



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 10:42 PM EDT

PDB ID : 1AI9  
Title : CANDIDA ALBICANS DIHYDROFOLATE REDUCTASE  
Authors : Whitlow, M.; Howard, A.J.; Stewart, D.  
Deposited on : 1997-05-01  
Resolution : 1.85 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

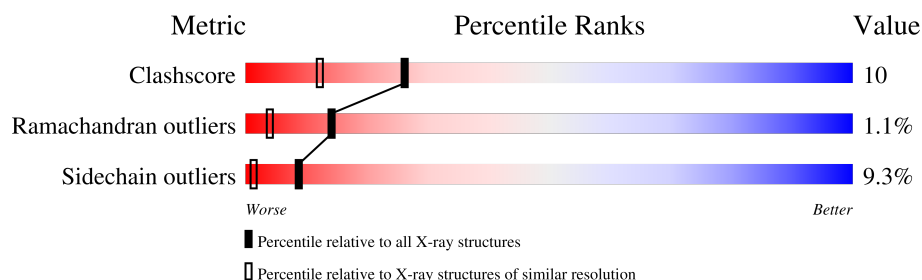
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	192	
1	B	192	

2 Entry composition ⓘ

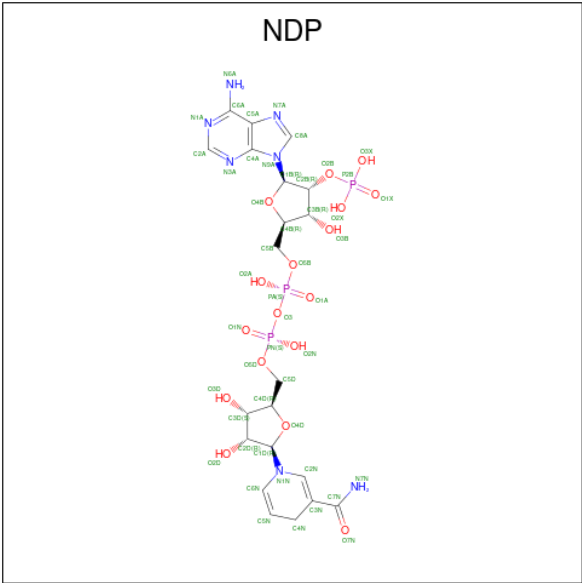
There are 3 unique types of molecules in this entry. The entry contains 3452 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	192	Total	C	N	O	S	0	10	0
			1597	1026	272	295	4			
1	B	192	Total	C	N	O	S	0	11	0
			1599	1022	271	302	4			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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 water.

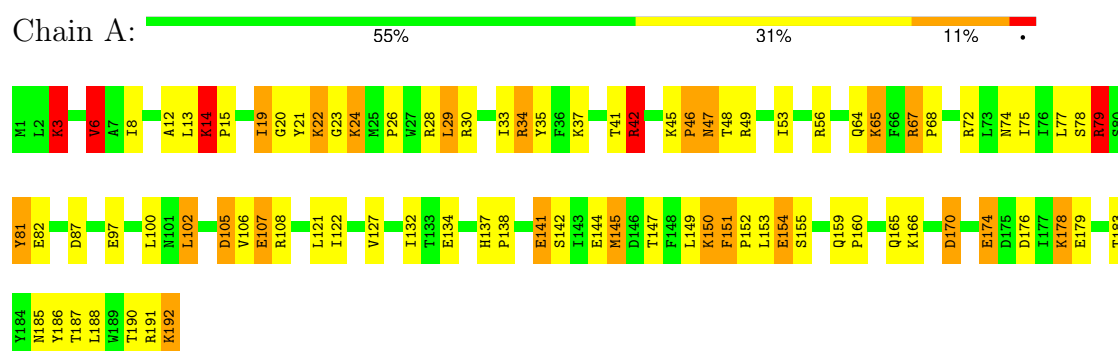
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total 70	O 70	0	0
3	B	90	Total 90	O 90	0	0

### 3 Residue-property plots

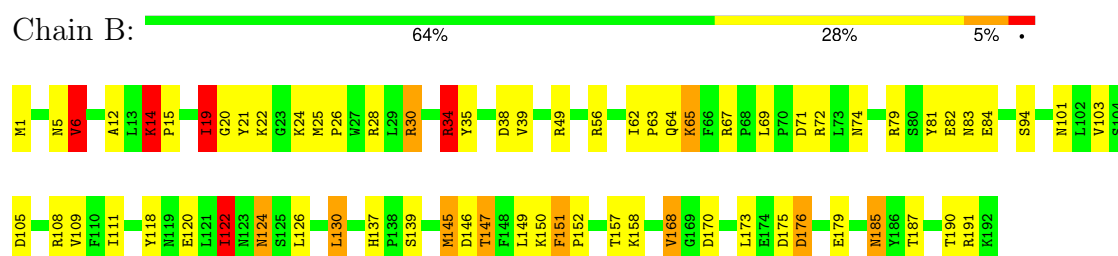
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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



#### • Molecule 1: DIHYDROFOLATE REDUCTASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.20Å 67.57Å 38.66Å 90.00° 93.06° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85	Depositor
% Data completeness (in resolution range)	90.0 (10.00-1.85)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	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

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	1.34	5/1680 (0.3%)	2.19	72/2274 (3.2%)
1	B	1.34	1/1691 (0.1%)	2.06	58/2287 (2.5%)
All	All	1.34	6/3371 (0.2%)	2.12	130/4561 (2.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	GLU	CA-CB	-6.09	1.40	1.53
1	A	107	GLU	CD-OE2	-5.89	1.19	1.25
1	A	35	TYR	CG-CD2	5.76	1.46	1.39
1	B	120	GLU	CD-OE1	-5.69	1.19	1.25
1	A	174	GLU	CB-CG	-5.38	1.42	1.52
1	A	165	GLN	C-O	5.13	1.33	1.23

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	ARG	CD-NE-CZ	26.69	160.96	123.60
1	B	56	ARG	NE-CZ-NH2	20.62	130.61	120.30
1	A	122	ILE	CB-CG1-CD1	19.91	169.65	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	GLU	CA-CB-CG	17.79	152.54	113.40
1	A	34	ARG	NE-CZ-NH2	17.69	129.15	120.30
1	A	34	ARG	NE-CZ-NH1	-16.93	111.84	120.30
1	A	42[A]	ARG	CD-NE-CZ	14.76	144.26	123.60
1	A	42[B]	ARG	CD-NE-CZ	14.76	144.26	123.60
1	B	191	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	A	72	ARG	NE-CZ-NH1	12.17	126.39	120.30
1	A	56	ARG	CD-NE-CZ	12.16	140.62	123.60
1	B	108	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	A	28	ARG	CD-NE-CZ	11.33	139.46	123.60
1	A	191	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	B	108	ARG	NE-CZ-NH1	10.41	125.51	120.30
1	A	28	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	A	67	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	B	14	LYS	CA-CB-CG	9.71	134.76	113.40
1	B	56	ARG	NE-CZ-NH1	-9.67	115.46	120.30
1	B	72	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	A	30[A]	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	30[B]	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	151	PHE	CB-CG-CD2	-8.62	114.77	120.80
1	A	30[A]	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	30[B]	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	105	ASP	CB-CG-OD1	8.25	125.73	118.30
1	B	34[A]	ARG	CD-NE-CZ	7.93	134.70	123.60
1	B	34[B]	ARG	CD-NE-CZ	7.93	134.70	123.60
1	A	192	LYS	CA-CB-CG	7.70	130.33	113.40
1	B	179	GLU	OE1-CD-OE2	7.67	132.50	123.30
1	B	150[A]	LYS	CA-CB-CG	7.66	130.24	113.40
1	B	150[B]	LYS	CA-CB-CG	7.66	130.24	113.40
1	B	81	TYR	CB-CG-CD1	7.63	125.58	121.00
1	A	121	LEU	CB-CA-C	7.63	124.69	110.20
1	B	130	LEU	O-C-N	7.56	134.79	122.70
1	A	19	ILE	CA-CB-CG2	7.55	126.01	110.90
1	A	14	LYS	CA-CB-CG	7.47	129.83	113.40
1	B	34[A]	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	B	34[B]	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	B	105[A]	ASP	CB-CG-OD1	7.36	124.93	118.30
1	B	105[B]	ASP	CB-CG-OD1	7.36	124.93	118.30
1	A	6[A]	VAL	CA-CB-CG2	7.30	121.85	110.90
1	A	6[B]	VAL	CA-CB-CG2	7.30	121.85	110.90
1	A	105	ASP	N-CA-CB	-7.26	97.54	110.60
1	A	56	ARG	NE-CZ-NH1	7.24	123.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	TYR	CA-CB-CG	7.02	126.74	113.40
1	A	166	LYS	N-CA-CB	6.91	123.04	110.60
1	A	121	LEU	CB-CG-CD1	6.74	122.45	111.00
1	A	3	LYS	CB-CG-CD	6.67	128.95	111.60
1	B	34[A]	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	B	34[B]	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	6[A]	VAL	CA-CB-CG1	6.50	120.65	110.90
1	A	6[B]	VAL	CA-CB-CG1	6.50	120.65	110.90
1	B	34[A]	ARG	CG-CD-NE	6.45	125.34	111.80
1	B	34[B]	ARG	CG-CD-NE	6.45	125.34	111.80
1	A	179	GLU	OE1-CD-OE2	6.40	130.98	123.30
1	B	6[A]	VAL	CA-CB-CG2	6.33	120.39	110.90
1	B	6[B]	VAL	CA-CB-CG2	6.33	120.39	110.90
1	B	81	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	146	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	178	LYS	CB-CG-CD	6.25	127.86	111.60
1	A	145	MET	CA-CB-CG	6.23	123.89	113.30
1	A	106	VAL	N-CA-C	6.19	127.72	111.00
1	B	151	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	105	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	186	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	B	147	THR	CA-CB-CG2	6.12	120.98	112.40
1	B	6[A]	VAL	CA-CB-CG1	6.10	120.05	110.90
1	B	6[B]	VAL	CA-CB-CG1	6.10	120.05	110.90
1	A	188	LEU	O-C-N	6.05	132.38	122.70
1	A	154	GLU	CA-CB-CG	6.02	126.64	113.40
1	A	6[A]	VAL	CB-CA-C	5.96	122.72	111.40
1	A	6[B]	VAL	CB-CA-C	5.96	122.72	111.40
1	A	154	GLU	CB-CG-CD	5.92	130.18	114.20
1	A	42[A]	ARG	CG-CD-NE	5.91	124.21	111.80
1	A	42[B]	ARG	CG-CD-NE	5.91	124.21	111.80
1	B	67	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	185	ASN	O-C-N	5.84	132.04	122.70
1	B	79[A]	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	79[B]	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	100	LEU	CB-CA-C	5.79	121.20	110.20
1	A	81	TYR	N-CA-CB	5.76	120.98	110.60
1	B	105[A]	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	105[B]	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	145	MET	CB-CG-SD	-5.73	95.22	112.40
1	B	103	VAL	CA-CB-CG2	5.73	119.49	110.90
1	A	151	PHE	CB-CG-CD1	5.72	124.81	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	TYR	O-C-N	5.72	131.85	122.70
1	A	144	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	A	108	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	B	12	ALA	CB-CA-C	-5.57	101.75	110.10
1	A	79	ARG	CB-CA-C	5.55	121.51	110.40
1	B	84	GLU	N-CA-CB	-5.55	100.62	110.60
1	A	141	GLU	CA-CB-CG	5.54	125.60	113.40
1	B	30	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	64	GLN	CA-CB-CG	5.53	125.56	113.40
1	A	132	ILE	O-C-N	5.49	131.49	122.70
1	A	153	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	187	THR	CA-CB-CG2	5.43	120.00	112.40
1	B	19	ILE	CA-CB-CG2	5.40	121.69	110.90
1	A	77	LEU	CB-CG-CD2	5.39	120.16	111.00
1	A	67	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	49	ARG	O-C-N	5.37	131.29	122.70
1	B	30	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	B	122	ILE	CG1-CB-CG2	5.34	123.15	111.40
1	A	150	LYS	CB-CG-CD	5.31	125.42	111.60
1	A	29	LEU	CB-CA-C	5.31	120.29	110.20
1	A	154	GLU	CG-CD-OE2	5.30	128.89	118.30
1	A	102	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	190	THR	OG1-CB-CG2	5.26	122.09	110.00
1	A	24	LYS	CA-CB-CG	5.25	124.96	113.40
1	A	87	ASP	CB-CA-C	5.23	120.86	110.40
1	B	168	VAL	CG1-CB-CG2	-5.22	102.56	110.90
1	B	67	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	B	71	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	38	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	145	MET	CB-CG-SD	-5.17	96.89	112.40
1	B	176	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	191	ARG	NH1-CZ-NH2	-5.16	113.72	119.40
1	B	30	ARG	CG-CD-NE	5.16	122.63	111.80
1	B	118	TYR	CA-CB-CG	5.12	123.13	113.40
1	A	97	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	B	56	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	B	175	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	49	ARG	O-C-N	5.07	130.81	122.70
1	A	8	ILE	O-C-N	5.06	130.80	122.70
1	A	144	GLU	CB-CG-CD	5.04	127.81	114.20
1	A	56	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
1	B	190	THR	CA-CB-CG2	5.02	119.43	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	ARG	Sidechain
1	B	34[A]	ARG	Sidechain
1	B	34[B]	ARG	Sidechain

## 5.2 Too-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 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	1597	0	1641	36	0
1	B	1599	0	1627	34	0
2	A	48	0	26	1	0
2	B	48	0	26	0	0
3	A	70	0	0	0	0
3	B	90	0	0	4	0
All	All	3452	0	3320	69	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 10.

All (69) 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:176:ASP:H	1:A:185:ASN:HD21	1.18	0.89
1:B:28:ARG:HH21	1:B:30:ARG:HG2	1.38	0.88
1:A:176:ASP:H	1:A:185:ASN:ND2	1.75	0.83
1:B:124:ASN:HD22	1:B:126:LEU:H	1.29	0.81
1:B:19:ILE:HG22	1:B:147:THR:HG22	1.66	0.76
1:B:83:ASN:HD21	1:B:94:SER:H	1.31	0.74
1:B:83:ASN:ND2	1:B:94:SER:H	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HH11	1:A:79:ARG:HB2	1.58	0.68
1:A:14:LYS:HE2	1:A:134:GLU:HB3	1.75	0.68
1:B:39:VAL:HG22	1:B:168:VAL:HG13	1.77	0.67
1:A:19:ILE:HD13	1:A:149:LEU:HG	1.77	0.66
1:B:176:ASP:H	1:B:185:ASN:HD21	1.42	0.66
1:A:45:LYS:HB3	1:A:46:PRO:HD2	1.77	0.66
1:B:176:ASP:H	1:B:185:ASN:ND2	1.94	0.65
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.79	0.64
1:B:65:LYS:HD3	1:B:65:LYS:H	1.63	0.62
1:A:42[A]:ARG:HH21	1:A:170:ASP:H	1.46	0.62
1:A:6[A]:VAL:HG22	1:A:127:VAL:HG22	1.83	0.61
1:B:137:HIS:HD2	1:B:139:SER:H	1.51	0.59
1:B:109:VAL:HG12	3:B:246:HOH:O	2.02	0.58
1:B:20:GLY:O	1:B:145:MET:HB2	2.04	0.56
1:B:124:ASN:ND2	1:B:126:LEU:H	1.99	0.56
1:B:111[B]:ILE:HG13	3:B:246:HOH:O	2.04	0.56
1:A:64:GLN:HG2	1:A:65:LYS:HE3	1.87	0.56
1:A:45:LYS:HB2	1:A:48:THR:HG21	1.88	0.56
1:B:137:HIS:CD2	1:B:139:SER:H	2.24	0.56
1:B:6[B]:VAL:HG23	3:B:246:HOH:O	2.05	0.55
1:A:37[B]:LYS:NZ	1:A:41[B]:THR:HG21	2.22	0.54
1:A:37[B]:LYS:HD3	1:A:41[B]:THR:HG21	1.91	0.52
1:A:53[B]:ILE:HG22	1:A:75:ILE:HD12	1.93	0.51
1:A:6[B]:VAL:HG13	1:A:127:VAL:HG22	1.93	0.51
1:B:39:VAL:HG22	1:B:168:VAL:CG1	2.42	0.49
1:A:14:LYS:CB	1:A:15:PRO:HA	2.43	0.48
1:A:176:ASP:N	1:A:185:ASN:HD21	1.98	0.47
1:B:20:GLY:HA2	1:B:26:PRO:HD3	1.96	0.47
1:A:21:TYR:O	1:A:22:LYS:HB3	2.14	0.47
1:A:3:LYS:HE3	1:B:101:ASN:O	2.16	0.46
1:B:83:ASN:ND2	1:B:94:SER:N	2.60	0.46
1:B:158:LYS:HZ2	1:B:187:THR:HG21	1.80	0.46
1:B:28:ARG:NH2	1:B:30:ARG:HG2	2.18	0.46
1:B:122:ILE:CD1	1:B:152:PRO:HD2	2.46	0.46
1:B:25:MET:HA	1:B:26:PRO:HD3	1.80	0.45
1:B:5:ASN:ND2	3:B:297:HOH:O	2.44	0.44
1:A:29:LEU:O	1:A:33[A]:ILE:HG12	2.17	0.44
1:B:122:ILE:HD13	1:B:152:PRO:HD2	2.00	0.44
1:A:155:SER:O	1:A:192:LYS:HG2	2.17	0.44
1:A:45:LYS:HE2	1:A:107:GLU:HG3	2.00	0.43
1:A:67:ARG:HA	1:A:68:PRO:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HB2	1:A:47[A]:ASN:ND2	2.33	0.43
1:A:78:SER:HB3	1:A:81:TYR:CD2	2.54	0.43
1:B:14:LYS:CB	1:B:15:PRO:HA	2.48	0.43
1:B:21:TYR:CE2	1:B:22:LYS:HD3	2.54	0.42
1:B:62:ILE:HD13	1:B:69:LEU:HD21	2.00	0.42
1:B:122:ILE:HD12	1:B:151:PHE:HB3	2.01	0.42
1:B:65:LYS:H	1:B:65:LYS:CD	2.29	0.42
1:A:159:GLN:HB3	1:A:160:PRO:HD2	2.02	0.42
1:A:12:ALA:HB2	1:A:19:ILE:HD11	2.01	0.41
1:A:37[B]:LYS:HZ2	1:A:41[B]:THR:HG21	1.84	0.41
1:A:13:LEU:HB3	1:A:145:MET:HE3	2.02	0.41
1:B:19:ILE:HD13	1:B:149:LEU:HG	2.03	0.41
1:A:6[B]:VAL:HG13	1:A:127:VAL:HA	2.03	0.41
1:B:63:PRO:HB3	1:B:65:LYS:HE3	2.03	0.41
1:A:178:LYS:HD3	1:A:183:THR:OG1	2.22	0.40
1:B:149:LEU:HD22	1:B:151:PHE:CZ	2.56	0.40
1:A:151:PHE:HA	1:A:152:PRO:HD3	1.82	0.40
1:A:79:ARG:NH1	2:A:193:NDP:O2X	2.55	0.40
1:A:137:HIS:CG	1:A:138:PRO:HD2	2.56	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	200/192 (104%)	188 (94%)	8 (4%)	4 (2%)		
1	B	201/192 (105%)	195 (97%)	6 (3%)	0		
All	All	401/384 (104%)	383 (96%)	14 (4%)	4 (1%)		

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	GLU
1	A	142	SER
1	A	23	GLY
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	187/177 (106%)	166 (89%)	21 (11%)	6	1
1	B	188/177 (106%)	170 (90%)	18 (10%)	8	1
All	All	375/354 (106%)	336 (90%)	39 (10%)	9	1

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	6[A]	VAL
1	A	6[B]	VAL
1	A	14	LYS
1	A	22	LYS
1	A	24	LYS
1	A	42[A]	ARG
1	A	42[B]	ARG
1	A	47[A]	ASN
1	A	47[B]	ASN
1	A	65	LYS
1	A	74	ASN
1	A	79	ARG
1	A	82	GLU
1	A	102	LEU
1	A	105	ASP
1	A	147	THR
1	A	150	LYS
1	A	154	GLU
1	A	170	ASP

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Mol	Chain	Res	Type
1	A	174	GLU
1	B	1	MET
1	B	6[A]	VAL
1	B	6[B]	VAL
1	B	14	LYS
1	B	19	ILE
1	B	24	LYS
1	B	34[A]	ARG
1	B	34[B]	ARG
1	B	65	LYS
1	B	74	ASN
1	B	82[A]	GLU
1	B	82[B]	GLU
1	B	122	ILE
1	B	124	ASN
1	B	130	LEU
1	B	157	THR
1	B	170	ASP
1	B	173	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	159	GLN
1	A	185	ASN
1	B	5	ASN
1	B	83	ASN
1	B	89	ASN
1	B	101	ASN
1	B	123	ASN
1	B	124	ASN
1	B	137	HIS
1	B	159	GLN
1	B	185	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides 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	193	-	47,52,52	1.75	8 (17%)	61,80,80	1.61	14 (22%)
2	NDP	B	193	-	47,52,52	2.16	13 (27%)	61,80,80	1.55	13 (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
2	NDP	A	193	-	-	2/30/77/77	0/5/5/5
2	NDP	B	193	-	-	2/30/77/77	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	193	NDP	O4B-C1B	-6.14	1.32	1.40
2	A	193	NDP	C7N-C3N	4.96	1.59	1.48
2	B	193	NDP	C7N-C3N	4.71	1.58	1.48
2	A	193	NDP	PA-O3	-4.65	1.54	1.59
2	B	193	NDP	PN-O3	4.45	1.64	1.59
2	A	193	NDP	C4N-C3N	-4.40	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	193	NDP	C4N-C3N	-4.40	1.41	1.50
2	B	193	NDP	P2B-O2B	4.21	1.66	1.59
2	B	193	NDP	C1B-N9A	-4.09	1.39	1.49
2	B	193	NDP	PA-O3	3.38	1.63	1.59
2	B	193	NDP	C8A-N7A	-3.30	1.28	1.34
2	A	193	NDP	P2B-O2X	-3.19	1.43	1.54
2	A	193	NDP	C2A-N1A	3.06	1.39	1.33
2	A	193	NDP	C1B-N9A	-2.93	1.42	1.49
2	A	193	NDP	P2B-O2B	2.91	1.64	1.59
2	B	193	NDP	C4N-C5N	-2.73	1.41	1.49
2	B	193	NDP	PN-O2N	-2.68	1.42	1.55
2	A	193	NDP	C4N-C5N	-2.53	1.42	1.49
2	B	193	NDP	C3B-C2B	2.40	1.58	1.53
2	B	193	NDP	PA-O2A	-2.39	1.44	1.55
2	B	193	NDP	P2B-O3X	-2.16	1.46	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	193	NDP	O3D-C3D-C4D	3.69	121.67	111.08
2	B	193	NDP	C3N-C2N-N1N	-3.68	117.80	123.20
2	B	193	NDP	C5A-C6A-N6A	3.68	125.92	120.31
2	B	193	NDP	O4D-C1D-N1N	3.60	114.94	108.08
2	A	193	NDP	O3B-C3B-C2B	3.27	120.33	111.19
2	A	193	NDP	C1D-N1N-C2N	-3.25	115.79	121.14
2	B	193	NDP	O3B-C3B-C2B	3.23	120.23	111.19
2	B	193	NDP	C1D-N1N-C2N	-3.17	115.91	121.14
2	A	193	NDP	C4A-C5A-N7A	3.17	112.68	109.34
2	A	193	NDP	C6N-N1N-C2N	3.03	122.56	119.32
2	B	193	NDP	O7N-C7N-N7N	3.00	129.63	122.89
2	A	193	NDP	N6A-C6A-N1A	3.00	124.74	118.33
2	B	193	NDP	C4B-O4B-C1B	2.99	112.66	109.92
2	A	193	NDP	C4B-O4B-C1B	-2.98	107.19	109.92
2	A	193	NDP	O2B-P2B-O1X	-2.92	98.92	109.33
2	B	193	NDP	O7N-C7N-C3N	-2.62	115.96	120.90
2	B	193	NDP	C3B-C2B-C1B	-2.57	97.89	102.81
2	A	193	NDP	P2B-O2B-C2B	-2.55	116.61	123.43
2	A	193	NDP	O2B-C2B-C3B	2.49	120.62	111.68
2	A	193	NDP	O4B-C1B-C2B	2.38	110.67	106.61
2	B	193	NDP	O2N-PN-O3	2.35	113.61	107.27
2	A	193	NDP	O3X-P2B-O2X	2.21	116.07	107.80
2	A	193	NDP	O4B-C1B-N9A	-2.17	105.86	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	NDP	O2B-P2B-O1X	-2.16	101.63	109.33
2	B	193	NDP	O2X-P2B-O1X	2.16	119.23	110.83
2	B	193	NDP	O2X-P2B-O2B	-2.03	97.92	105.85
2	A	193	NDP	C5A-C6A-N6A	-2.03	117.22	120.31

There are no chirality outliers.

All (4) torsion outliers are listed below:

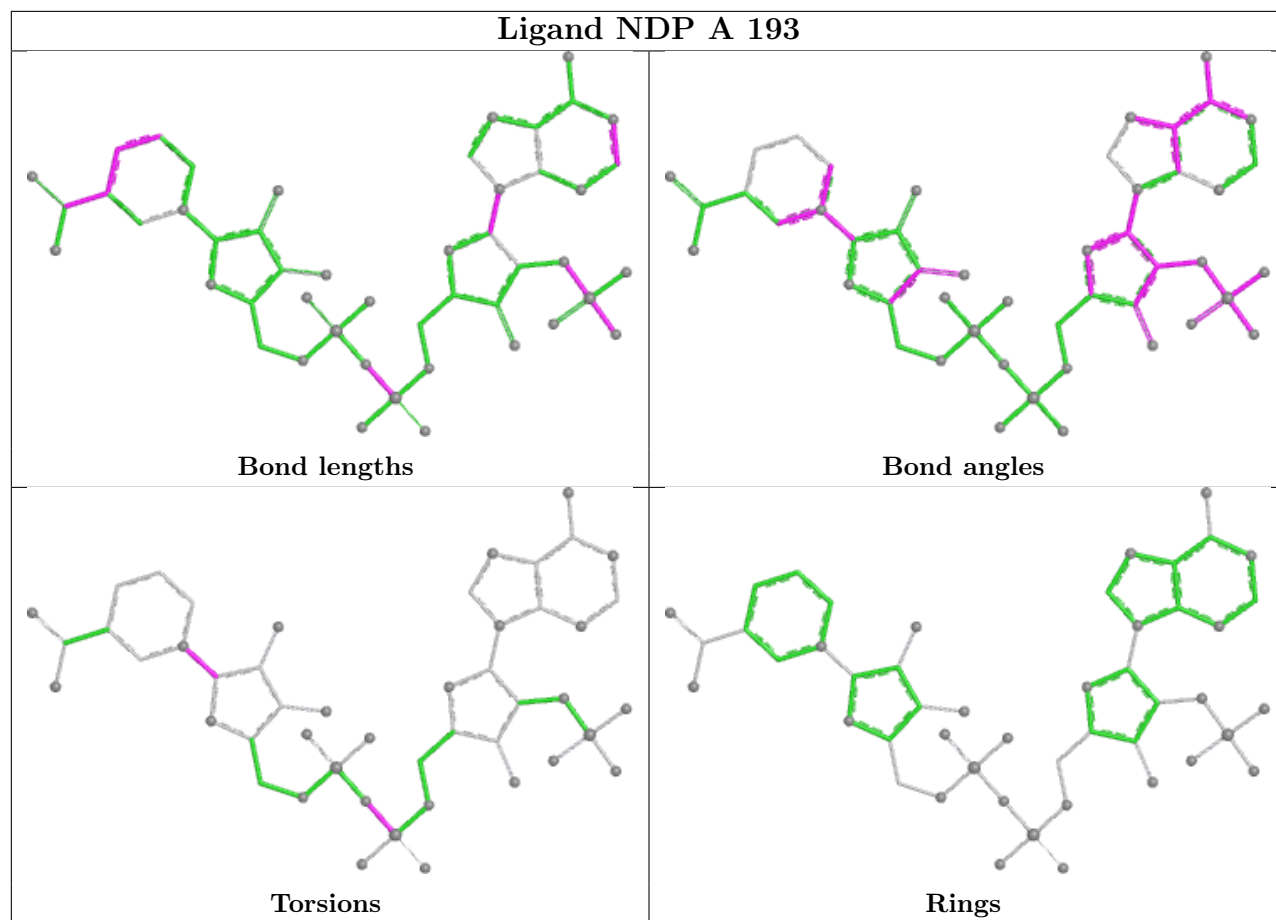
Mol	Chain	Res	Type	Atoms
2	A	193	NDP	O4D-C1D-N1N-C2N
2	B	193	NDP	O4D-C1D-N1N-C2N
2	A	193	NDP	PN-O3-PA-O2A
2	B	193	NDP	PN-O3-PA-O1A

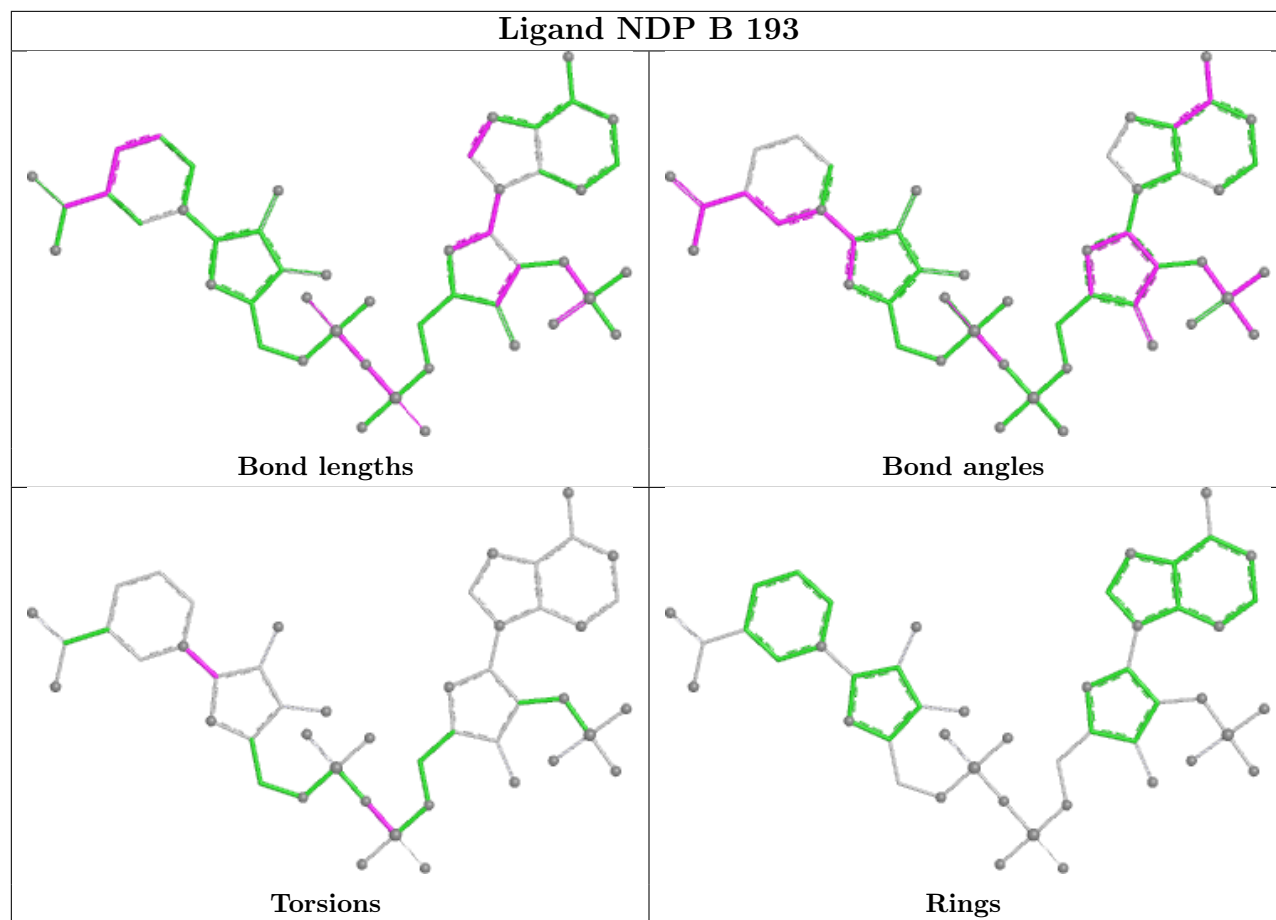
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	193	NDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.