



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:27 pm GMT

PDB ID : 3B5X  
Title : Crystal Structure of MsbA from Vibrio cholerae  
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Deposited on : 2007-10-26  
Resolution : 5.50 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	:	trunk28620
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)	:	recalc28949

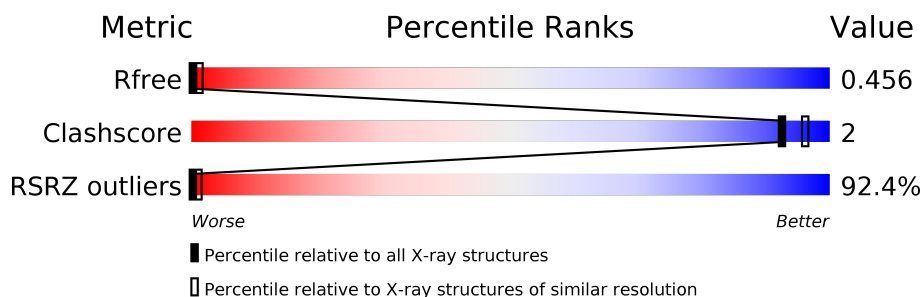
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.50 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	1052 (7.20-3.70)
Clashscore	112137	1021 (7.20-3.76)
RSRZ outliers	101464	1061 (7.20-3.70)

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	582	
1	B	582	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1144 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.

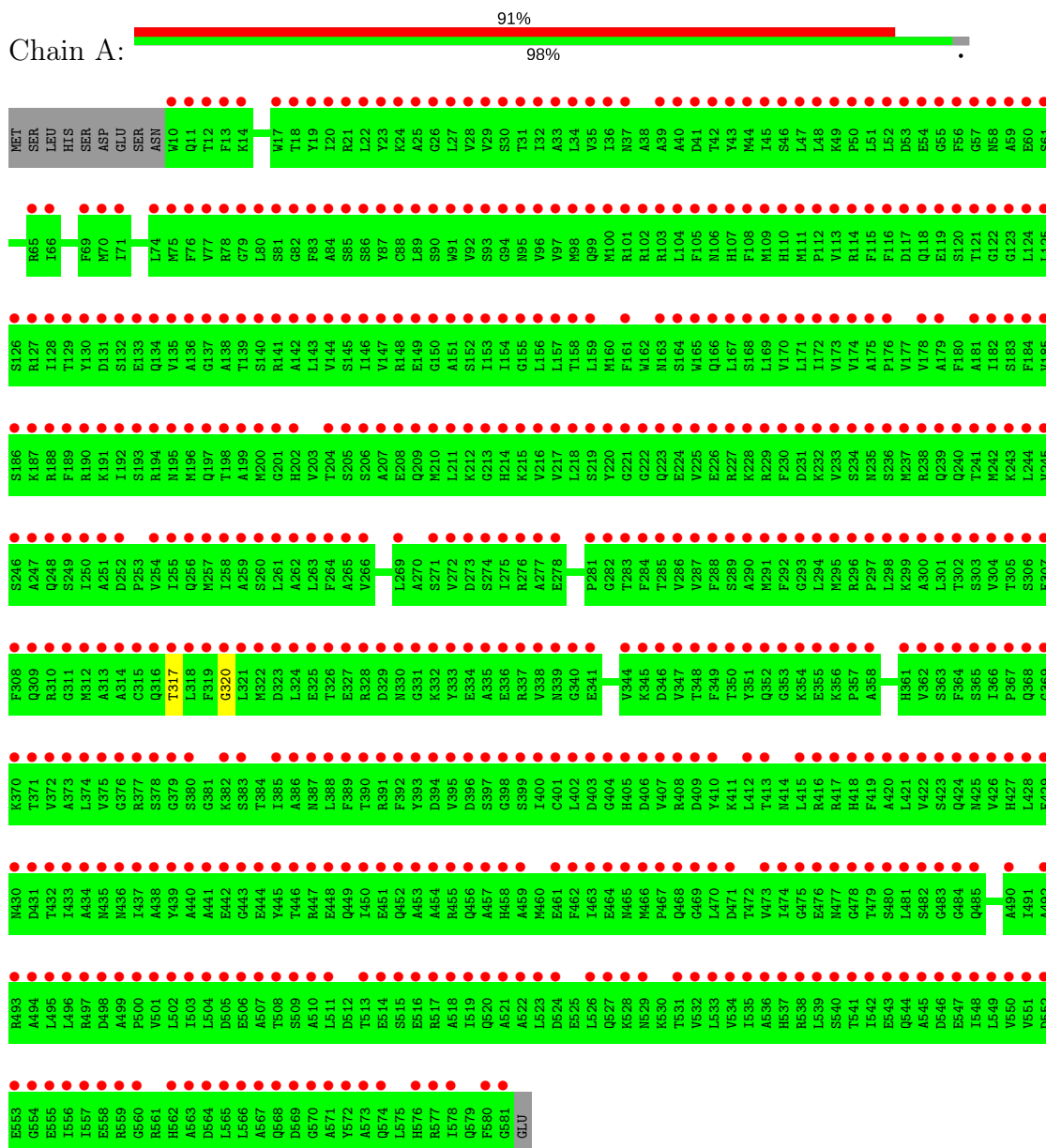
- Molecule 1 is a protein called Lipid A export ATP-binding/permease protein msbA.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	572	Total	C	0	0	572
			572	572			
1	B	572	Total	C	0	0	572
			572	572			

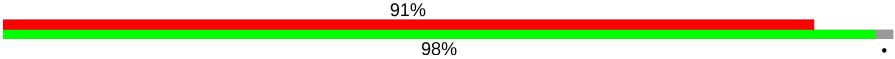
### 3 Residue-property plots

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: Lipid A export ATP-binding/permease protein msbA



- Molecule 1: Lipid A export ATP-binding/permease protein msbA

Chain B: 

V551	I491	Q368	T305	L244	F184	G123	S61
D552	A492	G369	S306	V245	V185	L124	N62
E553	R493	K370	E307	S246	S186	L125	
G554	T432	T371	F308	A247	K187	S126	R65
E555	I433	V372	Q309	Q248	R188	R127	I66
I556	L495	A373	R310	S249	F189	I128	L67
I557	N435						
E558	N436	L374	G311	T250	R190	T129	
D559	I437	V375	M312	A251	K191	Y130	M70
R559	A438	G376	A313	D252	I192	D131	L71
G560	P500	R377	A314	P253	S193	S132	L72
R561	V501	S378	C315	V254	R194	E133	G73
H562	L502	G379	Q316	T255	N195	Q134	L74
A663	F503	Q242	T317	Q256	M196	V135	M75
D664	L504	G381	L318	N257	Q197	A136	F76
L665	D505	E444	F319	L258	T198	G137	V77
L566	E506	L566	G320	A259	A199	A138	R78
A567	A507	T445	L321	S260	M200	T139	G79
Q568	T508	I385	M322	L261	G201	S140	L80
D669	S509	A386	D323	A262	H202	R141	S81
G570	A510	N387	L324	L263	V203	A142	G82
A571	L511	L388	E325	F264	T204	L143	F83
Y572	D512	F389	T326	A265	S205	V144	A84
A573	T513	T390	E327	V266	S206	S145	S85
A574	E514	R391	R328	L267	A207	I146	S86
L575	S515	D455	D329	F268	E208	V147	R87
H576	E516	Q456	N330	L269	Q209	R148	C88
R577	R517	A457	G331		M210	E149	L89
L578	A518	H458	K332	V272	L211	G150	S90
Q579	I519	D396	Y333	D273	K212	A151	W91
F580	Q520	S397	E334	S274	G213	S152	V92
G581	A521	G398	A335	L275	H214	I153	S93
	A522	S399	E336	R276	K215	I154	G94
	L523	I463	R337	A277	V216	G155	N95
	D524	C401	V338	E278	V217	L156	V96
	E525	N465	L402	L279	L218	L157	V97
	L526	D403	G340	T280	S219	T158	N98
	Q527	G404	E341	P281	Y220	L159	Q99
	K528	H405	V342	G282	G221	M160	M100
	N529	G469	D406	T283	G222	F161	R101
	K530	L470	V407	F284	Q223	W162	R102
	T531	D471	R408	T285	E224	N163	D41
	V532	T472	D409	V286	V225		L104
	L533	V473		V287	E226	Q166	F105
	V534	L474	L412	F288	R227	L167	M106
	I535	G475	T413	F289	K228	S168	H107
	L536	A536	N414	S289	R229	L169	F108
	H537	R415	L415	A290	F230	V170	S46
	R538	G478	R416	M291	D231	L171	M109
	L539	T479	R417	F292	L172	I171	H110
	S540	S480	H418	Q293	L232	G172	M111
	T541	L481	F419	L294	V233	V173	P112
	L542	S482	A420	M295	S234	V174	V113
	E543	G483	L421	K396	N235	A175	R114
	Q544	Q484	V422	P297	S236	P176	L52
	A545	R485	S423	L298	M237	V177	D53
	D546	R486	Q424	A300	R238	V178	E54
	E547	Q487	N425	L301	Q239	A179	G55
	L548	R488	V426	T302	Q240	F180	E119
	L549	V489	H427	S303	T241	A181	S120
	V550	A490	L428	V204	M242	I182	T121
					V243	S183	L122

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.59Å 150.42Å 148.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 5.50 19.97 – 5.50	Depositor EDS
% Data completeness (in resolution range)	84.0 (19.97-5.50) 84.0 (19.97-5.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 5.55Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.348 , 0.360 0.427 , 0.456	Depositor DCC
$R_{free}$ test set	740 reflections (9.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	215.7	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 82.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	1144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	309.0	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 30.55 % 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 1.2845e-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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	572	0	0	1	0
1	B	572	0	0	1	0
All	All	1144	0	0	2	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 2.

All (2) 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:317:THR:CA	1:A:320:GLY:CA	2.91	0.48
1:B:317:THR:CA	1:B:320:GLY:CA	2.92	0.48

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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, 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	572/582 (98%)	8.84	530 (92%) 0 1	309, 309, 309, 309	0
1	B	572/582 (98%)	8.15	527 (92%) 0 1	309, 309, 309, 309	0
All	All	1144/1164 (98%)	8.49	1057 (92%) 0 1	309, 309, 309, 309	0

The worst 5 of 1057 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	SER	35.3
1	A	31	THR	34.1
1	A	117	ASP	33.3
1	A	296	ARG	32.9
1	A	147	VAL	32.7

### 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.