



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:04 AM UTC

PDB ID : 1IA4 / pdb_00001ia4
Title : Candida albicans dihydrofolate reductase complex in which the dihydronicotinamide moiety of dihydro-nicotinamide-adenine-dinucleotide phosphate (NADPH) is displaced by 5-{[4-(4-MORPHOLINYL)PHENYL]SULFANYL}-2,4-QUINAZOLINEDIAMIN (GW2021)
Authors : Whitlow, M.; Howard, A.J.; Kuyper, L.F.
Deposited on : 2001-03-22
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)
Xtrriage (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

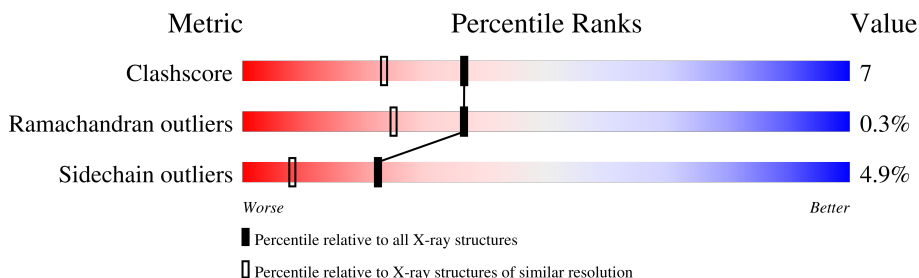
1 Overall quality at a glance

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	
1	B	192	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3659 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.

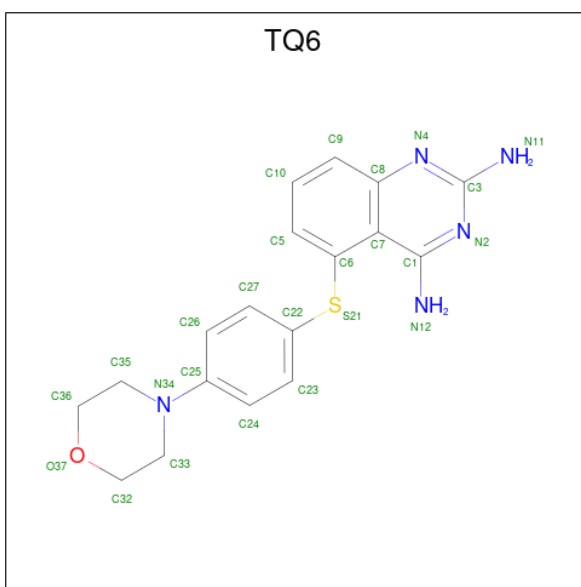
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	10	0
			1586	1017	271	294	4			
1	B	192	Total	C	N	O	S	0	12	0
			1594	1025	264	301	4			

- 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	C	N	O	P	0	0
			35	13	5	14	3		
2	B	1	Total	C	N	O	P	0	0
			39	15	5	16	3		

- Molecule 3 is 5-(4-MORPHOLIN-4-YL-PHENYLSULFANYL)-2,4-QUINAZOLINEDIAMINE (CCD ID: TQ6) (formula: $C_{18}H_{19}N_5OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			25	18	5	1	1		
3	B	1	Total	C	N	O	S	0	0
			25	18	5	1	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

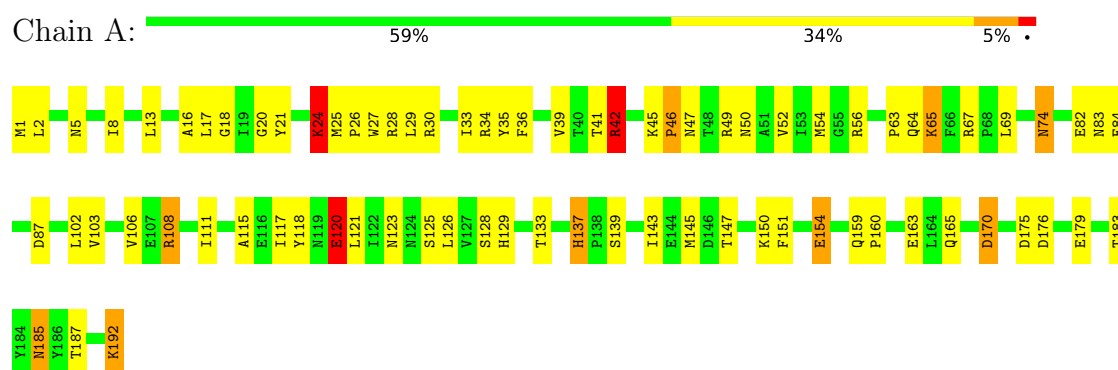
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	144	Total	O	0	8
			152	152		
5	B	175	Total	O	0	4
			179	179		

3 Residue-property plots

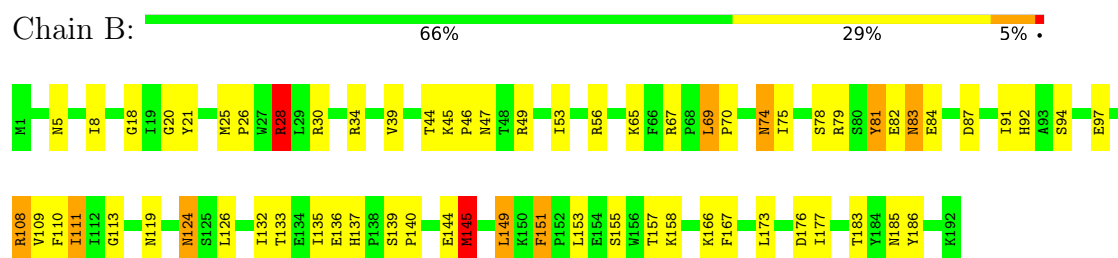
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	77.05 Å 67.09 Å 38.54 Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85	Depositor
% Data completeness (in resolution range)	97.6 (10.00-1.85)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3659	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: MES, TQ6, 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	1.55	10/1673 (0.6%)	2.04	58/2267 (2.6%)
1	B	1.51	8/1692 (0.5%)	1.96	48/2292 (2.1%)
All	All	1.53	18/3365 (0.5%)	2.00	106/4559 (2.3%)

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	4
1	B	0	1
All	All	0	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ILE	C-N	-6.96	1.25	1.33
1	B	92	HIS	N-CA	6.15	1.53	1.46
1	A	5	ASN	N-CA	6.08	1.53	1.46
1	A	36	PHE	N-CA	5.87	1.53	1.46
1	B	133	THR	CA-C	5.87	1.60	1.52
1	B	186	TYR	N-CA	5.80	1.53	1.46
1	B	8	ILE	CA-CB	5.70	1.61	1.54
1	A	111	ILE	N-CA	5.67	1.53	1.46
1	A	35	TYR	CA-C	5.57	1.59	1.52
1	A	133	THR	N-CA	5.36	1.52	1.46
1	A	185	ASN	CA-C	5.36	1.58	1.52
1	B	113	GLY	N-CA	5.23	1.50	1.45
1	A	129	HIS	N-CA	5.16	1.52	1.45
1	A	125	SER	C-O	5.16	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	GLU	N-CA	5.16	1.52	1.45
1	B	83	ASN	CA-CB	-5.11	1.45	1.53
1	B	132	ILE	CA-CB	5.08	1.60	1.54
1	A	50	ASN	N-CA	5.02	1.51	1.45

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	CD-NE-CZ	11.27	140.18	124.40
1	A	151	PHE	CA-CB-CG	10.62	124.42	113.80
1	B	151[A]	PHE	CA-CB-CG	10.48	124.28	113.80
1	B	151[B]	PHE	CA-CB-CG	10.48	124.28	113.80
1	A	108	ARG	NE-CZ-NH1	-9.54	111.96	121.50
1	A	8	ILE	CA-C-O	-9.18	110.20	120.84
1	B	145	MET	N-CA-C	8.22	121.75	108.76
1	A	67	ARG	CD-NE-CZ	8.19	135.87	124.40
1	A	111	ILE	CA-C-O	-8.09	111.57	120.71
1	B	97	GLU	CA-C-O	-7.99	112.09	120.55
1	A	154	GLU	CA-CB-CG	7.86	129.82	114.10
1	B	119	ASN	CB-CA-C	7.74	124.95	110.63
1	A	49	ARG	NE-CZ-NH2	-7.62	112.34	119.20
1	B	67	ARG	CB-CA-C	7.53	120.21	108.84
1	B	97	GLU	O-C-N	7.45	130.02	122.12
1	B	87	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	8	ILE	O-C-N	7.12	130.47	122.93
1	A	120	GLU	CA-CB-CG	7.09	128.28	114.10
1	A	84	GLU	CB-CG-CD	7.07	124.61	112.60
1	B	91	ILE	O-C-N	6.95	130.54	123.10
1	B	47	ASN	OD1-CG-ND2	6.95	129.55	122.60
1	B	75	ILE	CA-C-O	-6.92	112.83	120.72
1	B	149	LEU	O-C-N	6.90	131.16	123.16
1	A	67	ARG	CB-CA-C	6.87	119.18	108.88
1	B	145	MET	CA-CB-CG	6.84	127.78	114.10
1	A	128	SER	CA-C-O	-6.76	111.61	119.24
1	A	165	GLN	O-C-N	6.64	129.16	122.12
1	A	28	ARG	CD-NE-CZ	6.63	133.68	124.40
1	A	179	GLU	CB-CG-CD	6.63	123.87	112.60
1	A	151	PHE	O-C-N	6.52	129.29	121.60
1	A	54	MET	CA-C-O	-6.50	114.06	121.40
1	B	145	MET	CB-CG-SD	-6.47	93.28	112.70
1	B	135	ILE	O-C-N	6.45	129.77	122.93
1	A	192	LYS	CA-CB-CG	6.36	126.81	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ASN	CA-CB-CG	6.27	118.87	112.60
1	B	79	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	A	17	LEU	CB-CA-C	6.11	120.05	111.86
1	B	84	GLU	CB-CG-CD	6.11	122.99	112.60
1	A	160	PRO	CB-CA-C	-6.11	102.95	110.95
1	A	123	ASN	OD1-CG-ND2	6.10	128.70	122.60
1	A	34	ARG	CD-NE-CZ	6.08	132.91	124.40
1	A	35	TYR	O-C-N	6.01	128.26	122.07
1	B	108	ARG	NE-CZ-NH1	6.00	127.50	121.50
1	A	52	VAL	CA-C-O	-6.00	114.12	120.48
1	B	157	THR	CA-C-O	-5.98	113.90	120.36
1	B	18	GLY	CA-C-O	-5.96	116.15	121.64
1	B	81	TYR	O-C-N	5.92	129.57	122.94
1	B	49	ARG	O-C-N	5.92	129.91	123.10
1	B	167	PHE	CA-CB-CG	5.85	119.65	113.80
1	B	149	LEU	CA-C-O	-5.81	114.24	120.92
1	B	44	THR	CA-C-O	-5.80	113.30	119.97
1	A	69	LEU	CB-CA-C	5.77	119.16	109.69
1	A	175	ASP	CA-C-O	-5.77	114.47	121.28
1	B	39	VAL	CA-C-O	-5.76	114.75	120.85
1	B	133	THR	CA-CB-OG1	-5.75	100.98	109.60
1	B	56	ARG	CD-NE-CZ	5.74	132.43	124.40
1	B	18	GLY	O-C-N	5.73	128.81	122.96
1	A	42[A]	ARG	CA-C-O	5.70	127.46	121.19
1	A	42[B]	ARG	CA-C-O	5.70	127.46	121.19
1	A	82	GLU	CA-C-O	-5.69	114.54	121.36
1	B	109	VAL	CA-C-O	-5.66	114.45	120.39
1	A	108	ARG	NH1-CZ-NH2	5.61	126.60	119.30
1	B	69	LEU	CB-CA-C	5.61	118.42	109.62
1	A	67	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	A	87	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	83	ASN	CB-CA-C	5.53	119.35	110.29
1	A	108	ARG	CB-CG-CD	-5.53	98.59	111.30
1	A	39	VAL	O-C-N	5.52	127.52	121.83
1	B	56	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	A	187	THR	O-C-N	5.50	129.82	123.17
1	A	147	THR	N-CA-CB	-5.47	101.31	110.83
1	B	25	MET	N-CA-C	-5.45	102.78	109.65
1	B	111[A]	ILE	CA-C-O	-5.44	114.11	120.75
1	B	111[B]	ILE	CA-C-O	-5.44	114.11	120.75
1	A	126	LEU	O-C-N	5.43	128.95	122.27
1	A	45	LYS	CA-C-N	5.43	126.63	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	LYS	C-N-CA	5.43	126.63	119.84
1	A	150	LYS	CA-CB-CG	5.38	124.86	114.10
1	A	115	ALA	O-C-N	5.33	127.64	122.09
1	B	56	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	A	84	GLU	N-CA-CB	-5.31	101.59	110.99
1	B	158	LYS	CA-C-O	-5.29	114.66	120.69
1	B	183	THR	CA-CB-OG1	-5.29	101.67	109.60
1	B	82	GLU	N-CA-C	-5.27	102.25	110.42
1	B	177	ILE	CA-C-O	-5.27	115.59	121.23
1	A	118	TYR	O-C-N	5.26	127.49	122.07
1	A	74	ASN	CA-C-O	-5.26	114.70	120.43
1	A	28	ARG	N-CA-CB	5.20	119.35	110.87
1	B	70	PRO	CB-CA-C	-5.20	104.57	111.23
1	A	24	LYS	CA-CB-CG	5.19	124.49	114.10
1	B	75	ILE	O-C-N	5.17	128.41	123.14
1	A	83	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	183	THR	CA-CB-OG1	-5.16	101.87	109.60
1	A	46	PRO	N-CA-C	5.15	123.09	112.47
1	A	139	SER	N-CA-CB	-5.11	103.70	111.21
1	A	2	LEU	N-CA-CB	-5.10	102.54	110.55
1	B	28	ARG	N-CA-CB	5.10	119.18	110.87
1	B	97	GLU	CB-CG-CD	5.08	121.24	112.60
1	A	170	ASP	CA-CB-CG	5.08	117.67	112.60
1	B	69	LEU	N-CA-C	-5.07	102.17	109.48
1	A	192	LYS	N-CA-CB	5.07	119.11	110.50
1	B	83	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	5	ASN	N-CA-C	-5.03	102.26	110.20
1	A	47	ASN	CB-CA-C	5.03	118.12	111.14
1	B	110	PHE	N-CA-CB	5.01	118.42	110.55
1	A	137	HIS	O-C-N	5.01	125.36	121.85

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30[A]	ARG	Sidechain
1	A	30[B]	ARG	Sidechain
1	A	42[A]	ARG	Sidechain
1	A	42[B]	ARG	Sidechain
1	B	34	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	1586	0	1611	22	0
1	B	1594	0	1611	26	0
2	A	35	0	14	1	0
2	B	39	0	18	0	0
3	A	25	0	19	0	0
3	B	25	0	19	0	0
4	A	12	0	13	0	0
4	B	12	0	13	1	0
5	A	152	0	0	3	0
5	B	179	0	0	4	0
All	All	3659	0	3318	48	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 7.

All (48) 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:B:5[B]:ASN:ND2	5:B:283:HOH:O	1.84	1.07
1:B:5[B]:ASN:OD1	5:B:297:HOH:O	1.99	0.79
1:B:124:ASN:HD22	1:B:126:LEU:H	1.34	0.74
1:B:28:ARG:HH11	1:B:30:ARG:HG2	1.53	0.73
1:B:5[B]:ASN:ND2	1:B:108:ARG:HH11	1.87	0.72
1:B:5[B]:ASN:HD21	1:B:108:ARG:HH11	1.40	0.68
1:A:18:GLY:HA3	1:A:145:MET:HE3	1.77	0.67
1:A:13:LEU:HD23	1:A:145:MET:HE1	1.83	0.61
1:B:53:ILE:HB	1:B:111[A]:ILE:HD13	1.83	0.61
1:B:21:TYR:HB2	1:B:145:MET:HA	1.84	0.60
1:B:83:ASN:ND2	1:B:94:SER:H	2.00	0.59
1:B:137:HIS:HD2	1:B:139:SER:H	1.49	0.59
1:A:1:MET:HE1	1:A:106:VAL:HB	1.84	0.57
1:A:176:ASP:H	1:A:185:ASN:HD21	1.52	0.57
1:A:117:ILE:HG23	1:A:121[A]:LEU:HD12	1.87	0.55
1:B:69:LEU:HD22	4:B:202:MES:H82	1.88	0.54
1:A:41[B]:THR:HG21	5:A:446:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:HIS:CD2	1:B:139:SER:H	2.27	0.53
1:B:83:ASN:HD21	1:B:94:SER:H	1.55	0.53
1:B:151[A]:PHE:HB2	1:B:153:LEU:HD13	1.91	0.52
1:A:120:GLU:HG2	2:A:193:NDP:H61A	1.76	0.51
1:A:25:MET:HE2	1:A:27:TRP:HE1	1.76	0.51
1:B:176:ASP:H	1:B:185:ASN:ND2	2.08	0.50
1:A:176:ASP:H	1:A:185:ASN:ND2	2.10	0.49
1:A:65:LYS:H	1:A:65:LYS:CD	2.27	0.47
1:A:64:GLN:HG2	1:A:65:LYS:HE3	1.97	0.46
1:A:159:GLN:HE21	1:A:163:GLU:HG3	1.81	0.46
1:B:78:SER:HB3	1:B:81:TYR:CG	2.51	0.45
1:A:108:ARG:HD2	5:A:485:HOH:O	2.16	0.45
1:B:5[B]:ASN:ND2	1:B:108:ARG:NH1	2.62	0.45
1:B:176:ASP:H	1:B:185:ASN:HD21	1.64	0.44
1:A:21:TYR:O	1:A:24:LYS:HD2	2.18	0.44
1:A:18:GLY:HA3	1:A:145:MET:CE	2.45	0.44
1:B:20:GLY:HA2	1:B:26:PRO:HD3	1.99	0.44
1:B:45:LYS:HA	1:B:46:PRO:HD3	1.86	0.43
1:A:16:ALA:HB3	5:A:260[B]:HOH:O	2.19	0.43
1:B:30:ARG:NH1	5:B:339:HOH:O	2.52	0.43
1:A:20:GLY:HA2	1:A:26:PRO:HD3	2.01	0.42
1:A:20:GLY:O	1:A:145:MET:HG3	2.19	0.42
1:B:124:ASN:ND2	1:B:126:LEU:H	2.09	0.42
1:A:137:HIS:CD2	1:A:143:ILE:HD11	2.55	0.42
1:B:144:GLU:HB2	5:B:384:HOH:O	2.19	0.42
1:A:42[A]:ARG:NH1	1:A:170:ASP:H	2.18	0.41
1:B:139:SER:HA	1:B:140:PRO:HD2	1.86	0.41
1:A:29:LEU:O	1:A:33[A]:ILE:HG12	2.20	0.41
1:B:149:LEU:HD22	1:B:151[A]:PHE:CZ	2.56	0.41
1:A:29:LEU:O	1:A:33[B]:ILE:HG13	2.21	0.41
1:B:149:LEU:HD22	1:B:151[A]:PHE:CE1	2.56	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/192 (104%)	195 (98%)	4 (2%)	1 (0%)	24	13
1	B	202/192 (105%)	196 (97%)	6 (3%)	0	100	100
All	All	402/384 (105%)	391 (97%)	10 (2%)	1 (0%)	36	31

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	184/177 (104%)	175 (95%)	9 (5%)	22	8
1	B	186/177 (105%)	176 (95%)	10 (5%)	20	7
All	All	370/354 (104%)	351 (95%)	19 (5%)	22	7

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	63	PRO
1	A	65	LYS
1	A	74	ASN
1	A	102	LEU
1	A	103	VAL
1	A	120	GLU
1	A	154	GLU
1	A	192	LYS
1	B	28	ARG
1	B	65[A]	LYS
1	B	65[B]	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	74	ASN
1	B	124	ASN
1	B	145	MET
1	B	155	SER
1	B	166	LYS
1	B	173[A]	LEU
1	B	173[B]	LEU

Sometimes 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	123	ASN
1	A	159	GLN
1	A	185	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 [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
3	TQ6	B	196	-	28,28,28	1.57	4 (14%)	37,39,39	2.34	16 (43%)
2	NDP	A	193	-	37,37,52	2.08	9 (24%)	54,57,80	1.72	13 (24%)
4	MES	B	202	-	12,12,12	7.62	6 (50%)	15,16,16	1.79	2 (13%)
2	NDP	B	195	-	42,42,52	1.70	10 (23%)	60,65,80	1.38	13 (21%)
4	MES	A	201	-	12,12,12	7.76	6 (50%)	15,16,16	2.22	6 (40%)
3	TQ6	A	194	-	28,28,28	1.84	4 (14%)	37,39,39	2.35	17 (45%)

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
3	TQ6	B	196	-	-	2/8/16/16	0/4/4/4
2	NDP	A	193	-	-	4/27/43/77	0/3/3/5
4	MES	B	202	-	-	3/6/14/14	0/1/1/1
2	NDP	B	195	-	-	1/27/56/77	0/4/4/5
4	MES	A	201	-	-	3/6/14/14	0/1/1/1
3	TQ6	A	194	-	-	4/8/16/16	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	MES	C8-S	-25.85	1.41	1.77
4	B	202	MES	C8-S	-25.50	1.41	1.77
2	A	193	NDP	P2B-O2B	7.16	1.72	1.59
3	A	194	TQ6	C8-N4	6.24	1.47	1.37
2	A	193	NDP	PA-O3	-5.61	1.53	1.59
3	B	196	TQ6	C8-N4	5.20	1.45	1.37
3	A	194	TQ6	C35-N34	4.71	1.54	1.46
2	A	193	NDP	PN-O3	4.35	1.64	1.59
2	B	195	NDP	PN-O3	4.04	1.63	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	MES	C5-N4	3.74	1.57	1.46
2	B	195	NDP	C3B-C2B	3.68	1.61	1.53
2	B	195	NDP	C3B-C4B	3.61	1.62	1.53
2	B	195	NDP	P2B-O2B	3.60	1.65	1.59
4	A	201	MES	C7-N4	3.42	1.55	1.47
4	B	202	MES	C5-N4	3.33	1.55	1.46
4	A	201	MES	O1-C6	3.25	1.55	1.42
2	B	195	NDP	P2B-O2X	-3.17	1.43	1.54
3	B	196	TQ6	C33-N34	3.14	1.52	1.46
3	A	194	TQ6	C24-C25	3.02	1.45	1.39
2	A	193	NDP	P2B-O2X	-3.01	1.43	1.54
4	A	201	MES	O1-C2	2.83	1.53	1.42
4	B	202	MES	O1-C6	2.81	1.53	1.42
4	B	202	MES	C3-N4	2.76	1.54	1.46
4	B	202	MES	C7-N4	2.72	1.53	1.47
4	B	202	MES	O1-C2	2.62	1.52	1.42
2	B	195	NDP	PA-O1A	-2.58	1.41	1.50
2	B	195	NDP	PA-O3	2.46	1.62	1.59
2	A	193	NDP	C2A-N1A	2.42	1.38	1.33
3	A	194	TQ6	C33-N34	-2.40	1.42	1.46
2	B	195	NDP	PA-O2A	-2.37	1.44	1.55
4	A	201	MES	C3-N4	2.36	1.53	1.46
2	B	195	NDP	C6A-N1A	2.31	1.42	1.35
2	A	193	NDP	C3B-C2B	2.26	1.57	1.53
3	B	196	TQ6	C1-N2	-2.22	1.29	1.33
2	A	193	NDP	C4A-N9A	-2.19	1.33	1.37
3	B	196	TQ6	C3-N2	-2.19	1.31	1.35
2	B	195	NDP	O4B-C1B	-2.18	1.37	1.42
2	A	193	NDP	P2B-O3X	-2.12	1.46	1.54
2	A	193	NDP	PN-O2N	-2.11	1.45	1.55

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	196	TQ6	N11-C3-N2	5.98	126.18	117.22
3	A	194	TQ6	C32-C33-N34	5.64	120.60	109.93
4	A	201	MES	O1S-S-C8	5.54	115.10	106.73
3	B	196	TQ6	N4-C3-N2	-5.49	120.22	127.21
3	A	194	TQ6	C33-N34-C25	5.21	132.31	118.11
4	B	202	MES	O1S-S-C8	5.01	114.30	106.73
3	A	194	TQ6	N4-C3-N2	-4.26	121.79	127.21
2	A	193	NDP	O2B-P2B-O1X	-4.15	94.53	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	196	TQ6	O37-C32-C33	-3.99	103.18	111.77
2	A	193	NDP	P2B-O2B-C2B	-3.91	112.99	123.43
3	A	194	TQ6	O37-C36-C35	-3.79	103.60	111.77
2	A	193	NDP	O2X-P2B-O1X	3.76	125.50	110.83
3	B	196	TQ6	C35-N34-C33	3.69	119.87	111.57
3	A	194	TQ6	C24-C23-C22	3.57	124.59	120.48
3	A	194	TQ6	N12-C1-N2	-3.38	108.01	117.11
3	A	194	TQ6	C7-C1-N12	3.29	128.56	122.70
2	A	193	NDP	C1B-N9A-C8A	-3.23	119.92	127.09
4	A	201	MES	C2-C3-N4	3.23	115.02	110.12
3	B	196	TQ6	C32-C33-N34	-3.19	103.89	109.93
2	B	195	NDP	C2B-C3B-C4B	-3.02	95.50	101.99
3	B	196	TQ6	C26-C25-N34	-2.97	117.27	121.39
4	B	202	MES	O2S-S-O1S	-2.79	104.75	113.82
2	B	195	NDP	O4D-C1D-C2D	-2.78	100.97	105.76
3	B	196	TQ6	C24-C25-N34	2.77	125.24	121.39
2	A	193	NDP	O3B-C3B-C2B	2.75	118.89	111.19
2	B	195	NDP	C3B-C2B-C1B	-2.75	97.55	102.81
2	A	193	NDP	O2B-C2B-C1B	-2.74	100.43	110.05
3	B	196	TQ6	N11-C3-N4	-2.73	113.53	117.79
3	B	196	TQ6	C9-C8-C7	2.73	124.30	119.31
3	A	194	TQ6	C27-C22-C23	-2.72	114.42	118.85
4	A	201	MES	O2S-S-O1S	-2.69	105.08	113.82
2	A	193	NDP	N6A-C6A-N1A	2.65	124.28	118.38
3	A	194	TQ6	C27-C26-C25	2.60	123.60	120.30
2	A	193	NDP	O3B-C3B-C4B	-2.57	103.69	111.08
3	B	196	TQ6	C26-C27-C22	2.54	123.42	120.48
3	A	194	TQ6	C5-C6-C7	2.52	123.52	120.53
2	B	195	NDP	C2B-C1B-N9A	-2.51	109.62	113.75
3	B	196	TQ6	C3-N2-C1	2.45	123.72	116.72
3	B	196	TQ6	C36-C35-N34	2.44	114.55	109.93
2	B	195	NDP	O4B-C4B-C3B	-2.42	100.34	105.15
2	B	195	NDP	O4B-C1B-C2B	2.42	110.75	106.59
3	A	194	TQ6	C26-C25-C24	-2.40	114.60	119.18
2	B	195	NDP	C1D-C2D-C3D	-2.40	97.80	101.63
2	A	193	NDP	O3X-P2B-O2X	2.37	116.68	107.80
2	B	195	NDP	O2X-P2B-O1X	2.37	120.05	110.83
3	A	194	TQ6	C22-S21-C6	-2.34	99.21	103.71
3	B	196	TQ6	C23-C24-C25	2.29	123.20	120.30
2	A	193	NDP	C4A-N9A-C1B	2.28	131.97	126.63
2	A	193	NDP	C4A-N9A-C8A	2.26	108.11	105.74
4	A	201	MES	O2S-S-C8	2.26	110.14	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	193	NDP	C2B-C3B-C4B	-2.25	97.15	101.99
3	A	194	TQ6	C26-C25-N34	2.24	124.50	121.39
3	A	194	TQ6	C7-C8-N4	-2.21	118.15	122.45
4	A	201	MES	O3S-S-C8	2.19	110.30	106.00
2	B	195	NDP	C4A-C5A-N7A	-2.19	108.08	110.58
2	B	195	NDP	C5A-N7A-C8A	2.18	106.88	103.45
3	B	196	TQ6	C7-C1-N12	2.14	126.50	122.70
4	A	201	MES	O3S-S-O2S	-2.13	106.07	111.40
3	B	196	TQ6	C10-C9-C8	-2.12	117.19	120.09
3	A	194	TQ6	C35-N34-C25	-2.12	112.32	118.11
3	B	196	TQ6	N12-C1-N2	-2.12	111.41	117.11
2	A	193	NDP	C6A-C5A-N7A	-2.08	128.08	132.09
2	B	195	NDP	O2B-P2B-O1X	-2.07	101.97	109.33
3	A	194	TQ6	C9-C10-C5	-2.06	117.83	121.00
3	A	194	TQ6	C23-C22-S21	2.03	126.46	120.32
2	B	195	NDP	P2B-O2B-C2B	-2.02	118.03	123.43
2	B	195	NDP	O3D-C3D-C2D	-2.01	107.22	111.97

There are no chirality outliers.

All (17) torsion outliers are listed below:

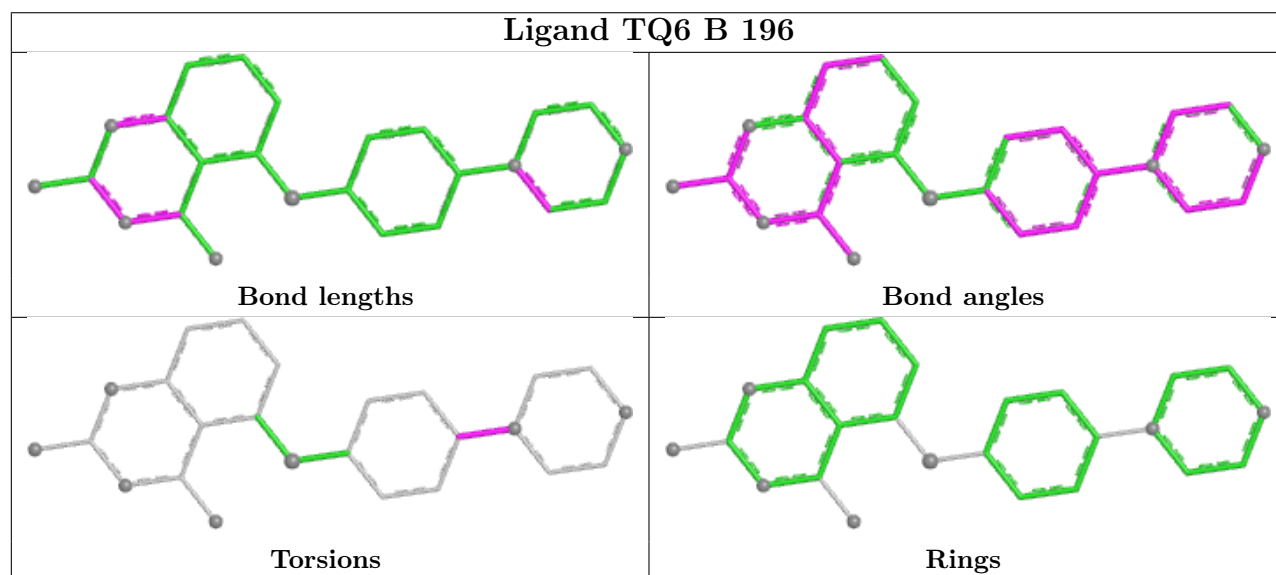
Mol	Chain	Res	Type	Atoms
2	A	193	NDP	C5D-O5D-PN-O3
2	A	193	NDP	C5D-O5D-PN-O2N
2	A	193	NDP	O4D-C4D-C5D-O5D
4	A	201	MES	C7-C8-S-O1S
4	A	201	MES	C7-C8-S-O3S
4	B	202	MES	C7-C8-S-O2S
3	A	194	TQ6	C24-C25-N34-C33
3	A	194	TQ6	C24-C25-N34-C35
3	A	194	TQ6	C26-C25-N34-C33
3	A	194	TQ6	C26-C25-N34-C35
3	B	196	TQ6	C24-C25-N34-C33
3	B	196	TQ6	C26-C25-N34-C33
4	A	201	MES	C7-C8-S-O2S
4	B	202	MES	C7-C8-S-O1S
2	A	193	NDP	C3D-C4D-C5D-O5D
4	B	202	MES	C7-C8-S-O3S
2	B	195	NDP	C2B-O2B-P2B-O3X

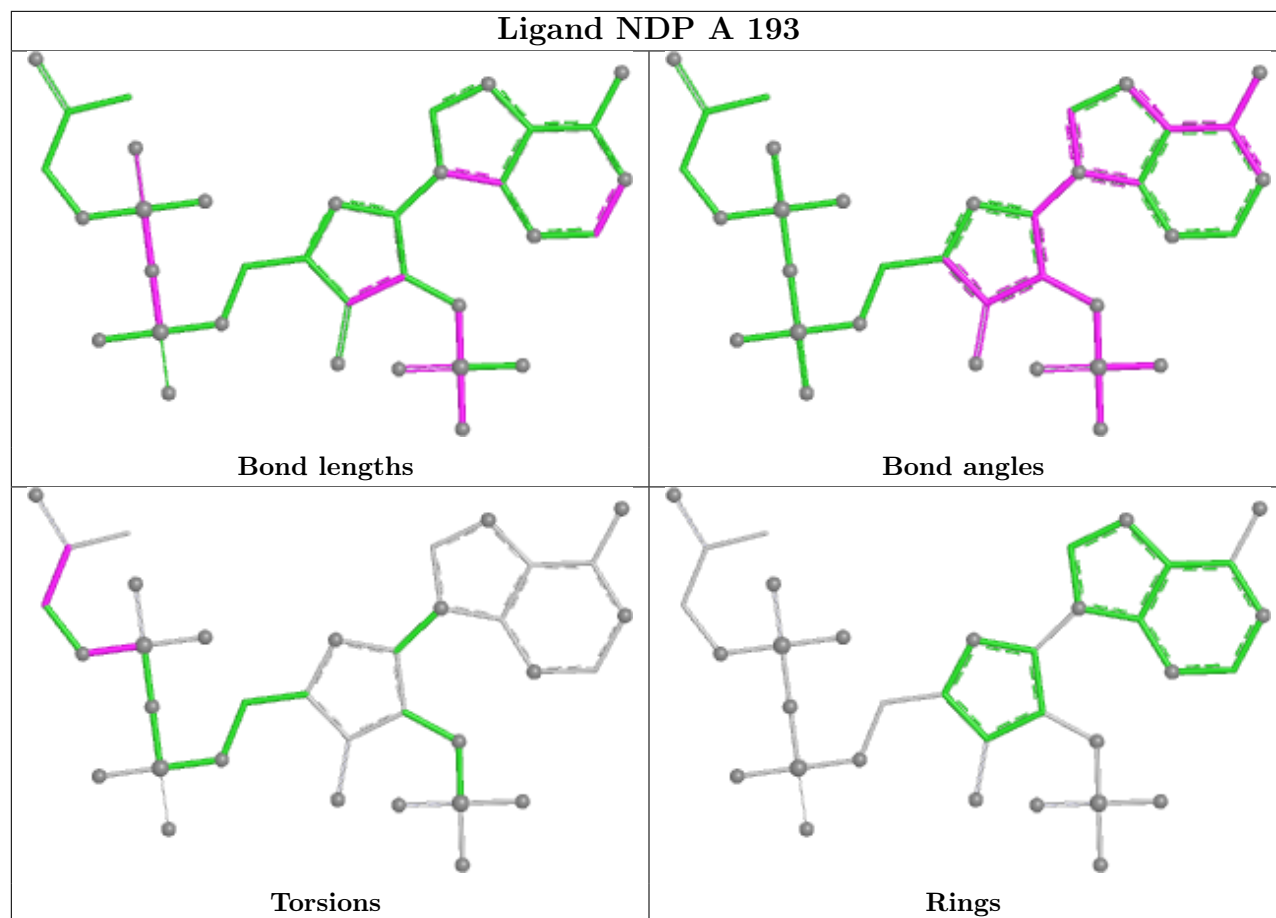
There are no ring outliers.

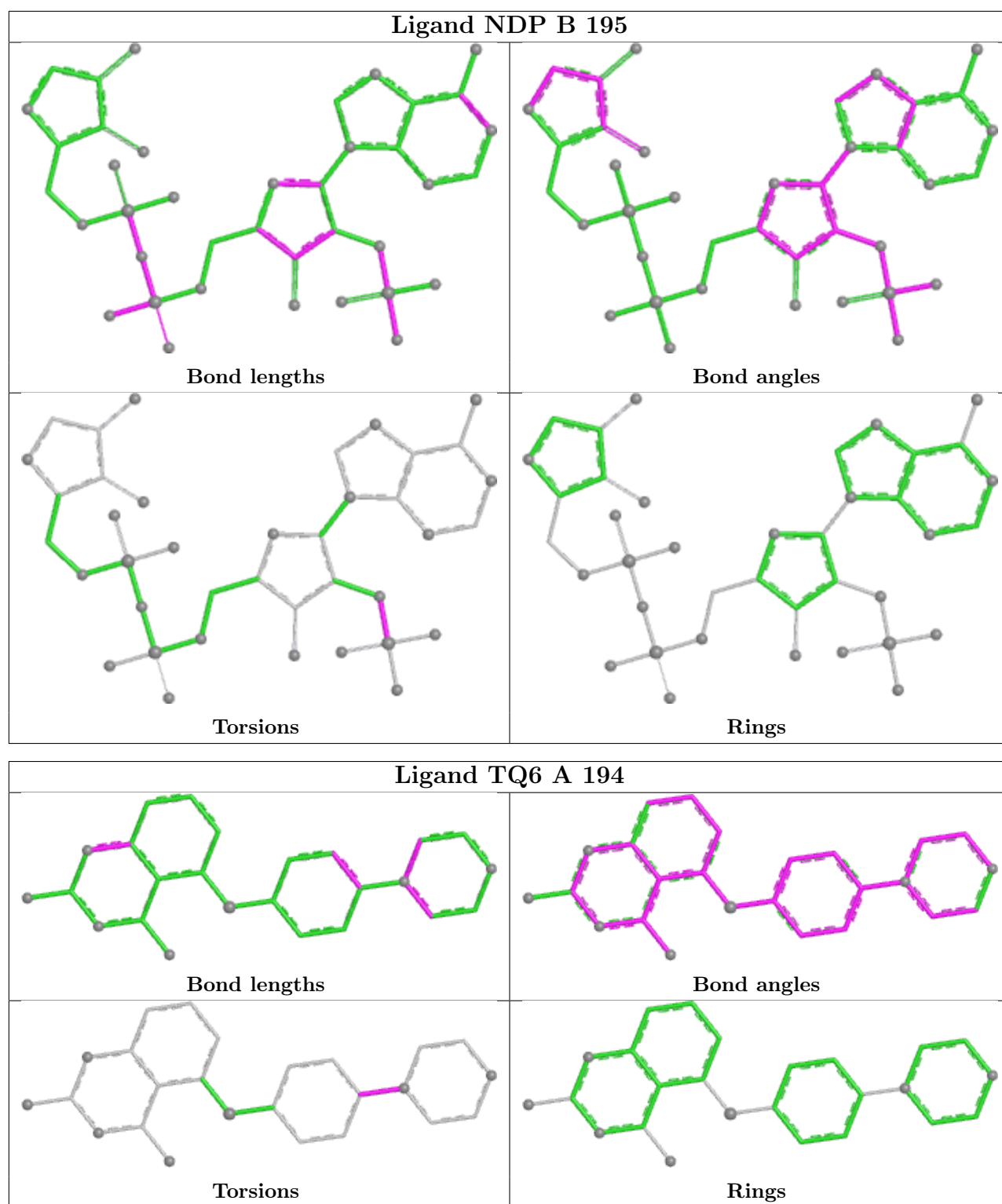
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	193	NDP	1	0
4	B	202	MES	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 ⓘ

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 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.