



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:00 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 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

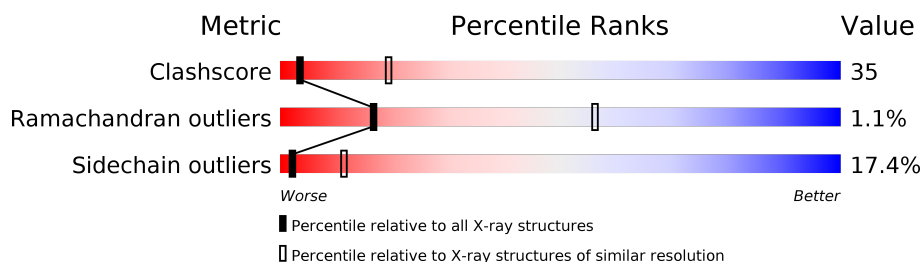
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

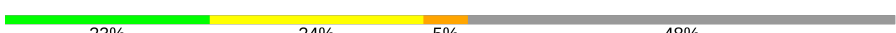
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (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 ≥ 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.

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 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 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 Ni 2 2	0	0
4	A	2	Total Ni 2 2	0	0
4	D	2	Total Ni 2 2	0	0
4	C	2	Total Ni 2 2	0	0

- Molecule 5 is water.


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

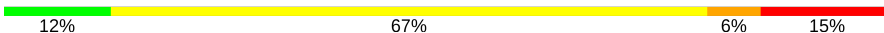
Note EDS was not executed.

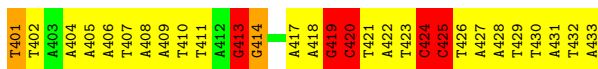
• Molecule 1: 33 BASE DNA CONTAINING TOXIN OPERATOR

Chain E: 

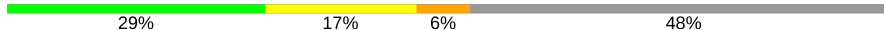


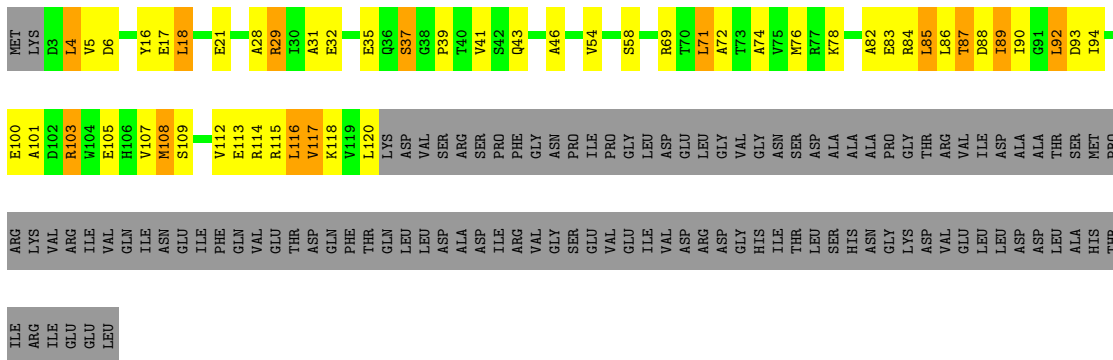
• Molecule 2: 33 BASE DNA CONTAINING TOXIN OPERATOR

Chain F: 



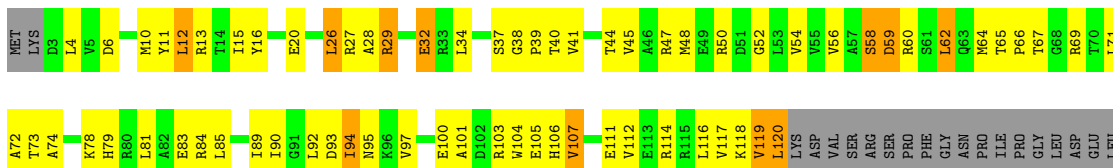
• Molecule 3: DIPHTHERIA TOX REPRESSOR

Chain A: 



• Molecule 3: DIPHTHERIA TOX REPRESSOR

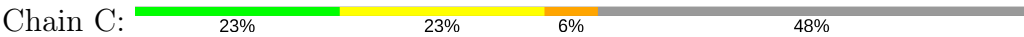
Chain B: 



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

ASP GLY HIS THR LEU SER HIS ASN GLY LYS ASP VAL GLU LEU LEU ASP LEU LEU ASP LEU LEU

● Molecule 3: DIPHTHERIA TOX REPRESSOR



MET LYS D3 L4 V5 D6 T7 T8 R13 Y16 E17 L18 E21 Q22 V23 T24 R27 A28 R29 I30 A31 E32 R33 L34 S37 Q38 P39 T40 V41 S42 Q43 T44 V45 A46 V54 V55 S58 D59 R60 R69 T70 L71 A72 M76 H79 A82 E83 R84 L85

L86 T87 D88 L89 I90 G91 L92 D93 I94 K96 V97 R103 M104 E105 H106 V107 M108 S109 D110 E111 V112 E113 R114 R115 L116 V117 K118 V119 L120 LYS ASP VAL SER ALA SER PRO PHE GLY ASN PRO ILE PRO GLY ASP LEU GLY VAL HIS ILE THR LEU SER ALA ALA PRO GLY

THR ARG VAL ILE LEU ASP ALA THR MET PRO LYS VAL ARG ILE GLU LEU THR ARG VAL ILE GLU LEU

ASP VAL GLU LEU ASP ASP LEU ALA HIS THR ARG ILE GLU LEU

● Molecule 3: DIPHTHERIA TOX REPRESSOR



MET LYS D3 L4 V5 D6 M10 Y11 L12 I15 V16 E17 E20 E21 L26 R27 A28 R29 E32 R33 L34 S37 Q38 T40 V41 S42 Q43 T44 V45 A46 R47 R48 E49 R50 D51 G52 L53 V54 A57 S58 D59 R60 R61 L62 Q63 M64 T67 R68 R69 T70 L71

A72 T73 H79 A82 E83 R84 L85 L86 T87 D88 I89 I90 G91 L92 D93 I94 N95 K96 V97 H98 D99 E100 A101 M104 E105 H106 V107 E111 R114 L115 L116 V117 K118 V119 L120 LYS ASP VAL SER ARG PRO PHE ASN GLY SER LEU ASP GLU LEU VAL

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

HIS ILE THR LEU SER HIS ASN GLY LYS ASP VAL GLU LEU LEU ASP ASP LEU LEU HIS THR ILE ARG ILE GLU LEU

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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 Too-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 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	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

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 35.

The worst 5 of 333 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: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 [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	
3	A	116/226 (51%)	102 (88%)	13 (11%)	1 (1%)	20	62
3	B	116/226 (51%)	102 (88%)	13 (11%)	1 (1%)	20	62
3	C	116/226 (51%)	104 (90%)	11 (10%)	1 (1%)	20	62
3	D	116/226 (51%)	104 (90%)	10 (9%)	2 (2%)	11	44
All	All	464/904 (51%)	412 (89%)	47 (10%)	5 (1%)	17	56

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 [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	
3	A	105/198 (53%)	87 (83%)	18 (17%)	2	12
3	B	105/198 (53%)	86 (82%)	19 (18%)	2	10
3	C	105/198 (53%)	87 (83%)	18 (17%)	2	12
3	D	105/198 (53%)	87 (83%)	18 (17%)	2	12
All	All	420/792 (53%)	347 (83%)	73 (17%)	2	11

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 [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](#)

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.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.