



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:35 PM GMT

PDB ID : 1BI2  
Title : STRUCTURE OF APO-AND HOLO-DIPHThERIA TOXIN REPRESSOR  
Authors : Pohl, E.; Hol, W.G.J.  
Deposited on : 1998-06-21  
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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

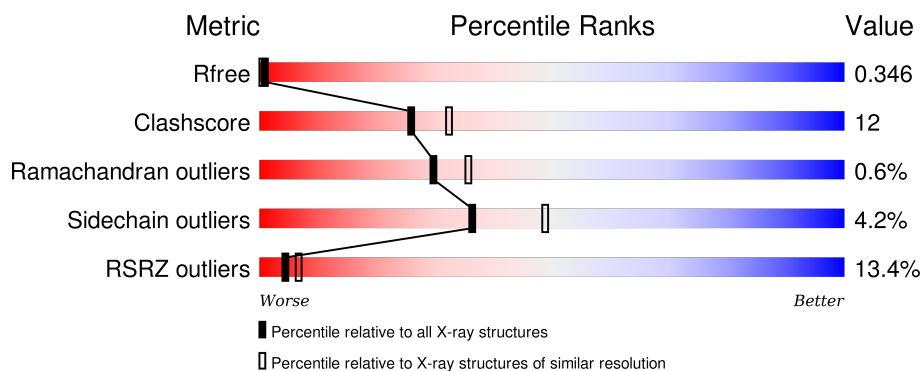
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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	226	
1	B	226	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3789 atoms, of which 932 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 DIPHTHERIA TOXIN REPRESSOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	H	N	O	S	0	0	0
			1951	995	346	283	321	6			
1	B	138	Total	C	H	N	O	S	0	0	0
			1337	670	252	198	211	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	103	Total	H	O	0	0
			309	206	103		
2	B	64	Total	H	O	0	0
			192	128	64		



- Molecule 1: DIPHTHERIA TOXIN REPRESSOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.00Å 63.00Å 216.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.30 27.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	88.9 (8.00-2.30) 83.4 (27.28-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.31Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.257 , 0.352 0.251 , 0.346	Depositor DCC
$R_{free}$ test set	894 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 82.8	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 19195 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3789	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.60 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.3240e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/1621	0.64	1/2204 (0.0%)
1	B	0.36	0/1098	0.61	0/1487
All	All	0.36	0/2719	0.63	1/3691 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	PRO	N-CA-CB	5.83	110.30	103.30

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	1605	346	1541	36	0
1	B	1085	252	1098	33	0
2	A	103	206	0	2	0
2	B	64	128	0	0	0
All	All	2857	932	2639	66	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 12.

All (66) 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:A:81:LEU:HB3	1:A:108:MET:HE1	1.70	0.72
1:B:117:VAL:HG11	1:B:140:VAL:HB	1.76	0.68
1:A:125:ARG:HH11	1:A:125:ARG:HG3	1.59	0.67
1:B:108:MET:CE	1:B:113:GLU:HG2	2.25	0.66
1:A:30:ILE:HD12	1:A:62:LEU:HD12	1.76	0.66
1:B:29:ARG:NH2	1:B:33:ARG:HH21	1.94	0.65
1:A:116:LEU:HA	1:A:119:VAL:HG22	1.81	0.63
1:A:152:VAL:CG1	1:A:202:ILE:HG21	2.29	0.62
1:A:108:MET:HE2	1:A:113:GLU:HG2	1.81	0.62
1:A:13:ARG:HG3	1:A:76:MET:HG2	1.83	0.60
1:B:108:MET:HE3	1:B:113:GLU:HG2	1.84	0.60
1:B:117:VAL:HG21	1:B:140:VAL:HG21	1.84	0.59
1:A:196:VAL:HG22	1:A:197:ASP:H	1.68	0.59
1:A:108:MET:CE	1:A:113:GLU:HG2	2.32	0.58
1:B:73:THR:HG23	1:B:133:PRO:HB2	1.85	0.58
1:B:77:ARG:O	1:B:81:LEU:HD22	2.04	0.57
1:A:160:PRO:HA	1:A:195:ILE:O	2.05	0.56
1:B:104:TRP:HA	1:B:107:VAL:HG22	1.88	0.56
1:A:44:THR:HG23	1:A:47:ARG:NH1	2.21	0.55
1:A:125:ARG:HG3	1:A:125:ARG:NH1	2.22	0.53
1:B:138:LEU:HD23	1:B:140:VAL:CG2	2.38	0.53
1:A:15:ILE:HG12	1:A:30:ILE:HD11	1.89	0.53
1:B:116:LEU:HA	1:B:119:VAL:HG22	1.92	0.52
1:A:107:VAL:O	1:B:103:ARG:NH1	2.44	0.51
1:A:73:THR:HG23	1:A:133:PRO:HB2	1.92	0.51
1:B:108:MET:HE2	1:B:113:GLU:HG2	1.92	0.50
1:A:196:VAL:HG22	1:A:197:ASP:N	2.27	0.50
1:B:30:ILE:HD12	1:B:62:LEU:HD12	1.93	0.50
1:B:125:ARG:HG3	1:B:125:ARG:HH11	1.76	0.49
1:A:187:ILE:HG12	1:A:206:HIS:HB3	1.94	0.49
1:B:80:ARG:HB3	1:B:132:ILE:HG12	1.94	0.49
1:B:81:LEU:HB2	1:B:108:MET:HE1	1.94	0.48
1:B:114:ARG:O	1:B:118:LYS:HG3	2.13	0.48
1:B:56:VAL:HG22	1:B:62:LEU:HD21	1.96	0.48
1:A:89:ILE:HG21	1:B:89:ILE:HG21	1.95	0.48
1:A:41:VAL:O	1:A:45:VAL:HG23	2.13	0.48
1:A:103:ARG:NH1	1:B:107:VAL:O	2.45	0.47
1:B:38:GLY:O	1:B:41:VAL:HG22	2.14	0.47
1:A:202:ILE:H	1:A:202:ILE:HD12	1.78	0.47
1:A:67:THR:HG21	2:A:389:HOH:O	2.16	0.46
1:A:80:ARG:HB3	1:A:132:ILE:HG12	1.97	0.46
1:B:138:LEU:HD23	1:B:140:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ALA:HB2	1:A:63:GLN:HG3	1.97	0.45
1:B:57:ALA:O	1:B:60:ARG:N	2.49	0.45
1:A:161:ARG:O	1:A:194:GLU:HA	2.17	0.45
1:A:152:VAL:HG13	1:A:202:ILE:HG21	1.98	0.44
1:A:84:ARG:HD2	1:A:125:ARG:O	2.17	0.44
1:A:77:ARG:O	1:A:81:LEU:HB2	2.17	0.44
1:B:47:ARG:HA	1:B:50:ARG:CZ	2.48	0.44
1:A:33:ARG:HA	2:A:424:HOH:O	2.18	0.43
1:A:163:VAL:O	1:A:192:GLU:HA	2.19	0.43
1:B:60:ARG:HA	1:B:60:ARG:HD3	1.93	0.42
1:A:217:LEU:HD22	1:A:221:ILE:HD11	2.01	0.42
1:B:15:ILE:HG12	1:B:30:ILE:HD11	2.02	0.42
1:B:47:ARG:HA	1:B:50:ARG:NH1	2.35	0.42
1:A:12:LEU:CD1	1:A:71:LEU:HD23	2.50	0.41
1:B:12:LEU:HB3	1:B:72:ALA:HB2	2.03	0.41
1:A:15:ILE:HG23	1:A:25:PRO:HB3	2.01	0.41
1:A:166:VAL:HG23	1:A:222:ARG:O	2.21	0.41
1:B:92:LEU:HD12	1:B:93:ASP:H	1.86	0.41
1:B:29:ARG:HH22	1:B:33:ARG:HE	1.68	0.41
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.91	0.40
1:A:14:THR:HG23	1:A:33:ARG:HG2	2.03	0.40
1:B:71:LEU:O	1:B:75:VAL:HG23	2.21	0.40
1:A:87:THR:CG2	1:A:97:VAL:HG21	2.51	0.40
1:B:87:THR:CG2	1:B:97:VAL:HG21	2.51	0.40

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
1	A	208/226 (92%)	196 (94%)	10 (5%)	2 (1%)	19 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	136/226 (60%)	130 (96%)	6 (4%)	0	100	100
All	All	344/452 (76%)	326 (95%)	16 (5%)	2 (1%)	30	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ALA
1	A	196	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	
1	A	168/198 (85%)	159 (95%)	9 (5%)	27	36
1	B	121/198 (61%)	118 (98%)	3 (2%)	55	73
All	All	289/396 (73%)	277 (96%)	12 (4%)	36	49

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	42	SER
1	A	58	SER
1	A	76	MET
1	A	81	LEU
1	A	125	ARG
1	A	140	VAL
1	A	166	VAL
1	A	212	GLU
1	B	43	GLN
1	B	76	MET
1	B	81	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	173	GLN
1	B	36	GLN
1	B	43	GLN
1	B	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](#)

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	214/226 (94%)	1.02	38 (17%) 2 3	8, 28, 71, 90	0
1	B	138/226 (61%)	0.49	9 (6%) 22 30	9, 23, 60, 83	0
All	All	352/452 (77%)	0.81	47 (13%) 4 7	8, 26, 67, 90	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	VAL	8.5
1	A	159	MET	7.8
1	A	207	ASN	7.3
1	B	4	LEU	6.5
1	A	4	LEU	6.3
1	A	156	ALA	6.0
1	A	160	PRO	5.9
1	A	190	GLY	5.8
1	A	152	VAL	5.5
1	A	196	VAL	5.3
1	A	157	THR	5.2
1	B	35	GLU	4.8
1	A	154	ASP	4.6
1	A	140	VAL	4.6
1	A	166	VAL	4.4
1	A	185	ALA	4.3
1	A	195	ILE	4.2
1	B	43	GLN	4.0
1	A	167	GLN	4.0
1	A	206	HIS	3.8
1	A	211	VAL	3.8
1	A	208	GLY	3.8
1	A	191	SER	3.5
1	A	158	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	197	ASP	3.1
1	A	202	ILE	2.9
1	A	165	ILE	2.9
1	A	201	HIS	2.8
1	A	193	VAL	2.8
1	A	214	LEU	2.7
1	A	187	ILE	2.7
1	A	205	SER	2.6
1	A	179	PHE	2.5
1	A	163	VAL	2.5
1	B	39	PRO	2.5
1	B	29	ARG	2.5
1	A	153	ILE	2.4
1	A	225	GLU	2.3
1	A	186	ASP	2.3
1	A	161	ARG	2.2
1	A	221	ILE	2.2
1	A	155	ALA	2.2
1	B	57	ALA	2.2
1	A	81	LEU	2.2
1	A	35	GLU	2.1
1	B	58	SER	2.1
1	B	47	ARG	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.