



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:33 AM GMT

PDB ID : 3B5W
Title : Crystal Structure of Eschericia coli MsbA
Authors : Ward, A.; Reyes, C.L.; Yu, J.; Roth, C.B.; Chang, G.
Deposited on : 2007-10-26
Resolution : 5.30 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
<http://wwpdb.org/validation/2016/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
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

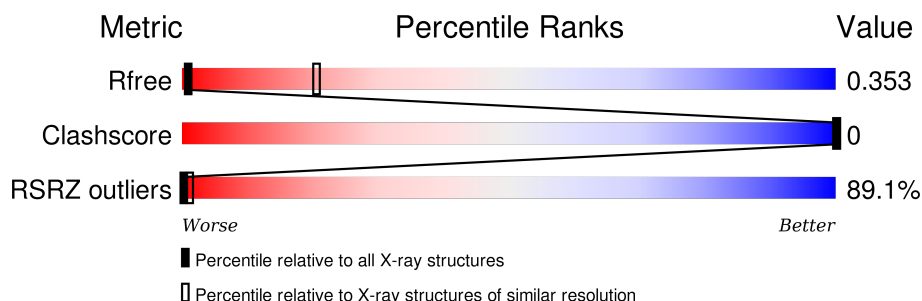
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.30 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}	91344	1162 (7.00-3.60)
Clashscore	102246	1007 (6.92-3.68)
RSRZ outliers	91569	1163 (7.00-3.60)

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 $\leq 5\%$. 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	<div> <div>90%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	B	582	<div> <div>89%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	C	582	<div> <div>89%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	D	582	<div> <div>90%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	E	582	<div> <div>86%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	F	582	<div> <div>86%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	G	582	<div> <div>84%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
1	H	582	<div> <div>86%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4576 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.

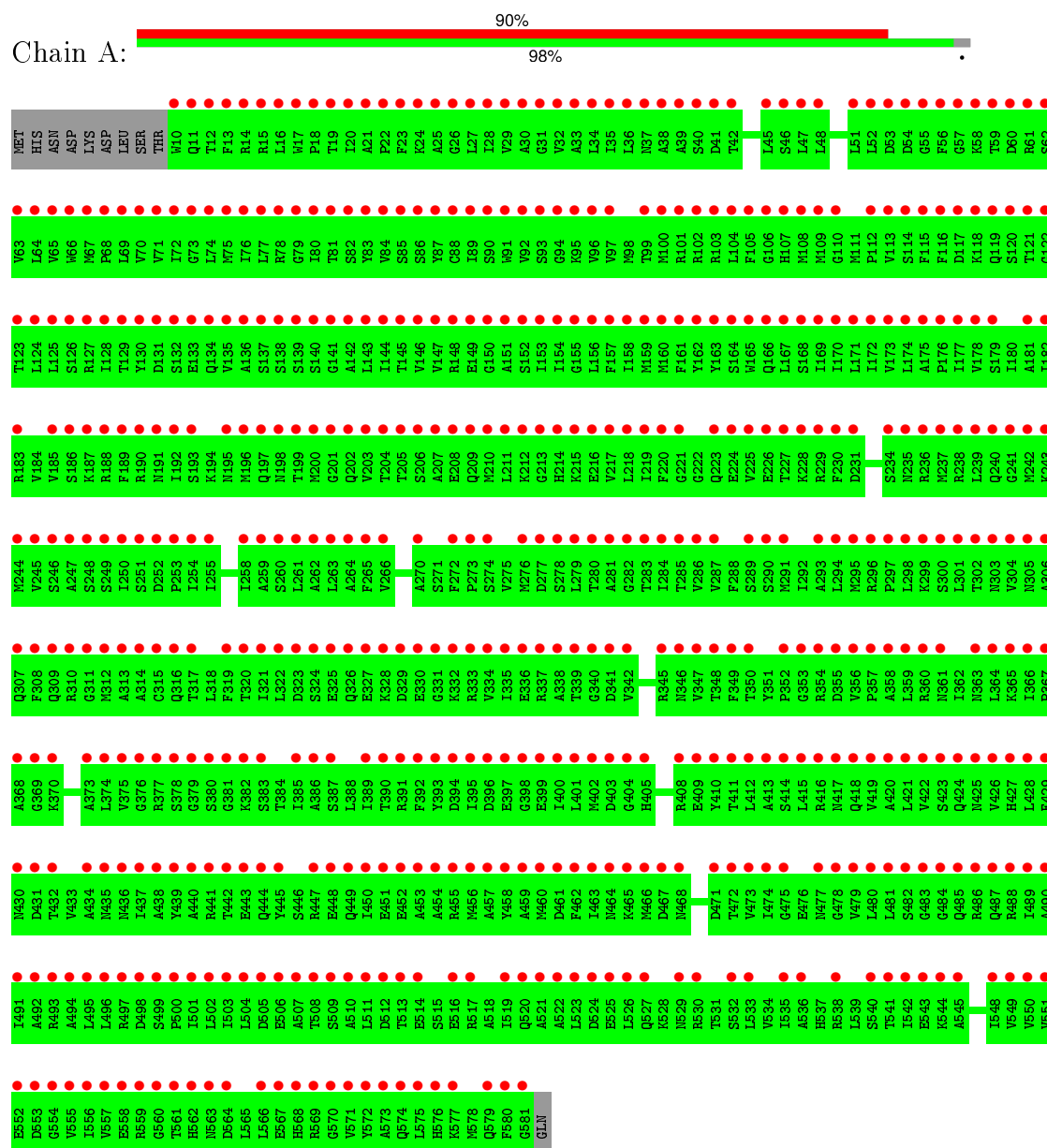
- Molecule 1 is a protein called Lipid A export ATP-binding/permease protein msbA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	572	Total C 572 572	0	0	572
1	B	572	Total C 572 572	0	0	572
1	C	572	Total C 572 572	0	0	572
1	D	572	Total C 572 572	0	0	572
1	E	572	Total C 572 572	0	0	572
1	F	572	Total C 572 572	0	0	572
1	G	572	Total C 572 572	0	0	572
1	H	572	Total C 572 572	0	0	572

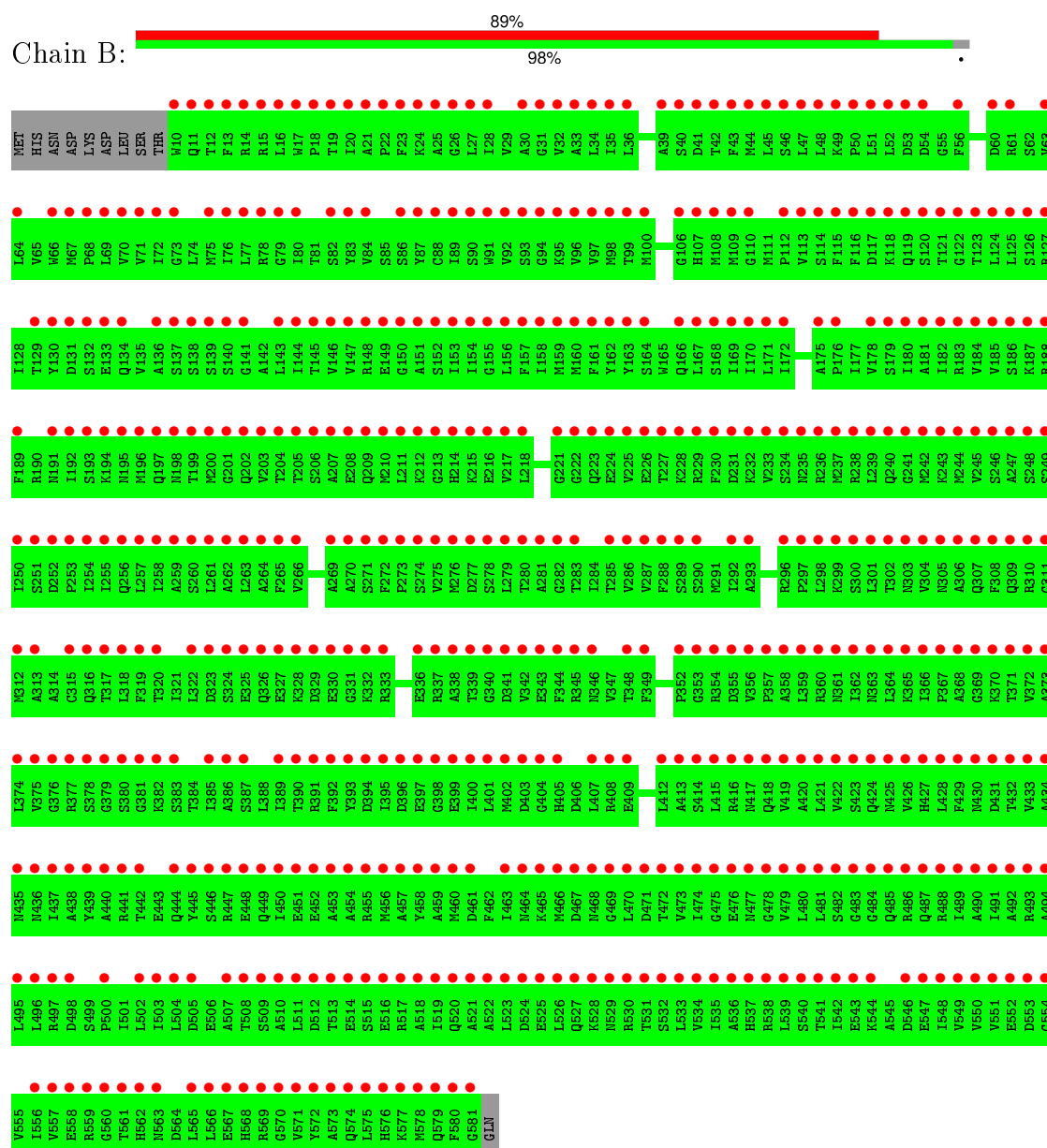
3 Residue-property plots

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

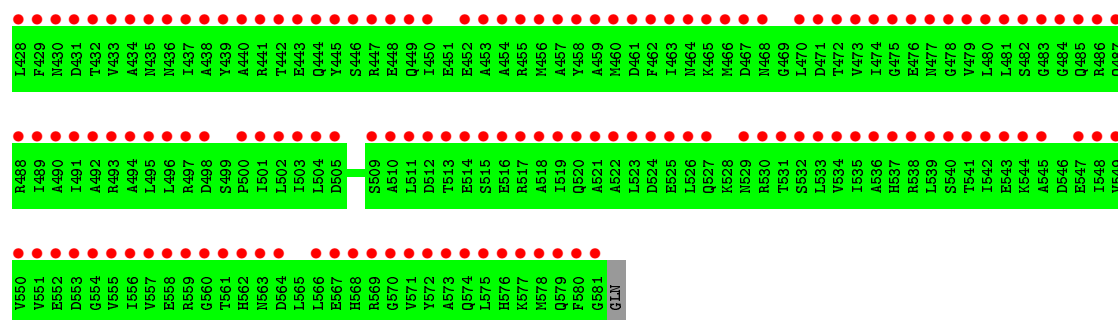
- Molecule 1: Lipid A export ATP-binding/permease protein msbA



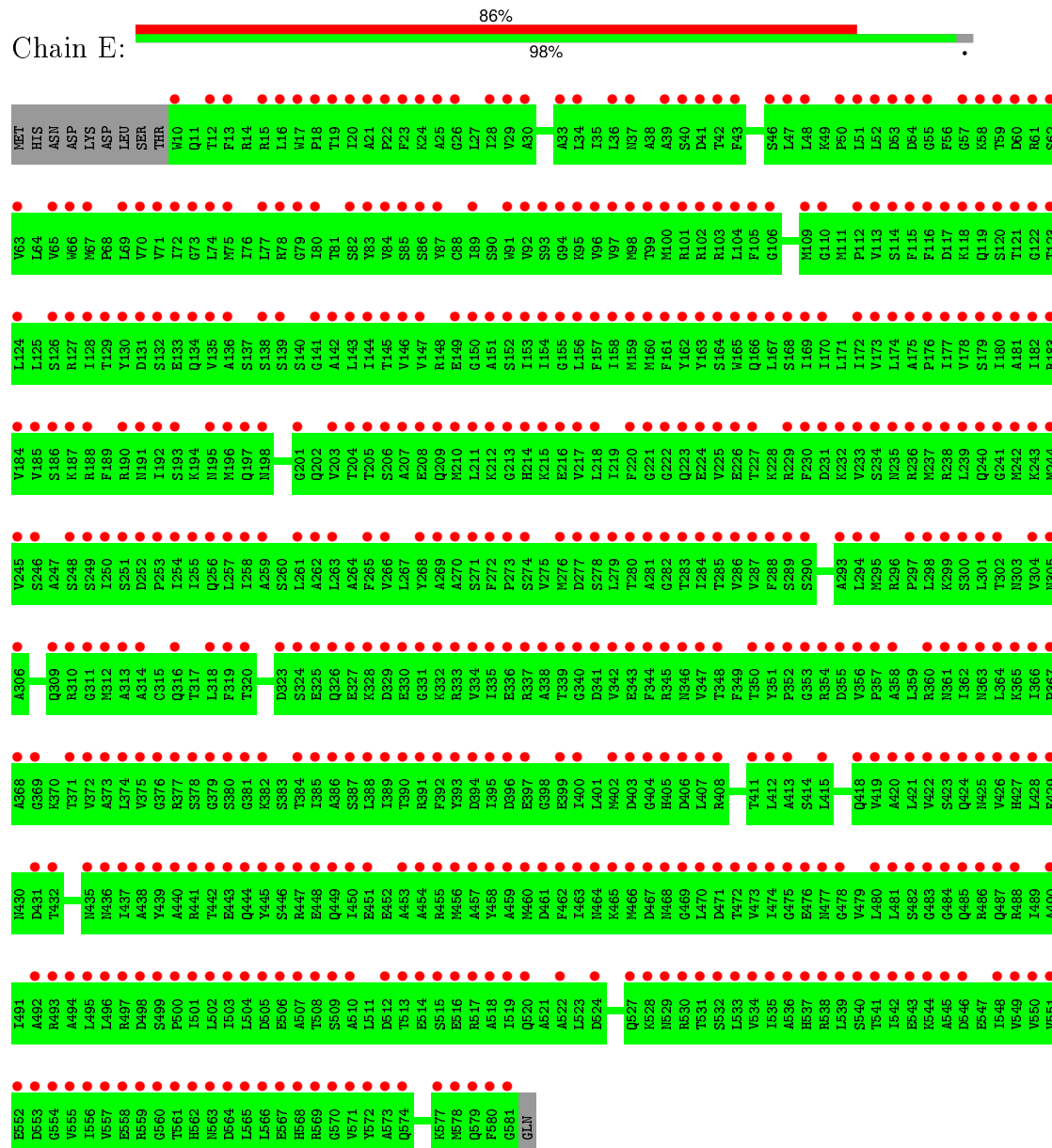
- Molecule 1: Lipid A export ATP-binding/permease protein msbA



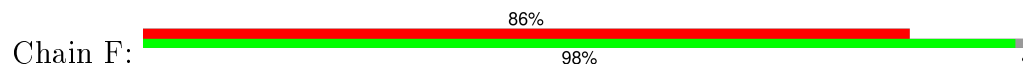




- Molecule 1: Lipid A export ATP-binding/permease protein msbA

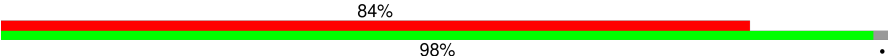


- Molecule 1: Lipid A export ATP-binding/permease protein msbA

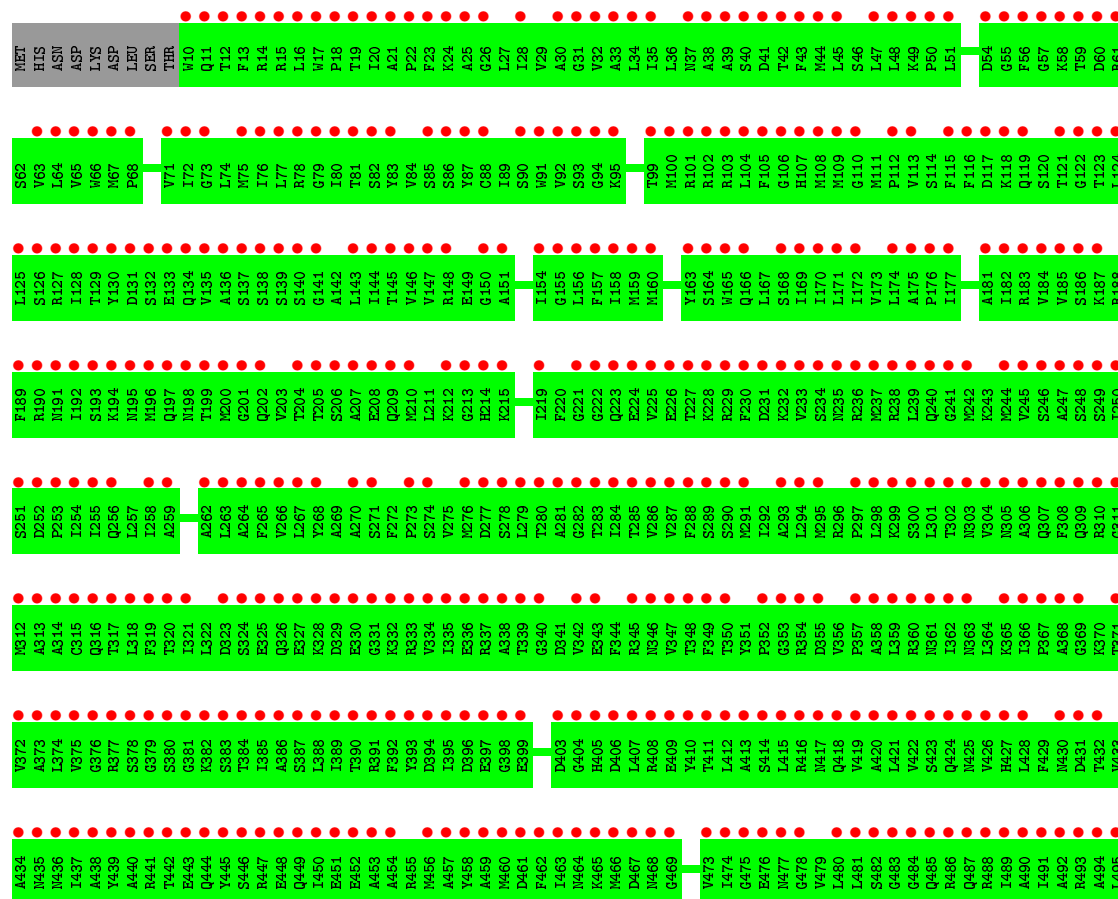


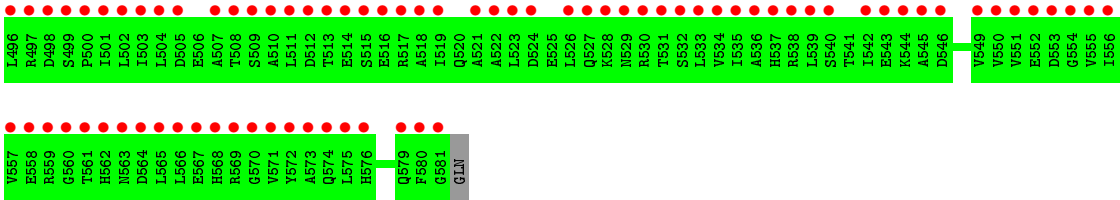
V549	F429	P367	A306	V245	R183	T121	R61
V550	M430	A368	Q307	S246	V184	G122	S62
V551	D431	G369	F308	A247	G369	T123	V63
A552	T432	K370	Q309	S248	S186	L124	L64
D553	V433	T371	R310	S249	K187	R127	V65
G554	A434	V372	G311	I250	R188		W66
V555	M435	A373	M312	S251	F189		M67
V556	M436	L374	A313	D252	R190	T129	P68
R559	R437	G375	C314	P253	M191	Y130	L69
	D498	A438	R354	I254	I192	X131	V70
	S499	Y439	R377	Q316	S193	S132	V71
T561	A440	S378	T317	Q256	K194	E133	O11
H562	R441	G379	L318	L257	M195	Q134	T12
N563	T442	S380	F319	I258	M196	F135	F13
D564	E443	G381	T320	A259	Q197	V135	R14
L565	Q444	K382	I321	S260	M198	A136	R15
L566	Y445	S383	L322	L261	T199	S137	I76
E567	S446	T384	D323	A262	W200	S138	L17
H568	R447	A386	S324	L263	Q201	S139	R78
R569	T508	E448	E325	A264	Q202	S140	T19
G570	S509	Q449	Q326	V203	W203	G141	I80
V571	A510	E451	E327	V265	T204	A143	T81
V572	L511	T390	K328	L267	T205	I144	S82
A573	E452	I389	D329	Y268	S206	T145	V84
Q574	T513		E330	A269	A207	V146	K24
L575	L514		D394	A270	E208	S86	G26
H576	S515	I395	K332	S271	Q209	V147	L27
K577	E516	D396	R333	F272	W210	G150	C88
M578	A457	E397	V334	P273	L211	A151	I89
Q579	A518	G398	I335	S274	K212	S152	S90
P580	I519	E399	E336	V275	G213	I153	W91
G581	Q460	L400	R337	M276	H214	I154	V92
GLN	D461	L401	A338	D277	K215	G155	S93
	A522	M402	T339	S278	E216	L156	G94
	L523	D403	G340	L279	V217	F157	K95
D524	M464	G404	E343	T280	L218	I158	V96
E525	K465	H405		A281	M159	V97	I37
L526	M466	D406		G282	M160	M98	A38
V527	D467	L407	R345	T283	F161	S161	T99
K528	M468	R408	N346	I284	Q223	Y162	M100
M529	Q469	E409	V347	T285	E224	G163	S40
R530	L470	Y410	T348	V286	V225	S164	D41
T531	D471	T411	F349	F287	E226	V165	R102
S532	T472	L412	L413	F288	T227	Q166	R103
L533	V473	A413	T350	S289	K228	L167	L104
V534	L474	S414	P352	S289	R229	S168	F105
T535	Q475	L415	G353	S290	F230	I169	G106
A536	E476	R416	R354	A293	D231	L170	H107
H537	M477	N417	D355		L294	I171	M108
R538	G478	V356	L294		M295	V172	R49
L539	V479	V419	P357	R296	F173	G110	F50
S540	L480	A420	A358	P297	L174	M111	P112
T541	L481	L421	L359	L298	K237	G175	V113
I542	T541	L481	L359	L298	R236	A175	P112
E543	S543	S423	N361	S300	L239	P176	L52
K544	G484	Q424	I362	L301	Q240	V177	D53
A545	Q485	N425	N363	T302	G241	V178	F115
D546	R486	V426	L364	N303	V242	S179	F116
E547	Q487	L427	K365	V304	K243	I180	D117
T548	R488	L428	L366	R205	V244	A181	K118
V549	F429	P367	A306	V245	R183	T121	R61

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

Chain G:  84% 98%

Met	His	Asn	Asp	Lys	Asp	Leu	Ser	Thr	W10	Q11	T12	F13	R14	R15	L16	W17	P18	T19	I20	A21	F22	F23	K24	A25	G26	L27	I28	V29	A30	G31	V32	A33	L34	I35	L36	V37	N37	A38	A39	S40	D41	T42	F43	M44	L45	S46	H47	M48	K49	P50	L51	L52	D53	S54	S55	F56	G57	K58	T59	Q119	S120																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	107.79Å 126.07Å 206.56Å 83.47° 76.25° 84.07°	Depositor
Resolution (Å)	19.98 – 5.30 19.98 – 5.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (19.98-5.30) 94.1 (19.98-5.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 5.23Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.276 , 0.311 0.357 , 0.353	Depositor DCC
R_{free} test set	2490 reflections (6.90%)	DCC
Wilson B-factor (Å ²)	260.4	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 74.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 36078 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4576	wwPDB-VP
Average B, all atoms (Å ²)	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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, 0.375 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).

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	0	0
1	B	572	0	0	0	0
1	C	572	0	0	0	0
1	D	572	0	0	0	0
1	E	572	0	0	0	0
1	F	572	0	0	0	0
1	G	572	0	0	0	0
1	H	572	0	0	0	0
All	All	4576	0	0	0	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 0.

There are no clashes within the asymmetric unit.

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, 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	572/582 (98%)	7.64	524 (91%) 0 1	223, 300, 343, 343	0
1	B	572/582 (98%)	8.16	518 (90%) 0 1	218, 299, 340, 343	0
1	C	572/582 (98%)	7.55	520 (90%) 0 1	227, 310, 343, 343	0
1	D	572/582 (98%)	7.52	523 (91%) 0 1	238, 308, 343, 343	0
1	E	572/582 (98%)	6.62	499 (87%) 0 1	243, 317, 343, 343	0
1	F	572/582 (98%)	6.53	502 (87%) 0 1	229, 311, 343, 343	0
1	G	572/582 (98%)	6.58	488 (85%) 0 1	245, 320, 343, 343	0
1	H	572/582 (98%)	6.51	502 (87%) 0 1	236, 317, 343, 343	0
All	All	4576/4656 (98%)	7.14	4076 (89%) 0 1	218, 311, 343, 343	0

The worst 5 of 4076 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	377	ARG	36.1
1	D	243	LYS	35.1
1	B	324	SER	34.4
1	C	236	ARG	34.0
1	B	524	ASP	32.9

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.