



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:30 am BST

PDB ID : 1VIV  
Title : Crystal structure of a hypothetical protein  
Authors : Structural GenomiX  
Deposited on : 2003-12-01  
Resolution : 2.60 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](mailto: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.

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

MolProbity : 4.02b-467  
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)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

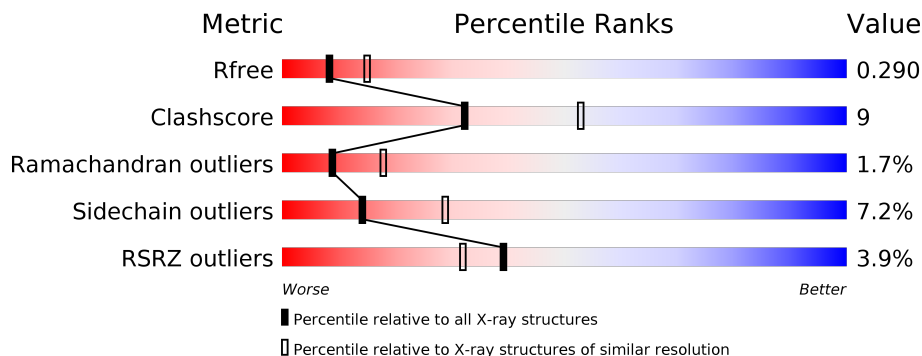
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	197	<p>3% (poor fit), 71% (0 outliers), 20% (1 outlier), 7% (2 outliers), 0% (3+ outliers)</p>
1	B	197	<p>4% (poor fit), 71% (0 outliers), 17% (1 outlier), 10% (2 outliers), 0% (3+ outliers)</p>

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 2758 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 protein yckF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	184	1360	859	230	263	8	0	1	0
1	B	177	1304	827	218	251	8	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP P42404
A	0	SER	-	cloning artifact	UNP P42404
A	1	LEU	-	cloning artifact	UNP P42404
A	186	GLU	-	cloning artifact	UNP P42404
A	187	GLY	-	cloning artifact	UNP P42404
A	188	GLY	-	cloning artifact	UNP P42404
A	189	SER	-	cloning artifact	UNP P42404
A	190	HIS	-	cloning artifact	UNP P42404
A	191	HIS	-	cloning artifact	UNP P42404
A	192	HIS	-	cloning artifact	UNP P42404
A	193	HIS	-	cloning artifact	UNP P42404
A	194	HIS	-	cloning artifact	UNP P42404
A	195	HIS	-	cloning artifact	UNP P42404
B	-1	MET	-	cloning artifact	UNP P42404
B	0	SER	-	cloning artifact	UNP P42404
B	1	LEU	-	cloning artifact	UNP P42404
B	186	GLU	-	cloning artifact	UNP P42404
B	187	GLY	-	cloning artifact	UNP P42404
B	188	GLY	-	cloning artifact	UNP P42404
B	189	SER	-	cloning artifact	UNP P42404
B	190	HIS	-	cloning artifact	UNP P42404
B	191	HIS	-	cloning artifact	UNP P42404
B	192	HIS	-	cloning artifact	UNP P42404
B	193	HIS	-	cloning artifact	UNP P42404
B	194	HIS	-	cloning artifact	UNP P42404

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Chain	Residue	Modelled	Actual	Comment	Reference
B	195	HIS	-	cloning artifact	UNP P42404

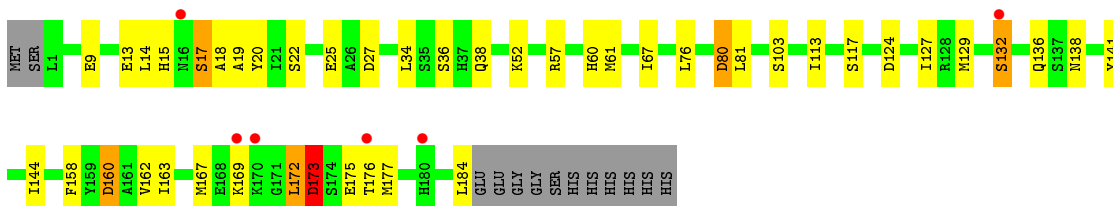
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	42	Total O 42 42	0	0
2	B	52	Total O 52 52	0	0

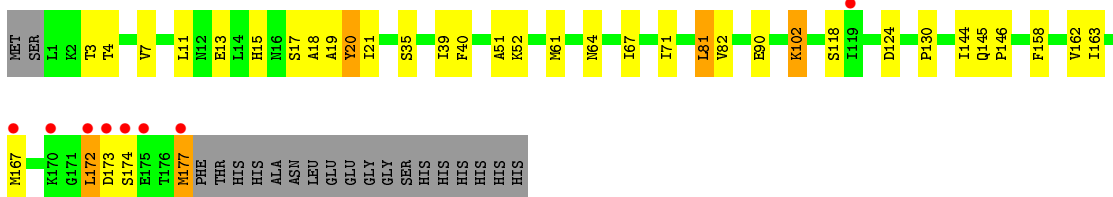
### 3 Residue-property plots [i](#)

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 protein yckF



- Molecule 1: Hypothetical protein yckF



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.36Å 71.36Å 245.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.68 – 2.60 35.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.68-2.60) 99.7 (35.68-2.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	11.55 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 4.0	Depositor
R, $R_{free}$	0.277 , 0.331 0.238 , 0.290	Depositor DCC
$R_{free}$ test set	584 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.0	Xtrriage
Anisotropy	0.529	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2758	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.48	0/1386	0.75	5/1874 (0.3%)
1	B	0.47	0/1324	0.70	1/1789 (0.1%)
All	All	0.48	0/2710	0.73	6/3663 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	80	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	160	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	124	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	173	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	124	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1360	0	1363	23	0
1	B	1304	0	1309	25	0
2	A	42	0	0	0	0
2	B	52	0	0	1	0
All	All	2758	0	2672	47	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 9.

All (47) 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:71:ILE:H	1:B:71:ILE:HD12	1.50	0.77
1:A:61:MET:HE1	1:A:163:ILE:HG23	1.68	0.75
1:B:61:MET:HE1	1:B:163:ILE:HG23	1.69	0.75
1:A:61:MET:CE	1:A:163:ILE:HG23	2.17	0.74
1:B:52:LYS:HG2	1:B:67:ILE:HD13	1.71	0.71
1:B:61:MET:HE3	1:B:163:ILE:HD12	1.77	0.67
1:A:127:ILE:HG22	1:A:129:MET:HE3	1.80	0.63
1:B:90:GLU:OE1	1:B:118:SER:OG	2.19	0.60
1:A:136:GLN:HG2	1:A:141:TYR:HD2	1.69	0.58
1:A:173:ASP:H	1:A:176:THR:CG2	2.17	0.57
1:B:3:THR:O	1:B:7:VAL:HG23	2.06	0.54
1:B:39:ILE:HG23	1:B:81:LEU:HD23	1.89	0.53
1:A:61:MET:HE3	1:A:163:ILE:HG23	1.92	0.52
1:B:145:GLN:HB2	1:B:146:PRO:HD2	1.92	0.52
1:A:136:GLN:HG2	1:A:141:TYR:CD2	2.45	0.51
1:A:57:ARG:HH11	1:A:60:HIS:HD2	1.59	0.51
1:B:40:PHE:HB2	1:B:82:VAL:HG22	1.92	0.51
1:B:71:ILE:CD1	1:B:71:ILE:H	2.21	0.50
1:B:61:MET:CE	1:B:163:ILE:HD12	2.41	0.50
1:B:51:ALA:HB2	2:B:201:HOH:O	2.11	0.49
1:A:173:ASP:H	1:A:176:THR:HG22	1.77	0.49
1:B:13:GLU:OE1	1:B:144:ILE:HG22	2.13	0.49
1:A:167:MET:HG2	1:A:172:LEU:HD12	1.95	0.49
1:A:127:ILE:HG22	1:A:129:MET:CE	2.43	0.48
1:A:132:SER:O	1:A:136:GLN:HG3	2.13	0.48
1:A:61:MET:HE3	1:A:163:ILE:HD12	1.96	0.47
1:B:17:SER:O	1:B:20:TYR:HB2	2.15	0.47
1:A:52:LYS:HG2	1:A:67:ILE:HD13	1.96	0.47
1:B:102:LYS:HA	1:B:102:LYS:NZ	2.31	0.46
1:A:160:ASP:O	1:A:163:ILE:HB	2.15	0.46
1:A:38:GLN:HB2	1:A:80:ASP:CG	2.37	0.45
1:B:17:SER:O	1:B:20:TYR:CB	2.66	0.44
1:A:15:HIS:NE2	1:B:15:HIS:NE2	2.53	0.44
1:A:113:ILE:HA	1:A:129:MET:O	2.18	0.43
1:A:76:LEU:HG	1:A:80:ASP:HB2	2.00	0.43
1:A:34:LEU:HD11	1:A:169:LYS:HD3	2.00	0.43
1:B:18:ALA:O	1:B:21:ILE:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:OG	1:B:130:PRO:HG2	2.19	0.42
1:B:61:MET:HE2	1:B:177:MET:HE3	2.01	0.42
1:B:158:PHE:O	1:B:162:VAL:HG23	2.20	0.42
1:B:173:ASP:CG	1:B:174:SER:H	2.24	0.41
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.94	0.41
1:B:167:MET:HG2	1:B:172:LEU:HD12	2.03	0.41
1:A:9:GLU:HG3	1:A:144:ILE:CD1	2.49	0.41
1:A:158:PHE:O	1:A:162:VAL:HG23	2.21	0.41
1:B:19:ALA:C	1:B:21:ILE:H	2.24	0.41
1:A:13:GLU:O	1:A:17:SER:OG	2.39	0.41

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	183/197 (93%)	174 (95%)	4 (2%)	5 (3%)	<b>5</b> <b>8</b>
1	B	175/197 (89%)	166 (95%)	8 (5%)	1 (1%)	25 47
All	All	358/394 (91%)	340 (95%)	12 (3%)	6 (2%)	<b>9</b> <b>18</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ALA
1	A	177	MET
1	B	20	TYR
1	A	20	TYR
1	A	19	ALA
1	A	117	SER

### 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	144/161 (89%)	131 (91%)	13 (9%)	9	18
1	B	136/161 (84%)	129 (95%)	7 (5%)	24	46
All	All	280/322 (87%)	260 (93%)	20 (7%)	14	29

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	17	SER
1	A	22	SER
1	A	25	GLU
1	A	36	SER
1	A	81	LEU
1	A	103	SER
1	A	132	SER
1	A	138	ASN
1	A	172	LEU
1	A	173	ASP
1	A	175	GLU
1	A	184	LEU
1	B	4	THR
1	B	35	SER
1	B	64	ASN
1	B	81	LEU
1	B	102	LYS
1	B	172	LEU
1	B	177	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	138	ASN

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Mol	Chain	Res	Type
1	B	28	GLN
1	B	32	HIS
1	B	114	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](#)

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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	184/197 (93%)	0.12	6 (3%) 46 39	25, 47, 74, 81	0
1	B	177/197 (89%)	0.27	8 (4%) 33 26	26, 52, 75, 103	0
All	All	361/394 (91%)	0.19	14 (3%) 39 32	25, 49, 74, 103	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	177	MET	5.0
1	B	173	ASP	3.0
1	B	174	SER	2.8
1	A	176	THR	2.7
1	B	175	GLU	2.5
1	A	169	LYS	2.3
1	A	132	SER	2.3
1	B	167	MET	2.3
1	A	170	LYS	2.2
1	B	119	ILE	2.2
1	B	172	LEU	2.2
1	A	16	ASN	2.1
1	B	170	LYS	2.1
1	A	180	HIS	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 carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.