



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:54 AM GMT

PDB ID : 1DDN  
Title : DIPHTHERIA TOX REPRESSOR (C102D MUTANT)/TOX DNA OPERATOR COMPLEX  
Authors : White, A.; Ding, X.; Vanderspek, J.C.; Murphy, J.R.; Ringe, D.  
Deposited on : 1998-06-23  
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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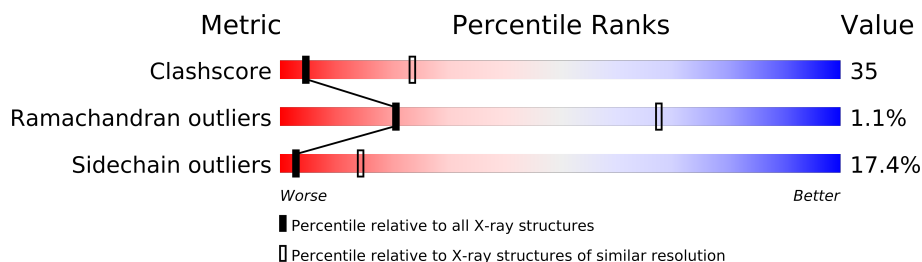
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 3.00 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))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	33	
2	F	33	
3	A	226	
3	B	226	
3	C	226	
3	D	226	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5135 atoms, of which 0 are hydrogen 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 DNA chain called 33 BASE DNA CONTAINING TOXIN OPERATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	33	Total	C	N	O	P	0	0	0
			672	327	114	199	32			

- Molecule 2 is a DNA chain called 33 BASE DNA CONTAINING TOXIN OPERATOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	33	Total	C	N	O	P	0	0	0
			675	327	123	193	32			

- Molecule 3 is a protein called DIPHTHERIA TOX REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	118	Total	C	N	O	S	0	0	0
			944	581	174	184	5			
3	B	118	Total	C	N	O	S	0	0	0
			944	581	174	184	5			
3	C	118	Total	C	N	O	S	0	0	0
			944	581	174	184	5			
3	D	118	Total	C	N	O	S	0	0	0
			944	581	174	184	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ASP	CYS	ENGINEERED	UNP P33120
B	102	ASP	CYS	ENGINEERED	UNP P33120
C	102	ASP	CYS	ENGINEERED	UNP P33120
D	102	ASP	CYS	ENGINEERED	UNP P33120

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total 2	Ni 2	0	0
4	A	2	Total 2	Ni 2	0	0
4	D	2	Total 2	Ni 2	0	0
4	C	2	Total 2	Ni 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	B	1	Total 1	O 1	0	0
5	C	1	Total 1	O 1	0	0
5	D	1	Total 1	O 1	0	0



GLY	ASP
VAL	GLY
ASN	HIS
ILE	ILE
SER	THR
ASP	LEU
ALA	SER
ALA	HIS
ALA	ASN
PRO	GLY
GLY	LYS
THR	ASP
ARG	VAL
VAL	GLU
ILE	LEU
ASP	LEU
ALA	ASP
ALA	ASP
THR	LEU
SER	ALA
MET	HIS
PRO	THR
ARG	ILE
LYS	ARG
VAL	ILE
ARG	ILE
ILE	GLU
VAL	GLU
GLN	LEU
ILE	ASN
ASN	GLU
GLU	ILE
ILE	PHE
GLN	GLN
VAL	VAL
GLU	GLU
THR	THR
ASP	ASP
GLN	GLN
PHE	THR
THR	THR
GLN	GLN
LEU	LEU
LEU	ASP
ALA	ASP
ASP	ILE
ARG	ARG
VAL	VAL
GLY	SER
SER	GLU
GLU	GLU
VAL	VAL
ILE	ILE
VAL	ASP
ASP	PRO
ARG	GLY


● Molecule 3: DIPHTHERIA TOX REPRESSOR

Chain C: 

MET	THR
LYS	ARG
D3	VAL
L4	ILE
V5	ASP
D6	ALA
T7	ALA
T8	THR
	SER
	MET
R13	PRO
	ARG
Y16	LYS
E17	VAL
L18	VAL
	ARG
E21	ILE
G22	VAL
V23	GLN
T24	ILE
	ASN
R27	GLU
A28	ILE
R29	PHE
T30	GLN
A31	VAL
E32	GLU
R33	THR
	ASP
S37	GLN
G38	PHE
P39	THR
T40	GLN
V41	LEU
S42	LEU
Q43	ASP
T44	ALA
V45	ASP
A46	ILE
	ARG
V54	VAL
V55	GLY
	ASN
S58	PRO
D59	ILE
R60	GLU
	VAL
R69	ASP
T70	ARG
L71	GLY
A72	VAL
	GLY
M76	ILE
	ASN
	THR
H79	LEU
	ASP
A82	ALA
E83	ALA
R84	ASN
L85	PRO
	GLY
	LYS

L86	THR
T87	ARG
D88	VAL
I89	ILE
I90	ASP
G91	ALA
L92	ALA
D93	THR
I94	SER
N95	MET
K96	PRO
V97	ARG
	LYS
R103	VAL
W104	VAL
E105	ARG
H106	ILE
V107	VAL
M108	GLN
S109	ILE
D110	ASN
E111	GLU
V112	ILE
E113	PHE
R114	GLN
R115	VAL
L116	GLU
V117	THR
K118	ASP
V119	THR
L120	GLN
	THR
LYS	LEU
ASP	LEU
VAL	LEU
SER	ASP
SER	ALA
ARG	Q43
PRO	V45
PHE	A46
GLY	R47
ASN	M48
PRO	E49
ILE	R50
ARG	D51
VAL	G52
GLY	L53
ASN	V54
VAL	
ASP	A57
THR	S58
GLY	D59
VAL	R60
GLY	S61
VAL	L62
GLY	Q63
THR	M64
LEU	
ASP	T67
ALA	G68
ALA	R69
PRO	T70
GLY	L71

● Molecule 3: DIPHTHERIA TOX REPRESSOR

Chain D: 

MET	THR
LYS	ARG
D3	VAL
L4	ILE
V5	ASP
D6	ALA
	ALA
M10	THR
Y11	SER
L12	MET
	PRO
I15	ARG
Y16	LYS
E17	VAL
	VAL
E20	ARG
E21	ILE
	ILE
L26	ASN
R27	GLU
A28	ILE
R29	PHE
	GLN
E32	VAL
R33	GLU
L34	THR
	ASP
S37	GLN
G38	PHE
P39	THR
T40	GLN
V41	LEU
S42	LEU
Q43	ASP
T44	ALA
V45	ASP
A46	ILE
R47	ARG
M48	VAL
E49	GLY
R50	ASN
D51	PRO
G52	ILE
L53	PRO
V54	VAL
	GLY
A57	SER
S58	GLY
D59	VAL
R60	VAL
S61	SER
L62	GLY
Q63	VAL
M64	GLY
	LEU
T67	ASP
G68	GLU
R69	GLY
T70	LEU
L71	VAL

A72	GLY
T73	ASN
H79	SER
	ASP
A82	ALA
E83	ALA
R84	PRO
L85	GLY
L86	LYS
T87	THR
D88	ARG
I89	VAL
Y90	GLU
G91	ILE
L92	ASP
D93	ALA
I94	THR
N95	SER
K96	MET
V97	PRO
H98	ARG
D99	ILE
E100	VAL
A101	ILE
	VAL
W104	GLN
E105	ILE
H106	ASN
V107	GLU
	ILE
E111	PHE
	GLN
R114	VAL
R115	GLU
L116	THR
V117	ASP
F118	GLN
V119	PHE
L120	THR
	GLN
LYS	LEU
ASP	LEU
VAL	SER
ARG	ALA
SER	ASP
PRO	ASP
PHE	ILE
GLY	ARG
ASN	VAL
PRO	GLY
ILE	SER
PRO	GLY
Q63	VAL
M64	GLY
	ILE
LEU	VAL
ASP	VAL
GLU	ASP
LEU	ARG
GLY	ASP
VAL	GLY

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.05Å 117.05Å 145.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	87.9 (8.00-3.00)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.240 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	E	0.81	3/752 (0.4%)	1.26	14/1159 (1.2%)
2	F	0.69	0/758	1.23	11/1168 (0.9%)
3	A	0.42	0/953	0.65	0/1288
3	B	0.39	0/953	0.61	0/1288
3	C	0.39	0/953	0.64	0/1288
3	D	0.39	0/953	0.63	0/1288
All	All	0.52	3/5322 (0.1%)	0.87	25/7479 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	5
2	F	0	6
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	317	DT	C5-C6	-6.29	1.29	1.34
1	E	317	DT	C5-C7	5.97	1.53	1.50
1	E	317	DT	N1-C6	-5.44	1.34	1.38

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	413	DG	O4'-C1'-N9	8.18	113.73	108.00
1	E	310	DG	O4'-C1'-N9	7.95	113.56	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	424	DC	C6-N1-C2	7.81	123.42	120.30
1	E	311	DG	N9-C1'-C2'	-7.70	97.97	112.60
2	F	419	DG	O4'-C1'-N9	7.43	113.20	108.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	310	DG	Sidechain
1	E	311	DG	Sidechain
1	E	316	DC	Sidechain
1	E	321	DC	Sidechain
1	E	322	DC	Sidechain

## 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	E	672	0	380	95	0
2	F	675	0	377	65	0
3	A	944	0	962	41	0
3	B	944	0	962	54	0
3	C	944	0	962	57	0
3	D	944	0	962	49	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	5135	0	4605	333	0

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 35.

The worst 5 of 333 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:327:DT:H2"	1:E:328:DA:H5"	1.24	1.15
1:E:328:DA:H2"	1:E:329:DT:H5"	1.15	1.14
3:C:27:ARG:HG3	3:C:27:ARG:HH11	1.10	1.14
1:E:330:DT:H2"	1:E:331:DT:H5"	1.25	1.13
1:E:301:DA:H2"	1:E:302:DT:H5"	1.33	1.11

There are no symmetry-related clashes.

## 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	
3	A	116/226 (51%)	102 (88%)	13 (11%)	1 (1%)	25	73
3	B	116/226 (51%)	102 (88%)	13 (11%)	1 (1%)	25	73
3	C	116/226 (51%)	104 (90%)	11 (10%)	1 (1%)	25	73
3	D	116/226 (51%)	104 (90%)	10 (9%)	2 (2%)	14	54
All	All	464/904 (51%)	412 (89%)	47 (10%)	5 (1%)	21	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	5	VAL
3	B	119	VAL
3	C	5	VAL
3	A	5	VAL
3	D	119	VAL

### 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	
3	A	105/198 (53%)	87 (83%)	18 (17%)	3	15
3	B	105/198 (53%)	86 (82%)	19 (18%)	2	13
3	C	105/198 (53%)	87 (83%)	18 (17%)	3	15
3	D	105/198 (53%)	87 (83%)	18 (17%)	3	15
All	All	420/792 (53%)	347 (83%)	73 (17%)	3	14

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	111	GLU
3	C	29	ARG
3	D	107	VAL
3	C	4	LEU
3	C	60	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	95	ASN
3	D	95	ASN

### 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 ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.