



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2017 – 11:45 PM EDT

PDB ID : 5C00
Title : MdbA protein, a thiol-disulfide oxidoreductase from *Corynebacterium diphtheriae*
Authors : OSIPIUK, J.; REARDON-ROBINSON, M.E.; TON-THAT, H.; JOACHIMIAK, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : unknown
Resolution : 1.77 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
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)	:	rb-20029824

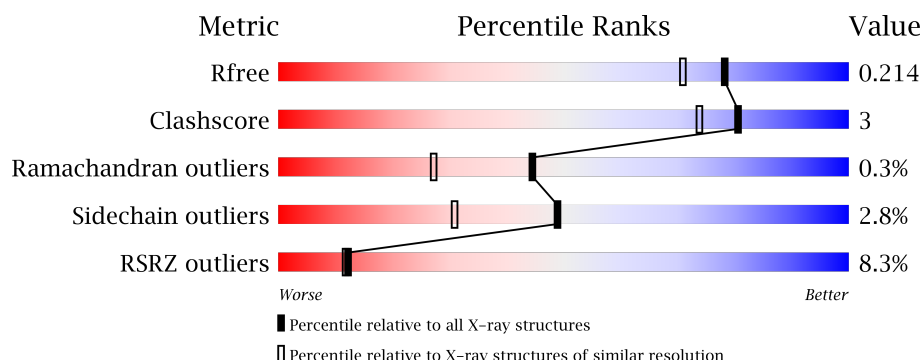
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	208	<div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	B	208	<div> <div>%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
1	C	208	<div> <div>7%</div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	D	208	<div> <div>23%</div> <div>83%</div> <div>8%</div> <div>.</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6756 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 MdbA protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	Se	0	14	0
			1632	1027	272	329	2	2			
1	B	202	Total	C	N	O	S	Se	0	12	0
			1628	1021	270	332	2	3			
1	C	197	Total	C	N	O	S	Se	0	12	0
			1580	989	260	326	2	3			
1	D	191	Total	C	N	O	S	Se	0	8	0
			1517	954	252	306	2	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	SER	-	expression tag	UNP Q6NFK7
A	38	ASN	-	expression tag	UNP Q6NFK7
A	39	ALA	-	expression tag	UNP Q6NFK7
B	37	SER	-	expression tag	UNP Q6NFK7
B	38	ASN	-	expression tag	UNP Q6NFK7
B	39	ALA	-	expression tag	UNP Q6NFK7
C	37	SER	-	expression tag	UNP Q6NFK7
C	38	ASN	-	expression tag	UNP Q6NFK7
C	39	ALA	-	expression tag	UNP Q6NFK7
D	37	SER	-	expression tag	UNP Q6NFK7
D	38	ASN	-	expression tag	UNP Q6NFK7
D	39	ALA	-	expression tag	UNP Q6NFK7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		
2	B	126	Total	O	0	1
			126	126		

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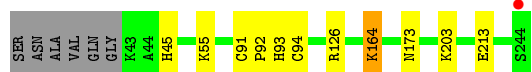
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	83	Total	O	0	0
			83	83		
2	D	67	Total	O	0	2
			68	68		

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.

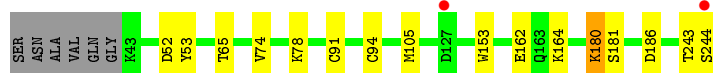
• Molecule 1: MdbA protein

Chain A: 




• Molecule 1: MdbA protein

Chain B: 




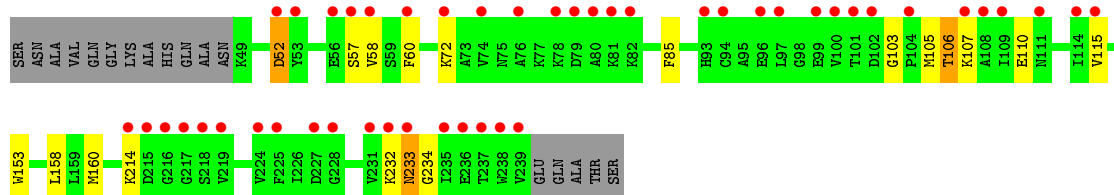
• Molecule 1: MdbA protein

Chain C: 



• Molecule 1: MdbA protein

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.53Å 76.62Å 72.59Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	34.00 – 1.77 33.88 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.00-1.77) 99.9 (33.88-1.77)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.162 , 0.210 0.172 , 0.214	Depositor DCC
R_{free} test set	3298 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.099 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6756	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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 [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	0.72	0/1700	0.81	0/2282
1	B	0.72	0/1689	0.84	0/2266
1	C	0.65	0/1639	0.78	1/2202 (0.0%)
1	D	0.58	0/1564	0.70	0/2099
All	All	0.67	0/6592	0.79	1/8849 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	119	ARG	NE-CZ-NH1	5.69	123.15	120.30

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	1632	0	1614	8	0
1	B	1628	0	1592	13	0
1	C	1580	0	1542	11	0
1	D	1517	0	1494	10	0
2	A	122	0	0	1	0
2	B	126	0	0	3	0
2	C	83	0	0	6	0
2	D	68	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6756	0	6242	39	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 3.

All (39) 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:D:72:LYS:HB3	1:D:115:VAL:HG13	1.84	0.59
1:C:161[A]:LYS:HE2	2:C:306:HOH:O	2.04	0.58
1:B:164[A]:LYS:HG2	2:B:340:HOH:O	2.05	0.57
1:C:225:PHE:CE2	1:C:230:GLU:HB2	2.40	0.57
1:B:74:VAL:HG13	2:B:348:HOH:O	2.05	0.56
1:D:106[A]:THR:HG23	1:D:107:LYS:HE2	1.88	0.55
1:C:158:LEU:C	1:C:158:LEU:HD23	2.27	0.55
1:D:103:GLY:O	1:D:106[A]:THR:HG22	2.08	0.54
1:B:105[B]:MSE:HE2	2:B:312:HOH:O	2.08	0.53
1:B:105[A]:MSE:HE2	1:B:153:TRP:HH2	1.75	0.52
1:A:45:HIS:CD2	1:A:173:ASN:HB3	2.45	0.51
1:B:91:CYS:HG	1:B:94:CYS:HG	1.44	0.51
1:A:203[A]:LYS:HE2	2:A:410:HOH:O	2.11	0.50
1:B:91:CYS:SG	1:B:94:CYS:SG	3.02	0.49
1:A:164:LYS:HD2	1:A:164:LYS:N	2.27	0.49
1:D:158:LEU:HD23	1:D:158:LEU:C	2.33	0.49
1:C:210:LYS:O	1:C:214:LYS:HG3	2.14	0.48
1:A:91:CYS:SG	1:A:94:CYS:SG	3.01	0.47
1:A:93[A]:HIS:ND1	1:B:52:ASP:OD1	2.48	0.47
1:C:161[B]:LYS:HG3	2:C:339:HOH:O	2.15	0.46
1:C:161[A]:LYS:HD2	2:C:350:HOH:O	2.16	0.45
1:B:243:THR:O	1:B:244:SER:CB	2.64	0.45
1:D:160[B]:MSE:HE3	2:D:347:HOH:O	2.15	0.45
1:A:91:CYS:CB	1:A:94:CYS:HG	2.30	0.44
1:C:187[A]:GLU:OE2	2:C:301:HOH:O	2.21	0.44
1:D:233:ASN:HB2	2:D:328:HOH:O	2.19	0.43
1:A:213:GLU:OE2	1:B:162:GLU:OE2	2.37	0.43
1:C:169:LYS:NZ	2:C:307:HOH:O	2.52	0.42
1:B:180:LYS:NZ	1:B:186[B]:ASP:OD1	2.42	0.42
1:D:158:LEU:O	1:D:158:LEU:HD23	2.20	0.41
1:B:53:TYR:CE1	1:B:181:SER:HB3	2.55	0.41
1:D:105:MSE:CE	1:D:153:TRP:HH2	2.34	0.41
1:C:47:ALA:O	1:C:48[A]:ASN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105[A]:MSE:HE2	1:B:153:TRP:CH2	2.54	0.41
1:A:126:ARG:CZ	1:C:169:LYS:HE2	2.51	0.41
1:C:55:LYS:NZ	2:C:304:HOH:O	2.53	0.41
1:B:164[B]:LYS:HB2	1:B:164[B]:LYS:HE2	1.73	0.40
1:D:52:ASP:OD1	1:D:52:ASP:N	2.55	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	214/208 (103%)	210 (98%)	4 (2%)	0	100	100
1	B	212/208 (102%)	208 (98%)	4 (2%)	0	100	100
1	C	207/208 (100%)	199 (96%)	7 (3%)	1 (0%)	32	16
1	D	197/208 (95%)	193 (98%)	3 (2%)	1 (0%)	32	16
All	All	830/832 (100%)	810 (98%)	18 (2%)	2 (0%)	44	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	234	GLY
1	C	234	GLY

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	176/164 (107%)	173 (98%)	3 (2%)	66	53
1	B	174/164 (106%)	171 (98%)	3 (2%)	66	53
1	C	170/164 (104%)	167 (98%)	3 (2%)	64	50
1	D	162/164 (99%)	152 (94%)	10 (6%)	21	6
All	All	682/656 (104%)	663 (97%)	19 (3%)	49	31

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	92	PRO
1	A	164	LYS
1	B	65	THR
1	B	78	LYS
1	B	180	LYS
1	C	78	LYS
1	C	85	PHE
1	C	100	VAL
1	D	52	ASP
1	D	57	SER
1	D	58	VAL
1	D	60	PHE
1	D	85	PHE
1	D	106[A]	THR
1	D	106[B]	THR
1	D	214	LYS
1	D	232	LYS
1	D	233	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	93	HIS

5.3.3 RNA

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	200/208 (96%)	-0.10	1 (0%) 90 90	15, 24, 40, 55	0
1	B	200/208 (96%)	-0.11	2 (1%) 82 83	15, 25, 38, 55	0
1	C	195/208 (93%)	0.40	15 (7%) 14 14	16, 35, 62, 89	0
1	D	189/208 (90%)	0.97	47 (24%) 1 1	18, 40, 78, 93	0
All	All	784/832 (94%)	0.28	65 (8%) 12 12	15, 29, 67, 93	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	97	LEU	7.2
1	D	238	TRP	7.0
1	D	114	ILE	6.7
1	C	97	LEU	5.8
1	D	235	ILE	5.6
1	D	78[A]	LYS	5.5
1	D	232	LYS	5.3
1	D	228	GLY	5.0
1	C	94	CYS	4.9
1	D	80	ALA	4.9
1	D	111	ASN	4.8
1	D	79	ASP	4.8
1	C	47	ALA	4.7
1	C	93	HIS	4.6
1	D	81	LYS	4.4
1	D	109	ILE	4.3
1	D	237	THR	4.0
1	D	100	VAL	3.9
1	D	227	ASP	3.8
1	A	244	SER	3.7
1	D	107	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	115	VAL	3.7
1	D	233	ASN	3.6
1	B	127	ASP	3.3
1	D	76	ALA	3.3
1	D	104	PRO	3.2
1	D	56	GLU	3.1
1	C	96[A]	GLU	3.1
1	D	96	GLU	3.0
1	D	53	TYR	3.0
1	D	239	VAL	3.0
1	D	217	GLY	2.9
1	C	79	ASP	2.9
1	D	236	GLU	2.9
1	D	82	LYS	2.9
1	D	52	ASP	2.8
1	D	99[A]	GLU	2.7
1	C	78	LYS	2.7
1	D	216	GLY	2.6
1	D	101	THR	2.6
1	C	95	ALA	2.6
1	D	224	VAL	2.5
1	D	93	HIS	2.5
1	D	57	SER	2.5
1	C	216	GLY	2.5
1	D	225	PHE	2.4
1	D	214	LYS	2.4
1	C	48[A]	ASN	2.4
1	D	219	VAL	2.4
1	D	60	PHE	2.4
1	D	102	ASP	2.4
1	D	58	VAL	2.3
1	D	74	VAL	2.3
1	D	231	VAL	2.3
1	C	235	ILE	2.3
1	C	217	GLY	2.3
1	B	244	SER	2.3
1	C	111	ASN	2.3
1	D	218	SER	2.1
1	D	72	LYS	2.1
1	D	108	ALA	2.1
1	C	227	ASP	2.1
1	D	94	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	215	ASP	2.0
1	C	233	ASN	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.