



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:32 PM UTC

PDB ID : 1IA3 / pdb_00001ia3
Title : Candida albicans dihydrofolate reductase complex in which the dihydronicotinamide moiety of dihydro-nicotinamide-adenine-dinucleotide phosphate (NADPH) is displaced by 5-[(4-TERT-BUTYLPHENYL)SULFANYL]-2,4-Q UINAZOLINEDIAMINE (GW995)
Authors : Whitlow, M.; Howard, A.J.; Kuyper, L.F.
Deposited on : 2001-03-22
Resolution : 1.78 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

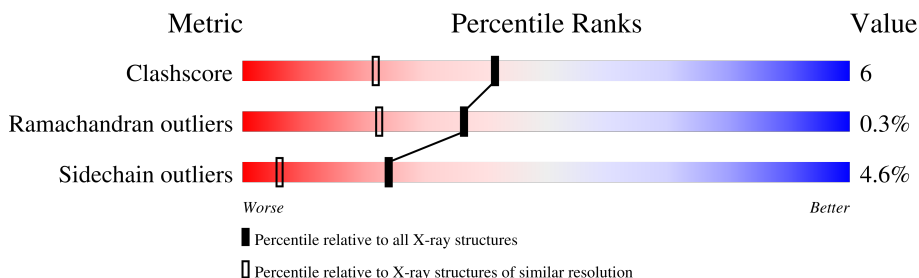
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)

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](#)

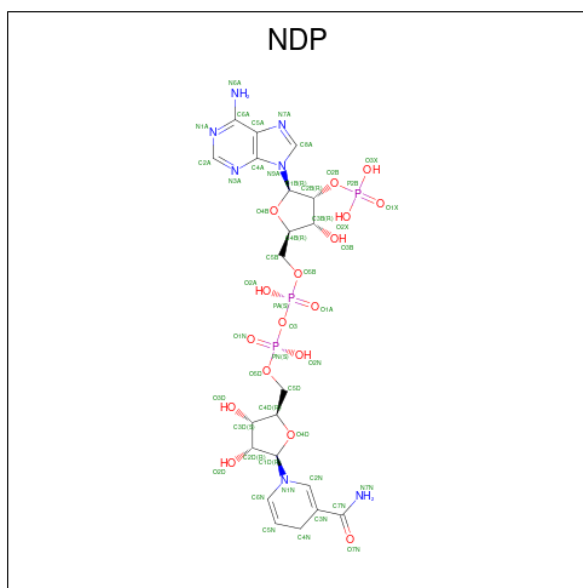
There are 5 unique types of molecules in this entry. The entry contains 3671 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

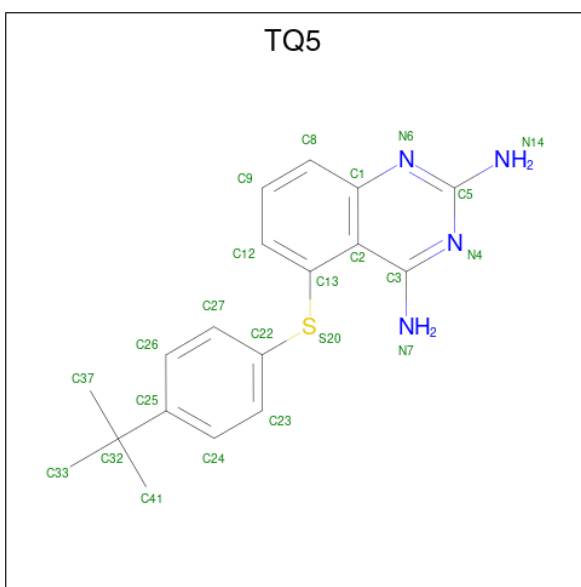
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	11	0
			1590	1019	271	296	4			
1	B	192	Total	C	N	O	S	0	11	0
			1591	1021	265	301	4			

- 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
			35	13	5	14	3		

- Molecule 3 is 5-[4-TERT-BUTYLPHENYLSULFANYL]-2,4-QUINAZOLINEDIAMINE (CCD ID: TQ5) (formula: $C_{18}H_{20}N_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			23	18	4	1		
3	B	1	Total	C	N	S	0	0
			23	18	4	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		

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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	156	Total	O	0	7
			163	163		
5	B	183	Total	O	0	4
			187	187		

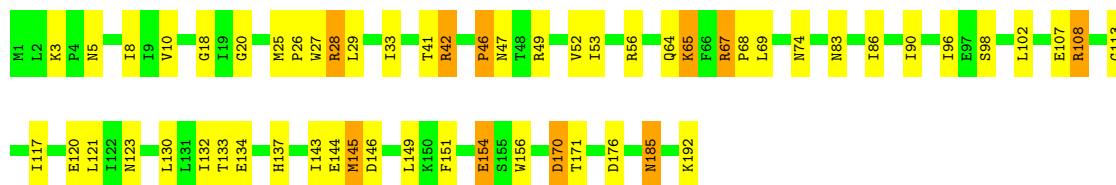
3 Residue-property plots

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.

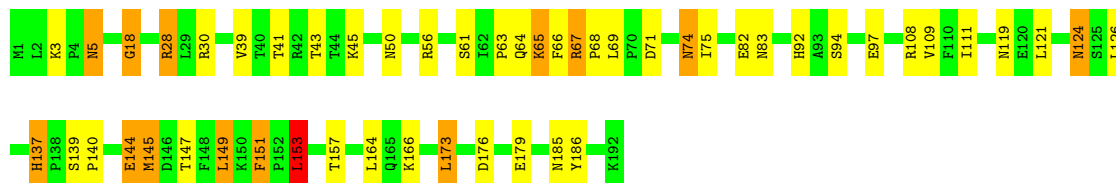
• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain A: 



• Molecule 1: DIHYDROFOLATE REDUCTASE

Chain B: 



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	76.91Å 67.28Å 38.49Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	10.00 – 1.78	Depositor
% Data completeness (in resolution range)	84.6 (10.00-1.78)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3671	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: TQ5, NDP, MES

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	1.51	5/1682 (0.3%)	1.94	34/2279 (1.5%)
1	B	1.54	4/1683 (0.2%)	1.83	33/2278 (1.4%)
All	All	1.53	9/3365 (0.3%)	1.88	67/4557 (1.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	TYR	N-CA	6.52	1.53	1.46
1	A	3	LYS	C-O	6.35	1.27	1.23
1	B	109	VAL	C-O	5.83	1.30	1.24
1	A	185	ASN	CA-C	5.55	1.59	1.52
1	A	52	VAL	C-N	-5.33	1.25	1.33
1	B	41	THR	CA-CB	5.21	1.61	1.53
1	B	92	HIS	N-CA	5.16	1.52	1.46
1	A	133	THR	N-CA	5.05	1.52	1.46
1	A	107	GLU	CA-CB	-5.01	1.47	1.53

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ARG	NE-CZ-NH2	-9.67	110.50	119.20
1	A	28	ARG	CD-NE-CZ	9.54	137.75	124.40
1	B	151	PHE	CA-CB-CG	9.39	123.19	113.80
1	A	154	GLU	CA-CB-CG	8.90	131.89	114.10
1	A	108	ARG	NE-CZ-NH1	-8.58	112.92	121.50
1	A	185	ASN	OD1-CG-ND2	8.30	130.90	122.60
1	A	151	PHE	CA-CB-CG	7.99	121.79	113.80
1	B	67	ARG	CB-CA-C	7.93	120.81	108.84
1	A	83	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	B	75	ILE	O-C-N	7.50	131.36	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	GLU	CB-CG-CD	7.50	125.34	112.60
1	B	137	HIS	O-C-N	7.37	127.01	121.85
1	A	52	VAL	CA-C-O	-7.22	112.82	120.48
1	B	74	ASN	CA-CB-CG	7.13	119.73	112.60
1	A	170	ASP	CA-CB-CG	7.04	119.64	112.60
1	B	3	LYS	O-C-N	6.99	126.84	121.88
1	B	75	ILE	CA-C-O	-6.85	113.20	120.39
1	B	149	LEU	O-C-N	6.84	131.10	123.16
1	A	67	ARG	CB-CA-C	6.72	119.29	108.87
1	B	119	ASN	CB-CA-C	6.59	123.33	110.67
1	B	145	MET	N-CA-CB	-6.59	99.21	111.13
1	A	192	LYS	CA-CB-CG	6.58	127.27	114.10
1	A	8	ILE	O-C-N	6.57	129.90	122.93
1	B	153	LEU	CB-CA-C	6.55	124.15	110.32
1	B	67	ARG	CD-NE-CZ	6.55	133.56	124.40
1	A	56	ARG	CD-NE-CZ	6.52	133.52	124.40
1	A	123	ASN	OD1-CG-ND2	6.47	129.07	122.60
1	A	49	ARG	NH1-CZ-NH2	6.46	127.70	119.30
1	B	151	PHE	CB-CA-C	6.39	117.57	108.68
1	A	5	ASN	CA-C-O	-6.34	113.46	120.69
1	A	47	ASN	CB-CA-C	6.31	119.91	111.14
1	B	71	ASP	O-C-N	6.15	129.69	122.00
1	B	157	THR	O-C-N	6.14	130.50	123.31
1	B	82	GLU	CA-C-O	-6.10	114.08	121.28
1	B	119	ASN	OD1-CG-ND2	-6.05	116.55	122.60
1	B	108	ARG	NE-CZ-NH1	6.00	127.50	121.50
1	B	50	ASN	OD1-CG-ND2	5.98	128.58	122.60
1	B	109	VAL	CA-C-O	-5.93	114.16	120.39
1	A	3	LYS	CB-CA-C	-5.87	107.03	111.20
1	B	108	ARG	NE-CZ-NH2	-5.86	113.93	119.20
1	B	147	THR	CA-CB-CG2	5.84	120.42	110.50
1	B	149	LEU	CA-C-O	-5.83	114.22	120.92
1	B	56	ARG	CD-NE-CZ	5.83	132.56	124.40
1	A	149	LEU	O-C-N	5.80	129.86	123.01
1	B	18	GLY	CA-C-O	-5.73	116.37	121.64
1	A	134	GLU	O-C-N	5.71	129.73	123.22
1	B	39	VAL	CA-C-O	-5.62	114.89	120.85
1	A	90	ILE	O-C-N	5.42	129.05	123.20
1	A	113	GLY	CA-C-O	-5.40	117.73	122.16
1	A	10	VAL	O-C-N	5.38	128.69	122.82
1	B	97	GLU	CB-CG-CD	5.35	121.69	112.60
1	B	43	THR	CA-CB-OG1	-5.34	101.59	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	GLU	N-CA-CB	5.33	119.22	110.90
1	B	147	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	42[A]	ARG	N-CA-C	5.17	117.73	110.23
1	A	42[B]	ARG	N-CA-C	5.17	117.73	110.23
1	A	132	ILE	CA-C-N	-5.17	115.32	122.30
1	A	132	ILE	C-N-CA	-5.17	115.32	122.30
1	A	144	GLU	N-CA-CB	5.16	117.95	109.95
1	A	171	THR	CA-CB-OG1	-5.14	101.89	109.60
1	B	82	GLU	N-CA-C	-5.10	101.96	110.17
1	B	45	LYS	CA-CB-CG	5.09	124.28	114.10
1	A	98	SER	CA-CB-OG	-5.08	100.94	111.10
1	B	61	SER	CB-CA-C	5.04	119.99	109.95
1	A	108	ARG	CB-CG-CD	-5.04	99.72	111.30
1	A	46	PRO	N-CA-C	5.03	122.83	112.47
1	A	146	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

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	1590	0	1613	21	0
1	B	1591	0	1615	22	0
2	A	35	0	14	0	0
2	B	35	0	14	0	0
3	A	23	0	20	1	0
3	B	23	0	20	0	0
4	A	12	0	13	1	0
4	B	12	0	13	1	0
5	A	163	0	0	2	0
5	B	187	0	0	2	0
All	All	3671	0	3322	43	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 6.

All (43) 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:28:ARG:HH11	1:B:30:ARG:HG2	1.44	0.81
1:B:124:ASN:HD22	1:B:126:LEU:H	1.31	0.78
1:A:25:MET:HE2	1:A:27:TRP:HE1	1.53	0.73
1:B:176:ASP:H	1:B:185:ASN:HD21	1.34	0.73
1:A:176:ASP:H	1:A:185:ASN:HD21	1.42	0.66
1:B:83:ASN:ND2	1:B:94:SER:H	1.95	0.64
1:B:137:HIS:HD2	1:B:139:SER:H	1.45	0.64
1:B:176:ASP:H	1:B:185:ASN:ND2	1.95	0.63
1:A:64:GLN:HG2	1:A:65:LYS:HE3	1.81	0.61
1:A:25:MET:HE2	1:A:27:TRP:NE1	2.16	0.60
1:B:137:HIS:CD2	1:B:139:SER:H	2.21	0.59
1:B:83:ASN:HD21	1:B:94:SER:H	1.51	0.58
1:B:69:LEU:HD22	4:B:202:MES:H82	1.85	0.58
1:A:176:ASP:H	1:A:185:ASN:ND2	2.02	0.57
1:B:18:GLY:HA3	1:B:145:MET:HE3	1.89	0.55
1:B:151:PHE:HB2	1:B:153:LEU:HD13	1.89	0.54
1:A:41[B]:THR:HG21	5:A:446:HOH:O	2.08	0.53
1:A:69:LEU:HD22	4:A:201:MES:H82	1.91	0.52
1:A:117:ILE:HG23	1:A:121[A]:LEU:HD12	1.92	0.51
1:A:20:GLY:HA2	1:A:26:PRO:HD3	1.93	0.49
1:B:67:ARG:HA	1:B:68:PRO:C	2.39	0.48
1:A:65:LYS:H	1:A:65:LYS:CD	2.26	0.48
1:A:42[A]:ARG:NH1	1:A:170:ASP:H	2.13	0.47
1:A:137:HIS:CD2	1:A:143:ILE:HD11	2.49	0.47
1:A:33[A]:ILE:HD12	3:A:194:TQ5:HC9	1.98	0.45
1:B:137:HIS:O	1:B:140:PRO:HD3	2.16	0.45
1:A:29:LEU:O	1:A:33[A]:ILE:HG12	2.17	0.45
1:A:53:ILE:HD13	1:A:96:ILE:HG13	1.98	0.44
1:A:67:ARG:HA	1:A:68:PRO:C	2.43	0.43
1:B:149:LEU:HD22	1:B:151:PHE:CZ	2.53	0.43
1:B:144:GLU:HB2	5:B:384:HOH:O	2.19	0.42
1:B:164:LEU:HG	1:B:173[A]:LEU:HD21	2.01	0.42
1:B:65[B]:LYS:HE3	1:B:66:PHE:CE2	2.54	0.42
1:A:28:ARG:HH21	1:A:28:ARG:HB3	1.85	0.42
1:B:111[B]:ILE:HD13	1:B:121:LEU:HG	2.01	0.41
1:A:25:MET:HA	1:A:26:PRO:HD3	1.83	0.41
1:B:5[B]:ASN:ND2	5:B:387:HOH:O	2.53	0.41
1:A:130:LEU:HG	1:A:156:TRP:CZ3	2.56	0.41
1:B:64:GLN:HG2	1:B:65[A]:LYS:NZ	2.36	0.41
1:B:63:PRO:HB3	1:B:65[A]:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLY:HA3	1:A:145:MET:HE3	2.03	0.40
1:A:108:ARG:HD2	5:A:485:HOH:O	2.20	0.40

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	201/192 (105%)	196 (98%)	4 (2%)	1 (0%)	24	11
1	B	201/192 (105%)	198 (98%)	3 (2%)	0	100	100
All	All	402/384 (105%)	394 (98%)	7 (2%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	PRO

5.3.2 Protein sidechains [i](#)

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	185/177 (104%)	178 (96%)	7 (4%)	29	9
1	B	186/177 (105%)	174 (94%)	12 (6%)	15	3
All	All	371/354 (105%)	352 (95%)	19 (5%)	24	5

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

Mol	Chain	Res	Type
1	A	65	LYS
1	A	74	ASN
1	A	86	ILE
1	A	102	LEU
1	A	120	GLU
1	A	145	MET
1	A	154	GLU
1	B	5[A]	ASN
1	B	5[B]	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	144	GLU
1	B	153	LEU
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	89	ASN
1	A	159	GLN
1	A	185	ASN
1	B	83	ASN
1	B	101	ASN
1	B	119	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 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$
2	NDP	A	193	-	37,37,52	1.37	4 (10%)	54,57,80	1.40	9 (16%)
4	MES	B	202	-	12,12,12	7.90	7 (58%)	15,16,16	2.38	5 (33%)
3	TQ5	A	194	-	25,25,25	1.77	5 (20%)	35,37,37	2.48	11 (31%)
4	MES	A	201	-	12,12,12	7.49	6 (50%)	15,16,16	2.39	6 (40%)
2	NDP	B	195	-	37,37,52	1.71	8 (21%)	54,57,80	1.20	5 (9%)
3	TQ5	B	196	-	25,25,25	1.56	3 (12%)	35,37,37	2.39	14 (40%)

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	-	-	3/27/43/77	0/3/3/5
4	MES	B	202	-	-	2/6/14/14	0/1/1/1
3	TQ5	A	194	-	-	0/10/10/10	0/3/3/3
4	MES	A	201	-	-	2/6/14/14	0/1/1/1
2	NDP	B	195	-	-	0/27/43/77	0/3/3/5
3	TQ5	B	196	-	-	0/10/10/10	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	MES	C8-S	-26.35	1.40	1.77
4	A	201	MES	C8-S	-24.75	1.42	1.77
2	B	195	NDP	PN-O3	5.19	1.65	1.59
3	A	194	TQ5	C24-C25	4.58	1.46	1.39
3	B	196	TQ5	C1-N6	4.52	1.44	1.37
4	A	201	MES	C5-N4	4.10	1.58	1.46
2	B	195	NDP	PA-O3	4.06	1.63	1.59
3	A	194	TQ5	C1-N6	3.92	1.43	1.37
4	A	201	MES	O1-C6	3.51	1.56	1.42
4	A	201	MES	O1-C2	3.42	1.55	1.42
3	A	194	TQ5	C3-N4	-3.34	1.27	1.33
2	A	193	NDP	P2B-O2B	3.26	1.65	1.59
4	B	202	MES	C3-N4	3.16	1.55	1.46
3	B	196	TQ5	C3-N4	-3.04	1.28	1.33
4	B	202	MES	C5-N4	3.04	1.55	1.46
4	B	202	MES	O1-C6	3.04	1.54	1.42
3	B	196	TQ5	C5-N4	-2.99	1.30	1.35
4	B	202	MES	O1-C2	2.93	1.54	1.42
2	B	195	NDP	O4B-C1B	-2.90	1.35	1.42
2	B	195	NDP	P2B-O2B	2.77	1.64	1.59
2	A	193	NDP	PA-O1A	-2.77	1.41	1.50
2	A	193	NDP	P2B-O2X	-2.68	1.44	1.54
4	B	202	MES	O2S-S	2.56	1.52	1.45
3	A	194	TQ5	C41-C32	2.52	1.61	1.53
4	B	202	MES	C7-N4	2.50	1.53	1.47
4	A	201	MES	C7-N4	2.49	1.53	1.47
2	A	193	NDP	C2A-N1A	2.38	1.38	1.33
2	B	195	NDP	C5A-C4A	-2.38	1.34	1.39
2	B	195	NDP	PA-O2A	-2.36	1.44	1.55
3	A	194	TQ5	C22-S20	2.29	1.82	1.77
2	B	195	NDP	PN-O2N	-2.26	1.44	1.55
4	A	201	MES	C3-N4	2.26	1.53	1.46
2	B	195	NDP	P2B-O3X	-2.20	1.46	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	202	MES	O1S-S-C8	6.90	117.15	106.73
3	B	196	TQ5	N6-C5-N4	-6.88	118.46	127.21
3	A	194	TQ5	C24-C23-C22	6.72	128.24	120.48
3	A	194	TQ5	N6-C5-N4	-6.08	119.48	127.21
3	B	196	TQ5	N14-C5-N4	5.92	126.10	117.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	MES	O1S-S-C8	5.15	114.51	106.73
3	A	194	TQ5	C27-C26-C25	4.68	127.63	121.17
3	A	194	TQ5	C27-C22-C23	-4.31	111.83	118.85
2	A	193	NDP	P2B-O2B-C2B	-4.26	112.06	123.43
3	B	196	TQ5	C27-C22-C23	-4.11	112.16	118.85
4	A	201	MES	C2-C3-N4	4.02	116.22	110.12
3	A	194	TQ5	C26-C25-C24	-4.01	112.05	118.03
3	B	196	TQ5	C26-C25-C24	-3.84	112.31	118.03
3	A	194	TQ5	C33-C32-C25	3.80	119.32	110.35
4	A	201	MES	O3S-S-C8	3.78	113.40	106.00
4	B	202	MES	O3S-S-C8	3.37	112.59	106.00
3	A	194	TQ5	C26-C25-C32	3.26	128.14	121.47
3	B	196	TQ5	C9-C8-C1	-3.11	115.84	120.09
3	A	194	TQ5	C23-C22-S20	2.90	129.07	120.32
3	B	196	TQ5	C26-C27-C22	2.86	123.78	120.48
3	A	194	TQ5	N14-C5-N4	2.86	121.51	117.22
3	B	196	TQ5	C5-N4-C3	2.80	124.72	116.72
3	A	194	TQ5	C41-C32-C33	-2.75	100.19	108.36
2	B	195	NDP	C2B-C1B-N9A	-2.73	109.26	113.75
3	B	196	TQ5	C8-C1-C2	2.72	124.29	119.31
2	A	193	NDP	O2B-P2B-O1X	-2.65	99.89	109.33
4	B	202	MES	O3S-S-O2S	-2.64	104.79	111.40
4	A	201	MES	O3S-S-O2S	-2.56	105.00	111.40
3	B	196	TQ5	C23-C24-C25	2.55	124.69	121.17
2	A	193	NDP	C6A-C5A-N7A	-2.42	127.43	132.09
2	A	193	NDP	O2X-P2B-O1X	2.42	120.26	110.83
2	A	193	NDP	O2N-PN-O3	2.40	113.77	107.27
2	A	193	NDP	C2B-C1B-N9A	-2.39	109.82	113.75
2	A	193	NDP	N6A-C6A-N1A	2.38	123.68	118.38
4	A	201	MES	C8-C7-N4	2.38	121.35	112.36
2	B	195	NDP	N9A-C8A-N7A	-2.33	110.63	113.94
2	A	193	NDP	C4A-C5A-N7A	2.31	113.23	110.58
4	A	201	MES	C7-N4-C3	2.28	117.31	111.24
4	B	202	MES	O2S-S-C8	-2.27	103.30	106.73
2	A	193	NDP	O2B-C2B-C1B	-2.26	102.09	110.05
3	B	196	TQ5	C27-C26-C25	2.21	124.21	121.17
2	B	195	NDP	C3B-C2B-C1B	-2.20	98.60	102.81
4	B	202	MES	O2S-S-O1S	-2.18	106.72	113.82
3	B	196	TQ5	C26-C25-C32	2.18	125.93	121.47
2	B	195	NDP	O4B-C1B-N9A	2.17	112.25	108.09
3	B	196	TQ5	C33-C32-C25	2.17	115.46	110.35
3	B	196	TQ5	N7-C3-N4	-2.10	111.45	117.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	194	TQ5	C5-N4-C3	2.10	122.72	116.72
3	B	196	TQ5	C2-C1-N6	-2.09	118.38	122.45
2	B	195	NDP	O4D-C4D-C3D	-2.03	100.72	109.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

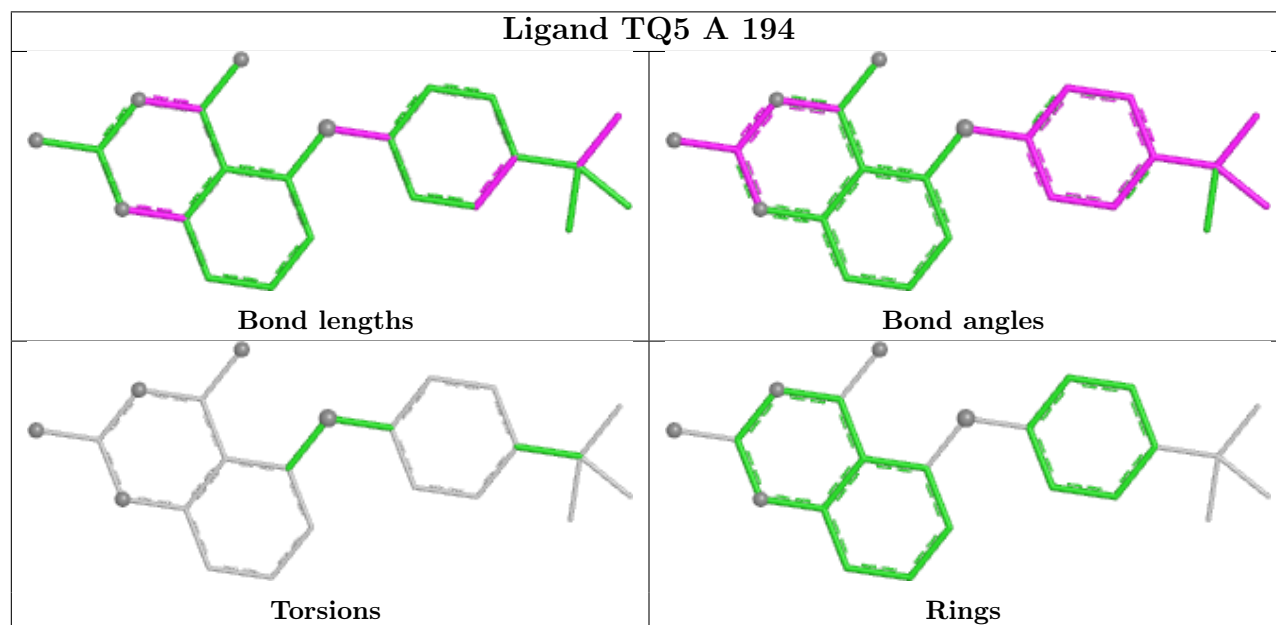
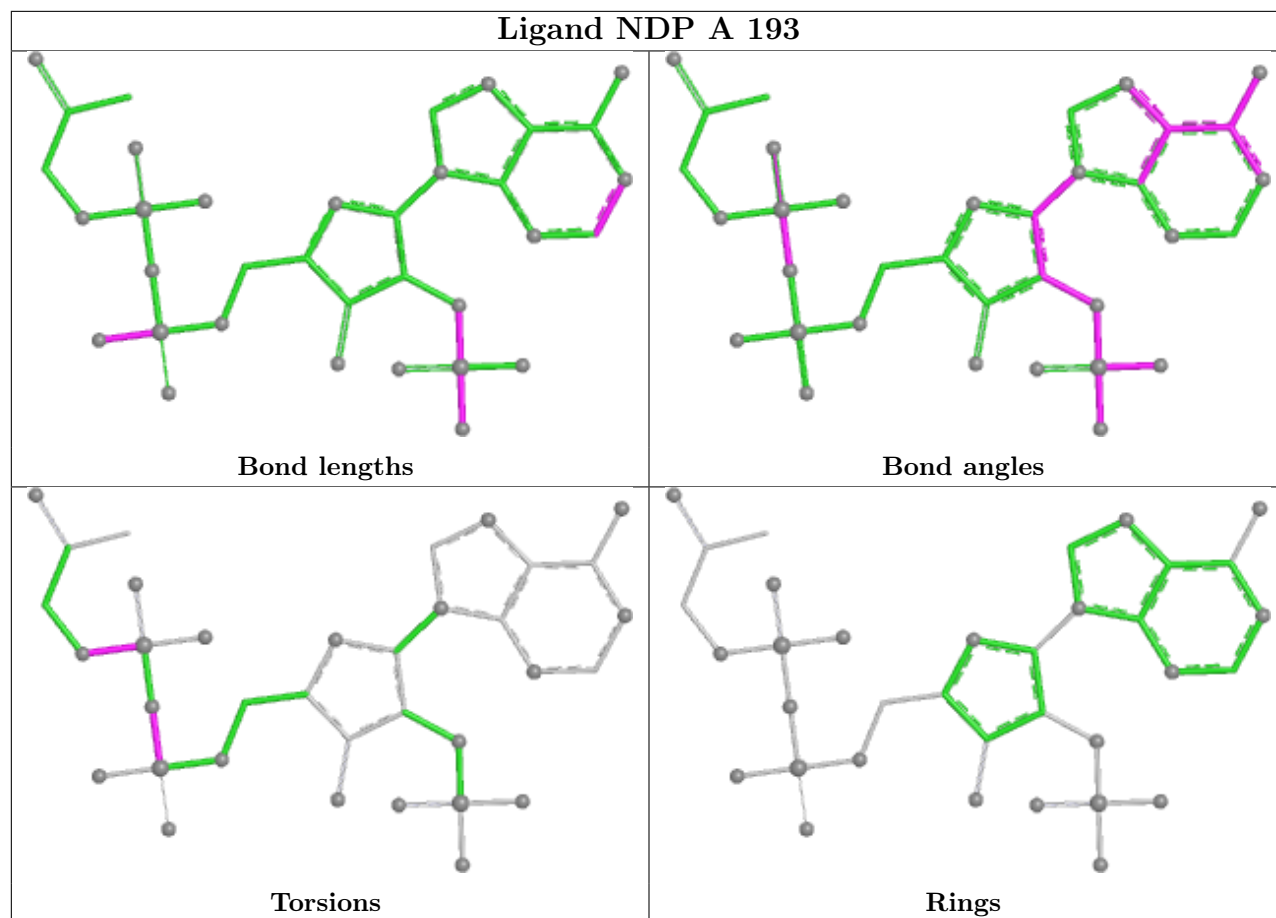
Mol	Chain	Res	Type	Atoms
2	A	193	NDP	C5D-O5D-PN-O1N
4	B	202	MES	C8-C7-N4-C3
4	B	202	MES	C8-C7-N4-C5
2	A	193	NDP	C5D-O5D-PN-O2N
4	A	201	MES	C8-C7-N4-C3
4	A	201	MES	C8-C7-N4-C5
2	A	193	NDP	PN-O3-PA-O2A

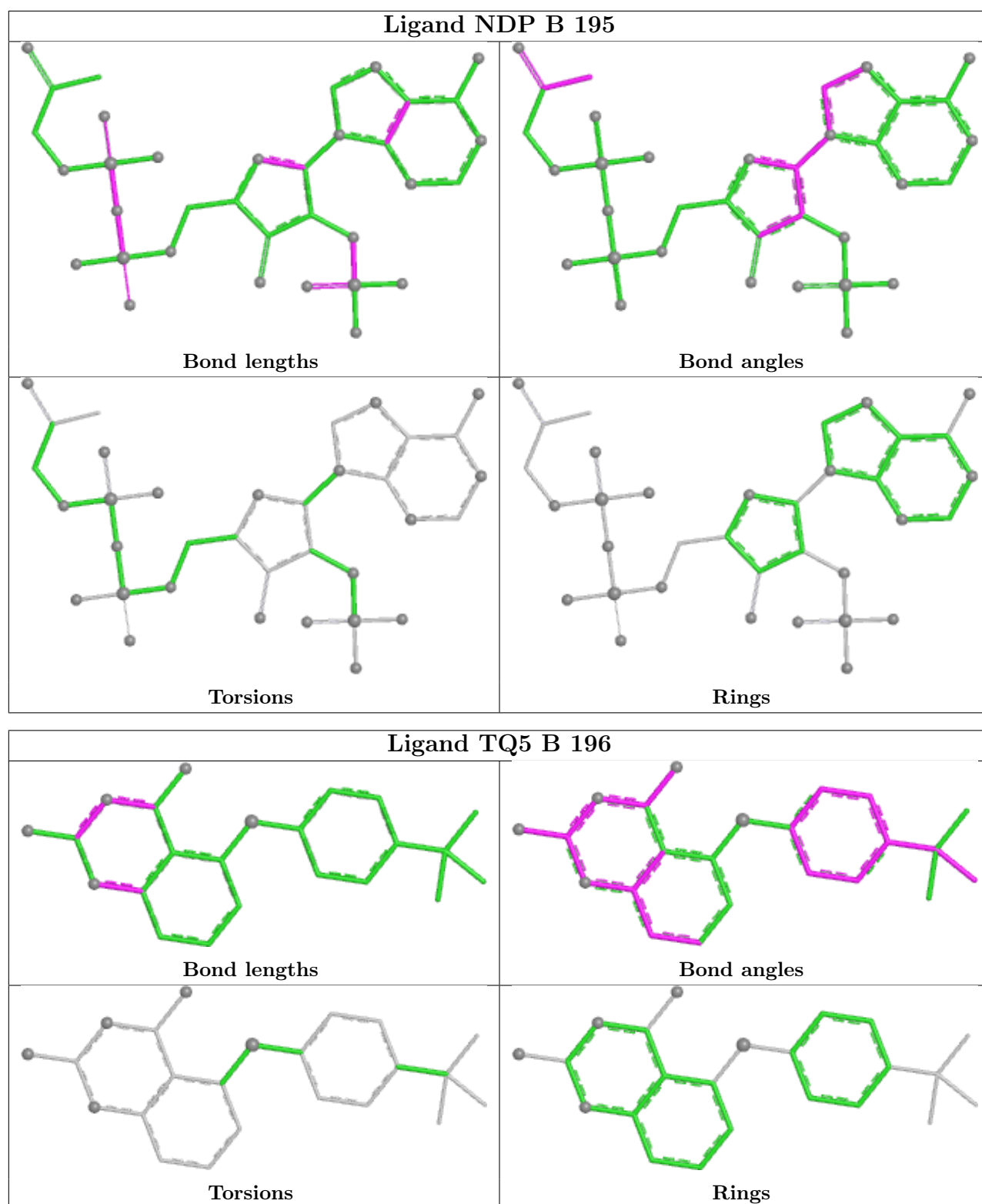
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	MES	1	0
3	A	194	TQ5	1	0
4	A	201	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.