



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:04 AM GMT

PDB ID : 1AOE
Title : CANDIDA ALBICANS DIHYDROFOLATE REDUCTASE COMPLEXED
WITH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOS-
PHATE (NADPH) AND 1,3-DIAMINO-7-(1-ETHYEPROPYE)-7H-PYRRA
LO-[3,2-F]QUINAZOLINE(GW345)
Authors : Whitlow, M.; Howard, A.J.; Stewart, D.
Deposited on : 1997-07-02
Resolution : 1.60 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>

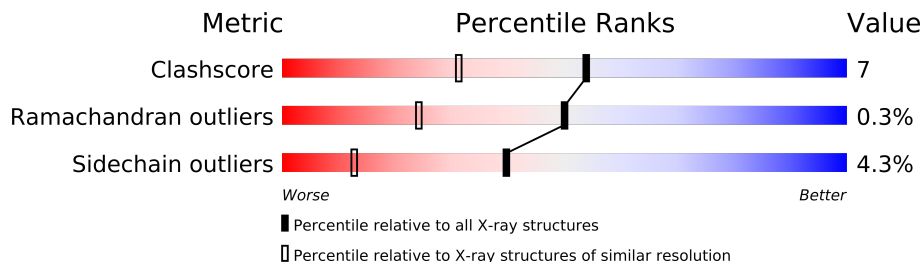
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.60 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	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)

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	192	
1	B	192	

2 Entry composition i

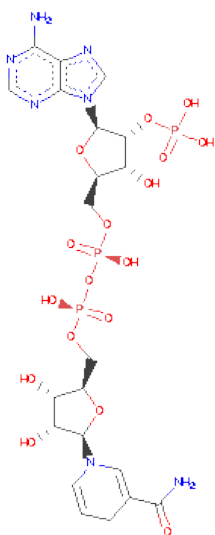
There are 4 unique types of molecules in this entry. The entry contains 3662 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

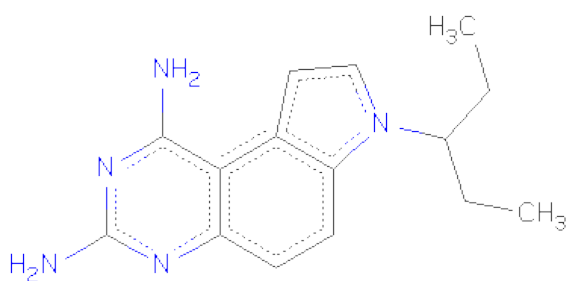
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	12	0
			1594	1023	271	296	4			
1	B	192	Total	C	N	O	S	0	10	0
			1588	1020	264	300	4			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 7-(1-ETHYL-PROPYL)-7H-PYRROLO-[3,2-F]QUINAZOLINE-1,3-DIAMINE (three-letter code: GW3) (formula: $C_{15}H_{19}N_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			20	15	5		
3	B	1	Total	C	N	0	0
			20	15	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	7
			164	164		
4	B	176	Total	O	0	4
			180	180		

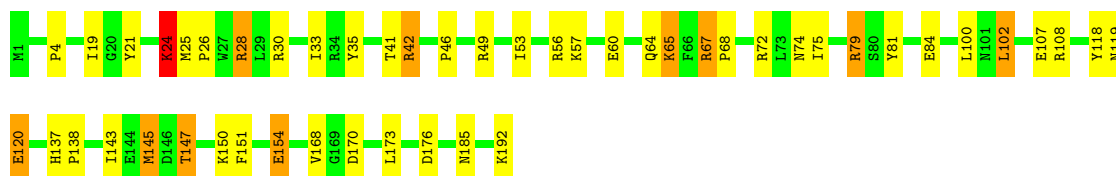
3 Residue-property plots

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: 



• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain B: 



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, α , β , γ	77.91Å 67.28Å 38.49Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60	Depositor
% Data completeness (in resolution range)	91.7 (10.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3662	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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, GW3

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	1.12	2/1690 (0.1%)	1.89	39/2290 (1.7%)
1	B	1.13	2/1675 (0.1%)	1.61	23/2267 (1.0%)
All	All	1.12	4/3365 (0.1%)	1.76	62/4557 (1.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	GLU	CD-OE2	-5.74	1.19	1.25
1	A	60	GLU	CD-OE2	-5.18	1.20	1.25
1	B	180	GLY	N-CA	5.13	1.53	1.46
1	A	107	GLU	CD-OE2	-5.11	1.20	1.25

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30[A]	ARG	NE-CZ-NH1	20.59	130.59	120.30
1	A	30[B]	ARG	NE-CZ-NH1	20.59	130.59	120.30
1	A	49	ARG	NE-CZ-NH2	-14.77	112.92	120.30
1	A	28	ARG	CD-NE-CZ	13.57	142.60	123.60
1	A	72	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	B	108	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	B	56	ARG	CD-NE-CZ	10.63	138.48	123.60
1	A	30[A]	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	A	30[B]	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	A	30[A]	ARG	CD-NE-CZ	9.97	137.56	123.60
1	A	30[B]	ARG	CD-NE-CZ	9.97	137.56	123.60
1	A	108	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	A	79[A]	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	A	79[B]	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	B	49	ARG	NE-CZ-NH2	-9.57	115.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	B	81	TYR	CB-CG-CD1	9.02	126.41	121.00
1	A	72	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	B	79	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	A	79[A]	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	79[B]	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	B	108	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	67	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	42[A]	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	A	42[B]	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	B	153	LEU	CB-CA-C	7.84	125.10	110.20
1	A	102	LEU	CA-CB-CG	7.73	133.08	115.30
1	A	56	ARG	CD-NE-CZ	7.68	134.35	123.60
1	A	118	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	42[A]	ARG	CA-CB-CG	7.54	129.99	113.40
1	A	42[B]	ARG	CA-CB-CG	7.54	129.99	113.40
1	B	67	ARG	CD-NE-CZ	7.46	134.05	123.60
1	A	56	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	B	34	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	154	GLU	CA-CB-CG	6.99	128.77	113.40
1	A	28	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	B	145	MET	CA-CB-CG	6.82	124.89	113.30
1	B	30	ARG	CD-NE-CZ	6.55	132.77	123.60
1	B	36	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	A	151	PHE	CB-CG-CD2	-6.50	116.25	120.80
1	B	79	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	35	TYR	CB-CG-CD1	-6.29	117.22	121.00
1	B	49	ARG	O-C-N	5.90	132.14	122.70
1	B	119	ASN	CB-CA-C	5.82	122.03	110.40
1	A	49	ARG	NH1-CZ-NH2	5.66	125.63	119.40
1	A	120	GLU	CA-CB-CG	5.62	125.77	113.40
1	B	81	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	B	35	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	B	185	ASN	O-C-N	5.48	131.46	122.70
1	A	81	TYR	CB-CG-CD1	5.32	124.19	121.00
1	A	151	PHE	CB-CG-CD1	5.29	124.50	120.80
1	A	147	THR	CA-CB-CG2	5.26	119.76	112.40
1	B	146	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	145	MET	CB-CG-SD	-5.24	96.67	112.40
1	A	84[A]	GLU	CB-CG-CD	5.20	128.25	114.20
1	A	84[B]	GLU	CB-CG-CD	5.20	128.25	114.20
1	A	145	MET	CG-SD-CE	5.18	108.48	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
1	B	72	ARG	O-C-N	5.15	130.94	122.70
1	A	24	LYS	CA-CB-CG	5.14	124.72	113.40
1	B	108	ARG	O-C-N	5.04	130.77	122.70
1	A	192	LYS	CA-CB-CG	5.04	124.48	113.40

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	1594	0	1620	24	0
1	B	1588	0	1613	21	1
2	A	48	0	26	1	0
2	B	48	0	26	0	0
3	A	20	0	19	1	0
3	B	20	0	19	1	0
4	A	164	0	0	3	1
4	B	180	0	0	2	0
All	All	3662	0	3323	46	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 7.

All (46) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:28:ARG:HH21	1:B:30:ARG:HG2	1.49	0.76
1:A:176:ASP:H	1:A:185:ASN:HD21	1.34	0.73
1:B:124:ASN:HD22	1:B:126:LEU:H	1.36	0.72
1:A:64:GLN:HG2	1:A:65:LYS:HE3	1.71	0.70
1:A:28:ARG:HH11	1:A:28:ARG:HB3	1.57	0.68
1:A:79[A]:ARG:NH1	4:A:492:HOH:O	2.04	0.68
1:B:137:HIS:HD2	1:B:139:SER:H	1.43	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:176:ASP:H	1:B:185:ASN:HD21	1.43	0.66
1:A:119:ASN:HB3	1:A:150:LYS:HE2	1.81	0.63
1:B:83:ASN:ND2	1:B:94:SER:H	1.99	0.61
1:B:176:ASP:H	1:B:185:ASN:ND2	1.99	0.60
1:A:65:LYS:HD2	1:A:65:LYS:H	1.68	0.59
1:A:176:ASP:H	1:A:185:ASN:ND2	2.03	0.56
1:A:33[A]:ILE:HD13	3:A:194:GW3:H8	1.87	0.56
1:B:137:HIS:CD2	1:B:139:SER:H	2.23	0.53
1:B:20:GLY:O	1:B:145:MET:HB2	2.09	0.52
1:A:21:TYR:HB3	1:A:24:LYS:HE3	1.90	0.52
1:A:65:LYS:H	1:A:65:LYS:CD	2.23	0.52
1:A:28:ARG:NH1	1:A:28:ARG:HB3	2.26	0.50
1:B:115:ALA:HB2	1:B:147:THR:HG23	1.92	0.50
1:A:42[A]:ARG:HH11	1:A:170:ASP:HB2	1.77	0.50
1:B:63:PRO:HB2	1:B:66:PHE:HD2	1.77	0.50
1:A:41[B]:THR:HG21	4:A:446:HOH:O	2.13	0.48
3:B:194:GW3:H303	3:B:194:GW3:C15	2.43	0.48
1:B:5:ASN:ND2	4:B:297:HOH:O	2.46	0.48
1:B:19:ILE:HG13	1:B:147:THR:HG22	1.95	0.47
1:B:124:ASN:ND2	1:B:126:LEU:H	2.10	0.47
1:B:83:ASN:HD21	1:B:94:SER:H	1.62	0.47
1:A:168:VAL:HG21	1:A:173:LEU:HD21	1.98	0.45
1:A:57:LYS:NZ	2:A:193:NDP:O3B	2.49	0.45
1:B:149:LEU:HD22	1:B:151:PHE:CZ	2.52	0.45
1:A:137:HIS:CD2	1:A:143:ILE:HD11	2.52	0.45
1:A:67:ARG:HA	1:A:68:PRO:C	2.37	0.44
1:A:19:ILE:HG13	1:A:147:THR:HG22	2.00	0.44
1:B:159:GLN:HB3	1:B:160:PRO:HD2	1.99	0.43
1:A:53[B]:ILE:HG22	1:A:75:ILE:HD12	2.00	0.43
1:A:25:MET:HA	1:A:26:PRO:HD3	1.79	0.42
1:B:67:ARG:HA	1:B:68:PRO:C	2.39	0.42
1:A:42[A]:ARG:NH1	1:A:170:ASP:H	2.18	0.42
1:A:4:PRO:CG	1:A:100:LEU:HD13	2.50	0.41
1:B:151:PHE:HB2	1:B:153:LEU:HD13	2.03	0.41
1:B:115:ALA:HB2	1:B:147:THR:CG2	2.51	0.41
1:A:150:LYS:HG3	4:A:233:HOH:O	2.21	0.40
1:B:80:SER:HB2	4:B:337:HOH:O	2.21	0.40
1:A:137:HIS:CG	1:A:138:PRO:HD2	2.56	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:87:ASP:OD2	4:A:288[A]:HOH:O[2_656]	2.03	0.17

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	202/192 (105%)	198 (98%)	3 (2%)	1 (0%)	38	13
1	B	200/192 (104%)	197 (98%)	3 (2%)	0	100	100
All	All	402/384 (105%)	395 (98%)	6 (2%)	1 (0%)	50	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	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	
1	A	186/177 (105%)	179 (96%)	7 (4%)	44	15
1	B	185/177 (104%)	174 (94%)	11 (6%)	28	6
All	All	371/354 (105%)	353 (95%)	18 (5%)	40	9

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

Mol	Chain	Res	Type
1	A	24	LYS
1	A	65	LYS
1	A	74	ASN
1	A	102	LEU

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Mol	Chain	Res	Type
1	A	120	GLU
1	A	145	MET
1	A	154	GLU
1	B	5	ASN
1	B	28	ARG
1	B	65[A]	LYS
1	B	65[B]	LYS
1	B	74	ASN
1	B	124	ASN
1	B	141[A]	GLU
1	B	141[B]	GLU
1	B	153	LEU
1	B	173[A]	LEU
1	B	173[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	159	GLN
1	A	185	ASN
1	B	5	ASN
1	B	83	ASN
1	B	101	ASN
1	B	123	ASN
1	B	124	ASN
1	B	137	HIS
1	B	185	ASN

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

4 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	193	-	52,52,52	1.54	11 (21%)	80,80,80	1.52	15 (18%)
3	GW3	A	194	-	22,22,22	4.09	6 (27%)	32,32,32	2.47	12 (37%)
2	NDP	B	193	-	52,52,52	1.50	10 (19%)	80,80,80	1.39	12 (15%)
3	GW3	B	194	-	22,22,22	4.04	4 (18%)	32,32,32	2.54	8 (25%)

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	193	-	-	0/35/77/77	0/3/5/5
3	GW3	A	194	-	-	0/4/8/8	0/0/3/3
2	NDP	B	193	-	-	0/35/77/77	0/3/5/5
3	GW3	B	194	-	-	0/4/8/8	0/0/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	194	GW3	C15-N16	-14.62	1.26	1.39
3	A	194	GW3	C15-N16	-14.13	1.26	1.39
3	A	194	GW3	C12-N16	-10.93	1.25	1.39
3	B	194	GW3	C12-N16	-9.65	1.27	1.39
3	B	194	GW3	C1-N6	5.80	1.47	1.37
2	A	193	NDP	C7N-C3N	4.39	1.57	1.47
2	B	193	NDP	C7N-C3N	3.93	1.56	1.47
3	A	194	GW3	C1-N6	3.76	1.44	1.37
2	A	193	NDP	PA-O3	-3.50	1.53	1.59
2	A	193	NDP	C4N-C3N	-3.48	1.43	1.50
2	B	193	NDP	P2B-O2B	3.47	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	194	GW3	C2-C1	-3.46	1.38	1.42
2	B	193	NDP	C4N-C3N	-3.45	1.43	1.50
2	A	193	NDP	P2B-O2B	3.38	1.70	1.59
2	B	193	NDP	C4N-C5N	-3.23	1.42	1.49
2	B	193	NDP	P2B-O2X	-2.91	1.44	1.54
2	A	193	NDP	P2B-O3X	-2.64	1.45	1.54
2	A	193	NDP	C2N-N1N	2.39	1.41	1.36
2	A	193	NDP	C4N-C5N	-2.32	1.44	1.49
2	B	193	NDP	C3B-C2B	2.28	1.58	1.53
2	A	193	NDP	C3B-C2B	2.21	1.58	1.53
2	A	193	NDP	C2A-N1A	2.19	1.38	1.33
3	B	194	GW3	C9-C8	2.16	1.41	1.34
2	B	193	NDP	PN-O2N	-2.14	1.45	1.55
3	A	194	GW3	C13-C2	-2.13	1.40	1.45
2	A	193	NDP	C1B-N9A	-2.10	1.42	1.48
2	A	193	NDP	C2N-C3N	2.09	1.38	1.34
3	A	194	GW3	C3-N4	-2.08	1.28	1.33
2	B	193	NDP	C6N-N1N	2.07	1.43	1.37
2	B	193	NDP	PA-O2A	-2.06	1.45	1.55
2	B	193	NDP	C1B-N9A	-2.04	1.42	1.48

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	194	GW3	C2-C1-N6	-8.88	117.56	124.02
3	A	194	GW3	C14-C13-C12	-5.80	101.25	106.20
3	A	194	GW3	C2-C1-N6	-5.67	119.90	124.02
3	A	194	GW3	N6-C5-N4	-5.25	119.24	127.54
2	B	193	NDP	C5N-C6N-N1N	-4.95	112.92	123.03
3	B	194	GW3	C3-C2-C1	4.54	117.45	114.81
3	A	194	GW3	C15-N16-C25	-4.53	120.73	125.41
2	A	193	NDP	C3N-C2N-N1N	-4.48	116.69	123.05
3	B	194	GW3	C8-C1-C2	4.36	124.17	120.25
2	A	193	NDP	PN-O3-PA	4.32	144.36	131.68
3	B	194	GW3	C14-C13-C12	-4.31	102.52	106.20
3	A	194	GW3	N19-C5-N4	3.99	124.07	117.19
3	B	194	GW3	N6-C5-N4	-3.86	121.44	127.54
2	A	193	NDP	O2B-P2B-O1X	-3.79	96.20	106.79
2	B	193	NDP	C4N-C5N-C6N	3.60	129.21	122.61
2	B	193	NDP	O4B-C1B-N9A	3.41	111.61	108.44
3	B	194	GW3	C9-C8-C1	-3.36	117.14	120.89
3	A	194	GW3	C9-C12-C13	-3.31	115.96	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	193	NDP	C1D-N1N-C2N	-3.25	115.49	121.02
2	A	193	NDP	C4N-C3N-C2N	3.16	125.53	121.68
2	A	193	NDP	C4A-C5A-N7A	3.15	112.22	109.52
2	B	193	NDP	O2B-P2B-O1X	-2.93	98.59	106.79
2	A	193	NDP	C5N-C6N-N1N	-2.83	117.25	123.03
3	A	194	GW3	C2-C13-C12	2.75	123.18	118.39
2	A	193	NDP	P2B-O2B-C2B	-2.70	116.27	121.96
2	B	193	NDP	O2X-P2B-O1X	2.68	119.19	110.44
2	B	193	NDP	C6N-N1N-C2N	2.59	122.83	119.44
3	A	194	GW3	C13-C12-N16	2.55	111.14	109.08
2	A	193	NDP	O4B-C1B-C2B	2.49	109.28	106.95
3	B	194	GW3	C14-C13-C2	2.48	135.67	131.52
2	B	193	NDP	P2B-O2B-C2B	-2.46	116.78	121.96
2	A	193	NDP	O4B-C1B-N9A	-2.45	106.16	108.44
3	A	194	GW3	C14-C13-C2	2.41	135.56	131.52
2	A	193	NDP	O4D-C1D-C2D	-2.35	101.20	106.60
3	A	194	GW3	C25-N16-C12	2.34	128.31	125.11
2	A	193	NDP	C6N-N1N-C2N	2.33	122.49	119.44
2	B	193	NDP	C8A-N9A-C4A	-2.30	105.14	106.90
2	B	193	NDP	O2N-PN-O3	2.27	115.93	105.14
2	B	193	NDP	O7N-C7N-C3N	-2.27	116.24	120.51
2	A	193	NDP	C4N-C5N-C6N	2.26	126.75	122.61
3	A	194	GW3	C5-N4-C3	2.25	124.50	116.50
3	A	194	GW3	C9-C8-C1	-2.24	118.39	120.89
2	A	193	NDP	O3X-P2B-O1X	2.24	117.76	110.44
2	B	193	NDP	C3N-C2N-N1N	-2.19	119.94	123.05
3	B	194	GW3	C15-N16-C25	-2.18	123.16	125.41
2	B	193	NDP	C5A-C6A-N6A	2.13	125.53	120.72
2	A	193	NDP	N6A-C6A-N1A	2.06	123.40	119.36

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.