



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:30 PM UTC

PDB ID : 1DDN / pdb\_00001ddn  
Title : DIPHTHERIA TOX REPRESSOR (C102D MUTANT)/TOX DNA OPERATOR COMPLEX  
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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](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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

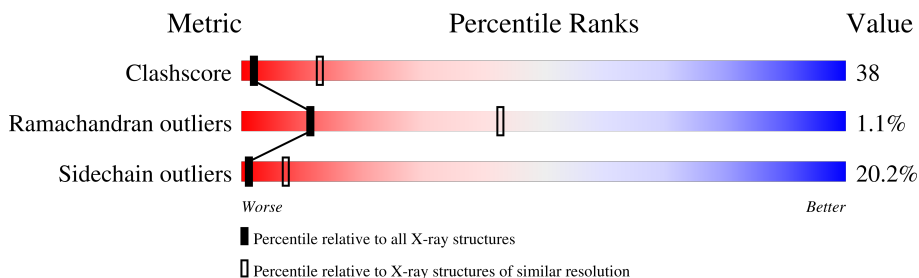
# 1 Overall quality at a glance

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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 of 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  $\leq 5\%$

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 [i](#)

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
			Total	C	N	O	P			
1	E	33	672	327	114	199	32	0	0	0

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

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

- Molecule 3 is a protein called DIPHTHERIA TOX REPRESSOR.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore 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.	Xtrriage
Total number of atoms	5135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.50	0/752	1.15	5/1159 (0.4%)
2	F	0.45	0/758	1.15	8/1168 (0.7%)
3	A	0.54	0/953	0.98	4/1288 (0.3%)
3	B	0.51	0/953	0.90	0/1288
3	C	0.51	0/953	0.98	3/1288 (0.2%)
3	D	0.51	0/953	0.92	2/1288 (0.2%)
All	All	0.51	0/5322	1.01	22/7479 (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

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	311	DG	N9-C1'-C2'	-10.35	97.97	113.50
1	E	317	DT	N1-C1'-C2'	-8.44	100.84	113.50
3	C	89	ILE	N-CA-C	8.30	118.33	110.53
3	A	89	ILE	N-CA-C	7.73	117.80	110.53
2	F	419	DG	N9-C1'-C2'	-7.36	102.46	113.50

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 [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	E	672	0	380	93	0
2	F	675	0	377	65	0
3	A	944	0	962	47	0
3	B	944	0	962	64	0
3	C	944	0	962	62	0
3	D	944	0	962	56	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	360	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 38.

The worst 5 of 360 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:307:DT:H2'	1:E:308:DT:H71	1.28	1.16
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

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%)	14	48
3	B	116/226 (51%)	102 (88%)	13 (11%)	1 (1%)	14	48
3	C	116/226 (51%)	104 (90%)	11 (10%)	1 (1%)	14	48
3	D	116/226 (51%)	104 (90%)	10 (9%)	2 (2%)	7	32
All	All	464/904 (51%)	412 (89%)	47 (10%)	5 (1%)	11	43

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%)	85 (81%)	20 (19%)	1	8
3	B	105/198 (53%)	83 (79%)	22 (21%)	1	6
3	C	105/198 (53%)	85 (81%)	20 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	105/198 (53%)	82 (78%)	23 (22%)	1	5
All	All	420/792 (53%)	335 (80%)	85 (20%)	1	7

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	108	MET
3	D	62	LEU
3	C	116	LEU
3	D	30	ILE
3	D	80	ARG

Sometimes 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 oligosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.