W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 02:49 am BST

PDB ID	:	3R6M
Title	:	Crystal structure of Vibrio parahaemolyticus YeaZ
Authors	:	Roujeinikova, A.; Aydin, I.
Deposited on	:	2011-03-21
Resolution	:	3.10 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:

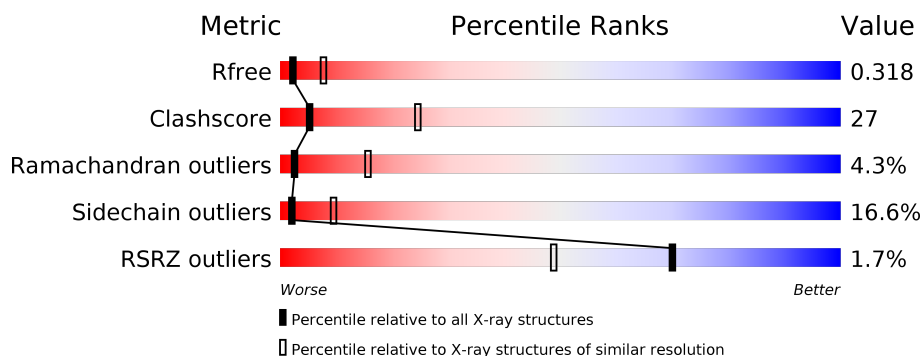|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	Percentile Ranks	Value
Rfree		0.318
Clashscore		27
Ramachandran outliers		4.3%
Sidechain outliers		16.6%
RSRZ outliers		1.7%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	213	2% / 55% / 38% / 7%
1	B	213	% / 54% / 38% / 7% ·
1	C	213	3% / 58% / 33% / 7% ·
1	D	213	55% / 35% / 8% ·

wwPDB X-ray Structure Validation Summary Report

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6162 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.
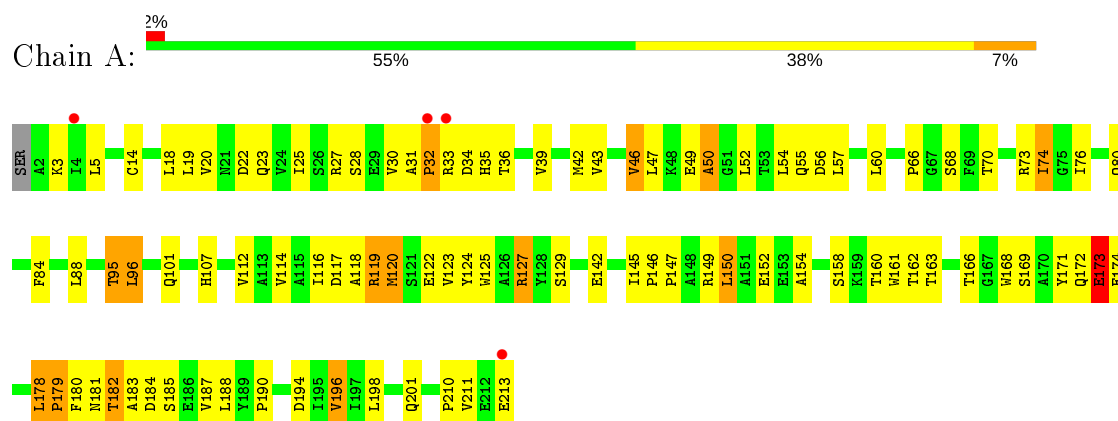
- Molecule 1 is a protein called YeaZ, resuscitation promoting factor.

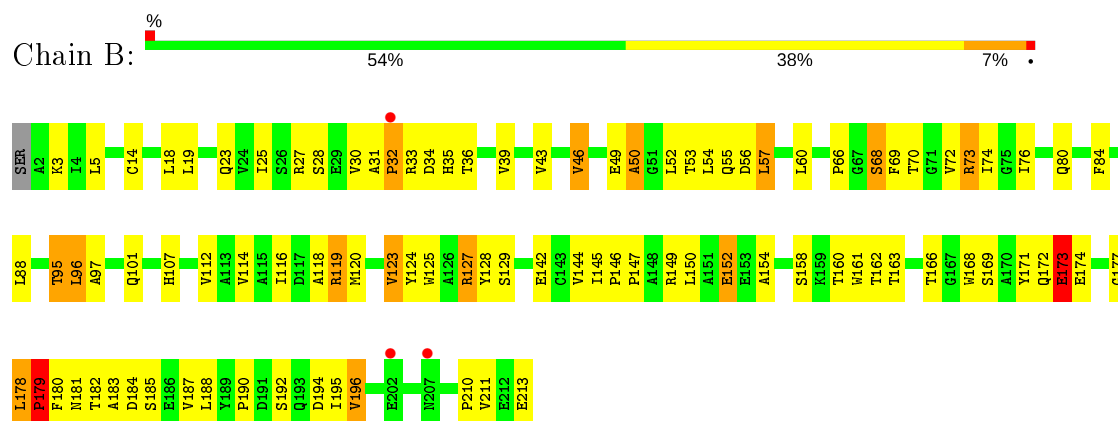| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1539	973	256	305	5			
1	B	212	Total	C	N	O	S	0	0	0
			1539	973	256	305	5			
1	C	212	Total	C	N	O	S	0	0	0
			1539	973	256	305	5			
1	D	212	Total	C	N	O	S	0	0	0
			1545	976	259	305	5			

3 Residue-property plots ⓘ

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.
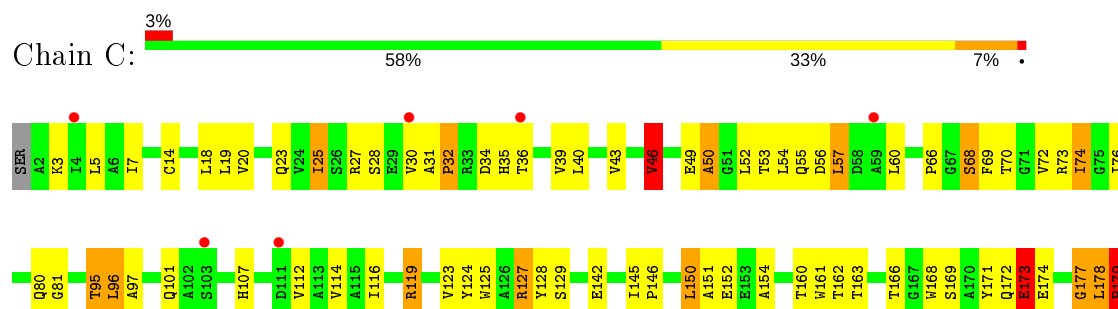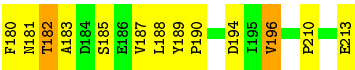
- Molecule 1: YeaZ, resuscitation promoting factor

- Molecule 1: YeaZ, resuscitation promoting factor

- Molecule 1: YeaZ, resuscitation promoting factor

F180 N181 T182 A183 D184 S185 E186 V187 L188 Y189 P190 D194 I195 V196 P210 E213

• Molecule 1: YeaZ, resuscitation promoting factor

Chain D:

55%   35%   8%

SER A2 K3 I4 L5 A6 I7 C14 L18 L19 V20 Q23 V24 I25 S26 R27 S28 E29 V30 A31 P32 R33 D34 H35 T36 V39 L40 V43 V46 E49 A50 G51 L52 T53 L54 Q55 D56 L57 L60 P66 G67 S68 F69 T70 G71 V72 R73 I74 G75 I76

Q80 G81 F84 T95 L96 A97 Q101 H107 V112 A113 V114 A115 I116 R119 V123 Y124 W125 A126 R127 Y128 S129 W136 E142 I145 P146 L150 A151 E152 E153 A154 T160 W161 T162 T163 T166 G167 W168 S169 A170 Y171 Q172 E173 E174 G177 L178 P179

F180 N181 T182 A183 D184 S185 E186 V187 L188 Y189 P190 D191 S192 Q193 D194 I195 V196 P210 E213

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.73Å 63.84Å 82.27Å 90.00° 104.94° 90.00°	Depositor
Resolution (Å)	79.49 – 3.10 49.78 – 3.10	Depositor EDS
% Data completeness (in resolution range)	89.9 (79.49-3.10) 90.0 (49.78-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$<I/\sigma(I)>$ [1]	2.37 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.239 , 0.294 0.262 , 0.318	Depositor DCC
R_{free} test set	687 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	97.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 94.6	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6162	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.18% 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 (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	0.74	0/1565	0.85	0/2140
1	B	0.77	0/1565	0.86	0/2140
1	C	0.71	0/1565	0.84	0/2140
1	D	0.71	0/1571	0.84	0/2147
All	All	0.73	0/6266	0.85	0/8567

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	1
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	PRO	Peptide
1	B	177	GLY	Peptide
1	B	179	PRO	Peptide
1	C	177	GLY	Peptide
1	C	179	PRO	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	1539	0	1458	83	1
1	B	1539	0	1458	83	1
1	C	1539	0	1458	76	1
1	D	1545	0	1469	89	1
All	All	6162	0	5843	319	2

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 27.

The worst 5 of 319 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:D:33:ARG:HH11	1:D:33:ARG:HG3	0.99	1.08
1:C:95:THR:HG22	1:C:190:PRO:HG3	1.40	1.03
1:A:95:THR:HG22	1:A:190:PRO:HG3	1.39	1.02
1:D:95:THR:HG22	1:D:190:PRO:HG3	1.41	0.97
1:A:119:ARG:HA	1:A:119:ARG:HH11	1.30	0.94

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:OG	1:B:158:SER:OG[1_545]	1.79	0.41
1:C:189:TYR:OH	1:D:189:TYR:OH[2_646]	2.13	0.07

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	210/213 (99%)	173 (82%)	28 (13%)	9 (4%)	2	16
1	B	210/213 (99%)	176 (84%)	25 (12%)	9 (4%)	2	16
1	C	210/213 (99%)	172 (82%)	29 (14%)	9 (4%)	2	16
1	D	210/213 (99%)	171 (81%)	30 (14%)	9 (4%)	2	16
All	All	840/852 (99%)	692 (82%)	112 (13%)	36 (4%)	2	16

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	ALA
1	B	50	ALA
1	B	154	ALA
1	C	50	ALA
1	C	154	ALA

5.3.2 Protein sidechains ⓘ

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	146/167 (87%)	123 (84%)	23 (16%)	2	11
1	B	146/167 (87%)	124 (85%)	22 (15%)	3	12
1	C	146/167 (87%)	121 (83%)	25 (17%)	2	9
1	D	147/167 (88%)	120 (82%)	27 (18%)	1	7
All	All	585/668 (88%)	488 (83%)	97 (17%)	2	9

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	196	VAL
1	C	68	SER
1	D	150	LEU
1	C	7	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	30	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	172	GLN
1	C	35	HIS
1	D	80	GLN
1	B	80	GLN
1	D	35	HIS

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, 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	212/213 (99%)	-0.11	4 (1%)	66	46	51, 88, 137, 160	0
1	B	212/213 (99%)	-0.14	3 (1%)	75	56	51, 88, 138, 158	0
1	C	212/213 (99%)	0.05	6 (2%)	53	30	52, 102, 164, 213	0
1	D	212/213 (99%)	-0.09	1 (0%)	91	81	49, 94, 148, 180	0
All	All	848/852 (99%)	-0.07	14 (1%)	70	49	49, 92, 150, 213	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	59	ALA	3.6
1	C	103	SER	3.0
1	C	4	ILE	2.9
1	B	32	PRO	2.9
1	C	111	ASP	2.5

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.