



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:50 am GMT

PDB ID : 1AF9  
Title : TETANUS NEUROTOXIN C FRAGMENT  
Authors : Umland, T.C.; Wingert, L.; Swaminathan, S.; Furey, W.F.; Schmidt, J.J.; Sax, M.  
Deposited on : 1997-03-24  
Resolution : 2.70 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

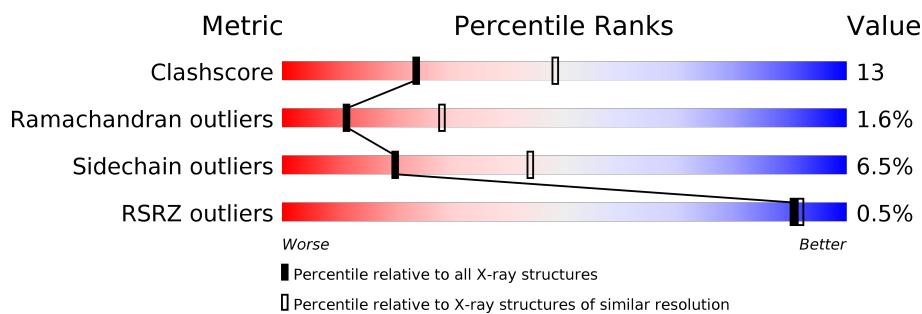
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	452	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3702 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 protein called TETANUS NEUROTOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3564	2282	597	676	9			

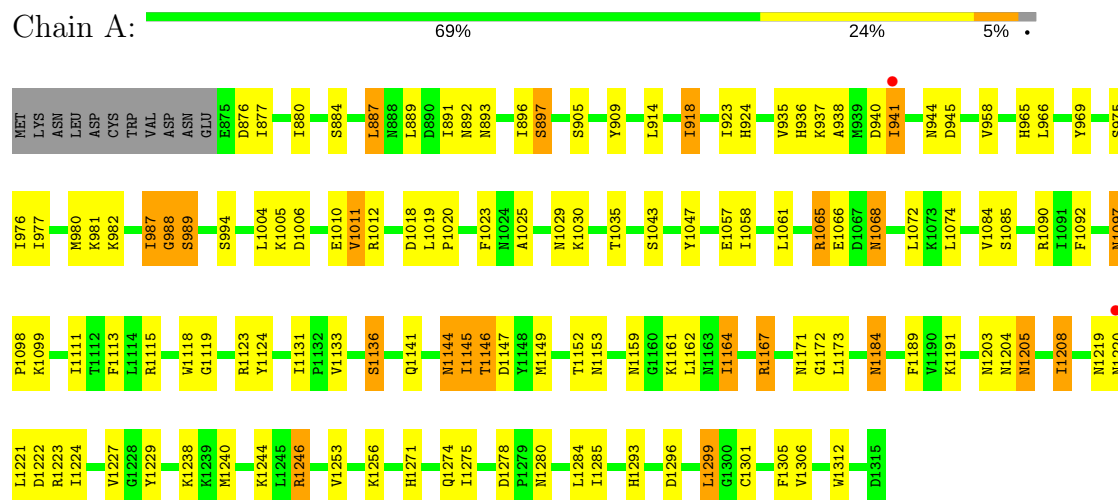
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	138	Total	O	0	0
			138	138		

### 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.

#### • Molecule 1: TETANUS NEUROTOXIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.40Å 79.70Å 91.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.70 34.11 – 2.57	Depositor EDS
% Data completeness (in resolution range)	95.4 (8.00-2.70) 89.1 (34.11-2.57)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.91 (at 2.57Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.161 , 0.245 0.160 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.59	0/3645	0.82	2/4945 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1167	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	982	LYS	N-CA-C	5.52	125.89	111.00

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	3564	0	3516	89	0
2	A	138	0	0	1	0
All	All	3702	0	3516	89	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 13.

All (89) 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:1224:ILE:HD13	1:A:1275:ILE:HD11	1.56	0.86
1:A:958:VAL:HG12	1:A:1084:VAL:HG23	1.59	0.85
1:A:938:ALA:O	1:A:941:ILE:HG22	1.79	0.82
1:A:937:LYS:HB3	1:A:941:ILE:CG2	2.20	0.71
1:A:989:SER:HB3	1:A:1066:GLU:HA	1.72	0.71
1:A:1113:PHE:CE1	1:A:1191:LYS:HG2	2.31	0.65
1:A:1159:ASN:HB3	1:A:1164:ILE:HG23	1.77	0.65
1:A:1123:ARG:HH11	1:A:1189:PHE:HE1	1.42	0.65
1:A:1221:LEU:O	1:A:1223:ARG:HG3	1.97	0.64
1:A:1274:GLN:NE2	1:A:1280:ASN:HD22	1.96	0.63
1:A:1090:ARG:HD2	1:A:1092:PHE:CZ	2.34	0.62
1:A:905:SER:HB3	1:A:936:HIS:HB3	1.82	0.62
1:A:1208:ILE:HD12	1:A:1238:LYS:HG2	1.81	0.62
1:A:1145:ILE:HG23	1:A:1146:THR:H	1.65	0.62
1:A:1293:HIS:O	1:A:1299:LEU:HD11	2.00	0.62
1:A:1146:THR:HG22	1:A:1229:TYR:HA	1.82	0.61
1:A:1043:SER:HA	1:A:1058:ILE:HG12	1.83	0.60
1:A:1159:ASN:HB3	1:A:1164:ILE:CG2	2.30	0.60
1:A:1006:ASP:OD2	1:A:1010:GLU:HB2	2.02	0.59
1:A:884:SER:O	1:A:1092:PHE:HA	2.03	0.58
1:A:958:VAL:HG12	1:A:1084:VAL:CG2	2.30	0.58
1:A:975:SER:HA	1:A:994:SER:HB3	1.86	0.57
1:A:988:GLY:HA3	1:A:1005:LYS:HD3	1.86	0.57
1:A:1066:GLU:HB2	2:A:1412:HOH:O	2.04	0.57
1:A:1097:ASN:HD21	1:A:1099:LYS:HB3	1.69	0.56
1:A:977:ILE:HG23	1:A:1072:LEU:HD23	1.87	0.56
1:A:891:ILE:HG21	1:A:914:LEU:HD13	1.89	0.55
1:A:1005:LYS:HA	1:A:1010:GLU:O	2.06	0.55
1:A:877:ILE:HA	1:A:880:ILE:HD12	1.88	0.54
1:A:887:LEU:HD11	1:A:935:VAL:HG11	1.89	0.54
1:A:1167:ARG:O	1:A:1167:ARG:HG3	2.08	0.53
1:A:891:ILE:HD12	1:A:896:ILE:HG12	1.91	0.52
1:A:1097:ASN:HB2	1:A:1098:PRO:HD2	1.92	0.52
1:A:1113:PHE:CD1	1:A:1191:LYS:HG2	2.45	0.52
1:A:1159:ASN:OD1	1:A:1161:LYS:HG2	2.10	0.51
1:A:1097:ASN:HD22	1:A:1099:LYS:H	1.58	0.51
1:A:1152:THR:HG22	1:A:1153:ASN:N	2.26	0.50
1:A:965:HIS:CD2	1:A:969:TYR:HE2	2.28	0.50
1:A:1246:ARG:NH2	1:A:1296:ASP:O	2.45	0.50
1:A:1271:HIS:HB2	1:A:1285:ILE:HG12	1.94	0.50
1:A:1035:THR:HB	1:A:1047:TYR:HB2	1.93	0.49
1:A:980:MET:HA	1:A:989:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:LYS:HG2	1:A:1118:TRP:HA	1.95	0.49
1:A:1205:ASN:N	1:A:1205:ASN:HD22	2.11	0.49
1:A:923:ILE:O	1:A:1085:SER:HA	2.13	0.49
1:A:1018:ASP:OD2	1:A:1025:ALA:HB1	2.13	0.49
1:A:889:LEU:HA	1:A:897:SER:O	2.13	0.49
1:A:1097:ASN:HD22	1:A:1099:LYS:N	2.09	0.49
1:A:1275:ILE:O	1:A:1278:ASP:HB2	2.13	0.48
1:A:1141:GLN:NE2	1:A:1172:GLY:HA2	2.28	0.48
1:A:941:ILE:O	1:A:941:ILE:HG23	2.13	0.48
1:A:1205:ASN:N	1:A:1205:ASN:ND2	2.62	0.47
1:A:937:LYS:HB3	1:A:941:ILE:HG23	1.97	0.47
1:A:1136:SER:O	1:A:1167:ARG:HD2	2.15	0.47
1:A:892:ASN:O	1:A:893:ASN:HB2	2.15	0.47
1:A:1224:ILE:CD1	1:A:1275:ILE:HD11	2.39	0.46
1:A:1131:ILE:HD12	1:A:1306:VAL:HG21	1.98	0.45
1:A:1012:ARG:HG3	1:A:1058:ILE:HA	1.97	0.45
1:A:876:ASP:O	1:A:880:ILE:HG13	2.17	0.45
1:A:909:TYR:N	1:A:909:TYR:CD1	2.85	0.45
1:A:1312:TRP:CD1	1:A:1312:TRP:C	2.90	0.45
1:A:1006:ASP:CG	1:A:1010:GLU:HB2	2.37	0.45
1:A:1145:ILE:O	1:A:1227:VAL:O	2.35	0.44
1:A:1149:MET:HB2	1:A:1284:LEU:HG	1.99	0.44
1:A:987:ILE:O	1:A:989:SER:N	2.50	0.44
1:A:1097:ASN:HB2	1:A:1098:PRO:CD	2.48	0.44
1:A:924:HIS:HD2	1:A:1085:SER:OG	2.01	0.44
1:A:1004:LEU:O	1:A:1011:VAL:HA	2.18	0.44
1:A:1019:LEU:HA	1:A:1020:PRO:HD3	1.87	0.44
1:A:1111:ILE:HD12	1:A:1244:LYS:HG2	1.99	0.44
1:A:1144:ASN:O	1:A:1147:ASP:HB2	2.18	0.44
1:A:1253:VAL:HB	1:A:1305:PHE:CE1	2.53	0.44
1:A:1299:LEU:HD13	1:A:1301:CYS:SG	2.58	0.43
1:A:1115:ARG:HD3	1:A:1119:GLY:O	2.18	0.43
1:A:1162:LEU:HB2	1:A:1164:ILE:HG22	2.00	0.43
1:A:918:ILE:HD13	1:A:918:ILE:HA	1.81	0.43
1:A:1023:PHE:CE2	1:A:1136:SER:HB2	2.54	0.42
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.66	0.42
1:A:944:ASN:ND2	1:A:1066:GLU:OE2	2.53	0.42
1:A:987:ILE:O	1:A:988:GLY:C	2.57	0.42
1:A:1068:ASN:OD1	1:A:1068:ASN:N	2.53	0.42
1:A:976:ILE:HG22	1:A:1074:LEU:CD2	2.49	0.42
1:A:1219:ASN:O	1:A:1220:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:ARG:HE	1:A:1065:ARG:HA	1.85	0.41
1:A:1203:ASN:O	1:A:1204:ASN:HB2	2.19	0.41
1:A:909:TYR:N	1:A:909:TYR:HD1	2.18	0.41
1:A:1240:MET:HA	1:A:1256:LYS:O	2.21	0.40
1:A:987:ILE:HG22	1:A:1005:LYS:HZ3	1.85	0.40
1:A:877:ILE:HD11	1:A:1099:LYS:HG2	2.04	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	439/452 (97%)	392 (89%)	40 (9%)	7 (2%)	11	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1145	ILE
1	A	1184	ASN
1	A	1136	SER
1	A	941	ILE
1	A	1124	TYR
1	A	989	SER
1	A	988	GLY

### 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	
1	A	397/408 (97%)	371 (94%)	26 (6%)	20	44

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	887	LEU
1	A	897	SER
1	A	918	ILE
1	A	940	ASP
1	A	945	ASP
1	A	981	LYS
1	A	987	ILE
1	A	1011	VAL
1	A	1029	ASN
1	A	1057	GLU
1	A	1061	LEU
1	A	1065	ARG
1	A	1068	ASN
1	A	1097	ASN
1	A	1133	VAL
1	A	1144	ASN
1	A	1146	THR
1	A	1164	ILE
1	A	1171	ASN
1	A	1173	LEU
1	A	1184	ASN
1	A	1205	ASN
1	A	1208	ILE
1	A	1222	ASP
1	A	1246	ARG
1	A	1299	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	892	ASN
1	A	924	HIS
1	A	965	HIS
1	A	1013	GLN
1	A	1029	ASN

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Mol	Chain	Res	Type
1	A	1078	ASN
1	A	1097	ASN
1	A	1120	ASN
1	A	1141	GLN
1	A	1163	ASN
1	A	1205	ASN
1	A	1274	GLN
1	A	1293	HIS

### 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 [i](#)

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

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	441/452 (97%)	-0.81	2 (0%) 90 92	2, 9, 45, 65	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	941	ILE	2.8
1	A	1220	ASN	2.4

### 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.