



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:04 PM GMT

PDB ID : 1DYR  
Title : THE STRUCTURE OF PNEUMOCYSTIS CARINII DIHYDROFOLATE  
REDUCTASE TO 1.9 ANGSTROMS RESOLUTION  
Authors : Champness, J.N.; Achari, A.; Ballantine, S.P.; Bryant, P.K.; Delves, C.J.;  
Stammers, D.K.  
Deposited on : 1994-09-14  
Resolution : 1.86 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

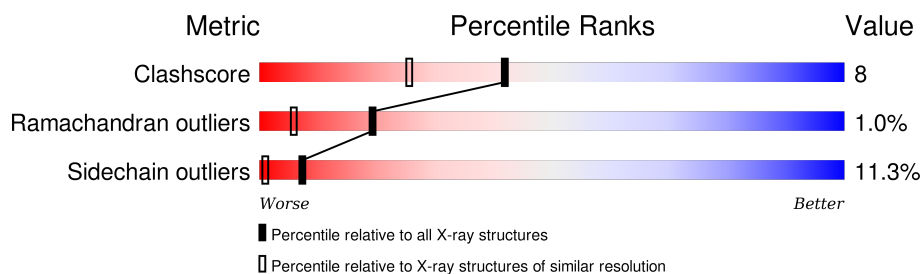
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (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. 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	A	206	

## 2 Entry composition [i](#)

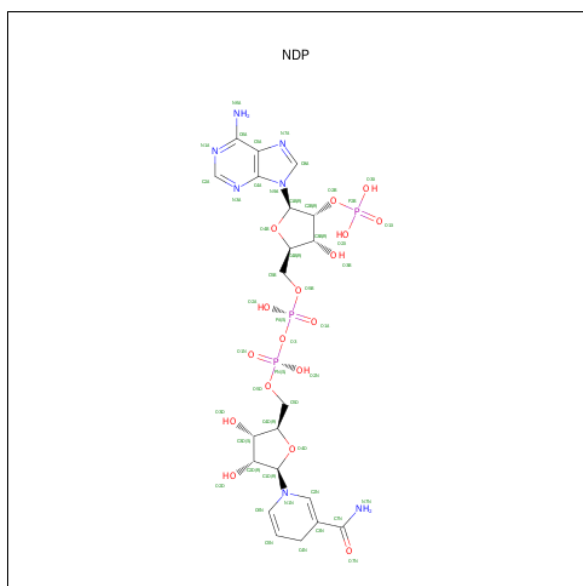
There are 4 unique types of molecules in this entry. The entry contains 1910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIHYDROFOLATE REDUCTASE.

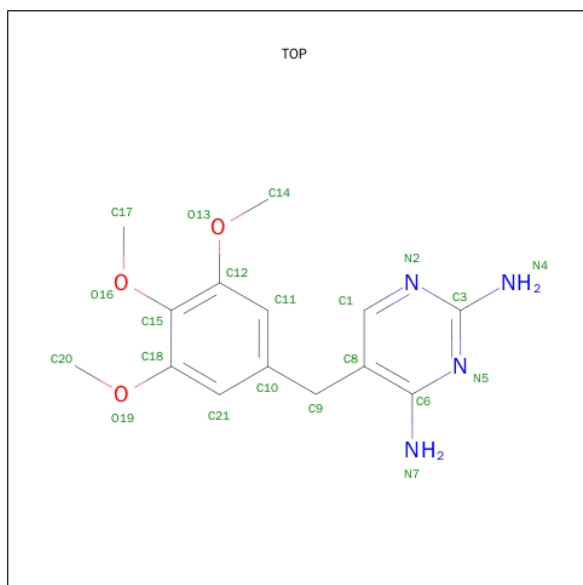
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1678	1081	287	304	6			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is TRIMETHOPRIM (three-letter code: TOP) (formula:  $C_{14}H_{18}N_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	14	4	3		

- Molecule 4 is water.

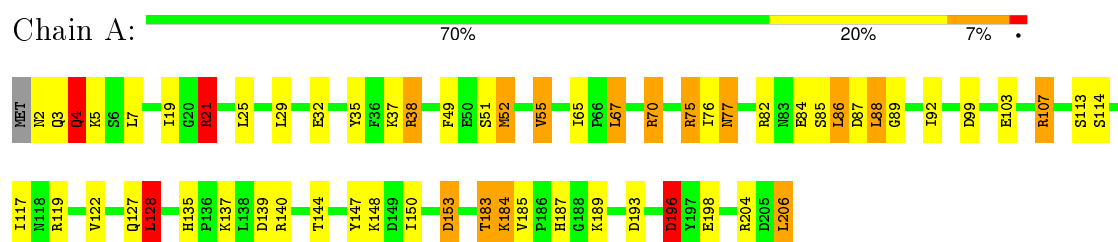
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		

### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: DIHYDROFOLATE REDUCTASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.90 Å   43.60 Å   37.60 Å 90.00°   117.70°   90.00°	Depositor
Resolution (Å)	10.00 – 1.86	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.86)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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: NDP, TOP

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	1.00	0/1720	1.75	39/2320 (1.7%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	-15.07	112.77	120.30
1	A	75	ARG	NE-CZ-NH1	13.70	127.15	120.30
1	A	119	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	A	35	TYR	CB-CG-CD2	10.49	127.30	121.00
1	A	119	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	52	MET	CA-CB-CG	9.21	128.95	113.30
1	A	107	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	38	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	A	153	ASP	CB-CG-OD1	8.61	126.05	118.30
1	A	82	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	A	21	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	35	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	A	55	VAL	CA-CB-CG1	7.58	122.28	110.90
1	A	75	ARG	CD-NE-CZ	7.52	134.13	123.60
1	A	140	ARG	CD-NE-CZ	6.49	132.68	123.60
1	A	87	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	140	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	A	84	GLU	CA-CB-CG	6.29	127.24	113.40
1	A	75	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	196	ASP	CB-CG-OD1	-6.16	112.75	118.30
1	A	103	GLU	CB-CG-CD	5.97	130.32	114.20
1	A	55	VAL	CB-CA-C	5.96	122.73	111.40
1	A	82	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	204	ARG	CB-CG-CD	-5.85	96.39	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	187	HIS	N-CA-CB	5.79	121.02	110.60
1	A	198	GLU	OE1-CD-OE2	5.68	130.11	123.30
1	A	153	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	128	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	70	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	139	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	140	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
1	A	140	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	86	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	67	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	193	ASP	CB-CG-OD1	-5.18	113.63	118.30
1	A	206	LEU	CB-CG-CD1	5.12	119.71	111.00
1	A	204	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	88	LEU	CA-CB-CG	5.00	126.81	115.30

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	1678	0	1681	26	1
2	A	48	0	26	3	0
3	A	21	0	18	3	0
4	A	163	0	0	8	2
All	All	1910	0	1725	29	2

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 8.

All (29) 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)
3:A:407:TOP:O19	3:A:407:TOP:H172	1.58	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ASP:HB3	4:A:707:HOH:O	1.65	0.96
1:A:153:ASP:CG	4:A:707:HOH:O	2.20	0.79
1:A:153:ASP:CB	4:A:707:HOH:O	2.25	0.75
1:A:122:VAL:HG13	1:A:128:LEU:HD13	1.71	0.71
3:A:407:TOP:O19	3:A:407:TOP:C17	2.37	0.69
1:A:135:HIS:HD2	1:A:137:LYS:H	1.41	0.68
1:A:38:ARG:HG2	4:A:764:HOH:O	2.01	0.60
1:A:32:GLU:HG2	1:A:144:THR:HG21	1.85	0.57
1:A:184:LYS:HB2	4:A:772:HOH:O	2.06	0.54
1:A:21:ARG:HA	1:A:153:ASP:OD1	2.11	0.51
1:A:189:LYS:HD3	1:A:196:ASP:HB3	1.92	0.50
1:A:127:GLN:OE1	2:A:391:NDP:H3B	2.11	0.50
2:A:391:NDP:H42N	3:A:407:TOP:H91	1.93	0.50
1:A:147:TYR:CE2	1:A:189:LYS:HE3	2.47	0.49
1:A:52:MET:HG3	1:A:76:ILE:HG13	1.93	0.49
1:A:148:LYS:HB3	1:A:150:ILE:HD11	1.94	0.49
1:A:38:ARG:NH2	1:A:185:VAL:HG22	2.28	0.48
1:A:21:ARG:NH2	4:A:543:HOH:O	2.46	0.47
1:A:3:GLN:O	1:A:4:GLN:HB2	2.15	0.45
1:A:5:LYS:HE3	1:A:117:ILE:HG22	1.98	0.45
1:A:75:ARG:O	1:A:77:ASN:ND2	2.49	0.45
1:A:38:ARG:NH2	1:A:184:LYS:O	2.41	0.45
1:A:19:ILE:O	2:A:391:NDP:H2N	2.17	0.44
1:A:89:GLY:HA2	1:A:92:ILE:HD12	2.00	0.43
1:A:38:ARG:NE	4:A:767:HOH:O	2.53	0.41
1:A:65:ILE:O	1:A:70:ARG:HD3	2.21	0.41
1:A:38:ARG:NH2	1:A:183:THR:HB	2.36	0.41
1:A:107:ARG:NH1	4:A:556:HOH:O	2.49	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
4:A:574:HOH:O	4:A:746:HOH:O[2_656]	2.01	0.19
1:A:99:ASP:OD1	4:A:722:HOH:O[2_656]	2.08	0.12

## 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	203/206 (98%)	195 (96%)	6 (3%)	2 (1%)	19 6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	85	SER

### 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	186/187 (100%)	165 (89%)	21 (11%)	7 1

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	GLN
1	A	7	LEU
1	A	21	ARG
1	A	25	LEU
1	A	29	LEU
1	A	37	LYS
1	A	49	PHE
1	A	51	SER

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Mol	Chain	Res	Type
1	A	55	VAL
1	A	67	LEU
1	A	77	ASN
1	A	86	LEU
1	A	88	LEU
1	A	113	SER
1	A	114	SER
1	A	128	LEU
1	A	183	THR
1	A	184	LYS
1	A	196	ASP
1	A	206	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	100	HIS
1	A	135	HIS
1	A	174	HIS
1	A	187	HIS
1	A	191	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](#)

2 ligands are 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$
2	NDP	A	391	-	42,52,52	1.28	4 (9%)	55,80,80	1.55	7 (12%)
3	TOP	A	407	-	22,22,22	1.21	1 (4%)	30,30,30	1.90	9 (30%)

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
2	NDP	A	391	-	-	0/30/77/77	0/5/5/5
3	TOP	A	407	-	-	0/10/10/10	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	391	NDP	C4N-C5N	-3.62	1.41	1.49
3	A	407	TOP	C3-N2	-3.53	1.30	1.35
2	A	391	NDP	P2B-O2X	-2.72	1.45	1.54
2	A	391	NDP	O4B-C1B	-2.22	1.38	1.41
2	A	391	NDP	P2B-O2B	2.03	1.66	1.60

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	407	TOP	C20-O19-C18	-4.86	110.17	117.54
3	A	407	TOP	N4-C3-N5	-3.00	112.23	117.20
3	A	407	TOP	C17-O16-C15	-2.93	107.12	114.82
2	A	391	NDP	C3B-C2B-C1B	-2.73	97.45	102.73
3	A	407	TOP	C8-C1-N2	-2.34	119.79	123.86
3	A	407	TOP	C3-N5-C6	-2.27	114.46	117.04
2	A	391	NDP	O2B-C2B-C3B	2.05	119.50	111.51
2	A	391	NDP	O7N-C7N-N7N	2.16	128.13	122.76
3	A	407	TOP	N4-C3-N2	2.25	119.42	117.39
3	A	407	TOP	N2-C3-N5	2.38	128.27	125.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	407	TOP	O13-C12-C15	2.40	119.59	115.26
3	A	407	TOP	C1-C8-C6	2.63	119.49	115.72
2	A	391	NDP	C4A-C5A-N7A	3.36	112.57	109.48
2	A	391	NDP	O3B-C3B-C2B	3.77	122.06	111.16
2	A	391	NDP	C4N-C5N-C6N	4.28	129.63	122.58
2	A	391	NDP	PN-O3-PA	6.15	150.00	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	391	NDP	3	0
3	A	407	TOP	3	0

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.