



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 12:02 pm BST

PDB ID : 5X90  
Title : Structure of DotL(656-783)-IcmS-IcmW-LvgA derived from Legionella pneumophila  
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Deposited on : 2017-03-04  
Resolution : 2.80 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

<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

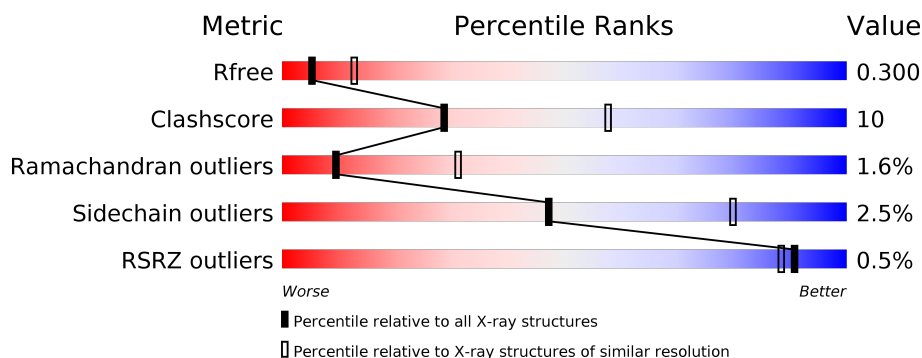
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	114	
1	E	114	
2	F	149	
3	G	108	
4	H	172	
5	B	148	

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Mol	Chain	Length	Quality of chain
6	C	107	<div><div></div><div>2%</div><div>69%</div><div>22%</div><div>6%</div></div>
7	D	171	<div><div></div><div>71%</div><div>27%</div><div></div></div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8058 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 IcmS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	113	Total	C	N	O	S	0	0	0
			849	540	135	165	9			
1	A	113	Total	C	N	O	S	0	0	0
			846	538	140	159	9			

- Molecule 2 is a protein called IcmW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	149	Total	C	N	O	S	0	0	0
			1153	739	195	215	4			

- Molecule 3 is a protein called IcmO (DotL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	108	Total	C	N	O	S	0	0	0
			768	489	133	145	1			

- Molecule 4 is a protein called Hypothetical virulence protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	167	Total	C	N	O	S	0	0	0
			1314	853	215	239	7			

- Molecule 5 is a protein called IcmW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	146	Total	C	N	O	S	0	0	0
			1093	705	188	196	4			

- Molecule 6 is a protein called IcmO (DotL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	101	Total	C	N	O	S	0	0	0
			717	455	124	137	1			

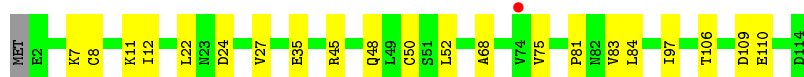
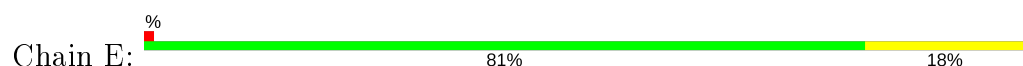
- Molecule 7 is a protein called Hypothetical virulence protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	171	Total	C	N	O	S	0	0	0
			1318	854	221	237	6			

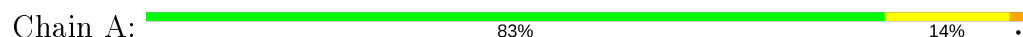
### 3 Residue-property plots [i](#)

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.

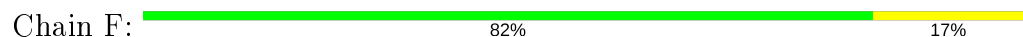
- Molecule 1: IcmS



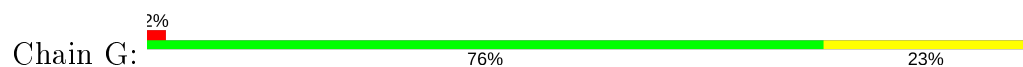
- Molecule 1: IcmS



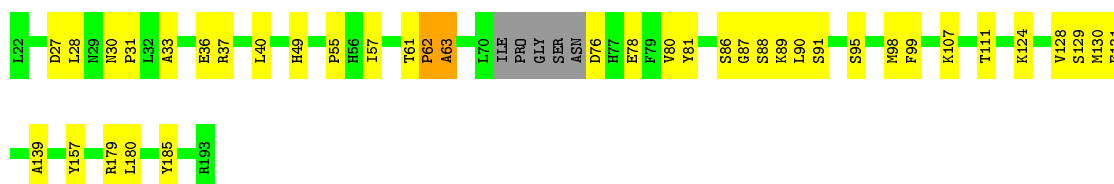
- Molecule 2: IcmW



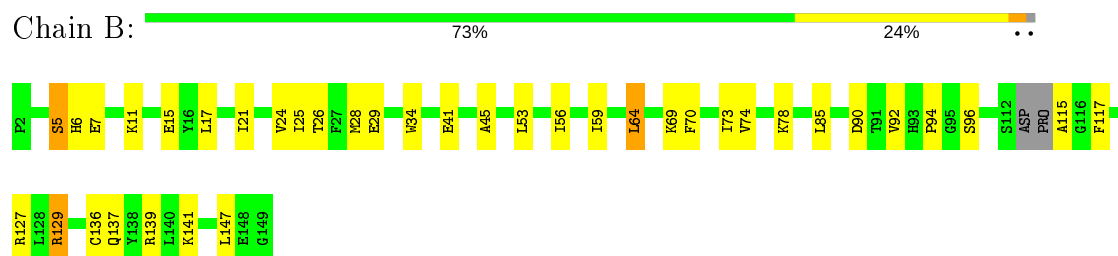
- Molecule 3: IcmO (DotL)



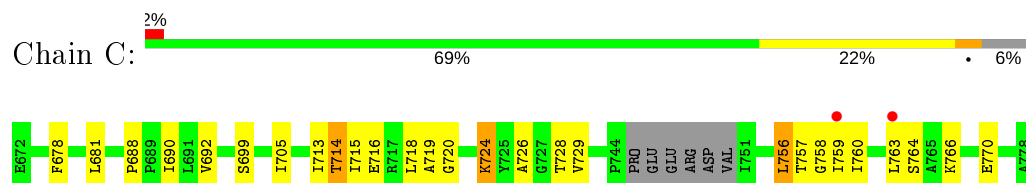
- Molecule 4: Hypothetical virulence protein



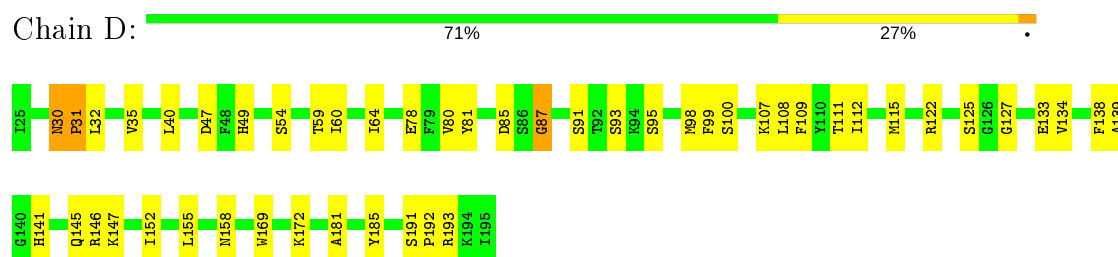
- Molecule 5: IcmW



- Molecule 6: IcmO (DotL)



- Molecule 7: Hypothetical virulence protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.32Å 152.32Å 74.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.43 – 2.80 49.86 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (41.43-2.80) 95.6 (49.86-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.252 , 0.295 0.256 , 0.300	Depositor DCC
$R_{free}$ test set	2034 reflections (3.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.034 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	8058	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

### 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	0.36	0/859	0.61	1/1162 (0.1%)
1	E	0.38	0/862	0.57	0/1166
2	F	0.46	3/1175 (0.3%)	0.56	2/1589 (0.1%)
3	G	0.31	0/779	0.46	0/1066
4	H	0.35	0/1351	0.55	1/1836 (0.1%)
5	B	0.31	0/1113	0.54	1/1507 (0.1%)
6	C	0.34	0/726	0.57	0/989
7	D	0.35	0/1356	0.54	0/1846
All	All	0.36	3/8221 (0.0%)	0.55	5/11161 (0.0%)

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
6	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	84	ARG	CZ-NH1	-5.67	1.25	1.33
2	F	84	ARG	NE-CZ	-5.56	1.25	1.33
2	F	84	ARG	CZ-NH2	-5.37	1.26	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	64	LEU	CA-CB-CG	7.37	132.25	115.30
1	A	103	ARG	NE-CZ-NH1	-5.38	117.61	120.30
2	F	63	LEU	CA-CB-CG	5.35	127.61	115.30
2	F	64	LEU	CA-CB-CG	5.30	127.50	115.30
4	H	76	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	720	GLY	Peptide
6	C	724	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	846	0	829	14	0
1	E	849	0	828	13	0
2	F	1153	0	1120	24	0
3	G	768	0	746	24	0
4	H	1314	0	1257	28	0
5	B	1093	0	1049	31	0
6	C	717	0	683	24	0
7	D	1318	0	1247	36	0
All	All	8058	0	7759	154	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.

The worst 5 of 154 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)
2:F:31:VAL:HG21	3:G:675:LEU:HD22	1.14	1.11
2:F:31:VAL:CG2	3:G:675:LEU:HD22	1.93	0.99
5:B:6:HIS:HE1	5:B:78:LYS:HD2	1.35	0.92
2:F:31:VAL:HG21	3:G:675:LEU:CD2	1.98	0.91
4:H:57:ILE:HD11	4:H:88:SER:HA	1.57	0.87

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	111/114 (97%)	105 (95%)	6 (5%)	0	100	100
1	E	111/114 (97%)	102 (92%)	9 (8%)	0	100	100
2	F	147/149 (99%)	134 (91%)	13 (9%)	0	100	100
3	G	106/108 (98%)	99 (93%)	6 (6%)	1 (1%)	17	46
4	H	163/172 (95%)	142 (87%)	16 (10%)	5 (3%)	4	14
5	B	142/148 (96%)	124 (87%)	15 (11%)	3 (2%)	7	23
6	C	97/107 (91%)	86 (89%)	8 (8%)	3 (3%)	4	14
7	D	169/171 (99%)	148 (88%)	16 (10%)	5 (3%)	4	15
All	All	1046/1083 (97%)	940 (90%)	89 (8%)	17 (2%)	9	31

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	130	MET
6	C	724	LYS
7	D	30	ASN
4	H	87	GLY
5	B	41	GLU

### 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	88/97 (91%)	85 (97%)	3 (3%)	37	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	90/97 (93%)	85 (94%)	5 (6%)	21	51
2	F	118/131 (90%)	116 (98%)	2 (2%)	60	87
3	G	73/91 (80%)	71 (97%)	2 (3%)	44	78
4	H	138/152 (91%)	135 (98%)	3 (2%)	52	83
5	B	106/130 (82%)	104 (98%)	2 (2%)	57	85
6	C	66/91 (72%)	65 (98%)	1 (2%)	65	89
7	D	133/151 (88%)	131 (98%)	2 (2%)	65	89
All	All	812/940 (86%)	792 (98%)	20 (2%)	47	80

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	27	ASP
4	H	37	ARG
5	B	129	ARG
3	G	716	GLU
3	G	764	SER

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

Mol	Chain	Res	Type
1	E	98	GLN
2	F	137	GLN
4	H	145	GLN
1	A	98	GLN
5	B	6	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	113/114 (99%)	-0.57	0 <span>100</span> <span>100</span>	38, 54, 73, 81	0
1	E	113/114 (99%)	-0.51	1 (0%) <span>84</span> <span>80</span>	31, 54, 75, 86	0
2	F	149/149 (100%)	-0.43	0 <span>100</span> <span>100</span>	35, 57, 86, 100	0
3	G	108/108 (100%)	-0.44	2 (1%) <span>66</span> <span>59</span>	46, 67, 98, 105	0
4	H	167/172 (97%)	-0.38	0 <span>100</span> <span>100</span>	32, 58, 97, 113	0
5	B	146/148 (98%)	-0.38	0 <span>100</span> <span>100</span>	41, 72, 96, 111	0
6	C	101/107 (94%)	-0.25	2 (1%) <span>65</span> <span>56</span>	46, 75, 110, 121	0
7	D	171/171 (100%)	-0.37	0 <span>100</span> <span>100</span>	39, 63, 102, 119	0
All	All	1068/1083 (98%)	-0.41	5 (0%) <span>91</span> <span>88</span>	31, 61, 100, 121	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	C	759	ILE	3.2
1	E	74	VAL	2.6
3	G	687	ALA	2.3
3	G	778	ALA	2.1
6	C	763	LEU	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.