



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:04 AM UTC

PDB ID : 1AI9 / pdb_00001ai9
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

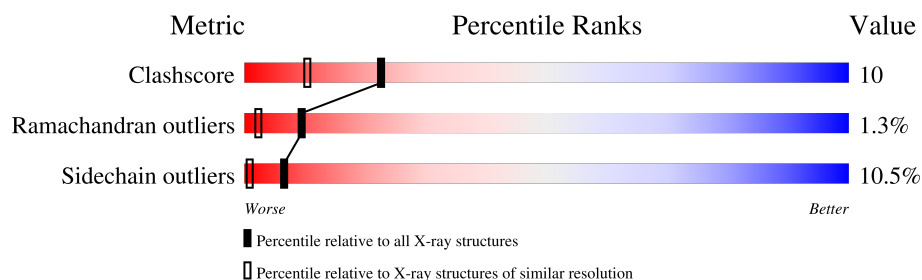
1 Overall quality at a glance

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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (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 ≥ 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.

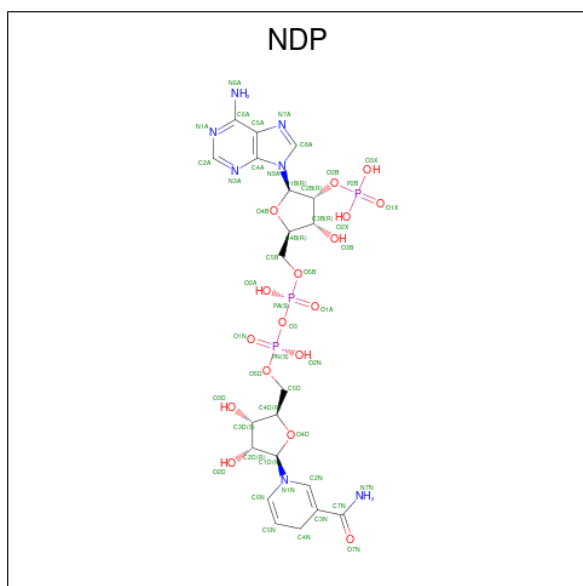
Mol	Chain	Length	Quality of chain
1	A	192	 43% 40% 15% .
1	B	192	 50% 36% 11% .

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

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



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

- Molecule 3 is water.

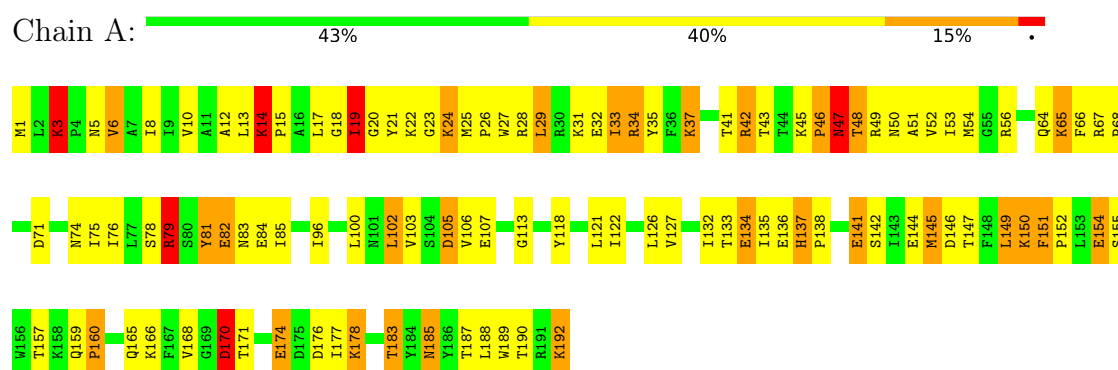
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total 70	O 70	0	0
3	B	90	Total 90	O 90	0	0

3 Residue-property plots

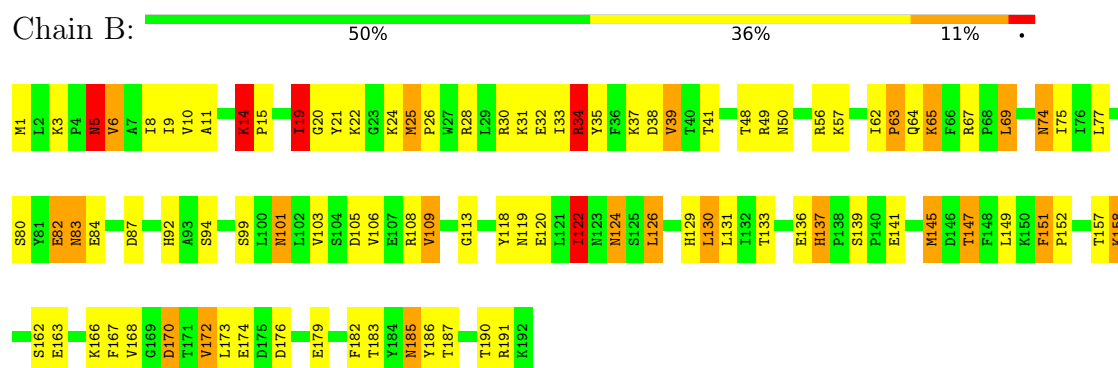
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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, α , β , γ	77.20 Å 67.57 Å 38.66 Å 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 ²)	16.0	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: 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	1.69	18/1680 (1.1%)	2.43	100/2274 (4.4%)
1	B	1.71	20/1691 (1.2%)	2.33	97/2287 (4.2%)
All	All	1.70	38/3371 (1.1%)	2.38	197/4561 (4.3%)

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 (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	GLU	CA-CB	-7.83	1.40	1.53
1	A	165	GLN	C-O	7.62	1.33	1.24
1	B	75	ILE	C-O	7.04	1.31	1.24
1	B	38	ASP	C-O	6.83	1.31	1.24
1	B	109	VAL	C-O	6.73	1.31	1.24
1	A	189	TRP	N-CA	6.59	1.54	1.46
1	B	92	HIS	C-O	6.34	1.31	1.24
1	A	54	MET	C-O	6.06	1.31	1.23
1	B	8	ILE	CA-C	5.97	1.59	1.52
1	B	120	GLU	N-CA	-5.96	1.38	1.46
1	B	186	TYR	C-O	5.85	1.31	1.23
1	B	56	ARG	CD-NE	-5.84	1.38	1.46
1	A	126	LEU	C-O	5.74	1.31	1.24
1	A	52	VAL	C-O	5.68	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	LEU	C-O	-5.66	1.17	1.24
1	A	3	LYS	CA-CB	5.66	1.57	1.52
1	A	33[A]	ILE	CA-CB	5.61	1.60	1.54
1	A	33[B]	ILE	CA-CB	5.61	1.60	1.54
1	A	145	MET	CA-CB	-5.60	1.43	1.53
1	B	33	ILE	N-CA	5.59	1.53	1.46
1	B	106	VAL	N-CA	5.55	1.52	1.46
1	B	162	SER	C-N	-5.52	1.26	1.33
1	A	5	ASN	C-O	5.41	1.30	1.23
1	A	157	THR	CA-CB	5.35	1.60	1.53
1	B	158	LYS	N-CA	5.33	1.52	1.46
1	B	129	HIS	N-CA	5.26	1.52	1.45
1	B	67	ARG	CA-CB	-5.22	1.46	1.53
1	A	85	ILE	C-O	5.20	1.29	1.24
1	A	14	LYS	CA-CB	-5.18	1.44	1.53
1	A	51	ALA	N-CA	5.13	1.52	1.46
1	B	133	THR	C-O	-5.12	1.17	1.24
1	A	50	ASN	N-CA	5.10	1.51	1.45
1	A	137	HIS	N-CA	5.09	1.51	1.46
1	B	11	ALA	N-CA	5.08	1.52	1.46
1	B	41	THR	CA-CB	5.06	1.61	1.53
1	B	136	GLU	N-CA	5.05	1.52	1.45
1	B	83	ASN	N-CA	5.02	1.52	1.46
1	A	122	ILE	CB-CG1	-5.00	1.43	1.53

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ILE	CB-CG1-CD1	26.59	169.65	113.80
1	B	56	ARG	CD-NE-CZ	26.12	160.96	124.40
1	A	174	GLU	CA-CB-CG	19.22	152.54	114.10
1	A	106	VAL	N-CA-C	12.76	127.72	108.71
1	B	56	ARG	NE-CZ-NH2	12.68	130.61	119.20
1	A	56	ARG	CD-NE-CZ	11.59	140.62	124.40
1	A	34	ARG	NE-CZ-NH2	11.05	129.15	119.20
1	B	167	PHE	CA-CB-CG	10.86	124.66	113.80
1	A	170	ASP	N-CA-C	10.77	124.10	111.71
1	A	28	ARG	CD-NE-CZ	10.76	139.46	124.40
1	A	154	GLU	CB-CG-CD	10.34	130.18	112.60
1	B	14	LYS	CA-CB-CG	10.33	134.76	114.10
1	B	151	PHE	CA-CB-CG	10.28	124.08	113.80
1	B	5	ASN	OD1-CG-ND2	10.19	132.78	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ARG	NE-CZ-NH1	-9.66	111.84	121.50
1	B	130	LEU	O-C-N	9.66	134.79	123.30
1	B	137	HIS	O-C-N	9.53	129.26	121.83
1	B	35	TYR	O-C-N	9.49	131.85	122.07
1	B	3	LYS	O-C-N	9.30	129.80	121.80
1	A	19	ILE	CA-CB-CG2	9.12	126.01	110.50
1	A	144	GLU	CB-CG-CD	8.95	127.81	112.60
1	B	87	ASP	CA-CB-CG	8.93	121.53	112.60
1	A	166	LYS	N-CA-CB	8.79	123.04	110.12
1	B	5	ASN	CA-CB-CG	-8.26	104.34	112.60
1	A	192	LYS	CA-CB-CG	8.11	130.33	114.10
1	A	132	ILE	O-C-N	7.91	131.49	123.18
1	A	66	PHE	CA-CB-CG	7.91	121.71	113.80
1	A	14	LYS	CA-CB-CG	7.87	129.83	114.10
1	B	129	HIS	CA-CB-CG	7.82	121.62	113.80
1	A	3	LYS	CB-CG-CD	7.67	128.95	111.30
1	A	3	LYS	N-CA-CB	-7.51	103.33	111.66
1	A	188	LEU	O-C-N	7.47	132.38	123.27
1	A	136	GLU	CB-CG-CD	7.45	125.26	112.60
1	A	8	ILE	O-C-N	7.42	130.80	122.93
1	B	34[A]	ARG	CD-NE-CZ	7.36	134.70	124.40
1	B	34[B]	ARG	CD-NE-CZ	7.36	134.70	124.40
1	B	19	ILE	N-CA-CB	-7.28	102.29	112.12
1	B	145	MET	N-CA-C	7.27	119.91	108.79
1	A	81	TYR	N-CA-CB	7.23	120.98	110.06
1	A	178	LYS	CB-CG-CD	7.20	127.86	111.30
1	B	185	ASN	O-C-N	7.20	132.04	123.33
1	A	81	TYR	CA-CB-CG	7.13	126.74	113.90
1	B	49	ARG	O-C-N	7.12	131.29	123.10
1	A	105	ASP	N-CA-CB	-7.02	97.54	110.32
1	A	8	ILE	CA-C-O	-7.02	112.70	120.84
1	A	118	TYR	O-C-N	7.00	129.28	122.07
1	A	82	GLU	CB-CG-CD	7.00	124.49	112.60
1	A	121	LEU	CB-CA-C	6.88	124.69	110.31
1	B	74	ASN	CA-CB-CG	6.87	119.47	112.60
1	B	67	ARG	CB-CA-C	6.81	119.12	108.84
1	A	49	ARG	CA-C-O	-6.80	113.71	121.40
1	A	174	GLU	CB-CG-CD	6.79	124.14	112.60
1	A	19	ILE	N-CA-CB	-6.71	104.35	112.33
1	B	99	SER	CA-CB-OG	6.71	124.51	111.10
1	B	179	GLU	CB-CG-CD	6.62	123.85	112.60
1	B	3	LYS	CA-C-O	-6.61	112.99	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ILE	N-CA-C	6.60	120.13	113.47
1	B	19	ILE	CA-CB-CG2	6.58	121.69	110.50
1	A	157	THR	CA-CB-OG1	-6.55	99.78	109.60
1	A	3	LYS	O-C-N	-6.54	118.52	121.53
1	A	185	ASN	OD1-CG-ND2	6.51	129.11	122.60
1	B	170	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	11	ALA	CA-C-O	-6.42	113.42	120.36
1	A	190	THR	OG1-CB-CG2	6.39	122.09	109.30
1	A	49	ARG	O-C-N	6.32	130.81	123.17
1	A	154	GLU	CA-CB-CG	6.27	126.64	114.10
1	A	5	ASN	CA-C-O	-6.26	114.27	121.47
1	A	83	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	B	147	THR	CA-CB-CG2	6.16	120.98	110.50
1	A	118	TYR	N-CA-CB	6.16	118.94	110.01
1	B	31	LYS	CA-C-N	6.16	128.53	120.28
1	B	31	LYS	C-N-CA	6.16	128.53	120.28
1	B	182	PHE	O-C-N	6.15	129.95	123.06
1	A	150	LYS	CB-CG-CD	6.14	125.42	111.30
1	B	6[A]	VAL	CA-C-O	6.14	127.85	120.67
1	B	6[B]	VAL	CA-C-O	6.14	127.85	120.67
1	A	171	THR	CA-CB-OG1	-6.10	100.45	109.60
1	B	56	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	47[A]	ASN	CA-CB-CG	6.01	118.61	112.60
1	A	47[B]	ASN	CA-CB-CG	6.01	118.61	112.60
1	B	130	LEU	CA-C-O	-5.99	113.89	120.36
1	B	84	GLU	N-CA-CB	-5.89	100.62	110.57
1	B	109	VAL	CA-C-O	-5.89	114.20	120.39
1	B	39	VAL	O-C-N	5.88	127.67	121.91
1	A	121	LEU	CA-C-O	5.86	126.58	119.38
1	A	149	LEU	O-C-N	5.86	129.92	123.01
1	A	54	MET	CA-C-N	5.84	128.00	120.64
1	A	54	MET	C-N-CA	5.84	128.00	120.64
1	A	177	ILE	CA-C-N	-5.83	114.95	123.00
1	A	177	ILE	C-N-CA	-5.83	114.95	123.00
1	B	6[A]	VAL	CA-CB-CG2	5.83	120.32	110.40
1	B	6[B]	VAL	CA-CB-CG2	5.83	120.32	110.40
1	A	145	MET	CB-CG-SD	-5.83	95.22	112.70
1	A	134	GLU	O-C-N	5.81	129.91	122.93
1	B	126	LEU	O-C-N	5.79	129.40	122.27
1	B	172	VAL	N-CA-CB	5.76	117.00	110.72
1	B	32	GLU	CA-C-O	-5.75	114.45	120.55
1	A	141	GLU	CA-CB-CG	5.75	125.60	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	GLU	CB-CA-C	5.74	119.90	110.88
1	B	74	ASN	O-C-N	5.74	129.75	123.27
1	B	64	GLN	CA-CB-CG	5.73	125.56	114.10
1	A	168	VAL	O-C-N	5.73	128.94	122.18
1	A	43	THR	CA-CB-OG1	-5.71	101.03	109.60
1	B	35	TYR	N-CA-C	-5.69	104.98	111.07
1	A	166	LYS	CA-C-O	-5.67	114.53	120.55
1	A	48	THR	CA-CB-OG1	-5.65	101.13	109.60
1	B	122	ILE	CB-CG1-CD1	5.65	125.66	113.80
1	A	14	LYS	CB-CA-C	5.64	118.34	109.37
1	A	141	GLU	CA-C-N	5.64	132.31	121.54
1	A	141	GLU	C-N-CA	5.64	132.31	121.54
1	A	96	ILE	CA-C-O	5.64	127.13	121.27
1	B	9	ILE	CA-CB-CG2	5.61	120.04	110.50
1	B	113	GLY	CA-C-N	5.61	131.79	121.70
1	B	113	GLY	C-N-CA	5.61	131.79	121.70
1	A	187	THR	CA-CB-CG2	5.59	120.00	110.50
1	A	183	THR	O-C-N	5.58	129.79	123.27
1	A	31	LYS	N-CA-CB	5.56	118.38	110.16
1	B	80	SER	CA-C-O	5.55	125.48	119.15
1	A	8	ILE	CA-C-N	-5.55	115.72	123.10
1	A	8	ILE	C-N-CA	-5.55	115.72	123.10
1	A	49	ARG	CD-NE-CZ	-5.54	116.64	124.40
1	A	146	ASP	CB-CA-C	5.54	118.86	109.55
1	A	76	ILE	CA-C-O	-5.54	114.58	120.39
1	B	119	ASN	CA-C-N	5.48	130.00	120.68
1	B	119	ASN	C-N-CA	5.48	130.00	120.68
1	A	160	PRO	CA-C-O	-5.48	115.06	122.08
1	B	105[A]	ASP	CA-C-N	-5.47	115.17	122.77
1	B	105[A]	ASP	C-N-CA	-5.47	115.17	122.77
1	B	105[B]	ASP	CA-C-N	-5.47	115.17	122.77
1	B	105[B]	ASP	C-N-CA	-5.47	115.17	122.77
1	A	24	LYS	CA-CB-CG	5.43	124.96	114.10
1	B	6[A]	VAL	CA-CB-CG1	5.43	119.62	110.40
1	B	6[B]	VAL	CA-CB-CG1	5.43	119.62	110.40
1	B	50	ASN	OD1-CG-ND2	5.42	128.03	122.60
1	A	183	THR	N-CA-CB	5.41	119.26	110.77
1	A	8	ILE	N-CA-C	-5.40	100.66	108.71
1	A	113	GLY	CA-C-N	5.39	131.41	121.70
1	A	113	GLY	C-N-CA	5.39	131.41	121.70
1	B	136	GLU	CB-CG-CD	5.39	121.76	112.60
1	B	82[A]	GLU	N-CA-CB	5.37	119.39	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82[B]	GLU	N-CA-CB	5.37	119.39	110.52
1	A	122	ILE	CA-C-N	-5.36	114.57	122.83
1	A	122	ILE	C-N-CA	-5.36	114.57	122.83
1	A	79	ARG	CB-CA-C	5.36	121.51	110.31
1	B	103	VAL	CA-CB-CG2	5.35	119.49	110.40
1	B	183	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	29	LEU	CB-CA-C	5.35	120.29	111.31
1	B	69	LEU	CB-CA-C	5.34	118.44	109.69
1	A	10	VAL	CA-C-N	5.33	130.51	123.05
1	A	10	VAL	C-N-CA	5.33	130.51	123.05
1	B	141[A]	GLU	CB-CG-CD	5.32	121.65	112.60
1	B	141[B]	GLU	CB-CG-CD	5.32	121.65	112.60
1	A	188	LEU	CA-C-O	-5.31	114.55	120.66
1	A	84	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	17	LEU	CB-CA-C	5.29	118.59	111.82
1	A	35	TYR	N-CA-C	-5.28	105.44	111.14
1	A	149	LEU	CA-C-O	-5.28	115.03	121.05
1	B	145	MET	CB-CG-SD	-5.27	96.89	112.70
1	A	151	PHE	CA-CB-CG	5.25	119.06	113.80
1	B	190	THR	CA-CB-CG2	5.25	119.43	110.50
1	B	32	GLU	O-C-N	5.24	127.67	122.12
1	B	122	ILE	CA-CB-CG1	-5.23	101.50	110.40
1	B	50	ASN	CA-CB-CG	5.22	117.83	112.60
1	A	102	LEU	N-CA-CB	-5.22	102.46	110.44
1	A	174	GLU	N-CA-CB	5.21	118.80	110.46
1	B	25	MET	CB-CA-C	5.21	116.22	108.87
1	B	48	THR	CA-CB-CG2	5.20	119.34	110.50
1	B	131	LEU	CA-C-O	-5.20	114.77	120.70
1	B	10	VAL	CA-C-O	-5.20	116.83	121.09
1	A	133	THR	CA-CB-OG1	-5.19	101.82	109.60
1	B	108	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	B	37	LYS	O-C-N	5.18	127.41	122.03
1	B	82[A]	GLU	CA-C-O	-5.17	115.06	120.80
1	B	82[B]	GLU	CA-C-O	-5.17	115.06	120.80
1	A	71	ASP	CA-C-O	-5.16	114.26	119.78
1	A	100	LEU	CB-CA-C	5.16	121.20	110.32
1	B	174[A]	GLU	CA-C-O	-5.15	115.55	121.47
1	B	174[B]	GLU	CA-C-O	-5.15	115.55	121.47
1	A	82	GLU	CA-CB-CG	5.14	124.38	114.10
1	B	8	ILE	O-C-N	5.14	128.38	122.93
1	B	8	ILE	CA-C-O	-5.13	114.89	120.84
1	B	118	TYR	CA-CB-CG	5.13	123.13	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	A	13	LEU	O-C-N	5.10	129.03	123.22
1	B	131	LEU	CA-C-N	-5.08	116.89	123.19
1	B	131	LEU	C-N-CA	-5.08	116.89	123.19
1	A	37[A]	LYS	CA-C-O	-5.08	115.47	120.70
1	A	37[B]	LYS	CA-C-O	-5.08	115.47	120.70
1	B	57	LYS	N-CA-CB	5.08	117.58	110.12
1	B	105[A]	ASP	CA-C-O	-5.06	113.64	119.56
1	B	105[B]	ASP	CA-C-O	-5.06	113.64	119.56
1	A	135	ILE	O-C-N	5.05	128.45	122.69
1	B	163	GLU	N-CA-CB	5.03	117.61	110.16
1	B	101	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	B	63	PRO	CA-C-N	5.02	131.12	121.54
1	B	63	PRO	C-N-CA	5.02	131.12	121.54
1	B	113	GLY	N-CA-C	5.00	118.10	111.70

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	39	0
1	B	1599	0	1627	32	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	2	0
All	All	3452	0	3320	70	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 (70) 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
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:A:25:MET:HE2	1:A:27:TRP:HE1	1.70	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: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:67:ARG:HA	1:A:68:PRO:C	2.39	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:18:GLY:HA3	1:A:145:MET:HE3	1.97	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:21:TYR:O	1:A:22:LYS:HB3	2.14	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:B:158:LYS:HZ2	1:B:187:THR:HG21	1.82	0.44
1:A:25:MET:HE2	1:A:27:TRP:NE1	2.32	0.43
1:A:45:LYS:HE2	1:A:107:GLU:HG3	2.00	0.43
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:1:MET:HE3	1:A:1:MET:HB2	1.95	0.41
1:A:37[B]:LYS:HZ2	1:A:41[B]:THR:HG21	1.84	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	146/192 (76%)	134 (92%)	8 (6%)	4 (3%)	4	0
1	B	178/192 (93%)	174 (98%)	4 (2%)	0	100	100
All	All	324/384 (84%)	308 (95%)	12 (4%)	4 (1%)	9	2

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%)	165 (88%)	22 (12%)	5	0
1	B	188/177 (106%)	167 (89%)	21 (11%)	6	1
All	All	375/354 (106%)	332 (88%)	43 (12%)	6	1

All (43) 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	19	ILE
1	A	24	LYS
1	A	42[A]	ARG
1	A	42[B]	ARG
1	A	47[A]	ASN

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Mol	Chain	Res	Type
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	103	VAL
1	A	105	ASP
1	A	147	THR
1	A	150	LYS
1	A	154	GLU
1	A	170	ASP
1	A	174	GLU
1	B	1	MET
1	B	5	ASN
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	166	LYS
1	B	170	ASP
1	B	172	VAL
1	B	173	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	101	ASN
1	A	159	GLN
1	A	185	ASN

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Mol	Chain	Res	Type
1	B	5	ASN
1	B	83	ASN
1	B	89	ASN
1	B	101	ASN
1	B	124	ASN
1	B	137	HIS
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	193	-	51,52,52	1.92	14 (27%)	71,80,80	1.37	11 (15%)
2	NDP	A	193	-	51,52,52	1.67	8 (15%)	71,80,80	1.50	13 (18%)

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	B	193	-	-	2/34/77/77	0/5/5/5
2	NDP	A	193	-	-	2/34/77/77	0/5/5/5

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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	O4B-C1B	-3.97	1.32	1.42
2	B	193	NDP	PA-O3	3.38	1.63	1.59
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	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	C1B-N9A	-2.37	1.39	1.46
2	B	193	NDP	C2A-N3A	-2.34	1.29	1.33
2	A	193	NDP	C2A-N3A	-2.19	1.30	1.33
2	B	193	NDP	P2B-O3X	-2.16	1.46	1.54
2	B	193	NDP	C2B-C1B	2.02	1.58	1.53

All (24) 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	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	C6N-N1N-C2N	3.03	122.56	119.32
2	B	193	NDP	O7N-C7N-N7N	3.00	129.63	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	193	NDP	C2B-C1B-N9A	-2.93	108.92	113.75
2	A	193	NDP	O2B-P2B-O1X	-2.92	98.92	109.33
2	A	193	NDP	N6A-C6A-N1A	2.86	124.74	118.38
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	C5A-C6A-N6A	-2.45	117.22	123.29
2	A	193	NDP	O4B-C1B-C2B	2.37	110.67	106.59
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	C4A-N9A-C8A	2.18	108.02	105.74
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

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

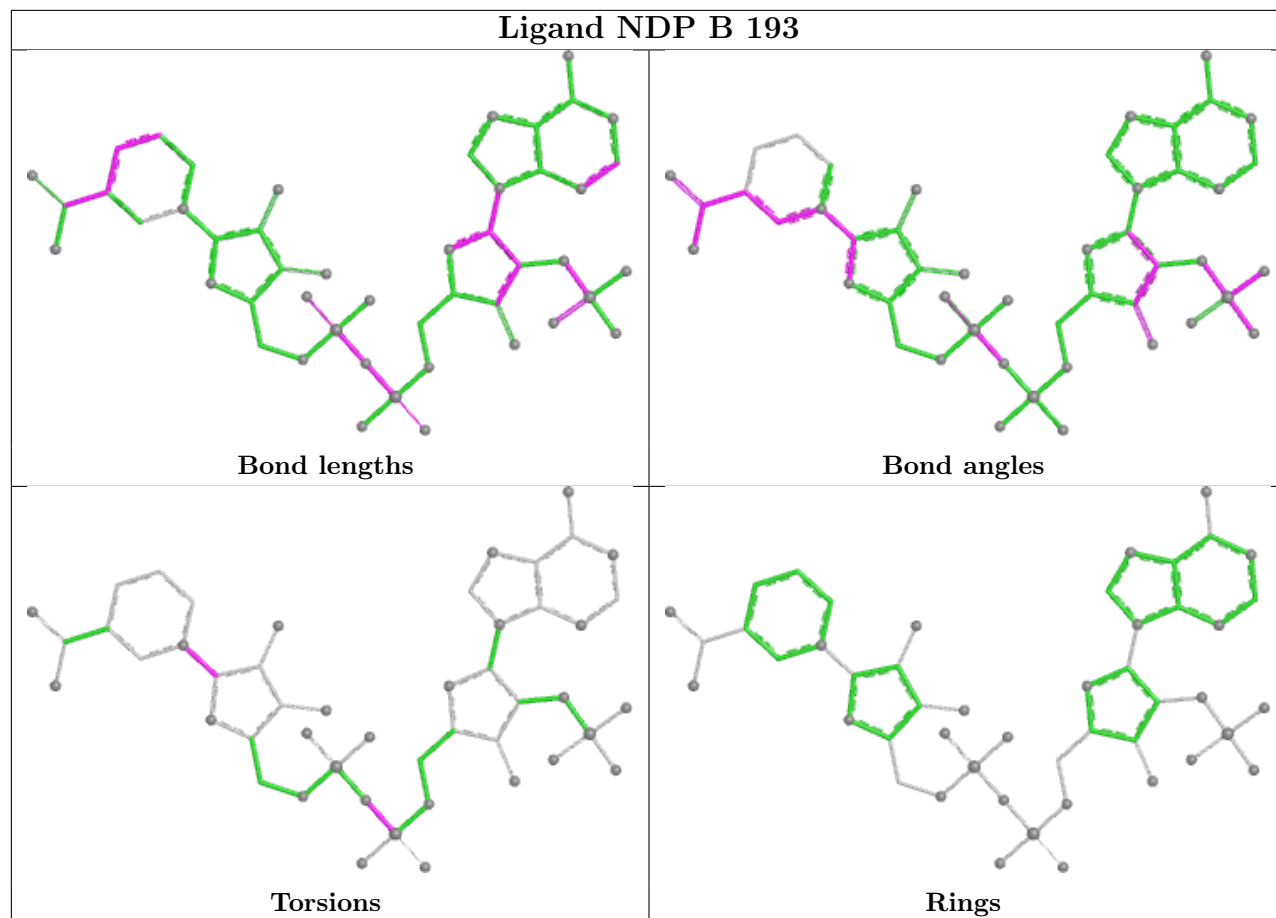
There are no ring outliers.

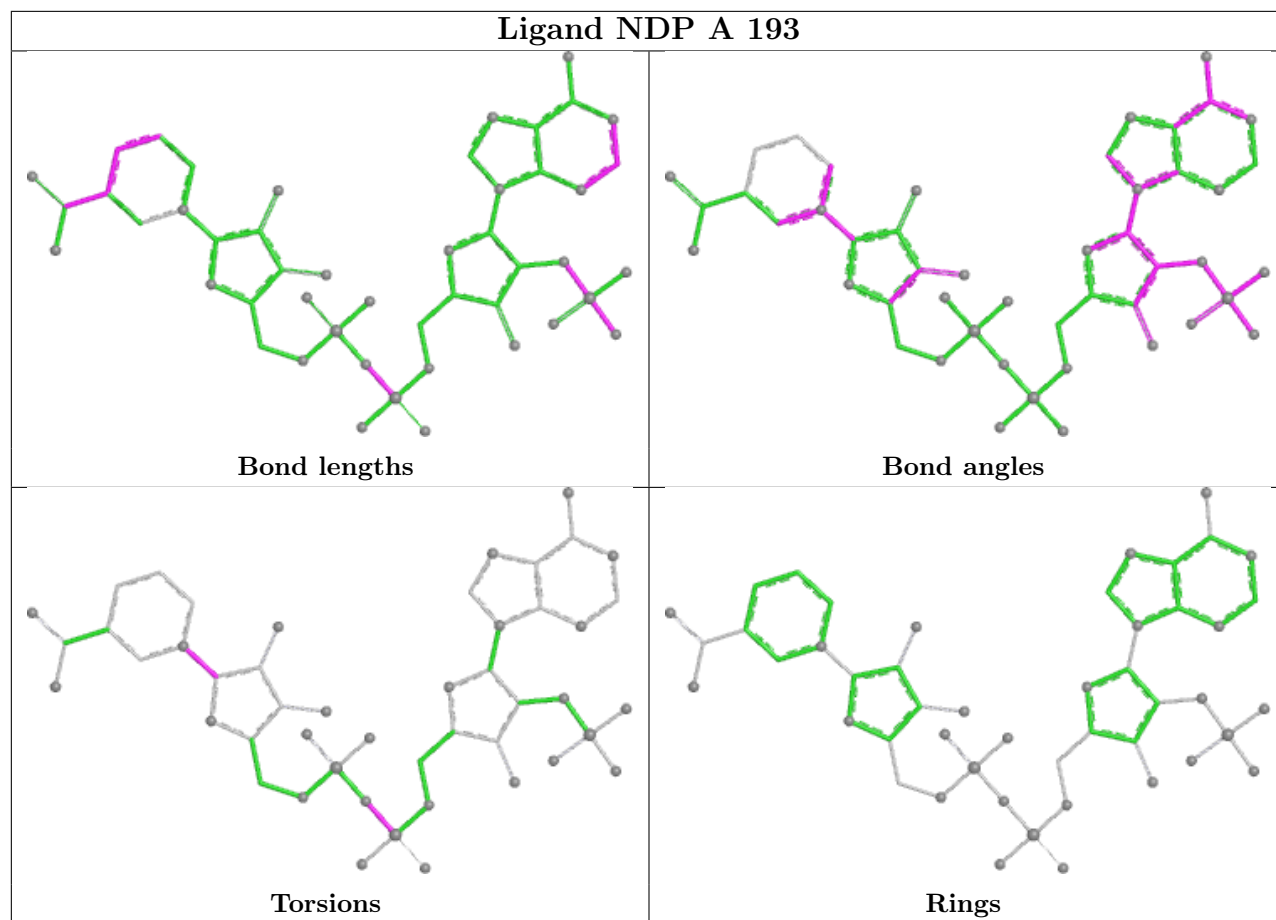
1 monomer is involved in 1 short contact:

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.