



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 04:04 AM EDT

PDB ID : 3U61 / pdb_00003u61
Title : Structure of T4 Bacteriophage Clamp Loader Bound To Closed Clamp, DNA and ATP Analog and ADP
Authors : Kelch, B.A.; Makino, D.L.; O'Donnell, M.; Kuriyan, J.
Deposited on : 2011-10-11
Resolution : 3.20 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
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 3.20 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

There are 8 unique types of molecules in this entry. The entry contains 16748 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 DNA polymerase accessory protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	305	Total	C	N	O	S	0	0	0
			2407	1525	412	454	16			
1	C	319	Total	C	N	O	S	0	0	0
			2503	1583	430	473	17			
1	D	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	E	294	Total	C	N	O	S	0	0	0
			2292	1451	394	432	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P04526
B	-3	PRO	-	expression tag	UNP P04526
B	-2	GLY	-	expression tag	UNP P04526
B	-1	GLY	-	expression tag	UNP P04526
B	0	SER	-	expression tag	UNP P04526
C	-4	GLY	-	expression tag	UNP P04526
C	-3	PRO	-	expression tag	UNP P04526
C	-2	GLY	-	expression tag	UNP P04526
C	-1	GLY	-	expression tag	UNP P04526
C	0	SER	-	expression tag	UNP P04526
D	-4	GLY	-	expression tag	UNP P04526
D	-3	PRO	-	expression tag	UNP P04526
D	-2	GLY	-	expression tag	UNP P04526
D	-1	GLY	-	expression tag	UNP P04526
D	0	SER	-	expression tag	UNP P04526
E	-4	GLY	-	expression tag	UNP P04526
E	-3	PRO	-	expression tag	UNP P04526
E	-2	GLY	-	expression tag	UNP P04526
E	-1	GLY	-	expression tag	UNP P04526
E	0	SER	-	expression tag	UNP P04526

- Molecule 2 is a protein called DNA polymerase accessory protein 62.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	178	Total	C	N	O	S	0	0	0
			1416	909	233	268	6			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	-	expression tag	UNP P04527
A	189	LEU	-	expression tag	UNP P04527
A	190	GLU	-	expression tag	UNP P04527
A	191	HIS	-	expression tag	UNP P04527
A	192	HIS	-	expression tag	UNP P04527
A	193	HIS	-	expression tag	UNP P04527
A	194	HIS	-	expression tag	UNP P04527
A	195	HIS	-	expression tag	UNP P04527
A	196	HIS	-	expression tag	UNP P04527
A	197	HIS	-	expression tag	UNP P04527
A	198	HIS	-	expression tag	UNP P04527
A	199	HIS	-	expression tag	UNP P04527
A	200	HIS	-	expression tag	UNP P04527

- Molecule 3 is a protein called DNA polymerase processivity component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	H	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	F	222	Total	C	N	O	Se	0	0	0
			1699	1083	280	330	6			

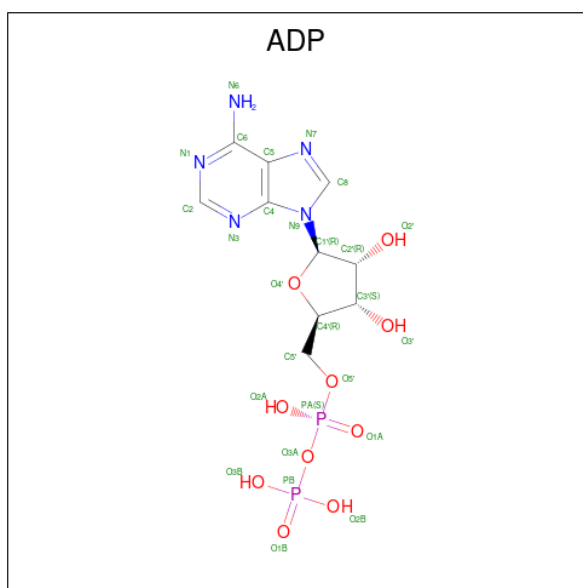
- Molecule 4 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	8	Total	C	N	O	P	0	0	0
			163	79	29	48	7			

- Molecule 5 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	8	Total	C	N	O	P	0	0	0
			162	77	31	46	8			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

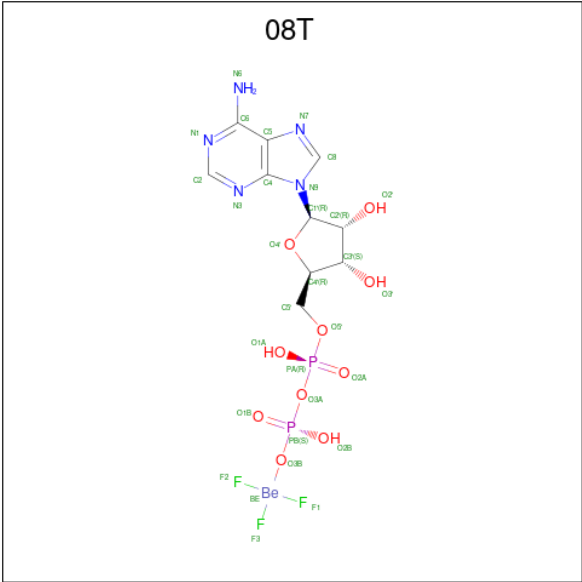


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is [[[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-tris(fluoranyl)beryllium (CCD ID: 08T) (formula: $C_{10}H_{14}BeF_3N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	C	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
8	D	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		

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	82.30Å 137.27Å 222.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 3.20	Depositor
% Data completeness (in resolution range)	96.2 (47.65-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.239 , 0.305	Depositor
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.483	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16748	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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
8	08T	D	700	7	31,33,33	2.97	14 (45%)	41,52,52	5.55	18 (43%)
6	ADP	B	700	-	28,29,29	1.68	6 (21%)	43,45,45	2.13	13 (30%)
8	08T	C	700	7	31,33,33	2.90	15 (48%)	41,52,52	5.22	14 (34%)

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
8	08T	D	700	7	-	2/16/38/38	0/3/3/3
6	ADP	B	700	-	-	7/16/32/32	0/3/3/3
8	08T	C	700	7	-	1/16/38/38	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	700	08T	F1-BE	-8.12	1.35	1.54
8	D	700	08T	F1-BE	-7.49	1.37	1.54
8	C	700	08T	F3-BE	-6.27	1.39	1.54
8	D	700	08T	F2-BE	-6.15	1.40	1.54
8	D	700	08T	F3-BE	-6.03	1.40	1.54
8	C	700	08T	F2-BE	-5.77	1.41	1.54
8	D	700	08T	C2'-C3'	-5.51	1.38	1.53
6	B	700	ADP	PA-O3A	5.34	1.65	1.59
8	C	700	08T	C2'-C3'	-4.94	1.40	1.53
8	D	700	08T	PB-O3A	-4.76	1.54	1.59
6	B	700	ADP	C5-C4	4.38	1.46	1.39
8	D	700	08T	C6-N6	4.19	1.44	1.34
8	C	700	08T	C6-N6	3.96	1.44	1.34
8	D	700	08T	C3'-C4'	-3.52	1.44	1.53
8	C	700	08T	C3'-C4'	-3.16	1.45	1.53
8	C	700	08T	PB-O3A	-3.08	1.56	1.59
8	C	700	08T	C5-N7	-3.06	1.33	1.39
8	D	700	08T	C5-N7	-3.01	1.33	1.39
8	D	700	08T	C8-N9	-2.84	1.32	1.37
8	C	700	08T	C4-N9	2.80	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	700	ADP	C5-N7	-2.67	1.34	1.39
8	C	700	08T	O4'-C4'	-2.58	1.39	1.45
8	C	700	08T	PA-O5'	-2.56	1.49	1.59
8	D	700	08T	C4-N9	2.55	1.43	1.37
8	C	700	08T	C4-N3	2.45	1.39	1.34
8	D	700	08T	C2'-C1'	-2.43	1.45	1.53
6	B	700	ADP	C8-N7	2.43	1.36	1.31
8	D	700	08T	O4'-C4'	-2.36	1.39	1.45
8	D	700	08T	C4-N3	2.35	1.38	1.34
8	C	700	08T	C2'-C1'	-2.28	1.46	1.53
6	B	700	ADP	C5-C6	2.28	1.47	1.41
8	D	700	08T	PA-O5'	-2.22	1.50	1.59
8	C	700	08T	C5-C4	2.21	1.43	1.39
8	C	700	08T	C8-N9	-2.14	1.33	1.37
6	B	700	ADP	C8-N9	-2.01	1.34	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	700	08T	C4-N9-C1'	-18.89	82.46	126.63
8	D	700	08T	C1'-N9-C8	17.29	165.48	127.09
8	C	700	08T	C4-N9-C1'	-16.83	87.26	126.63
8	C	700	08T	C1'-N9-C8	16.59	163.91	127.09
8	D	700	08T	C5-C4-N3	-14.02	107.41	126.72
8	D	700	08T	N3-C4-N9	13.46	150.06	127.17
8	C	700	08T	C5-C4-N3	-13.45	108.20	126.72
8	C	700	08T	N3-C4-N9	13.14	149.51	127.17
8	D	700	08T	C6-C5-C4	6.62	126.22	117.18
6	B	700	ADP	C5-C4-N3	-6.43	117.87	126.72
8	D	700	08T	C2-N3-C4	6.15	126.85	111.83
8	C	700	08T	C6-C5-C4	5.95	125.30	117.18
8	C	700	08T	C2-N3-C4	5.89	126.21	111.83
6	B	700	ADP	N3-C4-N9	5.55	136.61	127.17
8	C	700	08T	C3'-C2'-C1'	5.15	111.20	101.46
8	C	700	08T	N3-C2-N1	-4.67	121.51	128.58
8	D	700	08T	C6-C5-N7	-4.43	123.55	132.09
8	C	700	08T	C6-C5-N7	-4.36	123.69	132.09
8	D	700	08T	N3-C2-N1	-4.34	122.02	128.58
8	D	700	08T	O4'-C1'-C2'	-4.16	97.72	106.62
6	B	700	ADP	C2'-C1'-N9	-3.90	103.60	113.30
6	B	700	ADP	C2-N3-C4	3.86	121.27	111.83
8	D	700	08T	O4'-C1'-N9	-3.82	100.75	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	700	08T	C3'-C2'-C1'	3.56	108.20	101.46
6	B	700	ADP	N3-C2-N1	-3.38	123.47	128.58
8	C	700	08T	O4'-C1'-C2'	-3.31	99.54	106.62
8	C	700	08T	C5-C4-N9	-3.27	102.24	105.81
8	D	700	08T	C5-C4-N9	-3.21	102.31	105.81
8	C	700	08T	O5'-C5'-C4'	3.19	119.85	108.99
6	B	700	ADP	C4-N9-C8	3.00	108.89	105.74
6	B	700	ADP	C4-C5-N7	-2.91	107.26	110.58
6	B	700	ADP	N6-C6-N1	2.84	124.69	118.38
8	D	700	08T	C5-N7-C8	2.71	107.71	103.45
8	D	700	08T	C4-N9-C8	2.67	108.55	105.74
8	D	700	08T	O5'-C5'-C4'	2.63	117.95	108.99
6	B	700	ADP	O2A-PA-O1A	2.52	124.17	112.44
6	B	700	ADP	C5-N7-C8	2.51	107.39	103.45
8	C	700	08T	C5-N7-C8	2.33	107.11	103.45
8	D	700	08T	O4'-C4'-C5'	2.30	116.69	109.33
8	D	700	08T	N9-C8-N7	-2.29	110.69	113.94
8	D	700	08T	C5'-C4'-C3'	-2.22	107.21	115.21
6	B	700	ADP	N9-C8-N7	-2.11	110.94	113.94
6	B	700	ADP	C5-C6-N6	-2.07	118.17	123.29
6	B	700	ADP	O5'-PA-O1A	-2.06	100.77	108.94
8	C	700	08T	C4-N9-C8	2.04	107.88	105.74

There are no chirality outliers.

All (10) torsion outliers are listed below:

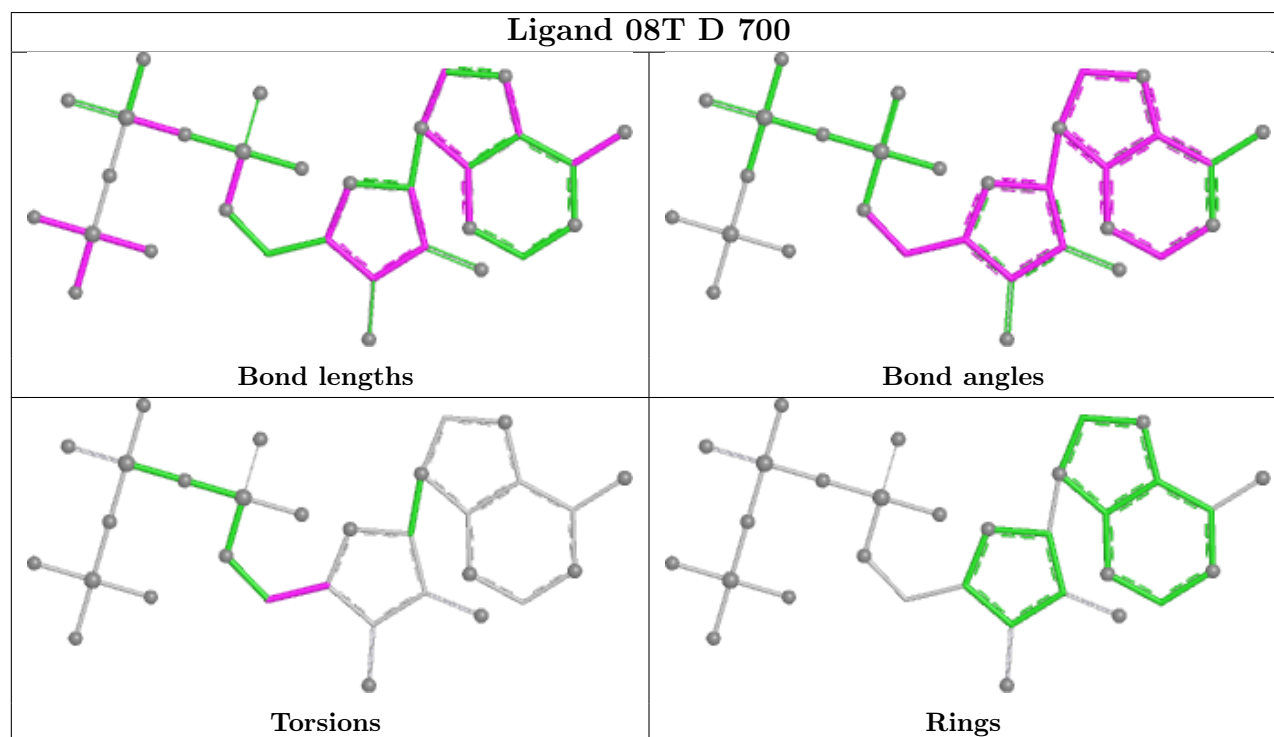
Mol	Chain	Res	Type	Atoms
6	B	700	ADP	PA-O3A-PB-O2B
6	B	700	ADP	PA-O3A-PB-O3B
6	B	700	ADP	C5'-O5'-PA-O1A
6	B	700	ADP	C5'-O5'-PA-O2A
6	B	700	ADP	C5'-O5'-PA-O3A
6	B	700	ADP	O4'-C4'-C5'-O5'
6	B	700	ADP	C3'-C4'-C5'-O5'
8	D	700	08T	O4'-C4'-C5'-O5'
8	D	700	08T	C3'-C4'-C5'-O5'
8	C	700	08T	C5'-O5'-PA-O1A

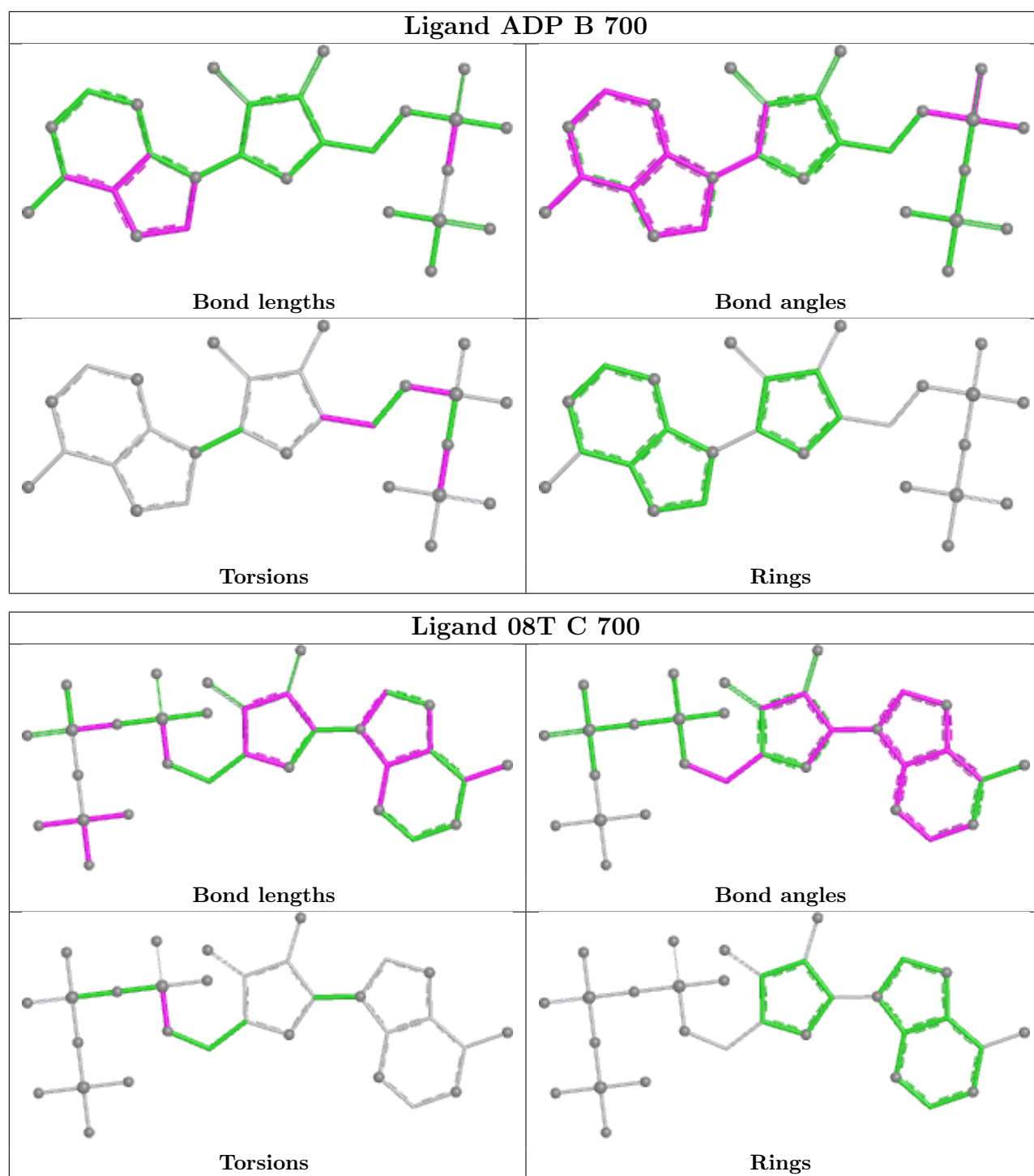
There are no ring outliers.

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 [i](#)

There are no chain breaks in this entry.

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.