



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 03:11 AM GMT

PDB ID : 4CD2
Title : LIGAND INDUCED CONFORMATIONAL CHANGES IN THE CRYSTAL
STRUCTURES OF PNEUMOCYSTIS CARINII DIHYDROFOLATE RE-
DUCTASE COMPLEXES WITH FOLATE AND NADP+
Authors : Cody, V.; Galitsky, N.; Rak, D.; Luft, J.R.; Pangborn, W.; Queener, S.F.
Deposited on : 1999-03-18
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

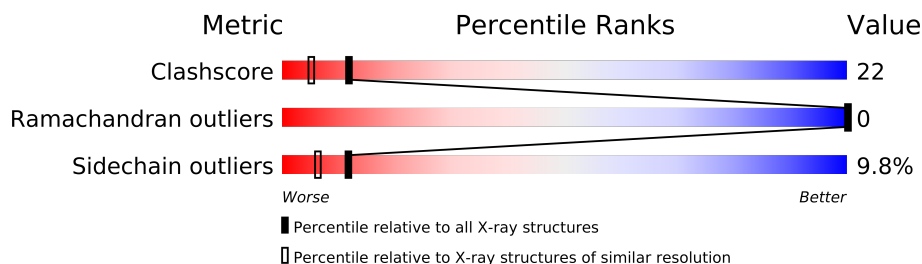
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	206	

2 Entry composition i

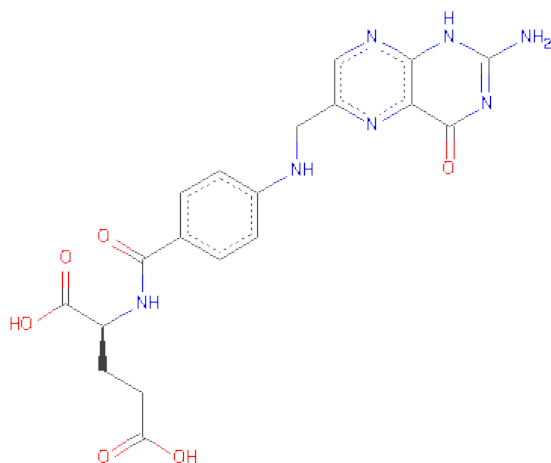
There are 3 unique types of molecules in this entry. The entry contains 1739 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	202	1652	1067	281	298	6	0	0	0

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: C₁₉H₁₉N₇O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	32	19	7	6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		

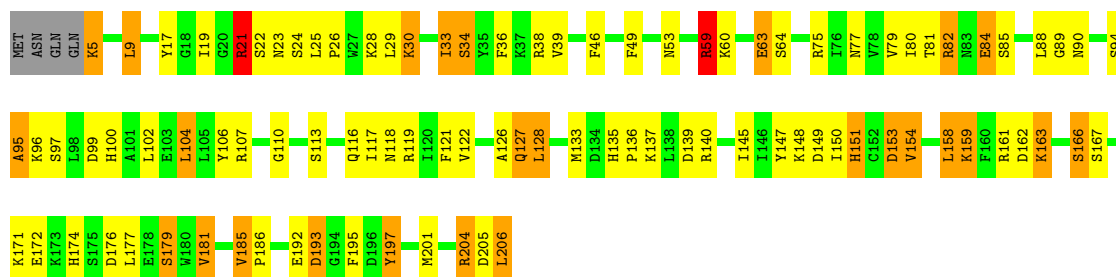
3 Residue-property plots

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.

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.05Å 61.51Å 85.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.3 (8.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1739	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: FOL

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	1.06	0/1694	2.16	64/2285 (2.8%)

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	18.11	129.35	120.30
1	A	75	ARG	NE-CZ-NH2	-17.32	111.64	120.30
1	A	59	ARG	CD-NE-CZ	17.16	147.63	123.60
1	A	139	ASP	CB-CG-OD1	15.26	132.04	118.30
1	A	59	ARG	NE-CZ-NH1	14.49	127.55	120.30
1	A	99	ASP	CB-CG-OD2	-14.43	105.31	118.30
1	A	204	ARG	NE-CZ-NH2	14.27	127.44	120.30
1	A	38	ARG	NE-CZ-NH1	-13.16	113.72	120.30
1	A	161	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	A	193	ASP	CB-CG-OD2	-10.52	108.83	118.30
1	A	162	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	A	204	ARG	CD-NE-CZ	9.18	136.45	123.60
1	A	82	ARG	CD-NE-CZ	8.95	136.12	123.60
1	A	107	ARG	NE-CZ-NH2	8.31	124.46	120.30
1	A	176	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	A	161	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	176	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	59	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	34	SER	CB-CA-C	7.30	123.97	110.10
1	A	158	LEU	CA-CB-CG	7.26	132.00	115.30
1	A	181	VAL	N-CA-CB	-6.84	96.45	111.50
1	A	21	ARG	NE-CZ-NH2	6.73	123.66	120.30
1	A	63	GLU	CG-CD-OE1	6.60	131.50	118.30
1	A	204	ARG	CG-CD-NE	6.56	125.58	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LEU	CA-CB-CG	6.56	130.38	115.30
1	A	162	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	205	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	A	204	ARG	NH1-CZ-NH2	-6.29	112.49	119.40
1	A	59	ARG	CG-CD-NE	6.21	124.83	111.80
1	A	64	SER	CB-CA-C	-6.04	98.61	110.10
1	A	85	SER	CB-CA-C	6.03	121.56	110.10
1	A	139	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	113	SER	N-CA-CB	-5.99	101.51	110.50
1	A	147	TYR	CB-CG-CD1	-5.84	117.49	121.00
1	A	9	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	95	ALA	CB-CA-C	5.76	118.74	110.10
1	A	63	GLU	C-N-CA	5.68	135.89	121.70
1	A	167	SER	N-CA-CB	5.62	118.93	110.50
1	A	75	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	5	LYS	CA-CB-CG	5.61	125.74	113.40
1	A	119	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	154	VAL	CB-CA-C	5.60	122.04	111.40
1	A	197	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	A	90	ASN	CB-CA-C	5.55	121.51	110.40
1	A	185	VAL	N-CA-CB	-5.47	99.47	111.50
1	A	121	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	A	30	LYS	CA-C-O	-5.42	108.73	120.10
1	A	63	GLU	CG-CD-OE2	-5.40	107.51	118.30
1	A	82	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	75	ARG	NH1-CZ-NH2	5.31	125.24	119.40
1	A	153	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	90	ASN	N-CA-CB	-5.26	101.12	110.60
1	A	179	SER	CB-CA-C	5.24	120.06	110.10
1	A	127	GLN	N-CA-CB	5.24	120.03	110.60
1	A	89	GLY	CA-C-O	5.20	129.96	120.60
1	A	84	GLU	CG-CD-OE2	-5.20	107.91	118.30
1	A	140	ARG	CA-CB-CG	5.18	124.79	113.40
1	A	192	GLU	CG-CD-OE2	-5.18	107.95	118.30
1	A	38	ARG	N-CA-CB	-5.17	101.30	110.60
1	A	181	VAL	CB-CA-C	5.13	121.15	111.40
1	A	193	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	159	LYS	CD-CE-NZ	-5.09	99.98	111.70
1	A	147	TYR	N-CA-CB	-5.04	101.52	110.60
1	A	89	GLY	CA-C-N	-5.02	106.16	117.20

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	A	1652	0	1658	71	0
2	A	32	0	17	2	0
3	A	55	0	0	1	0
All	All	1739	0	1675	73	0

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 22.

All (73) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:21:ARG:HG2	1:A:26:PRO:HB3	1.23	1.12
1:A:81:THR:HG23	1:A:84:GLU:HG3	1.37	1.03
1:A:206:LEU:HD12	1:A:206:LEU:H	1.30	0.97
1:A:21:ARG:HG2	1:A:26:PRO:CB	1.98	0.93
1:A:28:LYS:HG2	1:A:28:LYS:O	1.71	0.88
1:A:19:ILE:HD11	1:A:154:VAL:HG22	1.55	0.87
1:A:21:ARG:CG	1:A:26:PRO:HB3	2.05	0.86
1:A:39:VAL:HG22	1:A:181:VAL:HG22	1.59	0.85
1:A:19:ILE:HD11	1:A:154:VAL:CG2	2.07	0.84
1:A:21:ARG:HG3	1:A:22:SER:N	1.99	0.77
1:A:19:ILE:CD1	1:A:154:VAL:HG22	2.14	0.76
1:A:19:ILE:CG1	1:A:154:VAL:HG22	2.16	0.76
1:A:206:LEU:HD12	1:A:206:LEU:N	2.02	0.74
1:A:29:LEU:HD12	3:A:208:HOH:O	1.90	0.71
1:A:81:THR:HG23	1:A:84:GLU:CG	2.20	0.69
1:A:135:HIS:CD2	1:A:137:LYS:H	2.11	0.68
1:A:135:HIS:HD2	1:A:137:LYS:H	1.40	0.68
1:A:88:LEU:HD12	1:A:94:SER:HB3	1.81	0.62
1:A:46:PHE:CD2	1:A:49:PHE:CZ	2.88	0.62
1:A:46:PHE:HD2	1:A:49:PHE:CZ	2.18	0.61
1:A:23:ASN:ND2	1:A:24:SER:H	1.99	0.60
1:A:53:ASN:OD1	1:A:118:ASN:HB3	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:LYS:HD2	1:A:172:GLU:N	2.18	0.58
1:A:22:SER:HB3	1:A:151:HIS:CD2	2.40	0.57
1:A:21:ARG:HB2	1:A:151:HIS:O	2.06	0.56
1:A:59:ARG:NH1	1:A:60:LYS:HD3	2.21	0.56
1:A:33:ILE:HD12	1:A:36:PHE:HB3	1.88	0.55
1:A:28:LYS:O	1:A:29:LEU:HD23	2.07	0.55
1:A:135:HIS:CD2	1:A:137:LYS:HB2	2.41	0.55
1:A:163:LYS:O	1:A:166:SER:OG	2.22	0.55
1:A:19:ILE:HG13	1:A:154:VAL:HG22	1.90	0.54
1:A:133:MET:HE2	1:A:158:LEU:HD22	1.90	0.54
1:A:171:LYS:NZ	1:A:201:MET:H	2.07	0.53
1:A:21:ARG:HG2	1:A:26:PRO:CG	2.39	0.53
1:A:174:HIS:HE1	1:A:185:VAL:O	1.91	0.53
1:A:22:SER:HB3	1:A:151:HIS:NE2	2.25	0.52
1:A:177:LEU:C	1:A:177:LEU:HD23	2.31	0.50
1:A:19:ILE:CD1	1:A:126:ALA:HB2	2.40	0.50
1:A:19:ILE:HD11	1:A:126:ALA:HB2	1.95	0.49
1:A:28:LYS:CG	1:A:28:LYS:O	2.45	0.48
1:A:100:HIS:CD2	1:A:100:HIS:N	2.79	0.48
1:A:39:VAL:HG22	1:A:181:VAL:CG2	2.38	0.48
1:A:5:LYS:HE2	1:A:5:LYS:HB3	1.49	0.48
1:A:59:ARG:HG2	1:A:59:ARG:O	2.13	0.48
1:A:59:ARG:HD2	1:A:63:GLU:OE2	2.14	0.48
1:A:25:LEU:N	1:A:26:PRO:CD	2.77	0.47
1:A:127:GLN:HG2	1:A:127:GLN:O	2.15	0.46
1:A:171:LYS:HZ3	1:A:201:MET:H	1.63	0.46
1:A:21:ARG:CG	1:A:22:SER:N	2.72	0.46
1:A:151:HIS:CG	1:A:151:HIS:O	2.69	0.46
1:A:79:VAL:O	1:A:94:SER:HA	2.16	0.45
1:A:110:GLY:O	1:A:116:GLN:NE2	2.45	0.45
1:A:82:ARG:HG2	1:A:96:LYS:O	2.17	0.45
2:A:207:FOL:CG	2:A:207:FOL:O	2.66	0.44
1:A:145:ILE:N	1:A:145:ILE:HD13	2.33	0.44
1:A:150:ILE:HD11	1:A:195:PHE:HE1	1.82	0.44
1:A:21:ARG:HG2	1:A:26:PRO:HG3	1.99	0.43
1:A:137:LYS:HD2	1:A:137:LYS:HA	1.68	0.43
1:A:135:HIS:HD2	1:A:137:LYS:N	2.12	0.43
2:A:207:FOL:HG1	2:A:207:FOL:O	2.19	0.43
1:A:185:VAL:HA	1:A:186:PRO:HD3	1.86	0.43
1:A:145:ILE:O	1:A:197:TYR:HA	2.19	0.42
1:A:97:SER:OG	1:A:100:HIS:CD2	2.73	0.42
1:A:17:TYR:CZ	1:A:159:LYS:HA	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:LYS:HD3	1:A:150:ILE:HD11	2.02	0.41
1:A:102:LEU:O	1:A:106:TYR:CD2	2.74	0.41
1:A:174:HIS:CE1	1:A:185:VAL:O	2.73	0.41
1:A:135:HIS:HA	1:A:136:PRO:HD2	1.89	0.41
1:A:135:HIS:HD2	1:A:137:LYS:HB2	1.83	0.41
1:A:122:VAL:HG13	1:A:128:LEU:HD13	2.03	0.41
1:A:80:ILE:HA	1:A:95:ALA:O	2.21	0.41
1:A:171:LYS:C	1:A:171:LYS:HD2	2.41	0.41
1:A:117:ILE:HG21	1:A:117:ILE:HD13	1.91	0.40

There are no symmetry-related clashes.

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	
1	A	200/206 (97%)	194 (97%)	6 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	183/187 (98%)	165 (90%)	18 (10%)	12	6

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU

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Mol	Chain	Res	Type
1	A	21	ARG
1	A	30	LYS
1	A	33	ILE
1	A	34	SER
1	A	59	ARG
1	A	77	ASN
1	A	104	LEU
1	A	128	LEU
1	A	149	ASP
1	A	151	HIS
1	A	153	ASP
1	A	163	LYS
1	A	166	SER
1	A	179	SER
1	A	193	ASP
1	A	204	ARG
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	23	ASN
1	A	100	HIS
1	A	118	ASN
1	A	135	HIS
1	A	174	HIS

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$
2	FOL	A	207	-	34,34,34	1.51	6 (17%)	45,47,47	2.38	16 (35%)

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	FOL	A	207	-	-	0/22/22/22	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	207	FOL	C4-C4A	4.08	1.47	1.41
2	A	207	FOL	O4-C4	3.26	1.30	1.24
2	A	207	FOL	C2-NA2	-2.87	1.27	1.32
2	A	207	FOL	C4-N3	-2.70	1.32	1.37
2	A	207	FOL	O2-CT	-2.38	1.21	1.30
2	A	207	FOL	OE1-CD	2.03	1.29	1.22

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	FOL	OE2-CD-OE1	-7.17	105.06	123.30
2	A	207	FOL	O-C-N	-6.72	110.31	122.44
2	A	207	FOL	O2-CT-O1	3.85	132.78	124.07
2	A	207	FOL	C11-C-N	3.69	123.04	116.89
2	A	207	FOL	C15-C16-C11	3.27	124.66	120.76
2	A	207	FOL	O-C-C11	3.18	126.58	121.01
2	A	207	FOL	OE1-CD-CG	3.04	133.49	123.03
2	A	207	FOL	NA2-C2-N1	-3.01	114.54	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	207	FOL	O1-CT-CA	-2.98	110.96	121.86
2	A	207	FOL	CA-N-C	2.83	128.10	121.80
2	A	207	FOL	CB-CG-CD	-2.83	106.02	112.88
2	A	207	FOL	NA2-C2-N3	2.82	124.12	120.30
2	A	207	FOL	C2-N1-C8A	2.43	123.20	120.15
2	A	207	FOL	C15-C14-C13	-2.25	115.94	119.10
2	A	207	FOL	C8A-C4A-N5	2.10	123.00	120.45
2	A	207	FOL	OE2-CD-CG	2.04	121.43	114.22

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 ⓘ

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.