



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2023 – 11:26 PM EDT

PDB ID : 6N1S
Title : Toxoplasma gondii TS-DHFR in complex with selective inhibitor 29
Authors : Hopper, A.T.; Brockman, A.; Wise, A.; Gould, J.; Barks, J.; Radke, J.B.; Sibley, L.D.; Zou, Y.; Thomas, S.B.
Deposited on : 2018-11-11
Resolution : 3.00 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

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 3.00 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8426 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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	510	4080	2609	715	731	25	0	0	0
1	B	510	4082	2608	714	735	25	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q07422
A	?	-	ASN	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	TRP	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	THR	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	ASP	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	LYS	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422

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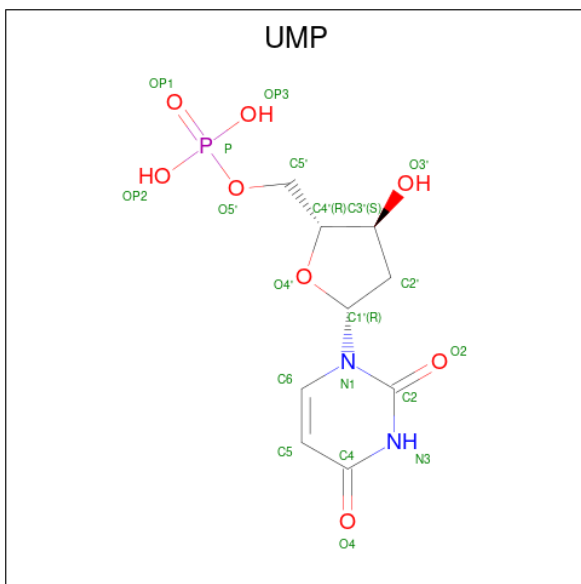
Chain	Residue	Modelled	Actual	Comment	Reference
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A	?	-	ALA	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	ALA	deletion	UNP Q07422
A	?	-	GLU	deletion	UNP Q07422
A	?	-	SER	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	VAL	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	PHE	deletion	UNP Q07422
A	?	-	CYS	deletion	UNP Q07422
A	?	-	PRO	deletion	UNP Q07422
A	?	-	GLU	deletion	UNP Q07422
A	?	-	LEU	deletion	UNP Q07422
A	?	-	GLY	deletion	UNP Q07422
A	?	-	ARG	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	ASN	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	TRP	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	LYS	deletion	UNP Q07422
B	?	-	THR	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	ASP	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422

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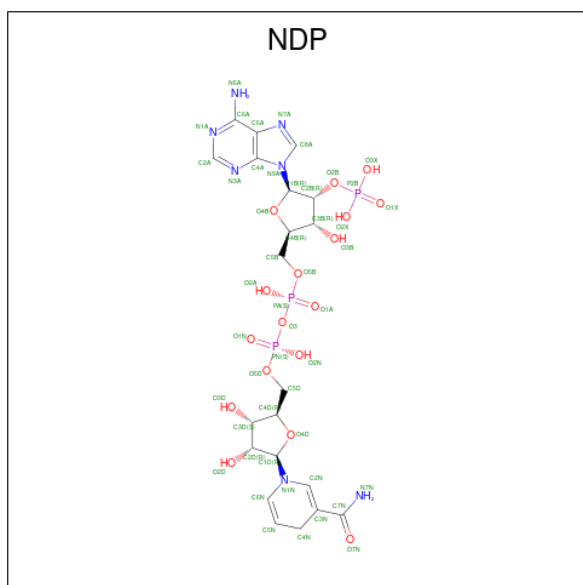
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422
B	?	-	GLN	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	ALA	deletion	UNP Q07422
B	?	-	GLU	deletion	UNP Q07422
B	?	-	SER	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	VAL	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	PHE	deletion	UNP Q07422
B	?	-	CYS	deletion	UNP Q07422
B	?	-	PRO	deletion	UNP Q07422
B	?	-	GLU	deletion	UNP Q07422
B	?	-	LEU	deletion	UNP Q07422
B	?	-	GLY	deletion	UNP Q07422
B	?	-	ARG	deletion	UNP Q07422

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



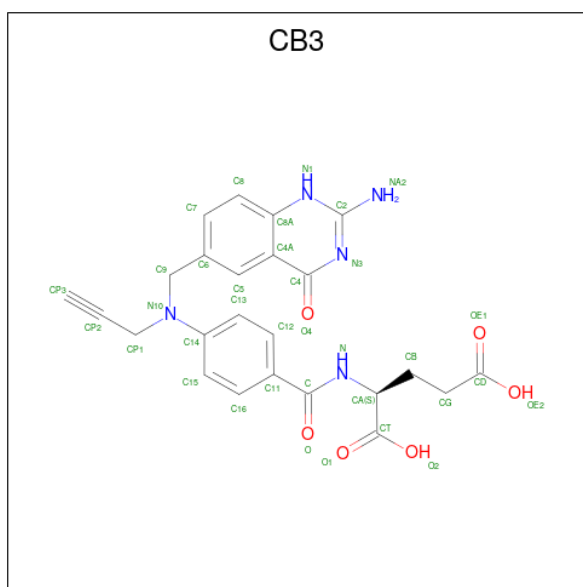
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



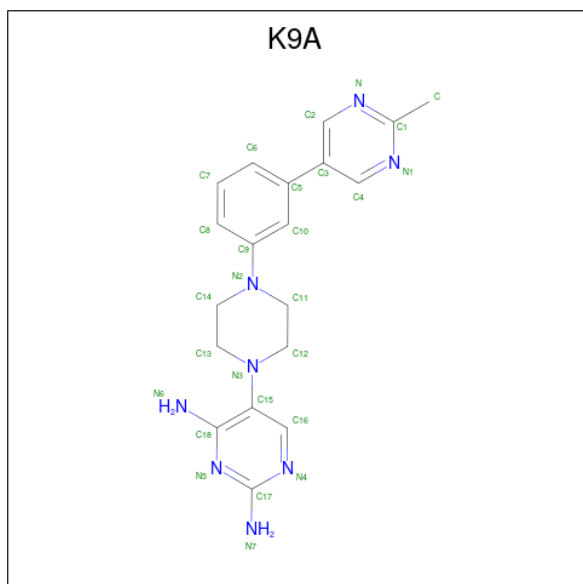
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	24	5	6		
4	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 5 is 5-{4-[3-(2-methylpyrimidin-5-yl)phenyl]piperazin-1-yl}pyrimidine-2,4-diamine (three-letter code: K9A) (formula: C₁₉H₂₂N₈).



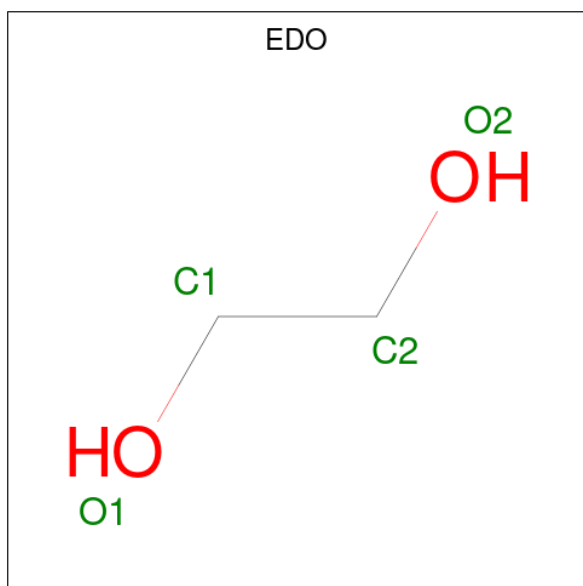
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			27	19	8		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
5	B	1	27	19	8	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	53.69Å 145.52Å 175.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 3.00	Depositor
% Data completeness (in resolution range)	87.7 (39.60-3.00)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.67 (at 3.01Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.241	Depositor
Wilson B-factor (Å ²)	43.6	Xtrriage
Anisotropy	0.246	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8426	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

9 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	UMP	B	701	-	21,21,21	0.34	0	31,31,31	0.41	0
3	NDP	B	702	-	45,52,52	0.61	0	53,80,80	0.67	1 (1%)
4	CB3	A	703	-	36,37,37	0.76	1 (2%)	46,51,51	1.88	5 (10%)
5	K9A	A	704	-	30,30,30	1.65	8 (26%)	38,42,42	2.07	16 (42%)
5	K9A	B	704	-	30,30,30	1.73	8 (26%)	38,42,42	2.24	18 (47%)
4	CB3	B	703	-	36,37,37	0.78	1 (2%)	46,51,51	1.93	5 (10%)
2	UMP	A	701	-	21,21,21	0.31	0	31,31,31	0.45	0
6	EDO	A	705	-	3,3,3	0.08	0	2,2,2	0.27	0
3	NDP	A	702	-	45,52,52	0.57	0	53,80,80	0.75	1 (1%)

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	UMP	B	701	-	-	2/10/22/22	0/2/2/2
3	NDP	B	702	-	-	2/30/77/77	0/5/5/5
4	CB3	A	703	-	-	4/27/28/28	0/3/3/3
5	K9A	A	704	-	-	2/12/22/22	0/4/4/4
5	K9A	B	704	-	-	2/12/22/22	0/4/4/4
4	CB3	B	703	-	-	9/27/28/28	0/3/3/3
2	UMP	A	701	-	-	1/10/22/22	0/2/2/2
6	EDO	A	705	-	-	1/1/1/1	-
3	NDP	A	702	-	-	3/30/77/77	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	K9A	C12-N3	4.06	1.53	1.46
5	B	704	K9A	C-C1	-3.43	1.39	1.49
5	A	704	K9A	C2-N	3.41	1.41	1.34
5	A	704	K9A	C-C1	-3.36	1.40	1.49
5	B	704	K9A	C2-N	3.35	1.41	1.34
5	B	704	K9A	C3-C5	-3.35	1.40	1.49
5	A	704	K9A	C12-N3	3.33	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	K9A	C4-N1	3.30	1.41	1.34
5	A	704	K9A	C3-C5	-3.19	1.41	1.49
5	A	704	K9A	C4-N1	3.13	1.41	1.34
5	A	704	K9A	C16-N4	2.91	1.40	1.34
5	A	704	K9A	C15-N3	-2.65	1.35	1.41
5	B	704	K9A	C16-N4	2.61	1.39	1.34
5	B	704	K9A	C15-N3	-2.57	1.35	1.41
5	B	704	K9A	C13-N3	2.36	1.50	1.46
4	B	703	CB3	C4-N3	2.27	1.37	1.33
5	A	704	K9A	C13-N3	2.11	1.50	1.46
4	A	703	CB3	C4-N3	2.10	1.36	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	CB3	C4A-C8A-N1	-9.55	118.42	123.60
4	A	703	CB3	C4A-C8A-N1	-9.27	118.56	123.60
4	A	703	CB3	C4A-C4-N3	-5.37	120.66	124.40
4	B	703	CB3	C4A-C4-N3	-5.35	120.67	124.40
5	B	704	K9A	N4-C17-N5	-4.48	120.25	125.70
5	B	704	K9A	C17-N5-C18	4.46	121.91	116.99
5	B	704	K9A	C12-N3-C15	4.42	126.74	116.27
5	B	704	K9A	C11-C12-N3	-4.07	102.79	110.70
5	A	704	K9A	C13-N3-C12	4.02	120.39	111.52
5	A	704	K9A	N4-C17-N5	-3.94	120.90	125.70
5	A	704	K9A	C17-N5-C18	3.69	121.07	116.99
5	B	704	K9A	C13-N3-C12	3.65	119.58	111.52
4	A	703	CB3	N1-C2-N3	-3.61	122.41	127.22
4	B	703	CB3	N1-C2-N3	-3.55	122.49	127.22
5	A	704	K9A	C11-C12-N3	-3.29	104.30	110.70
5	B	704	K9A	N1-C1-N	-3.06	120.35	125.51
5	A	704	K9A	N1-C1-N	-3.04	120.39	125.51
5	B	704	K9A	C11-N2-C9	3.04	126.31	118.09
5	A	704	K9A	C12-N3-C15	3.03	123.46	116.27
5	B	704	K9A	C2-N-C1	2.98	121.03	115.96
5	A	704	K9A	C4-N1-C1	2.96	121.00	115.96
5	A	704	K9A	C2-N-C1	2.94	120.97	115.96
5	B	704	K9A	C4-N1-C1	2.87	120.84	115.96
5	B	704	K9A	N6-C18-N5	2.86	121.07	117.03
5	A	704	K9A	N6-C18-N5	2.78	120.96	117.03
5	B	704	K9A	C-C1-N1	2.74	120.15	117.14
5	A	704	K9A	C12-C11-N2	-2.74	105.39	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	K9A	C3-C2-N	-2.68	119.91	124.32
5	B	704	K9A	C3-C2-N	-2.65	119.95	124.32
5	B	704	K9A	C3-C4-N1	-2.58	120.06	124.32
5	A	704	K9A	C3-C4-N1	-2.53	120.14	124.32
5	A	704	K9A	C-C1-N	2.47	119.85	117.14
5	A	704	K9A	C-C1-N1	2.39	119.76	117.14
4	A	703	CB3	C2-N3-C4	2.32	119.61	115.93
5	B	704	K9A	N7-C17-N5	2.29	120.82	117.25
3	B	702	NDP	C5A-C6A-N6A	2.24	123.76	120.35
5	B	704	K9A	C10-C9-N2	-2.23	118.93	121.33
4	B	703	CB3	C2-N3-C4	2.21	119.44	115.93
5	A	704	K9A	C11-N2-C9	2.20	124.04	118.09
5	B	704	K9A	C12-C11-N2	-2.16	106.50	110.70
5	B	704	K9A	C-C1-N	2.15	119.50	117.14
4	B	703	CB3	C2-N1-C8A	2.15	121.64	116.33
4	A	703	CB3	C2-N1-C8A	2.12	121.57	116.33
3	A	702	NDP	C5A-C6A-N6A	2.08	123.52	120.35
5	A	704	K9A	C16-N4-C17	2.03	120.19	116.44
5	B	704	K9A	C16-N4-C17	2.01	120.16	116.44

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	CB3	C11-C-N-CA
4	B	703	CB3	O-C-N-CA
4	B	703	CB3	C11-C-N-CA
4	A	703	CB3	O-C-N-CA
2	B	701	UMP	O4'-C4'-C5'-O5'
4	B	703	CB3	N-CA-CB-CG
4	B	703	CB3	CT-CA-CB-CG
2	B	701	UMP	C3'-C4'-C5'-O5'
5	A	704	K9A	C16-C15-N3-C13
5	B	704	K9A	C16-C15-N3-C13
3	A	702	NDP	O4D-C1D-N1N-C2N
6	A	705	EDO	O1-C1-C2-O2
3	A	702	NDP	C4D-C5D-O5D-PN
4	B	703	CB3	CB-CA-CT-O1
4	B	703	CB3	CB-CA-CT-O2
5	A	704	K9A	C18-C15-N3-C13
3	B	702	NDP	O4D-C1D-N1N-C2N
4	A	703	CB3	OE1-CD-CG-CB

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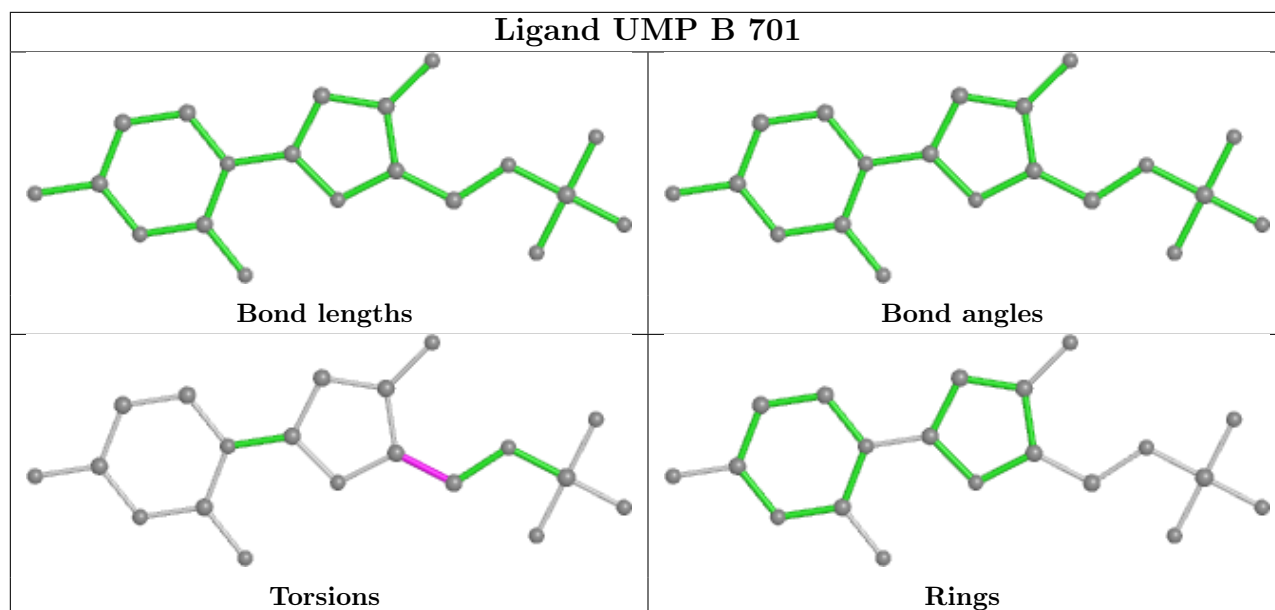
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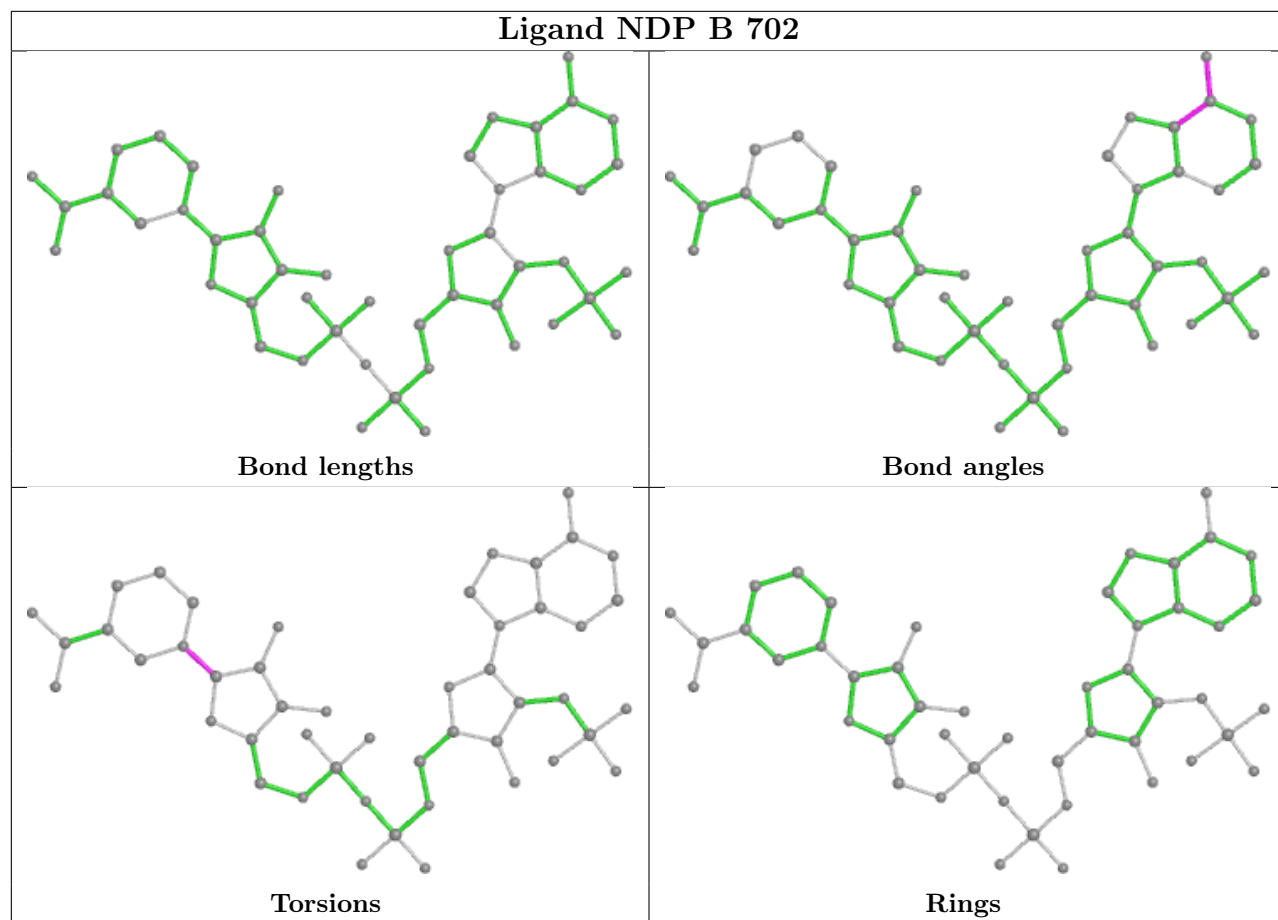
Mol	Chain	Res	Type	Atoms
3	B	702	NDP	C2D-C1D-N1N-C2N
4	A	703	CB3	OE2-CD-CG-CB
4	B	703	CB3	OE2-CD-CG-CB
5	B	704	K9A	C18-C15-N3-C13
4	B	703	CB3	OE1-CD-CG-CB
2	A	701	UMP	O4'-C4'-C5'-O5'
3	A	702	NDP	C3B-C4B-C5B-O5B
4	B	703	CB3	C6-C9-N10-C14

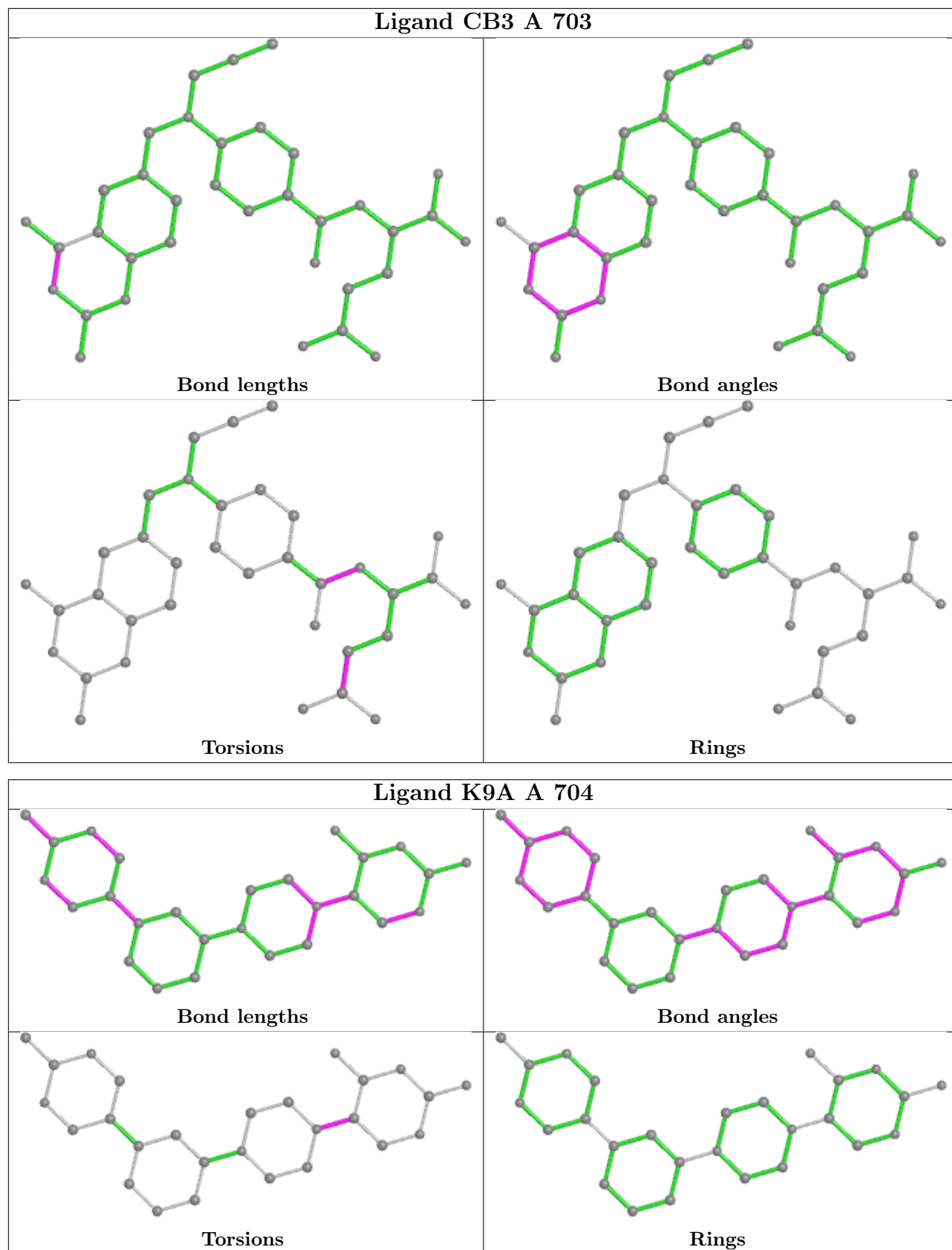
There are no ring outliers.

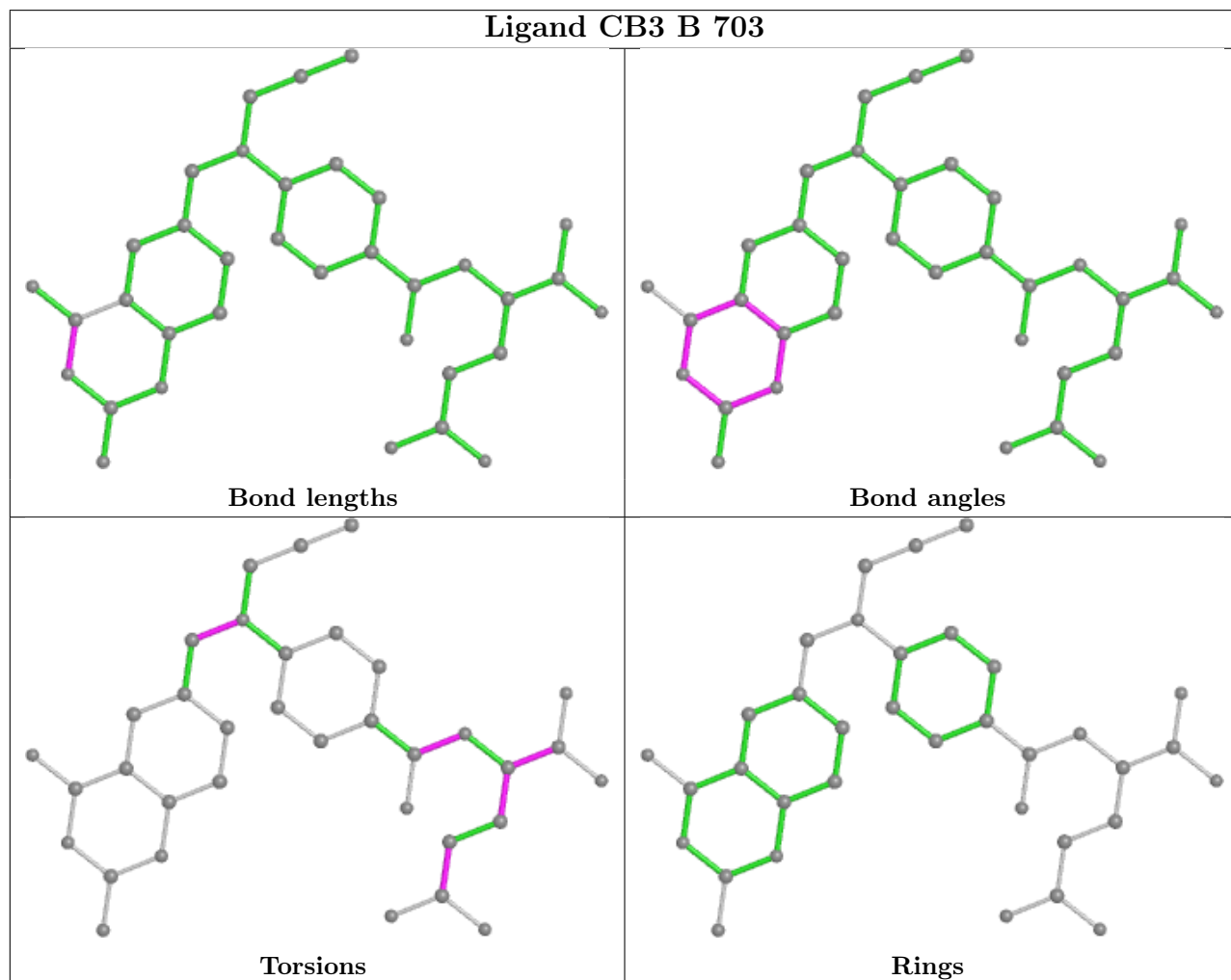
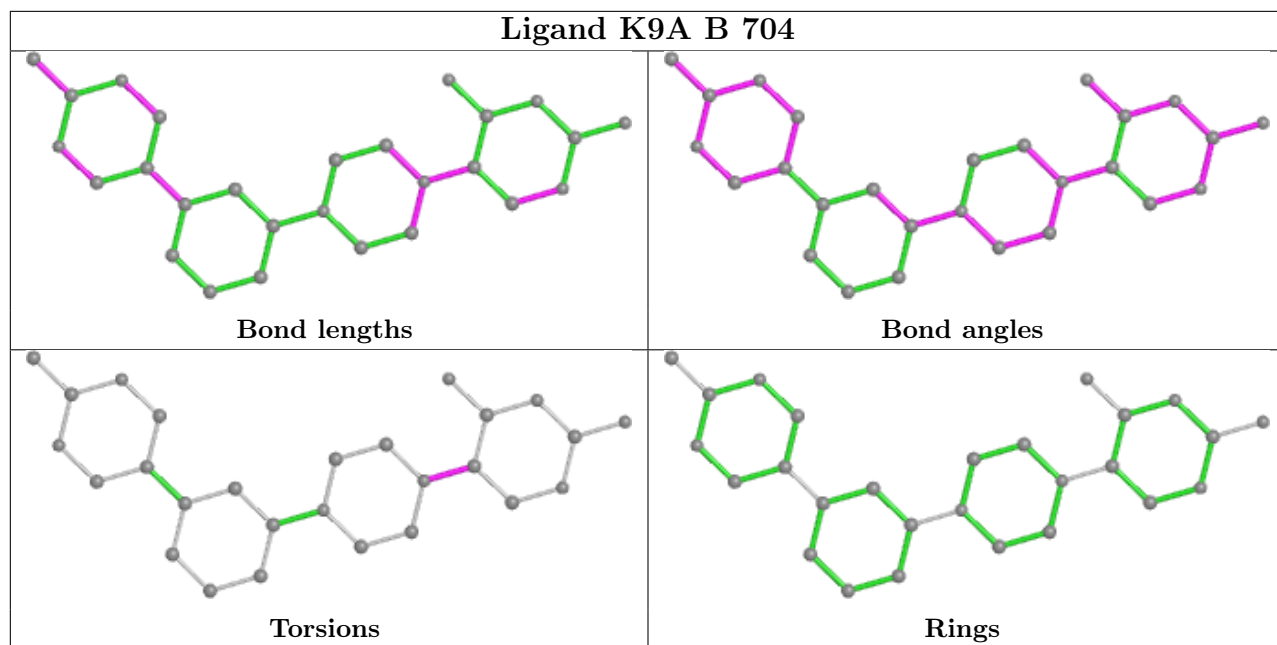
No monomer is involved in short contacts.

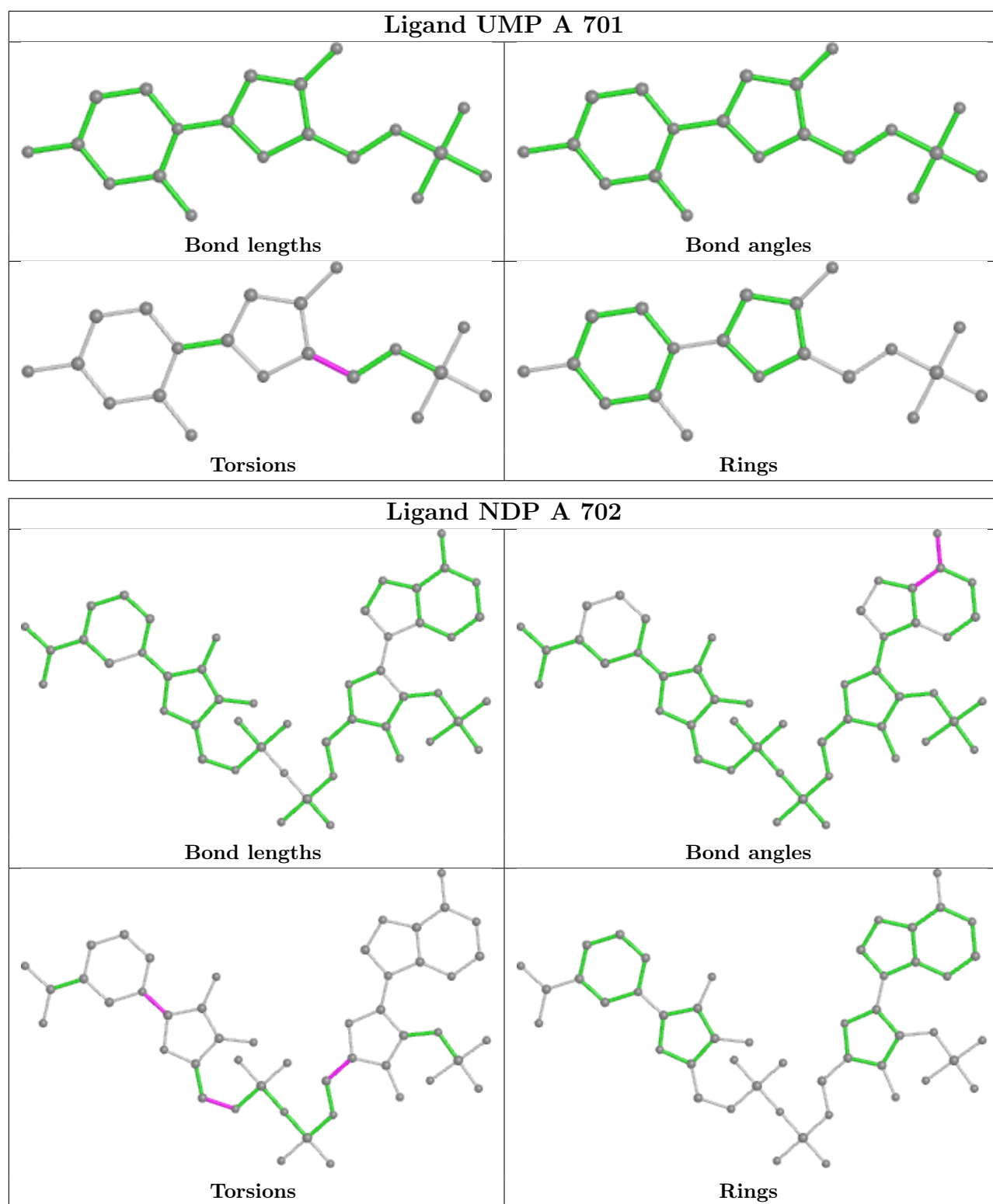
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.











4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	48:ARG	C	74:PHE	N	2.89
1	B	48:ARG	C	74:PHE	N	2.89

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.