



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 12:42 AM EDT

PDB ID : 3GFG  
Title : Structure of putative oxidoreductase yvaA from *Bacillus subtilis* in triclinic form  
Authors : Ramagopal, U.A.; Toro, R.; Gilmore, M.; Chang, S.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : unknown  
Resolution : 2.59 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

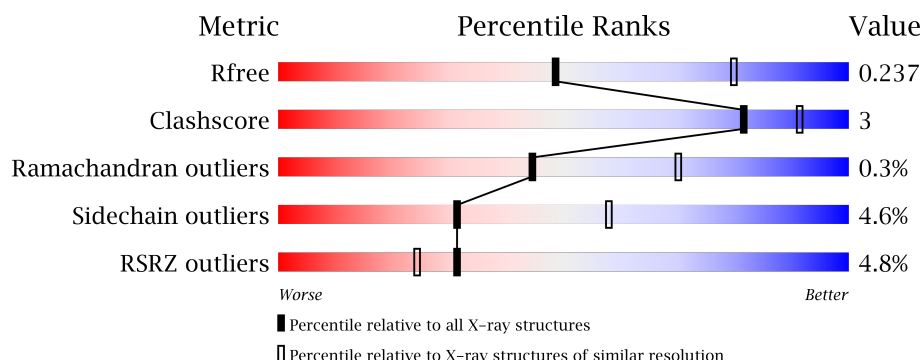
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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.




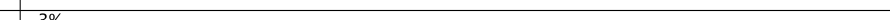

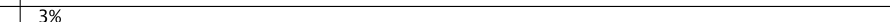

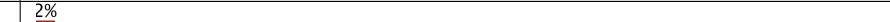

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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. 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	367	<div> <div>4%</div> <div>84% 8% 7%</div> </div>
1	B	367	<div> <div>%</div> <div>85% 10% 5%</div> </div>
1	C	367	<div> <div>4%</div> <div>84% 10% 6%</div> </div>
1	D	367	<div> <div>2%</div> <div>83% 8% 9%</div> </div>
1	E	367	<div> <div>2%</div> <div>84% 9% 7%</div> </div>

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Mol	Chain	Length	Quality of chain		
1	F	367		85%	8% • 7%
1	G	367		83%	9% • 7%
1	H	367		80%	13% 8%
1	I	367		83%	8% • 8%
1	J	367		87%	6% 7%
1	K	367		78%	13% • 8%
1	L	367		74%	17% • 9%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32457 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 Uncharacterized oxidoreductase yvaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2655	1675	449	522	9			
1	B	350	Total	C	N	O	S	0	3	0
			2763	1742	468	544	9			
1	C	346	Total	C	N	O	S	0	1	0
			2708	1709	460	530	9			
1	D	335	Total	C	N	O	S	0	1	0
			2622	1656	440	517	9			
1	E	342	Total	C	N	O	S	0	4	0
			2696	1701	458	528	9			
1	F	342	Total	C	N	O	S	0	2	0
			2674	1688	450	527	9			
1	G	340	Total	C	N	O	S	0	2	0
			2667	1683	451	524	9			
1	H	339	Total	C	N	O	S	0	1	0
			2653	1675	448	521	9			
1	I	336	Total	C	N	O	S	0	0	0
			2634	1661	444	520	9			
1	J	340	Total	C	N	O	S	0	0	0
			2650	1675	446	520	9			
1	K	337	Total	C	N	O	S	0	0	0
			2628	1659	441	519	9			
1	L	334	Total	C	N	O	S	0	0	0
			2591	1639	435	508	9			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP O32223
A	1	SER	-	EXPRESSION TAG	UNP O32223
A	2	LEU	-	EXPRESSION TAG	UNP O32223
A	359	GLU	-	EXPRESSION TAG	UNP O32223
A	360	GLY	-	EXPRESSION TAG	UNP O32223

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Chain	Residue	Modelled	Actual	Comment	Reference
A	361	HIS	-	EXPRESSION TAG	UNP O32223
A	362	HIS	-	EXPRESSION TAG	UNP O32223
A	363	HIS	-	EXPRESSION TAG	UNP O32223
A	364	HIS	-	EXPRESSION TAG	UNP O32223
A	365	HIS	-	EXPRESSION TAG	UNP O32223
A	366	HIS	-	EXPRESSION TAG	UNP O32223
B	0	MET	-	EXPRESSION TAG	UNP O32223
B	1	SER	-	EXPRESSION TAG	UNP O32223
B	2	LEU	-	EXPRESSION TAG	UNP O32223
B	359	GLU	-	EXPRESSION TAG	UNP O32223
B	360	GLY	-	EXPRESSION TAG	UNP O32223
B	361	HIS	-	EXPRESSION TAG	UNP O32223
B	362	HIS	-	EXPRESSION TAG	UNP O32223
B	363	HIS	-	EXPRESSION TAG	UNP O32223
B	364	HIS	-	EXPRESSION TAG	UNP O32223
B	365	HIS	-	EXPRESSION TAG	UNP O32223
B	366	HIS	-	EXPRESSION TAG	UNP O32223
C	0	MET	-	EXPRESSION TAG	UNP O32223
C	1	SER	-	EXPRESSION TAG	UNP O32223
C	2	LEU	-	EXPRESSION TAG	UNP O32223
C	359	GLU	-	EXPRESSION TAG	UNP O32223
C	360	GLY	-	EXPRESSION TAG	UNP O32223
C	361	HIS	-	EXPRESSION TAG	UNP O32223
C	362	HIS	-	EXPRESSION TAG	UNP O32223
C	363	HIS	-	EXPRESSION TAG	UNP O32223
C	364	HIS	-	EXPRESSION TAG	UNP O32223
C	365	HIS	-	EXPRESSION TAG	UNP O32223
C	366	HIS	-	EXPRESSION TAG	UNP O32223
D	0	MET	-	EXPRESSION TAG	UNP O32223
D	1	SER	-	EXPRESSION TAG	UNP O32223
D	2	LEU	-	EXPRESSION TAG	UNP O32223
D	359	GLU	-	EXPRESSION TAG	UNP O32223
D	360	GLY	-	EXPRESSION TAG	UNP O32223
D	361	HIS	-	EXPRESSION TAG	UNP O32223
D	362	HIS	-	EXPRESSION TAG	UNP O32223
D	363	HIS	-	EXPRESSION TAG	UNP O32223
D	364	HIS	-	EXPRESSION TAG	UNP O32223
D	365	HIS	-	EXPRESSION TAG	UNP O32223
D	366	HIS	-	EXPRESSION TAG	UNP O32223
E	0	MET	-	EXPRESSION TAG	UNP O32223
E	1	SER	-	EXPRESSION TAG	UNP O32223
E	2	LEU	-	EXPRESSION TAG	UNP O32223

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Chain	Residue	Modelled	Actual	Comment	Reference
E	359	GLU	-	EXPRESSION TAG	UNP O32223
E	360	GLY	-	EXPRESSION TAG	UNP O32223
E	361	HIS	-	EXPRESSION TAG	UNP O32223
E	362	HIS	-	EXPRESSION TAG	UNP O32223
E	363	HIS	-	EXPRESSION TAG	UNP O32223
E	364	HIS	-	EXPRESSION TAG	UNP O32223
E	365	HIS	-	EXPRESSION TAG	UNP O32223
E	366	HIS	-	EXPRESSION TAG	UNP O32223
F	0	MET	-	EXPRESSION TAG	UNP O32223
F	1	SER	-	EXPRESSION TAG	UNP O32223
F	2	LEU	-	EXPRESSION TAG	UNP O32223
F	359	GLU	-	EXPRESSION TAG	UNP O32223
F	360	GLY	-	EXPRESSION TAG	UNP O32223
F	361	HIS	-	EXPRESSION TAG	UNP O32223
F	362	HIS	-	EXPRESSION TAG	UNP O32223
F	363	HIS	-	EXPRESSION TAG	UNP O32223
F	364	HIS	-	EXPRESSION TAG	UNP O32223
F	365	HIS	-	EXPRESSION TAG	UNP O32223
F	366	HIS	-	EXPRESSION TAG	UNP O32223
G	0	MET	-	EXPRESSION TAG	UNP O32223
G	1	SER	-	EXPRESSION TAG	UNP O32223
G	2	LEU	-	EXPRESSION TAG	UNP O32223
G	359	GLU	-	EXPRESSION TAG	UNP O32223
G	360	GLY	-	EXPRESSION TAG	UNP O32223
G	361	HIS	-	EXPRESSION TAG	UNP O32223
G	362	HIS	-	EXPRESSION TAG	UNP O32223
G	363	HIS	-	EXPRESSION TAG	UNP O32223
G	364	HIS	-	EXPRESSION TAG	UNP O32223
G	365	HIS	-	EXPRESSION TAG	UNP O32223
G	366	HIS	-	EXPRESSION TAG	UNP O32223
H	0	MET	-	EXPRESSION TAG	UNP O32223
H	1	SER	-	EXPRESSION TAG	UNP O32223
H	2	LEU	-	EXPRESSION TAG	UNP O32223
H	359	GLU	-	EXPRESSION TAG	UNP O32223
H	360	GLY	-	EXPRESSION TAG	UNP O32223
H	361	HIS	-	EXPRESSION TAG	UNP O32223
H	362	HIS	-	EXPRESSION TAG	UNP O32223
H	363	HIS	-	EXPRESSION TAG	UNP O32223
H	364	HIS	-	EXPRESSION TAG	UNP O32223
H	365	HIS	-	EXPRESSION TAG	UNP O32223
H	366	HIS	-	EXPRESSION TAG	UNP O32223
I	0	MET	-	EXPRESSION TAG	UNP O32223

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Chain	Residue	Modelled	Actual	Comment	Reference
I	1	SER	-	EXPRESSION TAG	UNP O32223
I	2	LEU	-	EXPRESSION TAG	UNP O32223
I	359	GLU	-	EXPRESSION TAG	UNP O32223
I	360	GLY	-	EXPRESSION TAG	UNP O32223
I	361	HIS	-	EXPRESSION TAG	UNP O32223
I	362	HIS	-	EXPRESSION TAG	UNP O32223
I	363	HIS	-	EXPRESSION TAG	UNP O32223
I	364	HIS	-	EXPRESSION TAG	UNP O32223
I	365	HIS	-	EXPRESSION TAG	UNP O32223
I	366	HIS	-	EXPRESSION TAG	UNP O32223
J	0	MET	-	EXPRESSION TAG	UNP O32223
J	1	SER	-	EXPRESSION TAG	UNP O32223
J	2	LEU	-	EXPRESSION TAG	UNP O32223
J	359	GLU	-	EXPRESSION TAG	UNP O32223
J	360	GLY	-	EXPRESSION TAG	UNP O32223
J	361	HIS	-	EXPRESSION TAG	UNP O32223
J	362	HIS	-	EXPRESSION TAG	UNP O32223
J	363	HIS	-	EXPRESSION TAG	UNP O32223
J	364	HIS	-	EXPRESSION TAG	UNP O32223
J	365	HIS	-	EXPRESSION TAG	UNP O32223
J	366	HIS	-	EXPRESSION TAG	UNP O32223
K	0	MET	-	EXPRESSION TAG	UNP O32223
K	1	SER	-	EXPRESSION TAG	UNP O32223
K	2	LEU	-	EXPRESSION TAG	UNP O32223
K	359	GLU	-	EXPRESSION TAG	UNP O32223
K	360	GLY	-	EXPRESSION TAG	UNP O32223
K	361	HIS	-	EXPRESSION TAG	UNP O32223
K	362	HIS	-	EXPRESSION TAG	UNP O32223
K	363	HIS	-	EXPRESSION TAG	UNP O32223
K	364	HIS	-	EXPRESSION TAG	UNP O32223
K	365	HIS	-	EXPRESSION TAG	UNP O32223
K	366	HIS	-	EXPRESSION TAG	UNP O32223
L	0	MET	-	EXPRESSION TAG	UNP O32223
L	1	SER	-	EXPRESSION TAG	UNP O32223
L	2	LEU	-	EXPRESSION TAG	UNP O32223
L	359	GLU	-	EXPRESSION TAG	UNP O32223
L	360	GLY	-	EXPRESSION TAG	UNP O32223
L	361	HIS	-	EXPRESSION TAG	UNP O32223
L	362	HIS	-	EXPRESSION TAG	UNP O32223
L	363	HIS	-	EXPRESSION TAG	UNP O32223
L	364	HIS	-	EXPRESSION TAG	UNP O32223
L	365	HIS	-	EXPRESSION TAG	UNP O32223

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Chain	Residue	Modelled	Actual	Comment	Reference
L	366	HIS	-	EXPRESSION TAG	UNP O32223

- Molecule 2 is water.

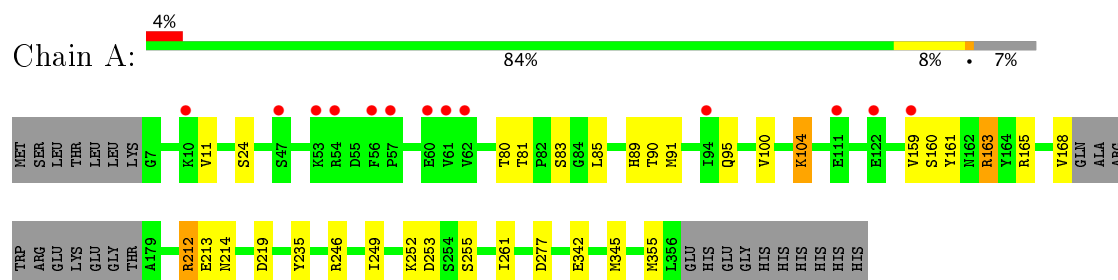
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	57	Total O 57 57	0	0
2	B	71	Total O 71 71	0	0
2	C	38	Total O 38 38	0	0
2	D	49	Total O 49 49	0	0
2	E	85	Total O 85 85	0	0
2	F	66	Total O 66 66	0	0
2	G	36	Total O 36 36	0	0
2	H	49	Total O 49 49	0	0
2	I	19	Total O 19 19	0	0
2	J	36	Total O 36 36	0	0
2	K	6	Total O 6 6	0	0
2	L	4	Total O 4 4	0	0



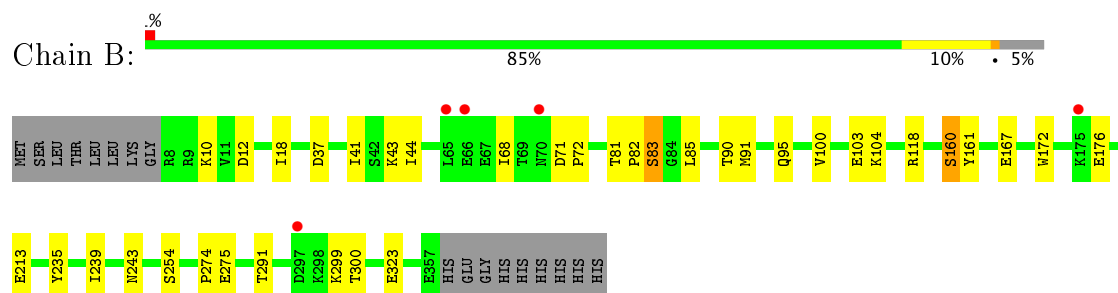
### 3 Residue-property plots [i](#)

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.

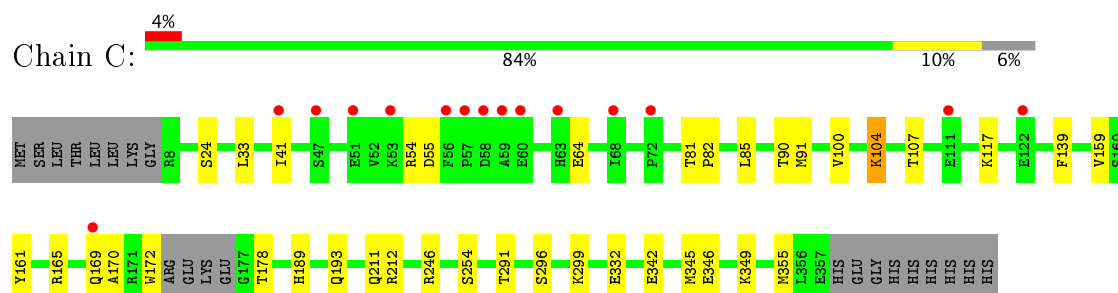
#### • Molecule 1: Uncharacterized oxidoreductase yvaA



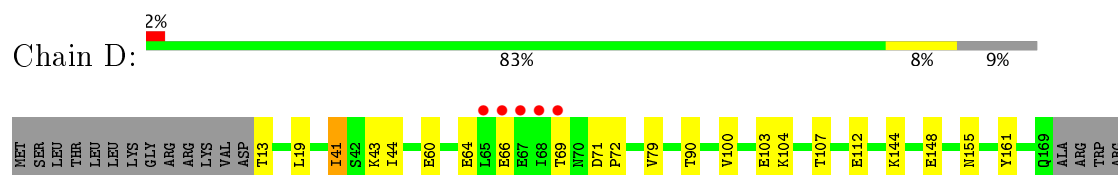
#### • Molecule 1: Uncharacterized oxidoreductase yvaA

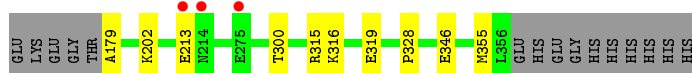


#### • Molecule 1: Uncharacterized oxidoreductase yvaA

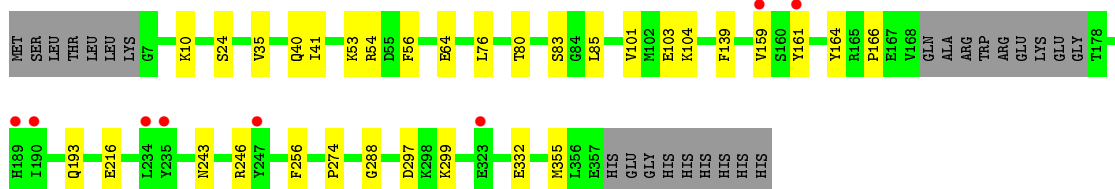
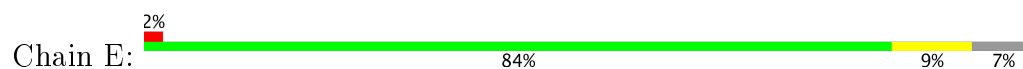


#### • Molecule 1: Uncharacterized oxidoreductase yvaA

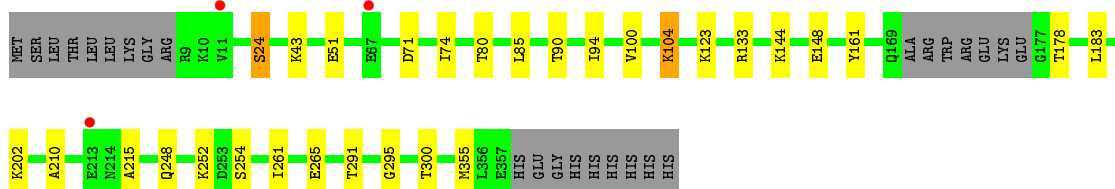
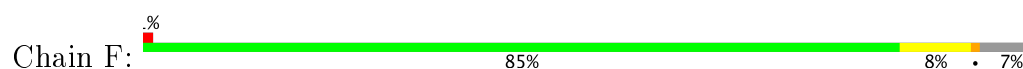




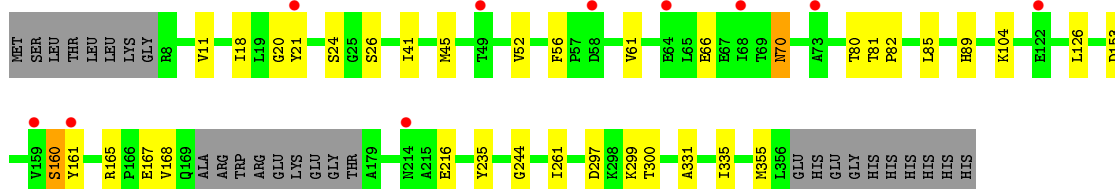
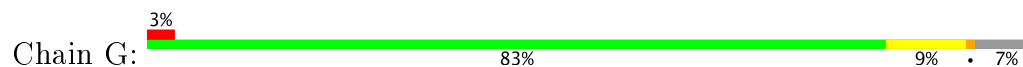
- Molecule 1: Uncharacterized oxidoreductase yvaA



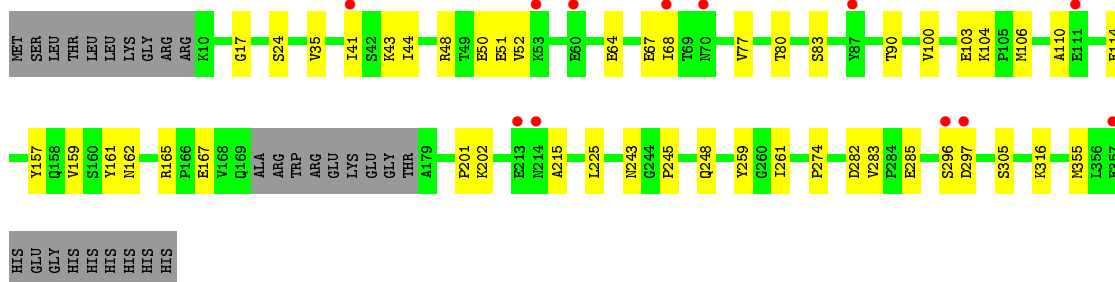
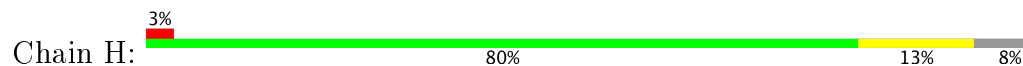
- Molecule 1: Uncharacterized oxidoreductase yvaA



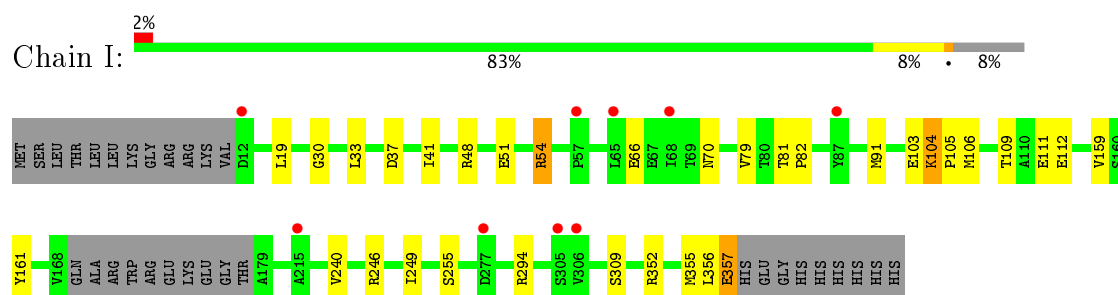
- Molecule 1: Uncharacterized oxidoreductase yvaA



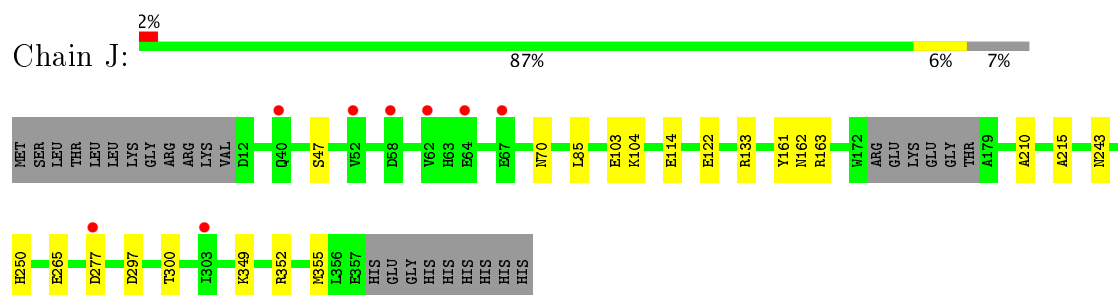
- Molecule 1: Uncharacterized oxidoreductase yvaA



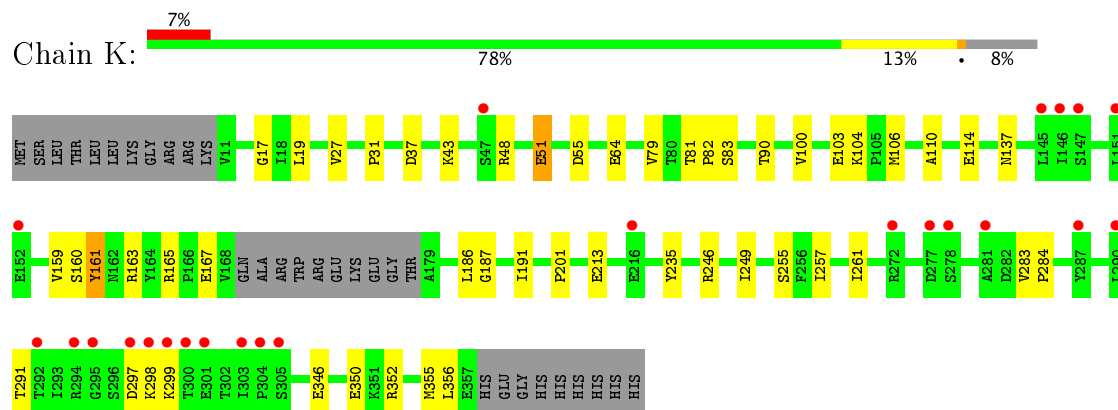
- Molecule 1: Uncharacterized oxidoreductase yvaA



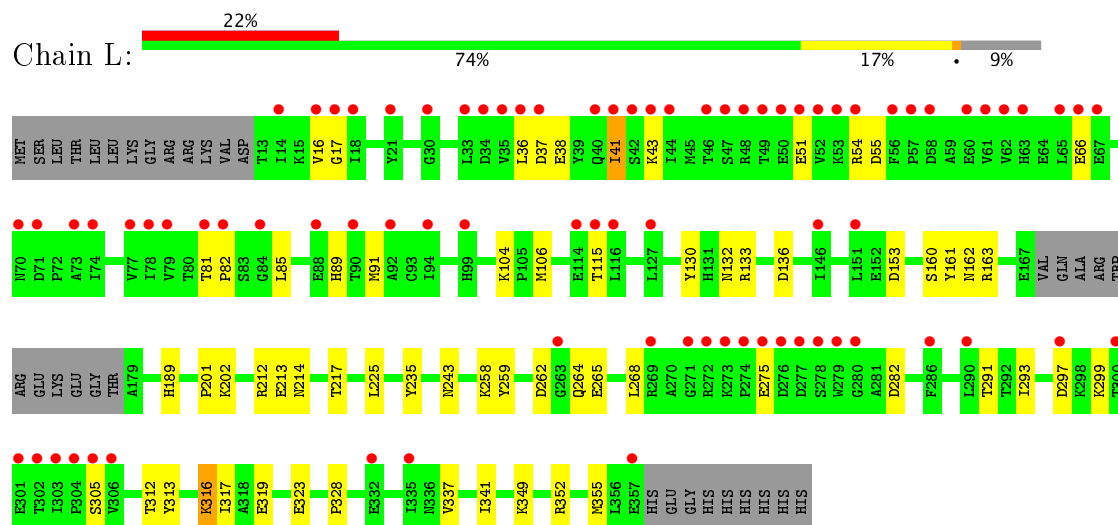
- Molecule 1: Uncharacterized oxidoreductase yvaA



- Molecule 1: Uncharacterized oxidoreductase yvaA



- Molecule 1: Uncharacterized oxidoreductase yvaA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.93Å 92.14Å 187.59Å 95.31° 94.19° 95.21°	Depositor
Resolution (Å)	45.41 – 2.59 44.55 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.41-2.59) 95.0 (44.55-2.59)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.182 , 0.236 0.184 , 0.237	Depositor DCC
$R_{free}$ test set	7368 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 30.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	32457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.87 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.9220e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.65	0/2704	0.66	0/3660
1	B	0.62	0/2824	0.68	0/3822
1	C	0.58	0/2762	0.64	0/3740
1	D	0.61	0/2674	0.68	0/3621
1	E	0.68	1/2757 (0.0%)	0.70	0/3730
1	F	0.66	0/2729	0.70	0/3695
1	G	0.61	0/2722	0.68	1/3685 (0.0%)
1	H	0.58	0/2705	0.65	0/3662
1	I	0.57	0/2683	0.66	0/3632
1	J	0.60	1/2701 (0.0%)	0.65	0/3660
1	K	0.49	0/2677	0.60	0/3627
1	L	0.49	0/2640	0.59	0/3577
All	All	0.60	2/32578 (0.0%)	0.66	1/44111 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	114	GLU	CG-CD	5.50	1.60	1.51
1	E	332	GLU	CG-CD	5.10	1.59	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	244	GLY	N-CA-C	-5.17	100.17	113.10

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	2655	0	2625	15	0
1	B	2763	0	2729	14	0
1	C	2708	0	2672	18	0
1	D	2622	0	2589	13	0
1	E	2696	0	2676	13	0
1	F	2674	0	2637	14	0
1	G	2667	0	2634	15	0
1	H	2653	0	2624	22	0
1	I	2634	0	2602	13	0
1	J	2650	0	2604	6	0
1	K	2628	0	2587	25	0
1	L	2591	0	2548	28	0
2	A	57	0	0	0	0
2	B	71	0	0	1	0
2	C	38	0	0	0	0
2	D	49	0	0	1	0
2	E	85	0	0	1	0
2	F	66	0	0	3	0
2	G	36	0	0	1	0
2	H	49	0	0	2	0
2	I	19	0	0	0	0
2	J	36	0	0	0	0
2	K	6	0	0	0	0
2	L	4	0	0	0	0
All	All	32457	0	31527	190	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 3.

The worst 5 of 190 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:I:356:LEU:O	1:I:357:GLU:HB2	1.78	0.81
1:J:210:ALA:HB1	1:J:215:ALA:HB3	1.65	0.79
1:L:41:ILE:HD12	1:L:41:ILE:H	1.48	0.78
1:E:40[A]:GLN:HE21	1:E:41:ILE:H	1.35	0.74
1:G:24:SER:HB2	1:G:80:THR:HB	1.70	0.74

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	336/367 (92%)	327 (97%)	9 (3%)	0	100	100
1	B	351/367 (96%)	336 (96%)	13 (4%)	2 (1%)	28	53
1	C	343/367 (94%)	331 (96%)	11 (3%)	1 (0%)	44	70
1	D	332/367 (90%)	317 (96%)	15 (4%)	0	100	100
1	E	342/367 (93%)	333 (97%)	9 (3%)	0	100	100
1	F	340/367 (93%)	329 (97%)	10 (3%)	1 (0%)	44	70
1	G	338/367 (92%)	322 (95%)	15 (4%)	1 (0%)	44	70
1	H	336/367 (92%)	325 (97%)	10 (3%)	1 (0%)	44	70
1	I	332/367 (90%)	317 (96%)	12 (4%)	3 (1%)	20	40
1	J	336/367 (92%)	319 (95%)	17 (5%)	0	100	100
1	K	333/367 (91%)	312 (94%)	20 (6%)	1 (0%)	44	70
1	L	330/367 (90%)	311 (94%)	18 (6%)	1 (0%)	44	70
All	All	4049/4404 (92%)	3879 (96%)	159 (4%)	11 (0%)	44	70

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	153	ASP
1	I	30	GLY
1	B	83	SER
1	C	170	ALA
1	L	106	MET

### 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	286/312 (92%)	274 (96%)	12 (4%)	34	62
1	B	297/312 (95%)	282 (95%)	15 (5%)	28	52
1	C	290/312 (93%)	278 (96%)	12 (4%)	35	63
1	D	283/312 (91%)	272 (96%)	11 (4%)	37	65
1	E	291/312 (93%)	279 (96%)	12 (4%)	35	63
1	F	287/312 (92%)	278 (97%)	9 (3%)	45	73
1	G	287/312 (92%)	272 (95%)	15 (5%)	27	52
1	H	286/312 (92%)	274 (96%)	12 (4%)	34	62
1	I	285/312 (91%)	274 (96%)	11 (4%)	37	65
1	J	283/312 (91%)	270 (95%)	13 (5%)	31	58
1	K	283/312 (91%)	267 (94%)	16 (6%)	24	47
1	L	276/312 (88%)	255 (92%)	21 (8%)	15	30
All	All	3434/3744 (92%)	3275 (95%)	159 (5%)	31	58

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	45	MET
1	H	161	TYR
1	L	104	LYS
1	G	104	LYS
1	G	216	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	40	GLN
1	G	70	ASN
1	K	231	GLN
1	D	158	GLN
1	J	207	ASN

### 5.3.3 RNA ⓘ

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 ⓘ

### 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<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	340/367 (92%)	0.45	13 (3%) 41 33	12, 21, 33, 54	0
1	B	350/367 (95%)	0.38	5 (1%) 75 71	12, 19, 33, 60	0
1	C	346/367 (94%)	0.48	15 (4%) 36 28	13, 21, 36, 54	0
1	D	335/367 (91%)	0.42	8 (2%) 59 52	11, 20, 32, 40	0
1	E	342/367 (93%)	0.47	8 (2%) 61 54	9, 18, 30, 51	0
1	F	342/367 (93%)	0.33	3 (0%) 84 81	12, 19, 31, 52	0
1	G	340/367 (92%)	0.49	10 (2%) 52 45	12, 20, 37, 52	0
1	H	339/367 (92%)	0.41	12 (3%) 44 36	11, 21, 32, 52	0
1	I	336/367 (91%)	0.33	9 (2%) 55 48	13, 22, 33, 46	0
1	J	340/367 (92%)	0.27	8 (2%) 59 52	13, 21, 33, 42	0
1	K	337/367 (91%)	0.50	24 (7%) 17 12	15, 23, 34, 52	0
1	L	334/367 (91%)	1.19	81 (24%) 1 0	15, 24, 35, 38	0
All	All	4081/4404 (92%)	0.48	196 (4%) 31 24	9, 21, 33, 60	0

The worst 5 of 196 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	53	LYS	5.9
1	L	42	SER	5.9
1	L	56	PHE	5.4
1	L	115	THR	5.0
1	L	49	THR	4.9

### 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 [i](#)

There are no carbohydrates 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.