



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:09 PM UTC

PDB ID : 1E7W / pdb_00001e7w
Title : One active site, two modes of reduction correlate the mechanism of leishmania pteridine reductase with pterin metabolism and antifolate drug resistance in trpanosomes
Authors : Gourley, D.G.; Hunter, W.N.
Deposited on : 2000-09-11
Resolution : 1.75 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

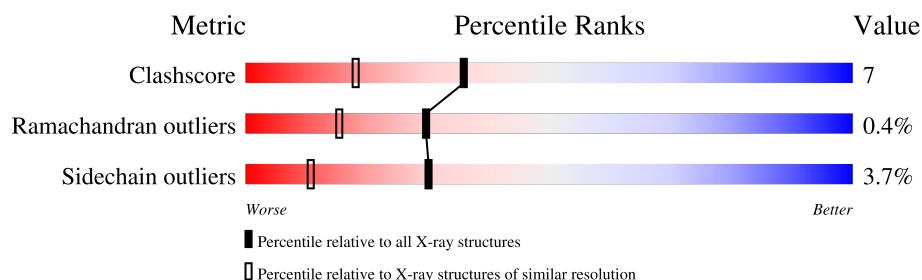
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)

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	291	
1	B	291	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MTX	B	301	-	-	X	-

2 Entry composition ⓘ

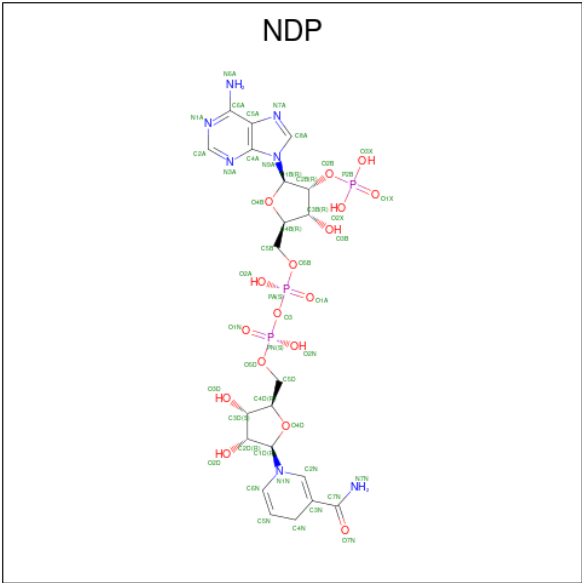
There are 5 unique types of molecules in this entry. The entry contains 4584 atoms, of which 0 are hydrogens and 0 are deuteriums.

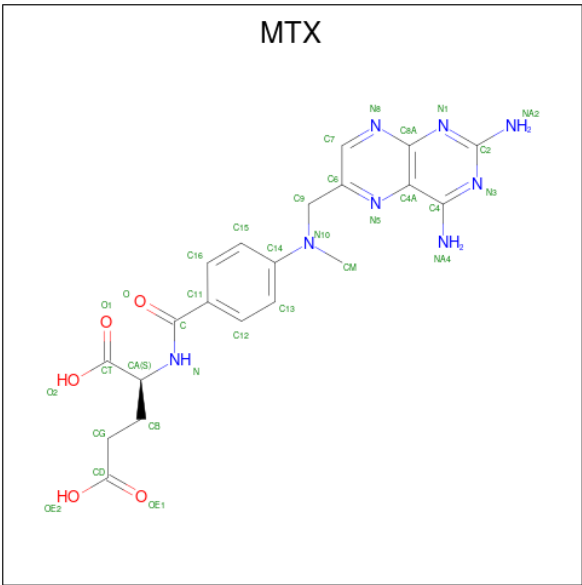
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PTERIDINE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	12	2	0
			1996	1260	353	372	11			
1	B	258	Total	C	N	O	S	20	1	0
			1938	1220	348	360	10			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	8	5		
3	B	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	265	Total	O	0	0
			265	265		
5	B	211	Total	O	0	0
			211	211		

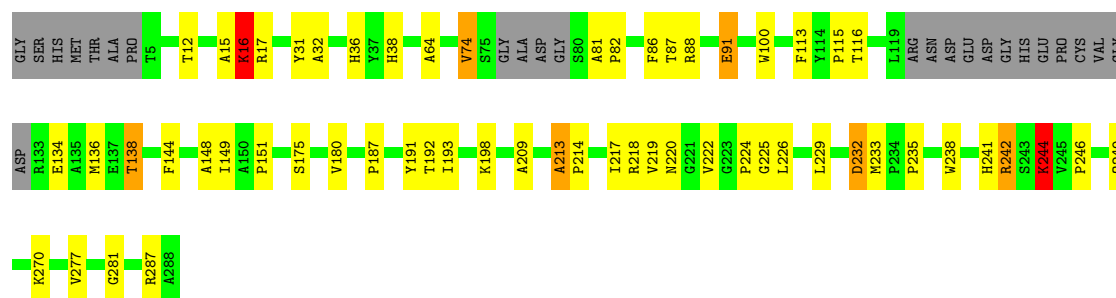
3 Residue-property plots

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.

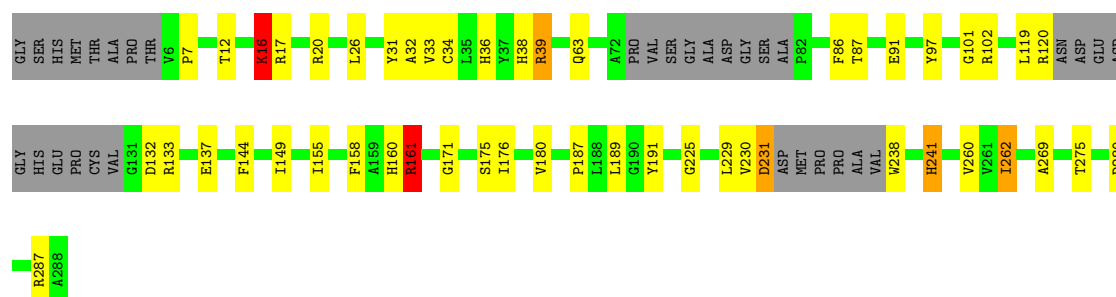
• Molecule 1: PTERIDINE REDUCTASE

Chain A: 



• Molecule 1: PTERIDINE 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 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	80.31 Å 80.80 Å 90.75 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75	Depositor
% Data completeness (in resolution range)	98.2 (30.00-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.45	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.244	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4584	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: MTX, EDO, 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	1.12	2/2044 (0.1%)	1.84	43/2786 (1.5%)
1	B	0.86	1/1976 (0.1%)	1.67	26/2684 (1.0%)
All	All	1.00	3/4020 (0.1%)	1.76	69/5470 (1.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	GLY	CA-C	8.96	1.57	1.51
1	A	219	VAL	N-CA	5.87	1.53	1.46
1	B	225	GLY	CA-C	5.61	1.55	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ARG	NE-CZ-NH2	10.83	128.94	119.20
1	A	218	ARG	CD-NE-CZ	8.10	135.74	124.40
1	B	132	ASP	CA-CB-CG	-8.06	104.54	112.60
1	A	242	ARG	CD-NE-CZ	7.71	135.19	124.40
1	A	88	ARG	NE-CZ-NH2	7.70	126.13	119.20
1	B	137	GLU	CB-CA-C	7.54	125.14	110.67
1	A	209	ALA	O-C-N	7.23	129.79	122.12
1	B	158	PHE	CA-CB-CG	7.11	120.91	113.80
1	A	115	PRO	CA-C-N	7.11	128.98	122.37
1	A	115	PRO	C-N-CA	7.11	128.98	122.37
1	A	287	ARG	NE-CZ-NH2	7.01	125.51	119.20
1	A	217	ILE	CA-C-O	-6.89	113.08	120.59
1	B	269	ALA	CA-C-O	6.85	128.99	120.15
1	A	244	LYS	O-C-N	6.85	131.83	122.37
1	A	113	PHE	CA-CB-CG	6.80	120.61	113.80
1	B	260	VAL	CA-C-O	6.71	127.97	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	ARG	CB-CA-C	6.63	122.89	110.63
1	A	270	LYS	N-CA-C	6.59	120.78	112.87
1	A	187	PRO	N-CA-C	6.57	121.53	111.15
1	B	187	PRO	N-CA-C	6.54	121.34	111.14
1	B	225	GLY	N-CA-C	-6.52	104.28	110.21
1	A	213	ALA	O-C-N	6.50	126.82	120.71
1	A	224	PRO	O-C-N	-6.46	115.09	122.91
1	B	287	ARG	NE-CZ-NH1	-6.46	115.04	121.50
1	A	209	ALA	CA-C-O	-6.43	113.73	120.55
1	B	161	ARG	CD-NE-CZ	-6.40	115.44	124.40
1	A	218	ARG	O-C-N	6.37	130.19	123.06
1	A	242	ARG	NE-CZ-NH1	6.31	127.81	121.50
1	B	175	SER	CA-CB-OG	6.30	123.70	111.10
1	A	244	LYS	CA-C-O	-6.23	111.75	119.28
1	A	225	GLY	N-CA-C	-6.15	104.61	110.21
1	A	31	TYR	O-C-N	6.03	129.77	122.96
1	B	280	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	32	ALA	N-CA-C	-6.01	99.48	109.46
1	A	32	ALA	N-CA-C	-6.00	99.88	109.96
1	A	218	ARG	NH1-CZ-NH2	6.00	127.10	119.30
1	B	187	PRO	O-C-N	5.98	130.27	123.03
1	A	222	VAL	CA-C-O	-5.94	114.06	120.36
1	A	187	PRO	CA-C-O	-5.93	114.66	121.36
1	B	171	GLY	N-CA-C	-5.91	103.46	112.51
1	A	64	ALA	N-CA-C	5.85	117.30	108.46
1	A	220	ASN	O-C-N	5.84	130.32	122.96
1	A	277	VAL	O-C-N	5.83	130.66	122.97
1	A	222	VAL	O-C-N	5.77	129.43	123.20
1	A	91	GLU	O-C-N	-5.72	115.23	122.27
1	A	17	ARG	CD-NE-CZ	5.70	132.39	124.40
1	A	88	ARG	O-C-N	5.64	128.10	122.12
1	B	33	VAL	N-CA-C	5.63	115.99	108.11
1	A	100	TRP	CA-C-N	5.62	131.93	120.80
1	A	100	TRP	C-N-CA	5.62	131.93	120.80
1	B	102	ARG	CD-NE-CZ	5.55	132.17	124.40
1	A	16	LYS	N-CA-CB	-5.52	101.99	111.21
1	A	86	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	16	LYS	N-CA-C	5.49	116.32	108.74
1	A	198	LYS	N-CA-C	-5.45	105.37	112.23
1	B	63	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	B	161	ARG	CG-CD-NE	5.33	123.73	112.00
1	A	192	THR	N-CA-C	5.26	117.42	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ALA	O-C-N	-5.22	115.45	122.19
1	A	281	GLY	O-C-N	-5.21	116.38	122.31
1	A	15	ALA	N-CA-C	5.18	117.83	111.82
1	A	224	PRO	CA-C-O	5.18	128.43	121.95
1	B	17	ARG	CD-NE-CZ	5.16	131.63	124.40
1	B	287	ARG	CB-CG-CD	5.16	123.16	111.30
1	A	116	THR	O-C-N	-5.14	117.44	121.19
1	B	34	CYS	CB-CA-C	5.13	118.51	110.19
1	B	160	HIS	CA-CB-CG	-5.08	108.72	113.80
1	B	241	HIS	CA-C-O	5.07	126.12	120.90
1	A	224	PRO	N-CA-CB	-5.01	98.68	103.39

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	1996	0	2008	27	0
1	B	1938	0	1950	29	0
2	A	48	0	26	0	0
2	B	48	0	25	0	0
3	A	33	0	20	7	0
3	B	33	0	18	10	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
5	A	265	0	0	6	1
5	B	211	0	0	8	2
All	All	4584	0	4065	59	2

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 (59) 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:244:LYS:HE2	1:A:244:LYS:HA	1.33	1.07
1:A:232:ASP:OD2	3:A:301:MTX:H7	1.77	0.84
1:A:244:LYS:HE2	1:A:244:LYS:CA	2.10	0.81
1:A:233:MET:HE1	1:A:241:HIS:CD2	2.17	0.79
1:B:191:TYR:OH	3:B:301:MTX:O2	2.07	0.72
1:B:39[A]:ARG:HG2	1:B:39[A]:ARG:HH11	1.58	0.69
1:A:87:THR:OG1	1:B:133:ARG:NH1	2.26	0.68
1:B:39[A]:ARG:HG2	1:B:39[A]:ARG:NH1	2.09	0.67
3:B:301:MTX:HG1	5:B:2130:HOH:O	1.95	0.66
1:A:136:MET:HE1	1:B:86:PHE:CE2	2.32	0.65
1:A:134:GLU:O	1:A:138:THR:HG23	1.97	0.64
1:B:238:TRP:HA	1:B:238:TRP:CE3	2.33	0.63
1:B:12:THR:HA	1:B:36:HIS:HB3	1.85	0.58
1:A:136:MET:HE1	1:B:86:PHE:CD2	2.39	0.58
1:A:144:PHE:CE2	1:A:193:ILE:HG23	2.39	0.57
3:B:301:MTX:CG	5:B:2130:HOH:O	2.53	0.57
1:B:26:LEU:HG	1:B:262:ILE:HD11	1.87	0.57
1:A:244:LYS:HA	1:A:244:LYS:CE	2.22	0.55
3:B:301:MTX:HB2	5:B:2130:HOH:O	2.07	0.55
1:A:191:TYR:OH	3:A:301:MTX:HA	2.07	0.54
1:A:144:PHE:CE2	1:B:149:ILE:CD1	2.91	0.54
1:A:175:SER:HB2	5:A:2224:HOH:O	2.09	0.53
1:A:74:VAL:HG23	5:A:2091:HOH:O	2.09	0.52
1:B:191:TYR:HE1	3:B:301:MTX:HG2	1.74	0.52
1:B:7:PRO:HB2	1:B:31:TYR:CE2	2.46	0.50
3:A:301:MTX:HG2	3:A:301:MTX:O	2.12	0.50
1:B:238:TRP:HZ3	1:B:241:HIS:CG	2.31	0.49
1:B:16:LYS:HA	1:B:20:ARG:HB2	1.95	0.48
1:A:87:THR:O	1:A:91:GLU:HG3	2.14	0.47
1:B:38:HIS:HD2	5:B:2204:HOH:O	1.98	0.46
1:B:230:VAL:O	1:B:231:ASP:C	2.57	0.46
1:A:148:ALA:C	1:A:151:PRO:HD2	2.41	0.46
1:A:38:HIS:HD2	5:A:2255:HOH:O	1.99	0.46
1:B:39[A]:ARG:HH11	1:B:39[A]:ARG:CG	2.23	0.46
1:A:149:ILE:CD1	1:B:144:PHE:CE2	2.99	0.46
1:A:226:LEU:HD22	3:A:301:MTX:HM2	1.97	0.46
1:A:81:ALA:HB1	1:A:82:PRO:CD	2.47	0.45
3:A:301:MTX:H15	3:A:301:MTX:HM1	1.55	0.45
1:A:213:ALA:N	1:A:214:PRO:CD	2.79	0.45
1:A:232:ASP:OD2	3:A:301:MTX:C7	2.59	0.45
1:A:12:THR:HA	1:A:36:HIS:HB3	1.98	0.45
3:B:301:MTX:HM1	3:B:301:MTX:H15	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HB2	1:A:238:TRP:CD1	2.53	0.43
3:A:301:MTX:H16	5:A:2259:HOH:O	2.18	0.43
1:A:74:VAL:O	5:A:2092:HOH:O	2.21	0.43
1:A:246:PRO:O	1:A:249:GLN:NE2	2.52	0.43
3:B:301:MTX:CB	5:B:2130:HOH:O	2.67	0.43
1:B:97:TYR:O	1:B:101:GLY:N	2.36	0.43
1:B:238:TRP:HD1	5:B:2038:HOH:O	2.00	0.43
1:B:191:TYR:OH	3:B:301:MTX:CT	2.66	0.42
1:B:191:TYR:HH	3:B:301:MTX:CT	2.25	0.42
1:B:161:ARG:HD2	5:B:2072:HOH:O	2.19	0.42
1:B:191:TYR:HE1	3:B:301:MTX:CG	2.33	0.42
1:B:87:THR:O	1:B:91:GLU:HG3	2.20	0.41
1:B:119:LEU:O	1:B:120:ARG:C	2.63	0.41
1:A:16:LYS:HG2	5:A:2003:HOH:O	2.20	0.41
1:B:230:VAL:HG22	5:B:2038:HOH:O	2.20	0.41
1:B:238:TRP:CZ3	1:B:241:HIS:CG	3.09	0.40
1:B:155:ILE:HG12	1:B:176:ILE:HD13	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2133:HOH:O	5:B:2131:HOH:O[2_555]	1.91	0.29
5:B:2148:HOH:O	5:B:2168:HOH:O[2_555]	2.16	0.04

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	263/291 (90%)	248 (94%)	14 (5%)	1 (0%)	30	15
1	B	251/291 (86%)	238 (95%)	12 (5%)	1 (0%)	30	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	514/582 (88%)	486 (95%)	26 (5%)	2 (0%)	30	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	B	180	VAL

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	210/225 (93%)	203 (97%)	7 (3%)	33	13
1	B	201/225 (89%)	192 (96%)	9 (4%)	24	7
All	All	411/450 (91%)	395 (96%)	16 (4%)	30	9

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	74	VAL
1	A	138	THR
1	A	232	ASP
1	A	235	PRO
1	A	242	ARG
1	A	244	LYS
1	B	16	LYS
1	B	39[A]	ARG
1	B	39[B]	ARG
1	B	161	ARG
1	B	189	LEU
1	B	229	LEU
1	B	231	ASP
1	B	262	ILE
1	B	275	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	108	ASN
1	A	241	HIS
1	A	249	GLN
1	B	108	ASN
1	B	249	GLN

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](#)

7 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	MTX	B	301	-	35,35,35	2.10	7 (20%)	47,49,49	3.88	12 (25%)
2	NDP	A	300	-	51,52,52	1.70	13 (25%)	71,80,80	2.07	18 (25%)
4	EDO	B	1289	-	3,3,3	0.75	0	2,2,2	0.78	0
3	MTX	A	301	-	35,35,35	1.70	7 (20%)	47,49,49	2.81	20 (42%)
4	EDO	A	1289	-	3,3,3	0.63	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	B	300	-	51,52,52	1.47	10 (19%)	71,80,80	2.04	20 (28%)
4	EDO	A	1290	-	3,3,3	0.42	0	2,2,2	0.28	0

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	MTX	B	301	-	-	9/25/25/25	0/3/3/3
2	NDP	A	300	-	-	2/34/77/77	0/5/5/5
4	EDO	B	1289	-	-	0/1/1/1	-
3	MTX	A	301	-	-	6/25/25/25	0/3/3/3
4	EDO	A	1289	-	-	0/1/1/1	-
2	NDP	B	300	-	-	3/34/77/77	0/5/5/5
4	EDO	A	1290	-	-	1/1/1/1	-

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	MTX	C7-N8	6.13	1.42	1.31
3	B	301	MTX	CM-N10	5.35	1.54	1.46
2	A	300	NDP	PA-O3	4.76	1.64	1.59
3	B	301	MTX	C6-N5	4.44	1.40	1.32
3	A	301	MTX	C7-N8	4.42	1.39	1.31
2	A	300	NDP	C4N-C3N	-4.13	1.42	1.50
3	B	301	MTX	CA-N	-3.89	1.37	1.45
3	A	301	MTX	CM-N10	3.64	1.51	1.46
2	B	300	NDP	C4N-C3N	-3.51	1.43	1.50
3	A	301	MTX	C11-C	-3.36	1.42	1.50
3	A	301	MTX	C6-N5	3.34	1.38	1.32
2	B	300	NDP	C5A-N7A	-3.34	1.33	1.39
2	A	300	NDP	P2B-O2B	3.30	1.65	1.59
3	A	301	MTX	C9-N10	-3.26	1.39	1.46
2	A	300	NDP	C7N-C3N	3.21	1.55	1.48
3	B	301	MTX	C11-C	-3.16	1.43	1.50
3	B	301	MTX	C9-N10	-3.12	1.40	1.46
2	A	300	NDP	PN-O2N	-3.11	1.40	1.55
2	B	300	NDP	C4N-C5N	-3.00	1.41	1.49
2	A	300	NDP	P2B-O3X	-2.99	1.43	1.54
2	A	300	NDP	C4A-N9A	-2.93	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	300	NDP	C6N-N1N	2.82	1.44	1.37
2	A	300	NDP	C6N-C5N	2.71	1.41	1.33
3	B	301	MTX	C2-N3	2.67	1.40	1.35
2	A	300	NDP	PA-O2A	-2.56	1.43	1.55
2	B	300	NDP	C4A-N9A	-2.53	1.32	1.37
2	A	300	NDP	C4N-C5N	-2.49	1.42	1.49
2	B	300	NDP	C7N-C3N	2.38	1.53	1.48
3	A	301	MTX	C2-N3	2.34	1.39	1.35
2	A	300	NDP	PN-O5D	2.30	1.68	1.59
2	B	300	NDP	PA-O2A	-2.30	1.44	1.55
2	B	300	NDP	P2B-O3X	-2.30	1.46	1.54
3	A	301	MTX	C9-C6	2.28	1.55	1.51
2	A	300	NDP	P2B-O2X	-2.15	1.46	1.54
2	B	300	NDP	P2B-O2B	2.08	1.63	1.59
2	B	300	NDP	PN-O5D	2.04	1.67	1.59
2	A	300	NDP	C5A-N7A	-2.03	1.35	1.39

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	MTX	CB-CA-N	12.95	136.53	110.91
3	B	301	MTX	CA-N-C	12.86	152.40	121.56
3	B	301	MTX	C9-N10-C14	10.88	133.36	120.17
2	B	300	NDP	O4B-C1B-N9A	8.73	124.86	108.09
2	A	300	NDP	O4B-C1B-N9A	7.34	122.19	108.09
3	B	301	MTX	N1-C2-N3	-7.24	118.00	127.21
3	A	301	MTX	C9-N10-C14	7.01	128.66	120.17
3	A	301	MTX	N1-C2-N3	-6.39	119.09	127.21
2	A	300	NDP	C4A-N9A-C8A	6.31	112.36	105.74
3	A	301	MTX	CG-CB-CA	5.95	124.14	113.16
3	B	301	MTX	C6-C9-N10	5.79	122.87	112.95
3	B	301	MTX	C2-N1-C8A	5.45	121.36	115.48
3	B	301	MTX	CM-N10-C14	-5.38	110.69	119.59
3	A	301	MTX	C2-N1-C8A	5.36	121.26	115.48
3	A	301	MTX	CA-N-C	5.09	133.77	121.56
3	A	301	MTX	CM-N10-C14	-5.01	111.30	119.59
2	B	300	NDP	C5A-C4A-N3A	-4.78	120.14	126.72
2	B	300	NDP	N3A-C4A-N9A	4.70	135.16	127.17
2	A	300	NDP	N9A-C8A-N7A	-4.62	107.38	113.94
3	B	301	MTX	N8-C8A-N1	4.38	120.55	115.77
3	A	301	MTX	O-C-C11	-3.91	113.14	120.90
3	A	301	MTX	C6-C7-N8	-3.87	119.42	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	MTX	C6-C7-N8	-3.86	119.44	123.14
3	A	301	MTX	CB-CA-N	3.77	118.37	110.91
2	A	300	NDP	C3N-C2N-N1N	-3.76	117.69	123.20
3	A	301	MTX	NA2-C2-N3	3.72	122.81	117.22
3	B	301	MTX	NA2-C2-N1	3.70	123.56	117.79
3	A	301	MTX	C7-C6-N5	3.63	123.23	120.87
2	A	300	NDP	O7N-C7N-C3N	-3.61	114.09	120.90
3	B	301	MTX	O-C-C11	-3.55	113.87	120.90
3	A	301	MTX	N8-C8A-N1	3.49	119.57	115.77
2	A	300	NDP	N3A-C4A-N9A	3.39	132.93	127.17
3	B	301	MTX	CB-CG-CD	3.37	121.49	112.49
2	A	300	NDP	O4D-C1D-N1N	3.31	114.40	108.08
2	B	300	NDP	C6A-C5A-C4A	3.30	121.68	117.18
2	B	300	NDP	N3A-C2A-N1A	-3.26	123.64	128.58
2	A	300	NDP	O2B-C2B-C1B	3.19	121.25	110.05
3	A	301	MTX	C16-C11-C12	3.03	122.42	118.57
2	B	300	NDP	C3B-C2B-C1B	2.96	108.48	102.81
2	B	300	NDP	C4A-N9A-C8A	2.86	108.75	105.74
2	B	300	NDP	C6A-C5A-N7A	-2.85	126.60	132.09
3	A	301	MTX	C4A-C4-NA4	-2.84	115.99	120.31
3	A	301	MTX	O2-CT-O1	2.78	130.39	124.08
2	B	300	NDP	O4B-C4B-C5B	2.78	118.23	109.33
2	A	300	NDP	C2B-C1B-N9A	2.75	118.28	113.75
2	A	300	NDP	O2B-P2B-O1X	-2.73	99.61	109.33
2	B	300	NDP	O3B-C3B-C2B	2.68	118.69	111.19
2	A	300	NDP	N3A-C2A-N1A	-2.67	124.53	128.58
3	A	301	MTX	O1-CT-CA	-2.65	113.70	122.26
2	B	300	NDP	O4D-C1D-N1N	2.63	113.10	108.08
2	A	300	NDP	C5A-C4A-N9A	-2.61	102.96	105.81
3	A	301	MTX	C13-C12-C11	-2.56	118.06	120.80
2	B	300	NDP	O3X-P2B-O2X	2.45	117.00	107.80
3	A	301	MTX	C15-C16-C11	-2.43	118.20	120.80
2	B	300	NDP	O7N-C7N-N7N	2.40	128.27	122.89
2	B	300	NDP	N9A-C8A-N7A	-2.35	110.60	113.94
2	A	300	NDP	C6A-C5A-N7A	-2.33	127.59	132.09
2	A	300	NDP	C6A-C5A-C4A	2.27	120.27	117.18
2	B	300	NDP	C4A-N9A-C1B	-2.23	121.42	126.63
2	B	300	NDP	C2A-N3A-C4A	2.22	117.26	111.83
2	B	300	NDP	C2A-N1A-C6A	2.20	122.35	118.73
2	A	300	NDP	O3X-P2B-O2X	2.17	115.93	107.80
2	B	300	NDP	O5B-C5B-C4B	-2.15	101.68	108.99
2	A	300	NDP	O4B-C4B-C5B	2.12	116.13	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	NDP	C3N-C2N-N1N	-2.11	120.11	123.20
3	A	301	MTX	CT-CA-N	-2.10	105.71	110.57
2	A	300	NDP	C3B-C2B-C1B	2.08	106.78	102.81
2	A	300	NDP	C1D-N1N-C2N	-2.05	117.76	121.14
2	B	300	NDP	O4B-C4B-C3B	2.05	109.23	105.15
3	A	301	MTX	NA4-C4-N3	2.00	122.49	117.11

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	MTX	CB-CA-N-C
3	B	301	MTX	CB-CA-N-C
3	B	301	MTX	C11-C-N-CA
3	A	301	MTX	C11-C-N-CA
2	A	300	NDP	O4D-C1D-N1N-C6N
2	B	300	NDP	C3B-C2B-O2B-P2B
3	A	301	MTX	CA-CB-CG-CD
2	B	300	NDP	O4D-C1D-N1N-C6N
3	A	301	MTX	N-CA-CT-O1
3	A	301	MTX	N-CA-CT-O2
3	B	301	MTX	CT-CA-N-C
3	A	301	MTX	C6-C9-N10-CM
3	B	301	MTX	N-CA-CB-CG
2	A	300	NDP	C3B-C2B-O2B-P2B
3	B	301	MTX	CA-CB-CG-CD
3	B	301	MTX	OE2-CD-CG-CB
3	B	301	MTX	OE1-CD-CG-CB
2	B	300	NDP	C2B-O2B-P2B-O3X
4	A	1290	EDO	O1-C1-C2-O2
3	B	301	MTX	CB-CA-CT-O1
3	B	301	MTX	CB-CA-CT-O2

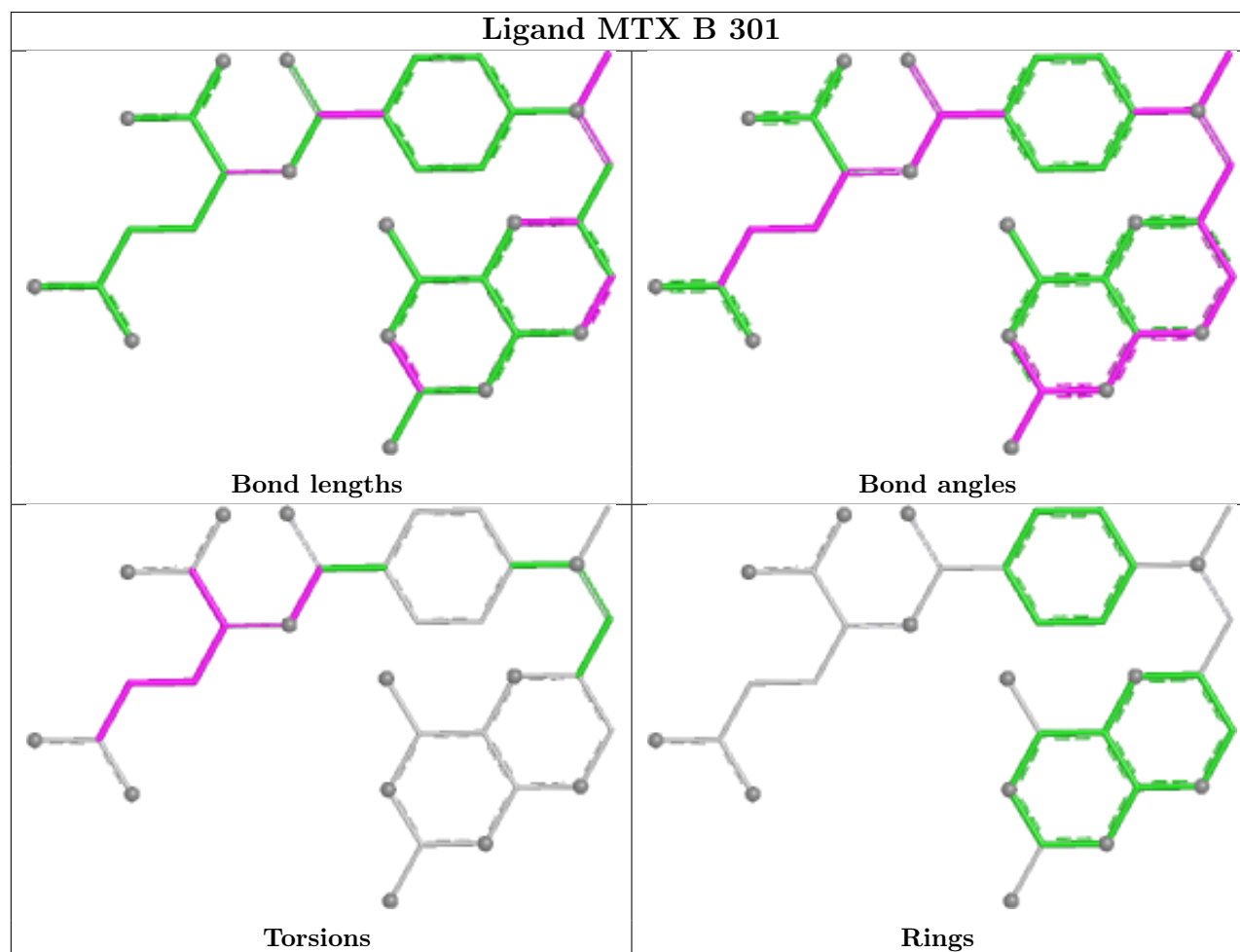
There are no ring outliers.

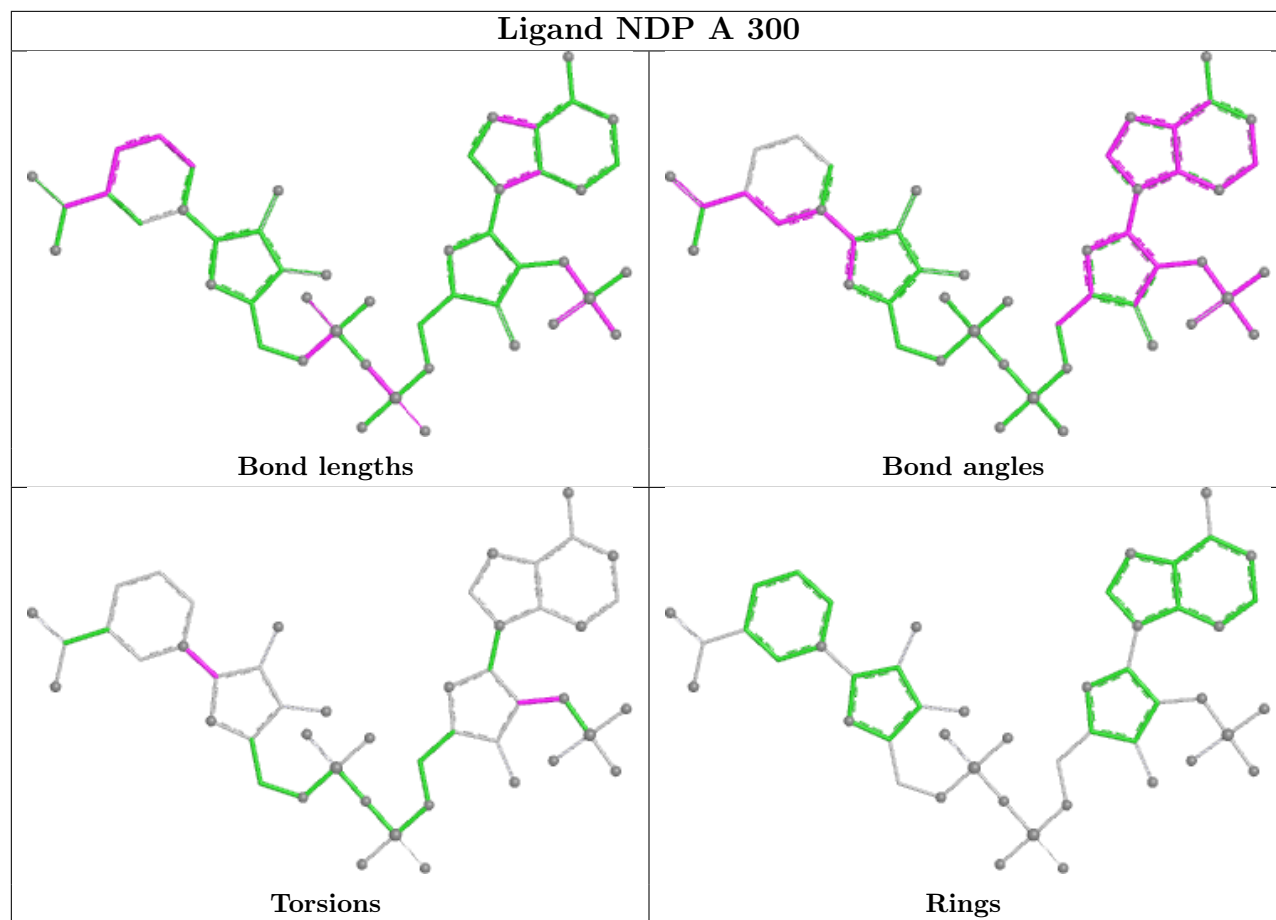
2 monomers are involved in 17 short contacts:

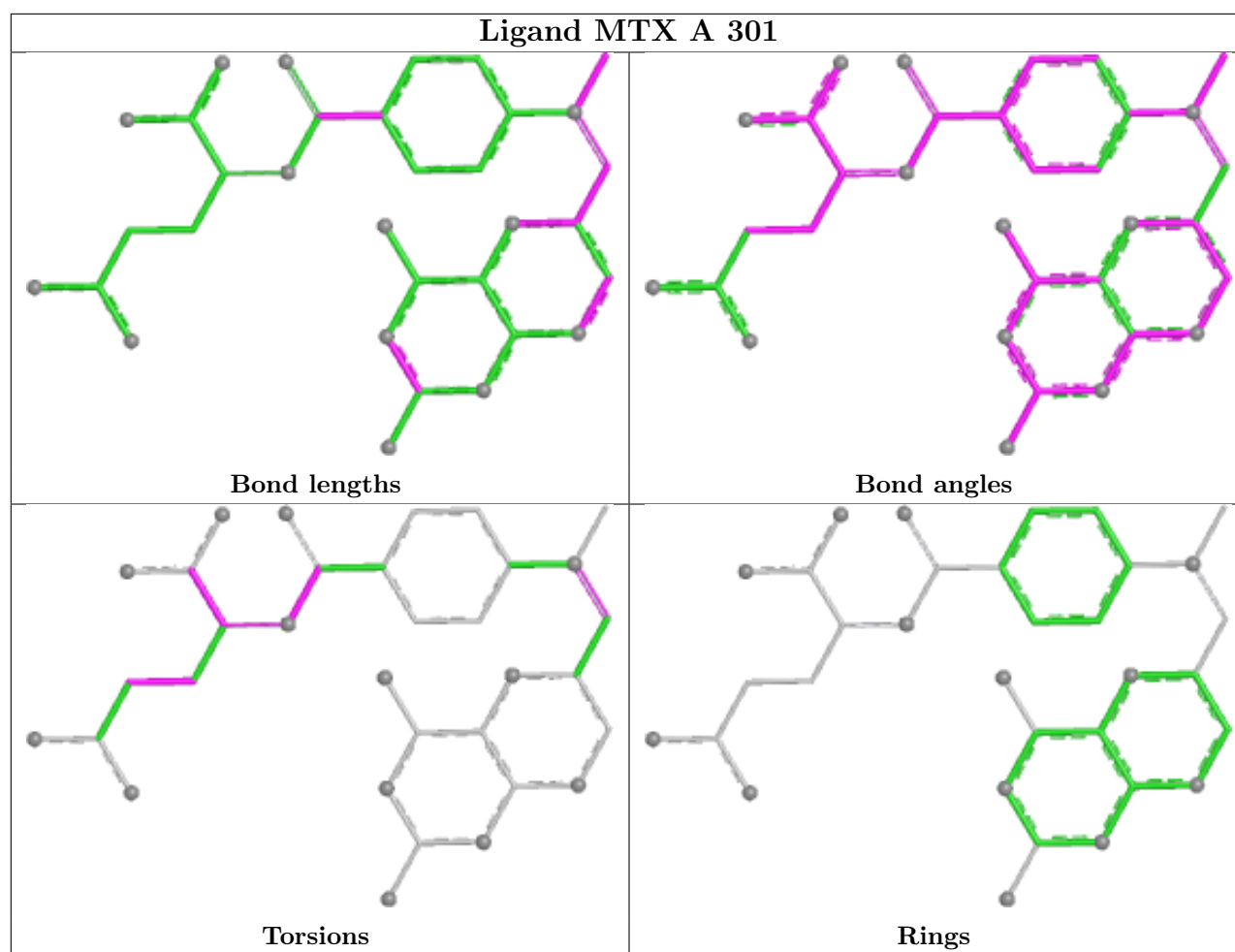
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	MTX	10	0
3	A	301	MTX	7	0

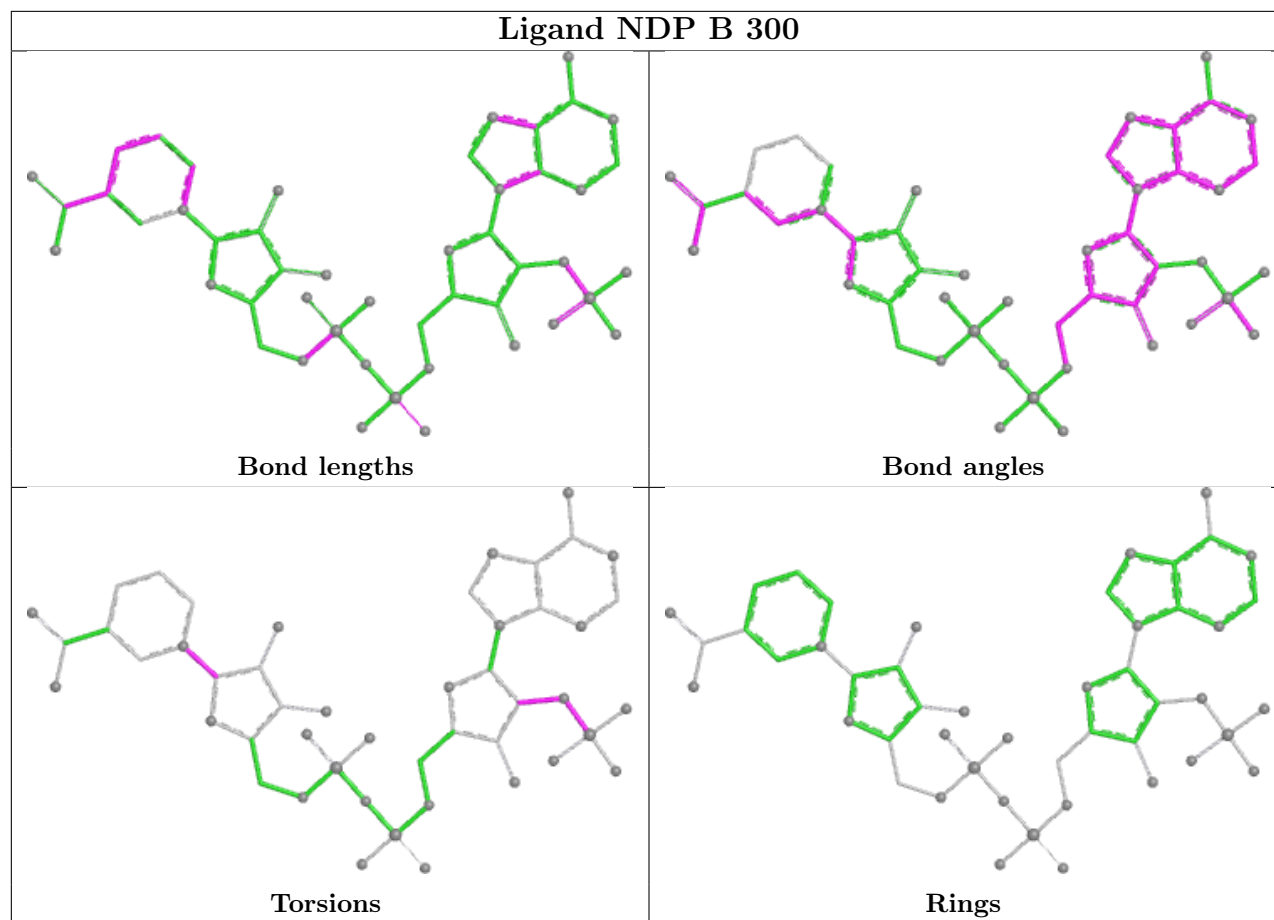
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.