



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:00 am BST

PDB ID : 4ML6  
Title : Disulfide isomerase from multidrug resistance IncA/C conjugative plasmid in reduced state  
Authors : Premkumar, L.; Kurth, F.; Neyer, S.; Martin, J.L.  
Deposited on : 2013-09-06  
Resolution : 2.30 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](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.

---

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

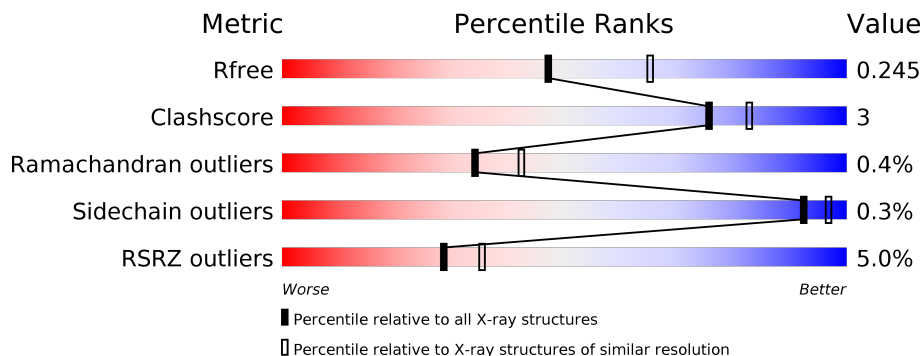
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	217	 5% 88% 5% 7%
1	B	217	 3% 87% 5% 7%
1	C	217	 2% 82% 12% 6%
1	D	217	 9% 83% 9% 7%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 12775 atoms, of which 6216 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 DsbP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	202	3102	985	1547	264	291	15	0	4	0
1	B	201	3111	983	1555	265	294	14	0	3	0
1	C	203	3139	990	1571	269	295	14	0	2	0
1	D	201	3097	981	1543	265	294	14	0	4	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP A6GV51
A	-1	ASN	-	EXPRESSION TAG	UNP A6GV51
A	0	ALA	-	EXPRESSION TAG	UNP A6GV51
B	-2	SER	-	EXPRESSION TAG	UNP A6GV51
B	-1	ASN	-	EXPRESSION TAG	UNP A6GV51
B	0	ALA	-	EXPRESSION TAG	UNP A6GV51
C	-2	SER	-	EXPRESSION TAG	UNP A6GV51
C	-1	ASN	-	EXPRESSION TAG	UNP A6GV51
C	0	ALA	-	EXPRESSION TAG	UNP A6GV51
D	-2	SER	-	EXPRESSION TAG	UNP A6GV51
D	-1	ASN	-	EXPRESSION TAG	UNP A6GV51
D	0	ALA	-	EXPRESSION TAG	UNP A6GV51

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	101	Total	O	0	0
			101	101		
2	B	72	Total	O	0	0
			72	72		

*Continued on next page...*

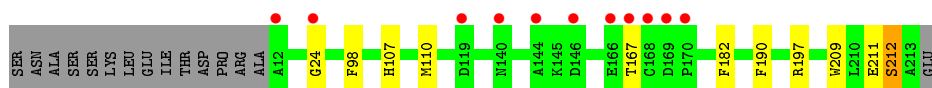
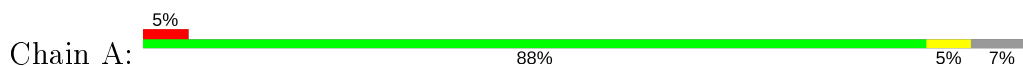
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
2	C	92	Total O 92 92	0	0
2	D	61	Total O 61 61	0	0

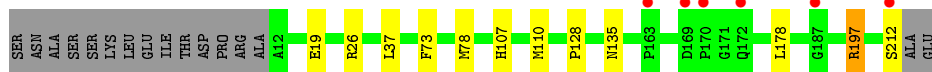
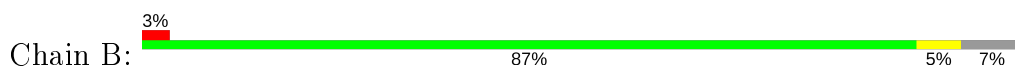
### 3 Residue-property plots [i](#)

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.

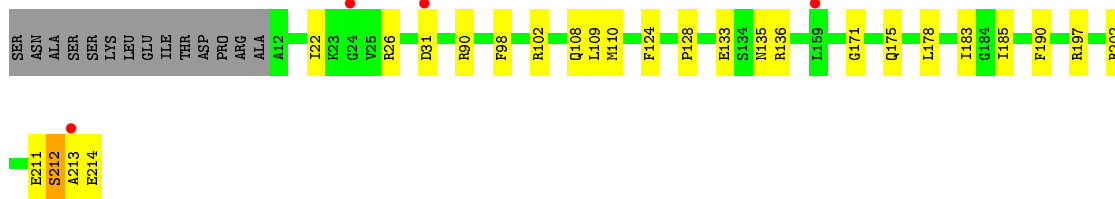
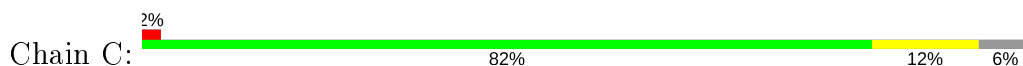
- Molecule 1: DsbP



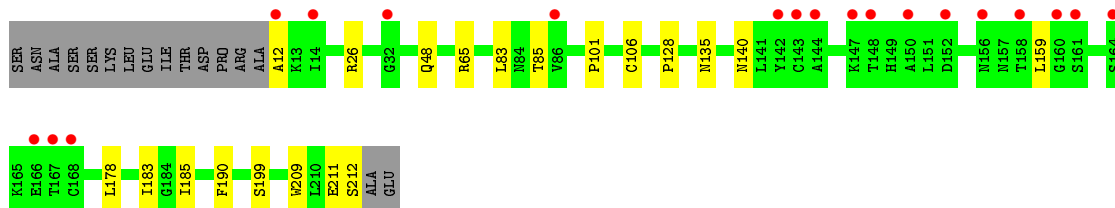
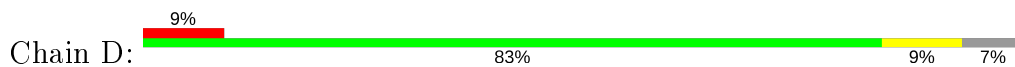
- Molecule 1: DsbP



- Molecule 1: DsbP



- Molecule 1: DsbP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.69Å 110.60Å 80.74Å 90.00° 96.83° 90.00°	Depositor
Resolution (Å)	33.78 – 2.30 39.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.78-2.30) 98.7 (39.81-2.30)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.07 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.190 , 0.244 0.191 , 0.245	Depositor DCC
$R_{free}$ test set	2155 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.7	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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 [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	0.62	0/1595	0.67	0/2157
1	B	0.58	0/1592	0.65	1/2151 (0.0%)
1	C	0.67	0/1602	0.73	2/2164 (0.1%)
1	D	0.60	2/1593 (0.1%)	0.63	0/2154
All	All	0.62	2/6382 (0.0%)	0.67	3/8626 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	106[A]	CYS	CB-SG	5.07	1.90	1.82
1	D	106[B]	CYS	CB-SG	5.07	1.90	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	C	197	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	197	ARG	NE-CZ-NH1	-5.25	117.68	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	1555	1547	1552	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1556	1555	1559	8	0
1	C	1568	1571	1572	17	0
1	D	1554	1543	1549	13	1
2	A	101	0	0	0	1
2	B	72	0	0	0	0
2	C	92	0	0	2	0
2	D	61	0	0	1	0
All	All	6559	6216	6232	39	1

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:140:ASN:ND2	1:D:159:LEU:O	2.29	0.65
1:C:90:ARG:NE	2:C:355:HOH:O	2.30	0.65
1:A:197:ARG:NH2	1:A:209:TRP:O	2.34	0.57
1:C:212:SER:HB3	1:C:213:ALA:HA	1.87	0.57
1:C:178:LEU:CD1	1:D:178:LEU:CD1	2.85	0.54
1:C:213:ALA:N	1:C:214:GLU:HA	2.23	0.54
1:C:108:GLN:OE1	1:C:202:ARG:NH1	2.42	0.53
1:C:133:GLU:OE2	1:C:136:ARG:NH2	2.35	0.53
1:D:185:ILE:O	2:D:332:HOH:O	2.19	0.53
1:D:185:ILE:HD12	1:D:190:PHE:CG	2.44	0.52
1:B:19:GLU:OE2	1:D:26:ARG:HD3	2.13	0.49
1:B:73:PHE:HD1	1:B:78:MET:HG2	1.78	0.49
1:A:211:GLU:O	1:A:212:SER:CB	2.62	0.47
1:D:101:PRO:HB3	1:D:159:LEU:HD12	1.95	0.47
1:C:26:ARG:NE	2:C:340:HOH:O	2.45	0.47
1:C:102:ARG:NH2	1:D:12:ALA:O	2.48	0.47
1:C:211:GLU:O	1:C:212:SER:CB	2.64	0.46
1:D:183:ILE:CD1	1:D:185:ILE:HD11	2.46	0.45
1:A:107:HIS:HA	1:A:110:MET:HE3	1.99	0.45
1:C:98:PHE:HB2	1:C:190:PHE:HB3	1.98	0.45
1:A:98:PHE:HB2	1:A:190:PHE:HB3	1.99	0.45
1:C:183:ILE:HD11	1:C:185:ILE:HD11	1.99	0.43
1:D:128:PRO:HB3	1:D:135:ASN:HA	2.01	0.43
1:D:83:LEU:O	1:D:85:THR:N	2.52	0.42
1:A:24:GLY:HA2	1:C:22:ILE:O	2.19	0.42
1:B:73:PHE:CD1	1:B:78:MET:HG2	2.54	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:LEU:C	1:C:109:LEU:HD23	2.39	0.42
1:D:211:GLU:O	1:D:212:SER:OG	2.28	0.42
1:C:171:GLY:O	1:C:175:GLN:HG2	2.19	0.42
1:B:128:PRO:HB3	1:B:135:ASN:HA	2.01	0.42
1:C:110:MET:HG2	1:C:124:PHE:CE1	2.54	0.42
1:C:213:ALA:N	1:C:214:GLU:CA	2.83	0.42
1:D:183:ILE:HD11	1:D:185:ILE:HD11	2.02	0.41
1:B:107:HIS:HA	1:B:110:MET:CE	2.51	0.40
1:C:128:PRO:HB3	1:C:135:ASN:HA	2.04	0.40
1:D:199:SER:HB2	1:D:209:TRP:CZ2	2.57	0.40
1:A:182:PHE:HB2	1:B:178:LEU:CD2	2.51	0.40
1:B:26:ARG:NH2	1:B:37:LEU:HD23	2.37	0.40
1:B:197:ARG:NH1	1:B:212:SER:HA	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:GLN:OE1	2:A:401:HOH:O[1_655]	2.19	0.01

## 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	204/217 (94%)	199 (98%)	3 (2%)	2 (1%)	15	17
1	B	202/217 (93%)	199 (98%)	3 (2%)	0	100	100
1	C	203/217 (94%)	200 (98%)	2 (1%)	1 (0%)	29	35
1	D	203/217 (94%)	200 (98%)	3 (2%)	0	100	100
All	All	812/868 (94%)	798 (98%)	11 (1%)	3 (0%)	34	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	SER
1	C	212	SER
1	A	167	THR

### 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	171/186 (92%)	171 (100%)	0	100	100
1	B	173/186 (93%)	173 (100%)	0	100	100
1	C	174/186 (94%)	173 (99%)	1 (1%)	86	94
1	D	172/186 (92%)	170 (99%)	2 (1%)	71	84
All	All	690/744 (93%)	687 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	31	ASP
1	D	65[A]	ARG
1	D	65[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	107	HIS
1	D	140	ASN
1	D	172	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

### 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, 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	202/217 (93%)	0.48	11 (5%) 25 32	21, 50, 91, 128	0
1	B	201/217 (92%)	0.20	6 (2%) 50 57	27, 48, 77, 106	0
1	C	203/217 (93%)	0.02	4 (1%) 65 71	20, 42, 80, 99	0
1	D	201/217 (92%)	0.57	19 (9%) 8 11	32, 63, 97, 117	0
All	All	807/868 (92%)	0.32	40 (4%) 28 35	20, 51, 91, 128	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	CYS	9.4
1	A	167	THR	5.4
1	B	170	PRO	4.9
1	D	168	CYS	4.9
1	D	161	SER	4.7
1	A	169	ASP	4.5
1	D	12	ALA	4.5
1	D	167	THR	4.3
1	A	166	GLU	4.1
1	B	169	ASP	3.6
1	D	150	ALA	3.5
1	D	166	GLU	3.0
1	D	144	ALA	3.0
1	D	143	CYS	2.9
1	A	170	PRO	2.8
1	D	147	LYS	2.7
1	C	159	LEU	2.7
1	B	172	GLN	2.7
1	D	160	GLY	2.6
1	D	86	VAL	2.5
1	A	144	ALA	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	24	GLY	2.5
1	B	187	GLY	2.4
1	A	146	ASP	2.4
1	A	12	ALA	2.4
1	D	142	TYR	2.4
1	D	156	ASN	2.3
1	B	163	PRO	2.3
1	D	152	ASP	2.2
1	C	31	ASP	2.2
1	D	14	ILE	2.2
1	D	164	SER	2.2
1	D	148	THR	2.2
1	A	24	GLY	2.2
1	B	212	SER	2.2
1	D	158	THR	2.1
1	C	213	ALA	2.1
1	A	119	ASP	2.1
1	D	32	GLY	2.0
1	A	140	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.