TAG	UNP O32152
A	75	HIS	-	EXPRESSION TAG	UNP O32152
A	76	HIS	-	EXPRESSION TAG	UNP O32152
A	77	SER	-	EXPRESSION TAG	UNP O32152
A	78	SER	-	EXPRESSION TAG	UNP O32152
A	79	GLY	_	EXPRESSION TAG	UNP O32152
A	80	VAL	-	EXPRESSION TAG	UNP O32152
A	81	ASP	-	EXPRESSION TAG	UNP O32152
A	82	LEU	-	EXPRESSION TAG	UNP O32152
A	83	GLY	-	EXPRESSION TAG	UNP O32152
A	84	THR	-	EXPRESSION TAG	UNP O32152
A	85	GLU	-	EXPRESSION TAG	UNP O32152
A	86	ASN	-	EXPRESSION TAG	UNP O32152
A	87	LEU	-	EXPRESSION TAG	UNP O32152
A	88	TYR	-	EXPRESSION TAG	UNP O32152
A	89	PHE	-	EXPRESSION TAG	UNP O32152
A	90	GLN	-	EXPRESSION TAG	UNP O32152
A	91	SER	-	EXPRESSION TAG	UNP O32152
A	92	ASN	-	EXPRESSION TAG	UNP O32152
A	93	ALA	-	EXPRESSION TAG	UNP O32152
A	166	MSE	MET	MODIFIED RESIDUE	UNP O32152

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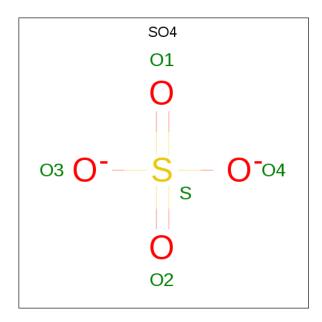


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Chain	Residue	Modelled	Actual	Comment	Reference
A	228	MSE	MET	MODIFIED RESIDUE	UNP O32152
В	70	MSE	-	EXPRESSION TAG	UNP O32152
В	71	HIS	_	EXPRESSION TAG	UNP O32152
В	72	HIS	_	EXPRESSION TAG	UNP O32152
В	73	HIS	-	EXPRESSION TAG	UNP O32152
В	74	HIS	-	EXPRESSION TAG	UNP O32152
В	75	HIS	-	EXPRESSION TAG	UNP O32152
В	76	HIS	-	EXPRESSION TAG	UNP O32152
В	77	SER	_	EXPRESSION TAG	UNP O32152
В	78	SER	-	EXPRESSION TAG	UNP O32152
В	79	GLY	-	EXPRESSION TAG	UNP O32152
В	80	VAL	-	EXPRESSION TAG	UNP O32152
В	81	ASP	-	EXPRESSION TAG	UNP O32152
В	82	LEU	-	EXPRESSION TAG	UNP O32152
В	83	GLY	-	EXPRESSION TAG	UNP O32152
В	84	THR	-	EXPRESSION TAG	UNP O32152
В	85	GLU	-	EXPRESSION TAG	UNP O32152
В	86	ASN	-	EXPRESSION TAG	UNP O32152
В	87	LEU	-	EXPRESSION TAG	UNP O32152
В	88	TYR	_	EXPRESSION TAG	UNP O32152
В	89	PHE	-	EXPRESSION TAG	UNP O32152
В	90	GLN	-	EXPRESSION TAG	UNP O32152
В	91	SER	-	EXPRESSION TAG	UNP O32152
В	92	ASN	-	EXPRESSION TAG	UNP O32152
В	93	ALA	=	EXPRESSION TAG	UNP O32152
В	166	MSE	MET	MODIFIED RESIDUE	UNP O32152
В	228	MSE	MET	MODIFIED RESIDUE	UNP O32152

 $\bullet$  Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0

### • Molecule 3 is water.

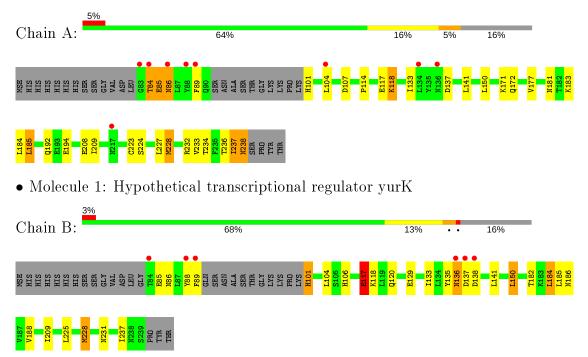
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	В	87	Total O 87 87	0	0



# 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: Hypothetical transcriptional regulator yurK





# 4 Data and refinement statistics (i)

Property	Value	Source		
Space group	P 1 21 1	Depositor		
Cell constants	$40.51 \text{\AA}  104.70 \text{Å}  40.54 \text{Å}$	Depositor		
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $118.58^{\circ}$ $90.00^{\circ}$	Depositor		
Resolution (Å)	35.60 - 1.80	Depositor		
resolution (A)	35.60 - 1.80	EDS		
% Data completeness	98.8 (35.60-1.80)	Depositor		
(in resolution range)	98.7 (35.60-1.80)	EDS		
$R_{merge}$	0.10	Depositor		
$\frac{\mathrm{R}_{sym}}{\langle I/\sigma(I)\rangle^{-1}}$	(Not available)	Depositor		
$< I/\sigma(I) > 1$	$1.26 \; ({\rm at} \; 1.79 {\rm \AA})$	Xtriage		
Refinement program	REFMAC 5.2.0019	Depositor		
D D.	0.194 , 0.230	Depositor		
$R, R_{free}$	0.196 , $0.199$	DCC		
$R_{free}$ test set	1366 reflections $(5.02\%)$	wwPDB-VP		
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage		
Anisotropy	0.062	Xtriage		
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.37,36.8	EDS		
L-test for twinning <sup>2</sup>	$< L >=0.47, < L^2>=0.30$	Xtriage		
	0.019 for -h-l,k,h			
	0.019  for  l,k,-h-l			
Estimated twinning fraction	0.039  for  h,-k,-h-l	Xtriage		
	0.042  for -h-l,-k,l			
	0.277  for  l,-k,h			
$F_o, F_c$ correlation	0.96	EDS		
Total number of atoms	2548	wwPDB-VP		
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP		

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.81% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



 $<sup>^{1}</sup>$ Intensities estimated from amplitudes.

## 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: SO4

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	Boı	nd lengths	Bond angles		
Moi Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	1.11	$2/1210 \ (0.2\%)$	1.03	2/1645~(0.1%)	
1	В	1.08	$2/1203 \ (0.2\%)$	1.06	3/1636 (0.2%)	
All	All	1.09	$4/2413 \ (0.2\%)$	1.04	5/3281 (0.2%)	

#### All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
1	A	208	GLU	CB-CG	5.32	1.62	1.52
1	В	188	VAL	CB-CG1	5.24	1.63	1.52
1	В	117	GLU	CD-OE1	5.22	1.31	1.25
1	A	224	SER	CB-OG	5.20	1.49	1.42

#### All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
1	В	228	MSE	CG-SE-CE	-12.02	72.45	98.90
1	A	228	MSE	CG-SE-CE	-11.56	73.48	98.90
1	A	185	LEU	CB-CG-CD2	-5.58	101.50	111.00
1	В	150	LEU	CB-CG-CD1	5.35	120.09	111.00
1	В	225	LEU	CB-CG-CD1	-5.17	102.20	111.00

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1183	0	1154	29	0
1	В	1176	0	1148	14	0
2	A	5	0	0	0	0
2	В	5	0	0	0	0
3	A	92	0	0	2	0
3	В	87	0	0	2	0
All	A11	2548	0	2302	42	0

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

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 9.

The worst 5 of 42 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{l}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:A:104:LEU:HD11	1:A:133:ILE:HG13	1.40	1.00
1:B:89:PHE:CZ	1:B:209:ILE:HD11	2.08	0.89
1:A:238:ASN:N	1:A:238:ASN:HD22	1.77	0.82
1:B:89:PHE:HZ	1:B:209:ILE:HD11	1.43	0.82
1:A:89:PHE:HZ	1:A:209:ILE:HD11	1.50	0.76

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	Perce	$_{ m ntiles}$
1	A	142/173 (82%)	134 (94%)	8 (6%)	0	100	100
1	В	141/173 (82%)	136 (96%)	4 (3%)	1 (1%)	22	10
All	All	283/346 (82%)	270 (95%)	12 (4%)	1 (0%)	34	21

All (1) Ramachandran outliers are listed below:



$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type
1	В	136	ASN

#### 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	136/157~(87%)	121 (89%)	15 (11%)	6 1		
1	В	136/157~(87%)	125 (92%)	11 (8%)	11 3		
All	All	272/314 (87%)	246 (90%)	26 (10%)	8 2		

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	LEU
1	A	238	ASN
1	В	184	LEU
1	A	228	MSE
1	A	237	ILE

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

Mol	Chain	${f Res}$	$\mathbf{Type}$
1	A	238	ASN
1	В	231	ASN
1	В	186	ASN
1	A	139	GLN
1	В	191	GLN

### 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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Mol Type Chain Res		Link	В	Bond lengths		Bond angles			
MIGI	Type	Chain	nes	SLINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	243	_	4,4,4	0.26	0	6,6,6	0.42	0
2	SO4	В	243	-	4,4,4	0.36	0	6,6,6	0.77	0

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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	144/173 (83%)	0.02	9 (6%) 20 15	19, 28, 53, 74	0
1	В	143/173~(82%)	-0.05	6 (4%) 36 30	19, 27, 52, 65	0
All	All	287/346 (82%)	-0.02	15 (5%) 27 22	19, 27, 53, 74	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	В	89	PHE	9.1
1	A	84	THR	7.9
1	A	88	TYR	7.7
1	A	89	PHE	6.5
1	В	84	THR	4.5

## 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)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	SO4	В	243	5/5	0.98	0.09	37,39,41,44	0
2	SO4	A	243	5/5	0.99	0.06	36,39,42,42	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

