Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:40 PM GMT

PDB ID	:	4J40
Title	:	Crystal structure of the dual-domain GGDEF-EAL module of FimX from Pseudomonas aeruginosa
Authors	:	Navarro, M.V.; De, N.; Bae, N.; Wang, Q.; Sondermann, H.
Deposited on	:	2013-02-06
Resolution	:	2.99 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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)	:	trunk26865
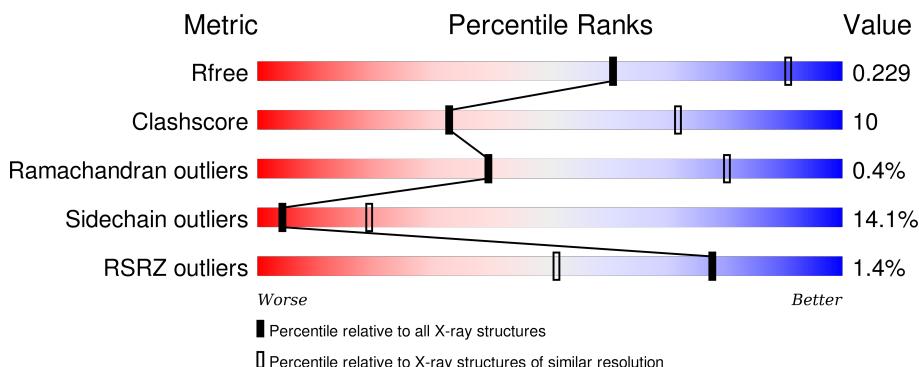
1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.99 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		0.229
Clashscore		10
Ramachandran outliers		0.4%
Sidechain outliers		14.1%
RSRZ outliers		1.4%

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	437	41% 14% • 43%
1	B	437	% 38% 17% • 43%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3916 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 FimX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			1958	1257	335	363	3			
1	B	251	Total	C	N	O	S	0	0	0
			1958	1257	335	363	3			
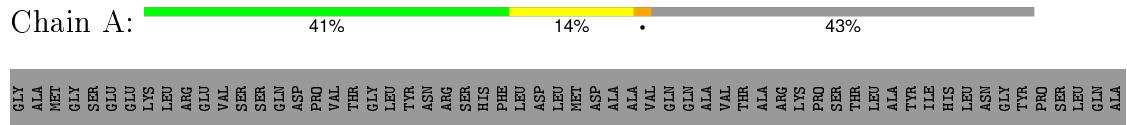
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLY	-	EXPRESSION TAG	UNP Q9HUK6
A	256	ALA	-	EXPRESSION TAG	UNP Q9HUK6
A	257	MET	-	EXPRESSION TAG	UNP Q9HUK6
A	258	GLY	-	EXPRESSION TAG	UNP Q9HUK6
A	259	SER	-	EXPRESSION TAG	UNP Q9HUK6
B	255	GLY	-	EXPRESSION TAG	UNP Q9HUK6
B	256	ALA	-	EXPRESSION TAG	UNP Q9HUK6
B	257	MET	-	EXPRESSION TAG	UNP Q9HUK6
B	258	GLY	-	EXPRESSION TAG	UNP Q9HUK6
B	259	SER	-	EXPRESSION TAG	UNP Q9HUK6
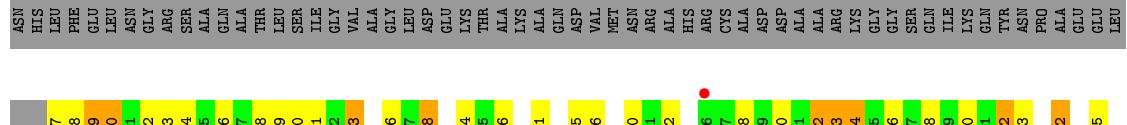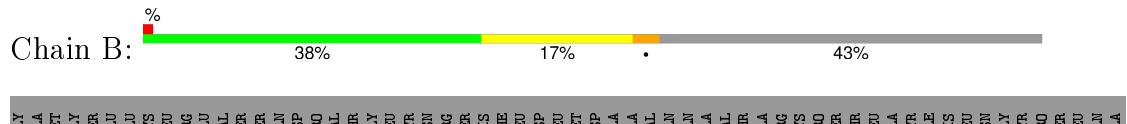
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: FimX

- Molecule 1: FimX

E629 I633 L634 L637 E643 Q644 Q645 S648 I649 V653 E654 L662 W663 T668 Y669 I670 Y673 Y674 L675 D683 S687 SER GLY ASP GLU

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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.25Å 106.25Å 193.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.36 – 2.99 26.80 – 2.99	Depositor EDS
% Data completeness (in resolution range)	90.0 (25.36-2.99) 90.0 (26.80-2.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	8.31 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.208 , 0.232 0.203 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (9.66%)	DCC
Wilson B-factor (Å^2)	79.4	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Outliers	1 of 20717 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3916	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.28	0/1999	0.46	0/2715
1	B	0.27	0/1999	0.48	0/2715
All	All	0.27	0/3998	0.47	0/5430

There are no bond length outliers.

There are no bond angle outliers.

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	1958	0	1973	41	0
1	B	1958	0	1973	54	0
All	All	3916	0	3946	82	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 10.

All (82) 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:A:496:ALA:HB2	1:B:654:GLU:HG2	1.63	0.81
1:A:674:TYR:O	1:B:440:ARG:NH2	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ARG:NH2	1:B:674:TYR:O	2.22	0.72
1:A:449:GLN:O	1:A:453:THR:OG1	2.08	0.71
1:B:439:GLN:OE1	1:B:482:ASN:ND2	2.25	0.69
1:A:673:TYR:HB2	1:B:492:GLU:HG2	1.73	0.69
1:B:522:ARG:HD2	1:B:558:PRO:HG2	1.74	0.68
1:B:653:VAL:HG21	1:B:670:ILE:HG23	1.78	0.65
1:B:518:LEU:HD23	1:B:557:LEU:HD21	1.79	0.65
1:A:654:GLU:HG3	1:B:443:VAL:HB	1.80	0.63
1:B:515:ILE:HG23	1:B:557:LEU:HD22	1.82	0.62
1:B:444:ILE:HD13	1:B:500:ALA:HB2	1.82	0.61
1:B:534:LEU:HB2	1:B:566:ILE:HG22	1.83	0.59
1:B:545:LEU:HG	1:B:546:PRO:HD3	1.84	0.57
1:B:545:LEU:HD23	1:B:545:LEU:H	1.69	0.57
1:B:670:ILE:HG22	1:B:675:LEU:HD21	1.86	0.56
1:A:464:ILE:HD13	1:A:675:LEU:HD23	1.88	0.56
1:B:475:GLU:HA	1:B:531:PHE:HB2	1.88	0.55
1:A:676:GLN:HG3	1:A:684:TYR:CD2	2.43	0.54
1:A:595:SER:HA	1:A:616:LYS:HB3	1.90	0.53
1:A:539:LEU:HD21	1:A:578:ALA:HA	1.89	0.53
1:B:552:LEU:HB2	1:B:553:LYS:HZ2	1.75	0.52
1:A:489:PRO:HB2	1:A:492:GLU:HB2	1.91	0.51
1:B:466:LEU:HD11	1:B:670:ILE:HD12	1.93	0.51
1:A:511:ILE:O	1:A:515:ILE:HG12	2.11	0.51
1:A:676:GLN:HA	1:B:440:ARG:HB3	1.93	0.51
1:B:629:GLU:O	1:B:633:ILE:HG12	2.11	0.51
1:A:654:GLU:HG2	1:B:496:ALA:HB2	1.93	0.50
1:A:495:HIS:HE1	1:B:619:GLY:HA3	1.76	0.50
1:A:534:LEU:HB2	1:A:566:ILE:HG22	1.94	0.50
1:A:659:LEU:HD12	1:A:675:LEU:HD11	1.94	0.49
1:B:490:PRO:HA	1:B:493:PHE:CD2	2.48	0.49
1:B:595:SER:HA	1:B:616:LYS:HB3	1.94	0.49
1:A:653:VAL:HG22	1:A:662:LEU:HD12	1.94	0.48
1:B:522:ARG:HA	1:B:526:HIS:O	2.13	0.48
1:A:536:SER:O	1:A:540:GLN:HG3	2.14	0.48
1:B:466:LEU:HD13	1:B:663:TRP:HD1	1.79	0.47
1:A:492:GLU:HG2	1:B:673:TYR:HB2	1.95	0.47
1:A:437:ALA:HA	1:A:438:ALA:HA	1.60	0.47
1:B:670:ILE:CG2	1:B:675:LEU:HD21	2.45	0.47
1:B:466:LEU:HD13	1:B:663:TRP:CD1	2.50	0.46
1:A:472:GLU:HB2	1:A:528:THR:HG22	1.97	0.46
1:B:450:ALA:HA	1:B:453:THR:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:LEU:HD21	1:A:581:LEU:HD23	1.98	0.46
1:A:490:PRO:HA	1:A:493:PHE:CE2	2.50	0.46
1:A:625:LEU:HD21	1:A:634:LEU:HD12	1.97	0.46
1:B:448:GLN:HG3	1:B:502:LEU:HD21	1.97	0.45
1:B:558:PRO:O	1:B:561:SER:HB3	2.17	0.45
1:B:458:LEU:HA	1:B:458:LEU:HD12	1.83	0.45
1:A:498:LYS:HB3	1:B:623:GLN:HG3	1.98	0.44
1:A:444:ILE:HD13	1:A:500:ALA:HB2	2.00	0.44
1:A:458:LEU:HD13	1:A:509:TRP:HZ3	1.81	0.44
1:B:649:ILE:HG12	1:B:669:TYR:HB2	1.99	0.44
1:A:653:VAL:HG21	1:A:670:ILE:HB	1.99	0.44
1:A:492:GLU:CG	1:B:673:TYR:HB2	2.47	0.44
1:B:490:PRO:O	1:B:494:LEU:HB2	2.18	0.44
1:B:512:LEU:HA	1:B:512:LEU:HD12	1.79	0.43
1:B:502:LEU:HD12	1:B:502:LEU:HA	1.88	0.42
1:A:557:LEU:HA	1:A:558:PRO:HD3	1.89	0.42
1:B:442:ASP:O	1:B:446:ILE:HG13	2.19	0.42
1:A:492:GLU:HG3	1:B:654:GLU:OE2	2.19	0.42
1:A:442:ASP:O	1:A:446:ILE:HG13	2.18	0.42
1:B:653:VAL:HG22	1:B:662:LEU:HD12	2.00	0.42
1:A:676:GLN:HG3	1:A:684:TYR:HD2	1.82	0.42
1:A:541:ASP:HA	1:A:542:PRO:HD3	1.72	0.42
1:A:446:ILE:O	1:A:450:ALA:N	2.53	0.42
1:B:548:LEU:HD11	1:B:564:PHE:CZ	2.55	0.42
1:A:544:LEU:O	1:A:548:LEU:HB2	2.20	0.41
1:B:437:ALA:HA	1:B:438:ALA:HA	1.55	0.41
1:A:649:ILE:HG12	1:A:669:TYR:HB2	2.03	0.41
1:B:547:TRP:O	1:B:550:VAL:HG22	2.20	0.41
1:A:518:LEU:O	1:A:522:ARG:HB2	2.20	0.41
1:B:625:LEU:HA	1:B:625:LEU:HD23	1.90	0.41
1:B:662:LEU:HB2	1:B:670:ILE:HD11	2.03	0.41
1:A:495:HIS:CE1	1:B:619:GLY:HA3	2.56	0.41
1:B:494:LEU:HD13	1:B:494:LEU:HA	1.85	0.41
1:A:456:PHE:HB2	1:A:509:TRP:CH2	2.55	0.41
1:B:541:ASP:HA	1:B:542:PRO:HD3	1.81	0.41
1:B:607:LEU:HD13	1:B:607:LEU:HA	1.92	0.41
1:B:464:ILE:HG12	1:B:675:LEU:HD23	2.02	0.40
1:B:456:PHE:CE1	1:B:480:LEU:HD13	2.57	0.40
1:B:553:LYS:H	1:B:553:LYS:CE	2.35	0.40

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	249/437 (57%)	235 (94%)	13 (5%)	1 (0%)	39	80
1	B	249/437 (57%)	231 (93%)	17 (7%)	1 (0%)	39	80
All	All	498/874 (57%)	466 (94%)	30 (6%)	2 (0%)	39	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	645	GLN
1	B	503	ALA

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	209/351 (60%)	186 (89%)	23 (11%)	8	30
1	B	209/351 (60%)	173 (83%)	36 (17%)	2	12
All	All	418/702 (60%)	359 (86%)	59 (14%)	4	19

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	LEU
1	A	453	THR
1	A	471	HIS
1	A	476	VAL

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Mol	Chain	Res	Type
1	A	484	GLN
1	A	488	VAL
1	A	502	LEU
1	A	539	LEU
1	A	548	LEU
1	A	550	VAL
1	A	557	LEU
1	A	562	LEU
1	A	575	LEU
1	A	576	LYS
1	A	581	LEU
1	A	626	ASN
1	A	628	VAL
1	A	634	LEU
1	A	637	LEU
1	A	645	GLN
1	A	654	GLU
1	A	668	THR
1	A	676	GLN
1	B	439	GLN
1	B	440	ARG
1	B	449	GLN
1	B	451	LEU
1	B	453	THR
1	B	458	LEU
1	B	471	HIS
1	B	476	VAL
1	B	488	VAL
1	B	492	GLU
1	B	493	PHE
1	B	494	LEU
1	B	498	LYS
1	B	502	LEU
1	B	512	LEU
1	B	521	HIS
1	B	528	THR
1	B	545	LEU
1	B	553	LYS
1	B	561	SER
1	B	577	GLN
1	B	579	LYS
1	B	580	GLN

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Mol	Chain	Res	Type
1	B	588	LEU
1	B	610	LEU
1	B	624	ASP
1	B	628	VAL
1	B	634	LEU
1	B	637	LEU
1	B	643	GLU
1	B	645	GLN
1	B	648	SER
1	B	668	THR
1	B	670	ILE
1	B	675	LEU
1	B	683	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	HIS
1	A	623	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)

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(Å²)	Q<0.9
1	A	251/437 (57%)	-0.19	2 (0%)	87	67	52, 76, 121, 180	0
1	B	251/437 (57%)	-0.04	5 (1%)	68	39	58, 93, 136, 191	0
All	All	502/874 (57%)	-0.11	7 (1%)	78	51	52, 86, 129, 191	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	525	GLY	3.3
1	B	556	ARG	2.6
1	B	526	HIS	2.4
1	B	486	GLN	2.3
1	A	524	LYS	2.1
1	A	481	LEU	2.1
1	B	533	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.