



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:10 AM GMT

PDB ID : 1ZTT  
Title : Netropsin bound to d(CTTAATTCGAATTAAG) in complex with MMLV RT catalytic fragment  
Authors : Goodwin, K.D.; Long, E.C.; Georgiadis, M.M.  
Deposited on : 2005-05-27  
Resolution : 1.85 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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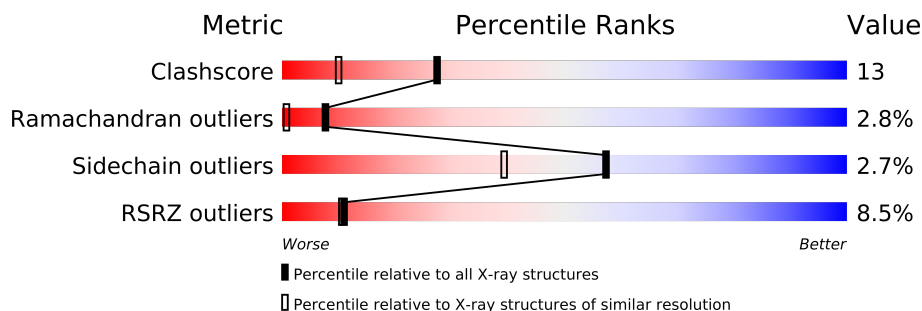
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 1.85 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	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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.

Mol	Chain	Length	Quality of chain
1	B	8	
2	G	8	
3	A	255	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NT	G	301	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 2679 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 5'-D(\*CP\*TP\*TP\*AP\*AP\*TP\*TP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	8	Total	C	N	O	P	0	0	0
			157	78	24	48	7			

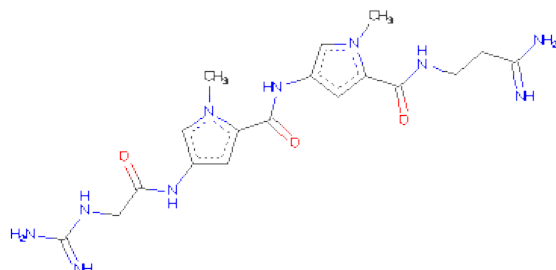
- Molecule 2 is a DNA chain called 5'-D(P\*GP\*AP\*AP\*TP\*TP\*AP\*AP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	P	0	0	0
			168	80	34	46	8			

- Molecule 3 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	255	Total	C	N	O	S	0	0	0
			2041	1311	356	367	7			

- Molecule 4 is NETROPSIN (three-letter code: NT) (formula: C<sub>18</sub>H<sub>26</sub>N<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			31	18	10	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	262	Total	O	0	0
			262	262		
5	B	7	Total	O	0	0
			7	7		
5	G	13	Total	O	0	0
			13	13		

### 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 errors 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: 5'-D(\*CP\*TP\*TP\*AP\*AP\*TP\*TP\*C)-3'

Chain B: 

G1  
T2  
T3  
A4  
A5  
T6  
T7  
C8
































- Molecule 2: 5'-D(P\*GP\*AP\*AP\*TP\*TP\*AP\*AP\*G)-3'






Chain G: 

G9  
A10  
A11  
T12  
T13  
A14  
A15  
G16

- Molecule 3: Reverse transcriptase

Chain A: 

T24 I61 Y64 Q68 E69 A70 R71 L72 G73 I74 K75 P76 L99 P100 V101 K102 K103 P104 G105 T106 N107 D108 Y109 R110 P111 V112 E117 P132 L136 S137 G138 L139 P140 V148 H161 P162 T163 S164 Q165 M172 R173 D174 P175 E176 M177 G178 I179 S180 Q182

L183 T184 W185 D206 D209 Q213 V223 L227 Q237 R241 L250 L272 L273 K274 E275 G276 Q277 R278

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.57Å 145.61Å 46.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.50 – 1.85 43.67 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.50-1.85) 94.9 (43.67-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 1.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.220 , 0.246 0.236 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 32107 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2679	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	B	0.26	0/174	0.68	0/266
2	G	0.25	0/189	0.68	0/290
3	A	0.30	0/2097	0.60	0/2858
All	All	0.30	0/2460	0.62	0/3414

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	B	157	0	94	9	1
2	G	168	0	91	5	1
3	A	2041	0	2056	46	0
4	G	31	0	25	0	0
5	A	262	0	0	1	0
5	B	7	0	0	0	0
5	G	13	0	0	0	0
All	All	2679	0	2266	60	1

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 13.

All (60) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:6:DT:H2''	1:B:7:DT:H5''	1.39	1.02
3:A:173:ARG:HH11	3:A:173:ARG:HB2	1.28	0.97
1:B:7:DT:H2''	1:B:8:DC:H5'	1.45	0.95
3:A:103:LYS:HZ3	3:A:103:LYS:H	1.17	0.89
3:A:74:ILE:HG23	3:A:111:PRO:HG3	1.51	0.89
3:A:103:LYS:HB2	3:A:104:PRO:HD3	1.54	0.88
1:B:6:DT:H2''	1:B:7:DT:C5'	2.07	0.84
1:B:6:DT:C2'	1:B:7:DT:H5''	2.08	0.82
3:A:174:ASP:H	3:A:178:GLY:HA3	1.45	0.80
1:B:3:DT:H2''	1:B:4:DA:H5'	1.72	0.72
3:A:68:GLN:O	3:A:72:LEU:HD13	1.91	0.70
2:G:13:DT:H2''	2:G:14:DA:H5'	1.72	0.69
3:A:173:ARG:NH1	3:A:173:ARG:HB2	2.05	0.69
2:G:9:DG:H2''	2:G:10:DA:C8	2.29	0.67
3:A:61:ILE:HD11	3:A:117:GLU:HG3	1.74	0.66
3:A:161:HIS:CD2	3:A:163:THR:H	2.15	0.65
3:A:103:LYS:N	3:A:103:LYS:HZ3	1.94	0.60
1:B:7:DT:H2''	1:B:8:DC:C5'	2.27	0.59
3:A:206:ASP:HB3	3:A:250:LEU:HD13	1.86	0.58
3:A:103:LYS:NZ	3:A:103:LYS:H	1.97	0.56
3:A:104:PRO:HD2	3:A:108:ASP:OD2	2.05	0.56
3:A:272:LEU:H	3:A:278:ARG:HH11	1.52	0.56
2:G:12:DT:H2''	2:G:13:DT:H5'	1.87	0.56
3:A:179:ILE:HG21	3:A:183:LEU:HD21	1.87	0.56
3:A:161:HIS:HD2	3:A:163:THR:H	1.53	0.55
2:G:12:DT:H2''	2:G:13:DT:C5'	2.37	0.55
3:A:138:GLY:O	3:A:140:PRO:HD3	2.07	0.54
3:A:101:VAL:HG12	3:A:103:LYS:NZ	2.24	0.53
3:A:227:LEU:C	3:A:227:LEU:HD13	2.30	0.52
3:A:173:ARG:HG3	3:A:174:ASP:N	2.24	0.51
3:A:209:ASP:O	3:A:213:GLN:HG2	2.11	0.51
3:A:148:VAL:HG22	3:A:227:LEU:HD23	1.91	0.51
3:A:277:GLN:O	3:A:278:ARG:HB2	2.12	0.49
3:A:174:ASP:N	3:A:178:GLY:HA3	2.22	0.48
3:A:173:ARG:HH11	3:A:173:ARG:CB	2.14	0.48
3:A:274:LYS:HG2	3:A:275:GLU:HG3	1.96	0.48
3:A:75:LYS:HB3	3:A:76:PRO:HD3	1.95	0.47
3:A:237:GLN:O	3:A:241:ARG:HG3	2.14	0.47
3:A:174:ASP:O	3:A:176:GLU:N	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:139:LEU:HD22	5:A:516:HOH:O	2.12	0.47
3:A:103:LYS:HB2	3:A:104:PRO:CD	2.34	0.46
2:G:13:DT:H2''	2:G:14:DA:C5'	2.43	0.46
3:A:213:GLN:HA	3:A:213:GLN:NE2	2.30	0.46
3:A:179:ILE:N	3:A:179:ILE:HD12	2.31	0.45
1:B:1:DC:H2'	1:B:2:DT:H72	1.99	0.45
1:B:7:DT:C2'	1:B:8:DC:H5'	2.31	0.44
3:A:101:VAL:HG21	3:A:112:VAL:HG21	2.00	0.44
3:A:172:TRP:CD1	3:A:179:ILE:HD13	2.53	0.44
3:A:179:ILE:HD12	3:A:179:ILE:H	1.81	0.43
3:A:132:PRO:O	3:A:136:LEU:HD23	2.19	0.43
3:A:165:GLN:HG2	3:A:185:TRP:O	2.20	0.42
3:A:102:LYS:O	3:A:103:LYS:C	2.57	0.42
3:A:176:GLU:HB2	3:A:177:MET:H	1.57	0.42
3:A:103:LYS:HD3	3:A:110:ARG:CZ	2.51	0.41
3:A:101:VAL:HG12	3:A:102:LYS:N	2.36	0.41
3:A:70:ALA:HA	3:A:109:TYR:CE2	2.56	0.40
3:A:213:GLN:HA	3:A:213:GLN:HE21	1.85	0.40
1:B:5:DA:H2''	1:B:6:DT:H5'	2.02	0.40
3:A:179:ILE:CG2	3:A:180:SER:N	2.85	0.40
3:A:179:ILE:H	3:A:179:ILE:CD1	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:8:DC:O3'	2:G:9:DG:P[2_765]	1.60	0.60

## 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	253/255 (99%)	236 (93%)	10 (4%)	7 (3%)	<b>8</b> <b>1</b>

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	102	LYS
3	A	104	PRO
3	A	108	ASP
3	A	223	VAL
3	A	103	LYS
3	A	181	GLY
3	A	175	PRO

### 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	224/224 (100%)	218 (97%)	6 (3%)	57	39

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	64	TYR
3	A	99	LEU
3	A	139	LEU
3	A	173	ARG
3	A	176	GLU
3	A	177	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	84	GLN
3	A	144	GLN
3	A	161	HIS
3	A	213	GLN
3	A	237	GLN
3	A	245	GLN

### 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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NT	G	301	-	32,32,32	1.95	10 (31%)	38,44,44	1.49	8 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NT	G	301	-	-	0/21/27/27	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	301	NT	C9-N6	3.99	1.46	1.35
4	G	301	NT	C18-N9	3.58	1.35	1.27
4	G	301	NT	C11-C12	3.38	1.43	1.39
4	G	301	NT	C15-N8	3.35	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	301	NT	C7-C4	3.17	1.43	1.38
4	G	301	NT	C5-C4	3.08	1.42	1.39
4	G	301	NT	C17-C18	3.01	1.54	1.51
4	G	301	NT	C3-N4	2.49	1.41	1.35
4	G	301	NT	C6-N5	2.13	1.41	1.36
4	G	301	NT	C5-C6	2.10	1.41	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	301	NT	C7-C4-N4	3.18	132.74	122.40
4	G	301	NT	C14-N7-C12	2.66	128.35	125.59
4	G	301	NT	C13-C10-N6	2.58	130.76	122.40
4	G	301	NT	C11-C12-N7	2.52	109.68	108.09
4	G	301	NT	C5-C4-N4	-2.46	121.06	129.27
4	G	301	NT	C13-N7-C12	-2.39	105.97	108.70
4	G	301	NT	O1-C3-C2	2.38	125.60	120.66
4	G	301	NT	O3-C15-N8	-2.11	117.92	122.50

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 ⓘ

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(Å²)	Q<0.9	
1	B	8/8 (100%)	0.10	0	100	100	37, 42, 47, 51	0
2	G	8/8 (100%)	-0.08	0	100	100	23, 37, 44, 49	0
3	A	255/255 (100%)	0.33	23 (9%)	10	9	12, 22, 63, 87	0
All	All	271/271 (100%)	0.31	23 (8%)	11	10	12, 22, 61, 87	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	179	ILE	10.2
3	A	107	ASN	9.0
3	A	105	GLY	8.5
3	A	177	MET	7.5
3	A	180	SER	7.0
3	A	178	GLY	6.7
3	A	106	THR	6.1
3	A	104	PRO	5.9
3	A	103	LYS	5.8
3	A	175	PRO	5.0
3	A	102	LYS	4.0
3	A	64	TYR	4.0
3	A	101	VAL	3.9
3	A	100	PRO	3.8
3	A	108	ASP	3.7
3	A	174	ASP	3.6
3	A	176	GLU	3.2
3	A	110	ARG	2.9
3	A	109	TYR	2.4
3	A	173	ARG	2.4
3	A	99	LEU	2.3
3	A	24	THR	2.3
3	A	278	ARG	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NT	G	301	31/31	0.20	2.38	53,57,63,64	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.