



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 05:47 am BST

PDB ID : 4P9U
Title : FadR, Fatty Acid Responsive Transcription Factor from *Vibrio cholerae*, in Complex with DNA
Authors : Kull, F.J.; Shi, W.
Deposited on : 2014-04-05
Resolution : 3.21 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 ⓘ symbol.

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

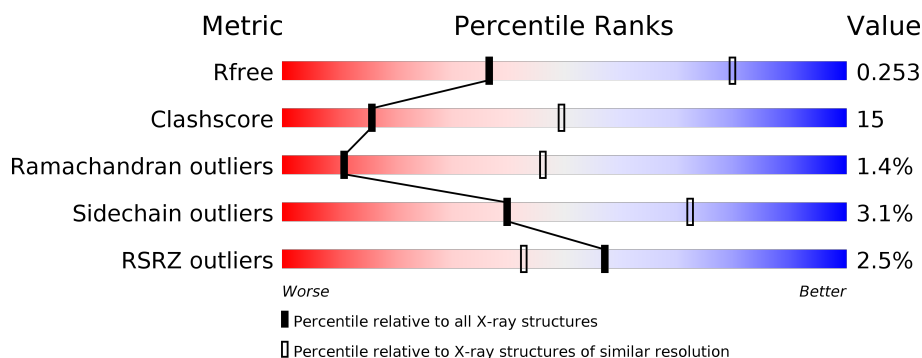
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. 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	272	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>.</div> </div> </div>
1	B	272	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>..</div> </div> </div>
1	E	272	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>.</div> </div> </div>
1	F	272	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>..</div> </div> </div>
2	C	31	<div> <div></div> <div> <div>35%</div> <div>65%</div> </div> </div>
2	G	31	<div> <div></div> <div> <div>35%</div> <div>65%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	31	 68%32%
3	H	31	 65%35%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11346 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 Fatty acid metabolism regulator protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	272	Total	C	N	O	S	0	0	0
			2201	1407	377	407	10			
1	F	272	Total	C	N	O	S	0	0	0
			2201	1407	377	407	10			
1	A	272	Total	C	N	O	S	0	0	0
			2201	1407	377	407	10			
1	B	272	Total	C	N	O	S	0	0	0
			2201	1407	377	407	10			

- Molecule 2 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	31	Total	C	N	O	P	0	0	0
			637	303	126	177	31			
2	C	31	Total	C	N	O	P	0	0	0
			637	303	126	177	31			

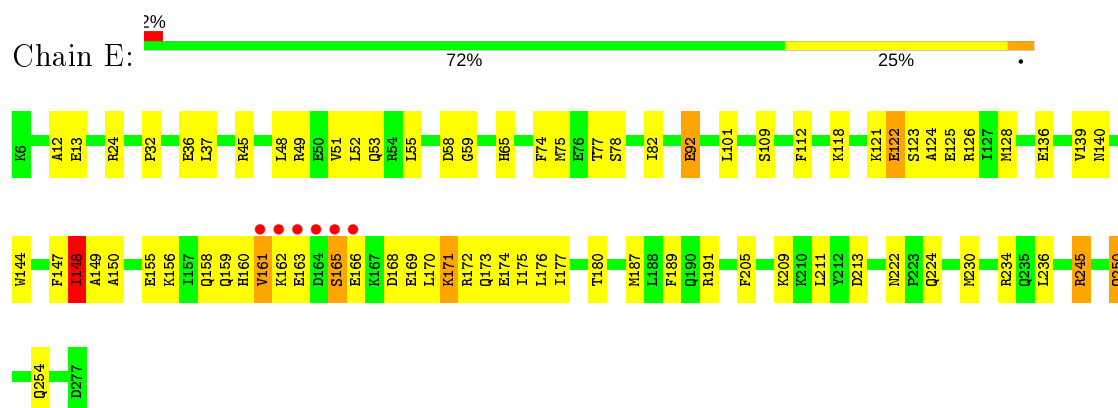
- Molecule 3 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	31	Total	C	N	O	P	0	0	0
			634	305	103	195	31			
3	D	31	Total	C	N	O	P	0	0	0
			634	305	103	195	31			

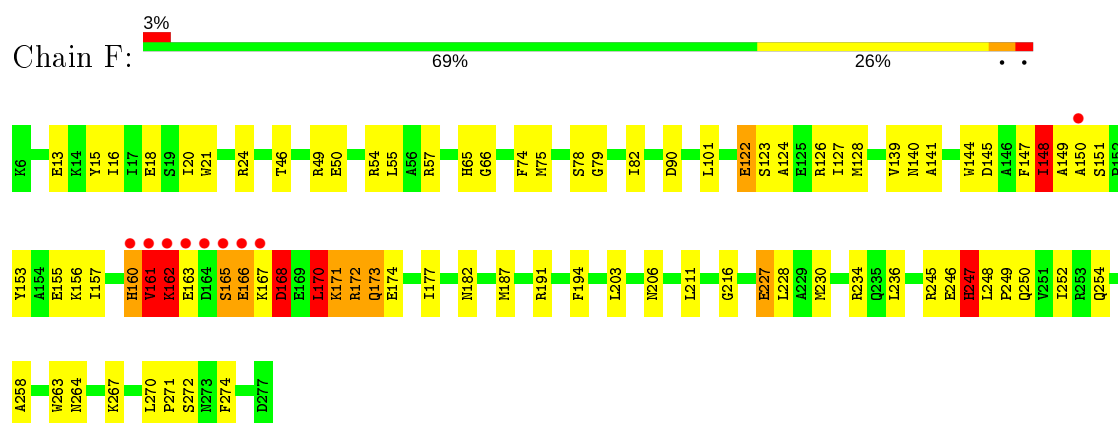
3 Residue-property plots

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.

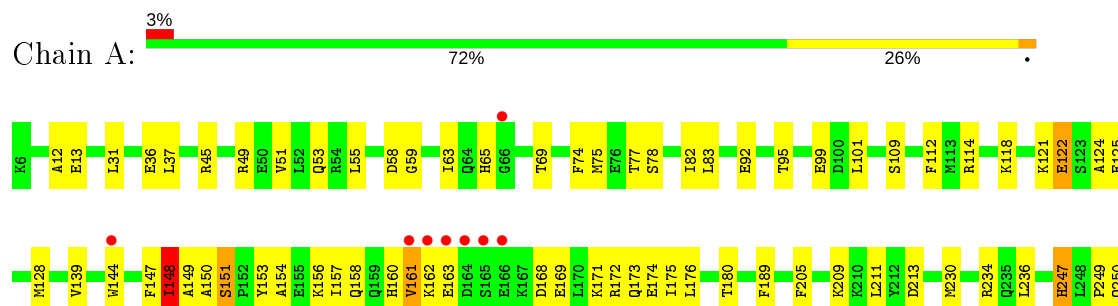
- Molecule 1: Fatty acid metabolism regulator protein

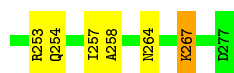


- Molecule 1: Fatty acid metabolism regulator protein

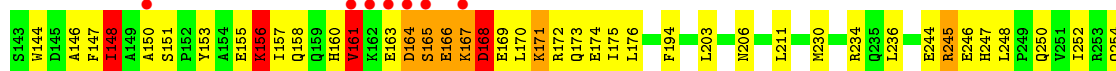
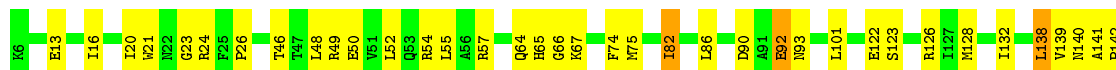


- Molecule 1: Fatty acid metabolism regulator protein





- Molecule 1: Fatty acid metabolism regulator protein



- Molecule 2: DNA (31-MER)



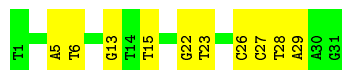
- Molecule 2: DNA (31-MER)



- Molecule 3: DNA (31-MER)



- Molecule 3: DNA (31-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.60Å 94.70Å 101.70Å 89.80° 114.60° 116.50°	Depositor
Resolution (Å)	19.89 – 3.21 19.89 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.89-3.21) 98.4 (19.89-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.15 (at 3.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.218 , 0.252 0.221 , 0.253	Depositor DCC
R_{free} test set	1995 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	1.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.438 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11346	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.34	0/2250	0.63	2/3041 (0.1%)
1	B	0.40	0/2250	0.74	6/3041 (0.2%)
1	E	0.32	0/2250	0.61	0/3041
1	F	0.52	5/2250 (0.2%)	0.92	15/3041 (0.5%)
2	C	0.60	0/717	0.96	0/1103
2	G	0.60	0/717	0.95	0/1103
3	D	0.62	0/707	1.15	0/1090
3	H	0.62	0/707	1.15	0/1090
All	All	0.46	5/11848 (0.0%)	0.83	23/16550 (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	1
1	B	0	3
1	E	0	2
1	F	0	6
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	161	VAL	CA-CB	7.21	1.69	1.54
1	F	162	LYS	CB-CG	-7.05	1.33	1.52
1	F	160	HIS	CA-CB	5.42	1.65	1.53
1	F	160	HIS	CA-C	5.28	1.66	1.52
1	F	161	VAL	N-CA	5.02	1.56	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	168	ASP	CB-CG-OD2	-12.29	107.24	118.30
1	F	172	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	F	160	HIS	CB-CA-C	11.20	132.81	110.40
1	F	162	LYS	CB-CA-C	-9.43	91.54	110.40
1	F	168	ASP	CB-CG-OD1	9.21	126.59	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	122	GLU	Peptide
1	E	148	ILE	Peptide
1	F	148	ILE	Peptide
1	F	161	VAL	Peptide
1	F	162	LYS	Peptide

5.2 Too-close contacts ⓘ

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	2201	0	2185	61	1
1	B	2201	0	2185	77	0
1	E	2201	0	2185	60	1
1	F	2201	0	2185	96	0
2	C	637	0	347	13	0
2	G	637	0	347	14	0
3	D	634	0	356	10	0
3	H	634	0	356	10	0
All	All	11346	0	10146	312	1

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 15.

The worst 5 of 312 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:171:LYS:HG3	1:B:174:GLU:HB2	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:TYR:HD1	1:F:156:LYS:HE2	1.39	0.87
1:E:148:ILE:HD13	1:E:150:ALA:HB2	1.57	0.86
1:F:122:GLU:HG2	1:F:126:ARG:HH12	1.44	0.82
1:F:160:HIS:CD2	1:F:162:LYS:HE2	2.17	0.78

All (1) 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:E:24:ARG:NH2	1:A:174:GLU:OE2[1_565]	2.15	0.05

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	270/272 (99%)	247 (92%)	20 (7%)	3 (1%)	14	51
1	B	270/272 (99%)	248 (92%)	16 (6%)	6 (2%)	6	35
1	E	270/272 (99%)	246 (91%)	22 (8%)	2 (1%)	22	61
1	F	270/272 (99%)	245 (91%)	21 (8%)	4 (2%)	10	44
All	All	1080/1088 (99%)	986 (91%)	79 (7%)	15 (1%)	11	46

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	148	ILE
1	F	148	ILE
1	F	162	LYS
1	F	165	SER
1	A	148	ILE

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	236 / 236 (100%)	232 (98%)	4 (2%)	60	83
1	B	236 / 236 (100%)	227 (96%)	9 (4%)	33	67
1	E	236 / 236 (100%)	230 (98%)	6 (2%)	47	77
1	F	236 / 236 (100%)	226 (96%)	10 (4%)	30	65
All	All	944 / 944 (100%)	915 (97%)	29 (3%)	40	72

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	245	ARG
1	A	114	ARG
1	B	171	LYS
1	F	247	HIS
1	A	122	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	160	HIS
1	F	254	GLN
1	B	158	GLN
1	F	158	GLN
1	A	247	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 ⓘ

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, 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	272/272 (100%)	0.01	8 (2%)	51	36	49, 72, 125, 186	0
1	B	272/272 (100%)	0.01	7 (2%)	56	40	50, 80, 144, 188	0
1	E	272/272 (100%)	0.03	6 (2%)	62	48	51, 71, 125, 187	0
1	F	272/272 (100%)	0.02	9 (3%)	46	30	52, 80, 141, 190	0
2	C	31/31 (100%)	-0.79	0	100	100	58, 103, 124, 129	0
2	G	31/31 (100%)	-0.69	0	100	100	59, 104, 123, 129	0
3	D	31/31 (100%)	-0.69	0	100	100	61, 95, 127, 135	0
3	H	31/31 (100%)	-0.72	0	100	100	60, 95, 126, 134	0
All	All	1212/1212 (100%)	-0.06	30 (2%)	57	43	49, 78, 135, 190	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	SER	6.6
1	B	150	ALA	6.4
1	F	161	VAL	6.1
1	E	163	GLU	5.7
1	B	164	ASP	5.5

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 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.