



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:13 AM GMT

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 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/ValidationPDFNotes.html>

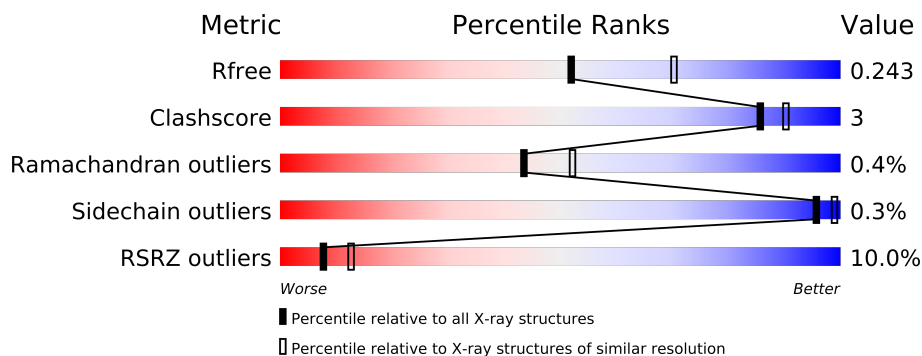
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	
1	C	217	
1	D	217	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12775 atoms, of which 6216 are hydrogens and 0 are deuterium.

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

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		

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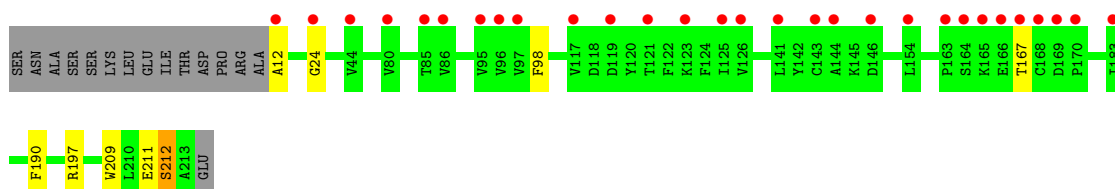
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	92	Total 92	O 92	0	0
2	D	61	Total 61	O 61	0	0

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: DsbP

Chain A: 



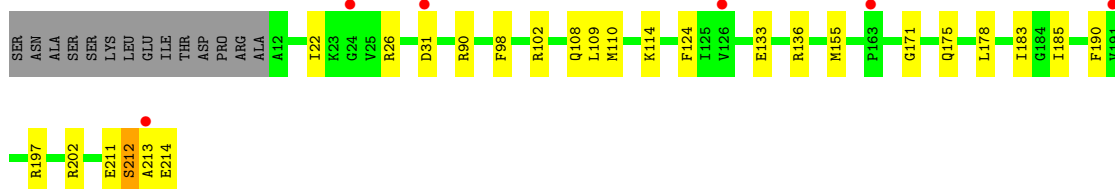
- Molecule 1: DsbP

Chain B: 



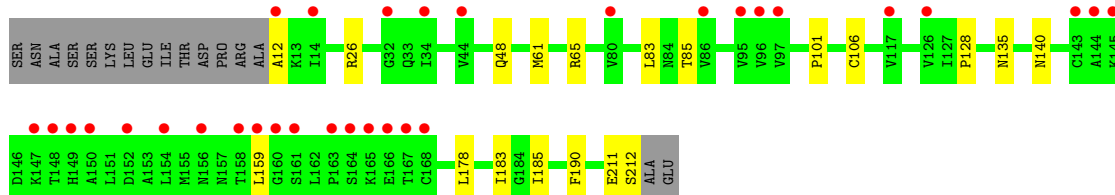
- Molecule 1: DsbP

Chain C: 



- Molecule 1: DsbP

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	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
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.190 , 0.244 0.189 , 0.243	Depositor DCC
R_{free} test set	2153 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.798	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 41823 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12775	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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	0.62	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1555	1547	0	5	0
1	B	1556	1555	0	5	0
1	C	1568	1571	0	17	0
1	D	1554	1543	0	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	0	34	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (34) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:C:212:SER:HB3	1:C:213:ALA:HA	1.81	0.60
1:A:197:ARG:NH2	1:A:209:TRP:O	2.34	0.57
1:C:178:LEU:CD1	1:D:178:LEU:CD1	2.85	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	2.45	0.52
1:D:211:GLU:O	1:D:212:SER:OG	2.28	0.51
1:B:73:PHE:HD1	1:B:78:MET:HG2	1.77	0.50
1:C:213:ALA:N	1:C:214:GLU:HA	2.27	0.49
1:A:211:GLU:O	1:A:212:SER:CB	2.62	0.47
1:B:19:GLU:OE2	1:D:26:ARG:HD3	2.14	0.47
1:C:114:LYS:HD2	1:C:155:MET:HE1	1.95	0.47
1:D:101:PRO:HB3	1:D:159:LEU:HD12	1.96	0.47
1:C:26:ARG:NE	2:C:340:HOH:O	2.45	0.47
1:D:183:ILE:CD1	1:D:185:ILE:HD11	2.46	0.46
1:C:211:GLU:O	1:C:212:SER:CB	2.64	0.46
1:C:98:PHE:HB2	1:C:190:PHE:HB3	1.98	0.44
1:C:183:ILE:HD11	1:C:185:ILE:HD11	1.98	0.44
1:A:98:PHE:HB2	1:A:190:PHE:HB3	2.00	0.44
1:C:102:ARG:NH2	1:D:12:ALA:O	2.48	0.43
1:D:83:LEU:O	1:D:85:THR:N	2.52	0.42
1:C:109:LEU:C	1:C:109:LEU:HD23	2.39	0.42
1:D:183:ILE:HD11	1:D:185:ILE:HD11	2.01	0.42
1:A:24:GLY:HA2	1:C:22:ILE:O	2.19	0.42
1:D:128:PRO:HB3	1:D:135:ASN:HA	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:110:MET:HG2	1:C:124:PHE:CE1	2.55	0.42
1:C:213:ALA:N	1:C:214:GLU:CA	2.83	0.42
1:B:18:VAL:HG23	1:D:61:MET:HE3	2.02	0.42
1:A:12:ALA:O	1:B:102:ARG:NH1	2.50	0.42
1:C:171:GLY:O	1:C:175:GLN:HG2	2.21	0.41
1:B:107:HIS:HA	1:B:110:MET:CE	2.52	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	Distance(Å)	Clash(Å)
1:D:48:GLN:OE1	2:A:401:HOH:O[1_655]	2.19	0.01

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	204/217 (94%)	199 (98%)	3 (2%)	2 (1%)	22	23
1	B	202/217 (93%)	199 (98%)	3 (2%)	0	100	100
1	C	203/217 (94%)	200 (98%)	2 (1%)	1 (0%)	38	45
1	D	203/217 (94%)	200 (98%)	3 (2%)	0	100	100
All	All	812/868 (94%)	798 (98%)	11 (1%)	3 (0%)	43	52

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 ⓘ

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%)	92	97
1	D	172/186 (92%)	170 (99%)	2 (1%)	82	92
All	All	690/744 (93%)	687 (100%)	3 (0%)	96	98

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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	175	GLN
1	B	156	ASN
1	C	48	GLN
1	C	107	HIS
1	C	175	GLN
1	D	175	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	202/217 (93%)	0.79	29 (14%) 3 5	22, 51, 91, 128	0
1	B	201/217 (92%)	0.45	14 (6%) 16 23	27, 48, 77, 106	0
1	C	203/217 (93%)	0.28	6 (2%) 48 58	21, 43, 80, 99	0
1	D	201/217 (92%)	0.91	32 (15%) 3 4	32, 63, 97, 124	0
All	All	807/868 (92%)	0.61	81 (10%) 8 13	21, 52, 92, 128	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	CYS	7.6
1	D	167	THR	6.8
1	D	150	ALA	6.4
1	D	86	VAL	6.1
1	A	167	THR	5.6
1	A	80	VAL	5.0
1	A	86	VAL	4.9
1	B	170	PRO	4.8
1	D	12	ALA	4.7
1	D	144	ALA	4.7
1	D	168	CYS	4.6
1	D	148	THR	4.4
1	D	147	LYS	4.4
1	D	14	ILE	4.1
1	D	158	THR	4.1
1	D	161	SER	4.0
1	A	95	VAL	4.0
1	B	44	VAL	3.6
1	A	166	GLU	3.5
1	B	169	ASP	3.5
1	D	95	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	166	GLU	3.4
1	A	144	ALA	3.4
1	A	169	ASP	3.4
1	D	152	ASP	3.4
1	D	156	ASN	3.2
1	C	213	ALA	3.2
1	A	126	VAL	3.1
1	A	170	PRO	3.0
1	D	117	VAL	3.0
1	C	24	GLY	2.9
1	B	163	PRO	2.9
1	A	117	VAL	2.9
1	A	121	THR	2.8
1	C	31	ASP	2.8
1	D	154	LEU	2.8
1	D	160	GLY	2.8
1	A	12	ALA	2.8
1	B	86	VAL	2.8
1	D	96	VAL	2.8
1	A	163	PRO	2.8
1	A	164	SER	2.8
1	D	159	LEU	2.6
1	D	149	HIS	2.6
1	B	187	GLY	2.6
1	A	24	GLY	2.6
1	D	163	PRO	2.6
1	D	34	ILE	2.5
1	D	143	CYS	2.5
1	A	146	ASP	2.5
1	B	172	GLN	2.5
1	D	126	VAL	2.5
1	A	85	THR	2.4
1	B	167	THR	2.4
1	A	97	VAL	2.4
1	A	119	ASP	2.3
1	A	44	VAL	2.3
1	C	191	VAL	2.3
1	B	212	SER	2.3
1	A	96	VAL	2.3
1	D	145	LYS	2.3
1	D	164	SER	2.2
1	D	32	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	126	VAL	2.2
1	A	123	LYS	2.2
1	A	141	LEU	2.2
1	D	165	LYS	2.2
1	A	143	CYS	2.2
1	D	97	VAL	2.1
1	A	183	ILE	2.1
1	B	192	VAL	2.1
1	A	125	ILE	2.1
1	B	28	VAL	2.1
1	B	159	LEU	2.1
1	B	162	LEU	2.1
1	B	146	ASP	2.1
1	A	165	LYS	2.0
1	C	163	PRO	2.0
1	D	44	VAL	2.0
1	A	154	LEU	2.0
1	D	80	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.