



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 10:23 am BST

PDB ID : 1NB6
Title : HC-J4 RNA polymerase complexed with UTP
Authors : O'Farrell, D.J.; Trowbridge, R.; Rowlands, D.J.; Jaeger, J.
Deposited on : 2002-12-02
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.11

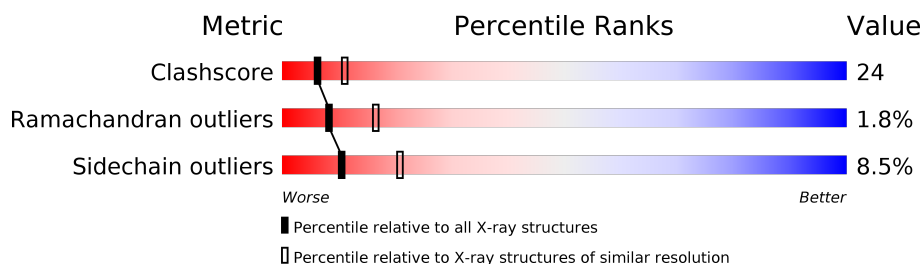
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 on 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	570	
1	B	570	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9453 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.

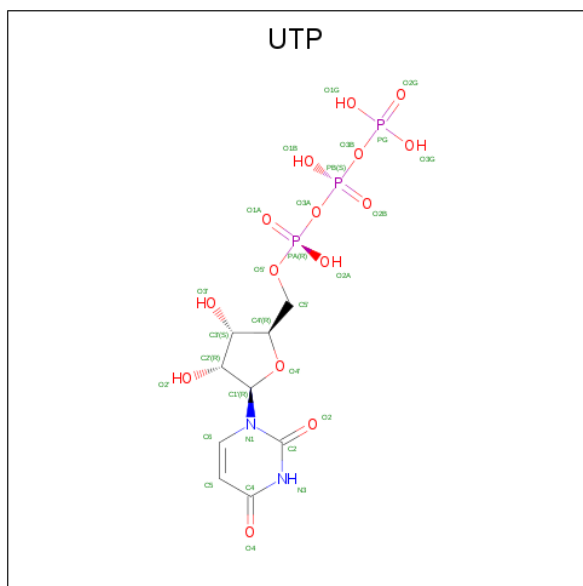
- Molecule 1 is a protein called polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4388	2763	777	816	32			
1	B	565	Total	C	N	O	S	0	0	0
			4381	2758	776	815	32			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	B	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 4 is water.

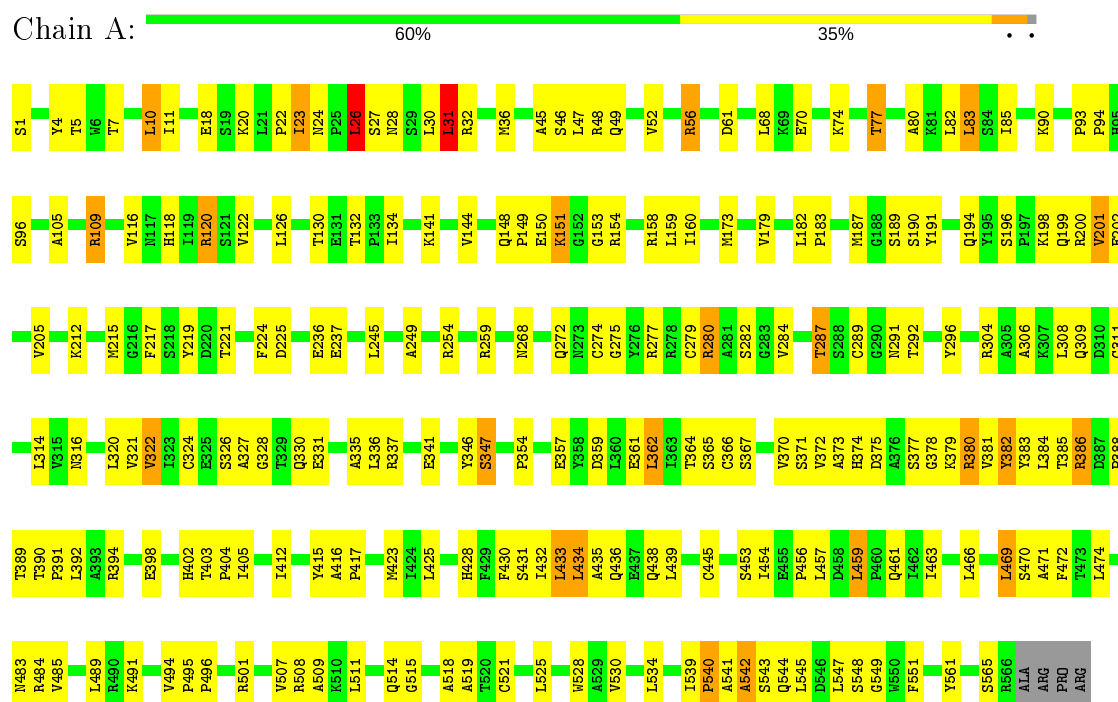
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	270	Total	O	0	0
			270	270		
4	B	352	Total	O	0	0
			352	352		

3 Residue-property plots

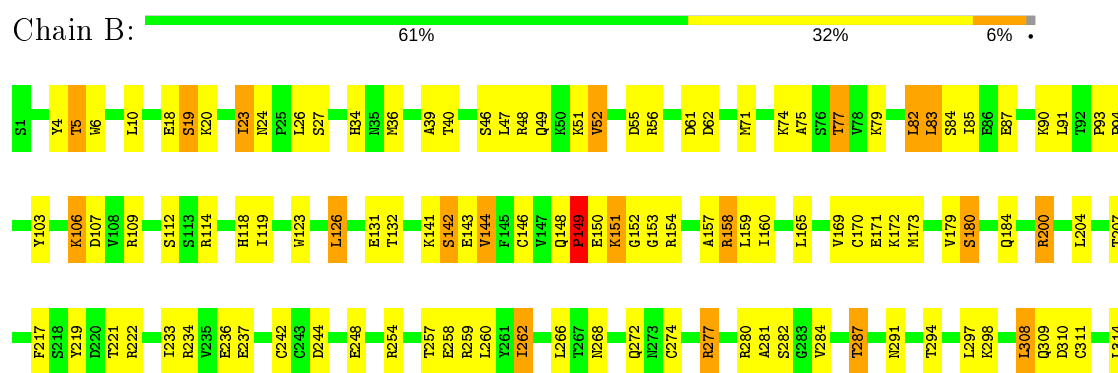
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: polypeptide



- Molecule 1: polypeptide



A416	L320	A417	V321	A418	V322	I323	C324	E325	S326	A327	Q330	E331	A335	L336	R337	A338	F339	T340	Y346	S347	P350	G351	D352	Q355	T364	S365	C366	S367	S368	V372	A373	H374	G378	L384	T390	P391	R394	E398	R401	P404	I405	N406	S407	W408	I412				
A416	P417	T418	R422	L425	F430	S431	I432	L433	L434	A435	Q436	E437	Q438	L439	E440	Q446	I447	Y448	G449	A450	G451	Y452	S453	I454	E455	P456	L459	P460	Q461	E464	R465	G468	I469	S470	L474	H475	S476	V485	A486	S487	C488	L489	R490	K491	L492	R505	S506	V507	R508
A509	K510	L511	L512	S513	Q514	Q515	A518	A519	T520	G521	G522	R523	V530	R531	P538	I539	P540	A541	A542	L545	D546	L547	S548	G549	W550	F551	Y555	S556	G557	G558	D559	S563	L564	S565	ARG	ALA	ARG	PRO	ARG										

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 21	Depositor
Cell constants a, b, c, α , β , γ	105.43Å 107.74Å 133.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 2.60	Depositor
% Data completeness (in resolution range)	95.1 (26.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9453	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: UTP, MN

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	0.64	1/4484 (0.0%)	0.83	5/6087 (0.1%)
1	B	0.69	2/4477 (0.0%)	0.85	3/6077 (0.0%)
All	All	0.66	3/8961 (0.0%)	0.84	8/12164 (0.1%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	SER	CB-OG	8.42	1.53	1.42
1	A	274	CYS	CB-SG	-6.32	1.71	1.82
1	B	242	CYS	CB-SG	-5.57	1.72	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	B	200	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	11	ILE	N-CA-C	-6.20	94.26	111.00
1	A	31	LEU	CA-CB-CG	6.13	129.39	115.30
1	A	277	ARG	NE-CZ-NH1	6.10	123.35	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	4388	0	4383	224	0
1	B	4381	0	4374	204	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	29	0	11	2	0
3	B	29	0	11	2	0
4	A	270	0	0	28	0
4	B	352	0	0	38	0
All	All	9453	0	8779	428	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 24.

The worst 5 of 428 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:109:ARG:HB2	1:B:109:ARG:NH1	1.63	1.12
1:B:141:LYS:NZ	1:B:158:ARG:HH12	1.55	1.04
1:B:148:GLN:HE21	1:B:153:GLY:HA3	1.18	1.03
1:A:547:LEU:HD12	1:A:565:SER:H	1.25	1.01
1:B:277:ARG:HE	1:B:281:ALA:HB2	1.22	0.98

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	564/570 (99%)	517 (92%)	38 (7%)	9 (2%)	9	19
1	B	563/570 (99%)	515 (92%)	37 (7%)	11 (2%)	7	14
All	All	1127/1140 (99%)	1032 (92%)	75 (7%)	20 (2%)	8	16

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	A	540	PRO
1	B	469	LEU
1	B	542	ALA
1	B	549	GLY

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	475/485 (98%)	443 (93%)	32 (7%)	16	33
1	B	474/485 (98%)	425 (90%)	49 (10%)	7	13
All	All	949/970 (98%)	868 (92%)	81 (8%)	10	21

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	ILE
1	B	112	SER
1	B	465	ARG
1	B	47	LEU
1	B	77	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	ASN
1	B	24	ASN
1	B	483	ASN
1	A	514	GLN
1	B	34	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
3	UTP	A	1700	2	26,30,30	2.29	6 (23%)	34,47,47	2.47	14 (41%)
3	UTP	B	2700	2	26,30,30	2.39	7 (26%)	34,47,47	1.67	6 (17%)

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	UTP	A	1700	2	-	8/22/38/38	0/2/2/2
3	UTP	B	2700	2	-	7/22/38/38	0/2/2/2

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2700	UTP	C6-C5	-8.15	1.30	1.52
3	A	1700	UTP	C6-C5	-7.87	1.31	1.52
3	B	2700	UTP	C2-N1	4.31	1.41	1.35
3	B	2700	UTP	C6-N1	-4.25	1.39	1.47
3	A	1700	UTP	C6-N1	-4.14	1.39	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1700	UTP	O3G-PG-O2G	-5.46	89.30	110.68
3	A	1700	UTP	O3G-PG-O3B	-4.71	88.83	104.64
3	A	1700	UTP	PB-O3B-PG	-4.30	118.06	132.83
3	A	1700	UTP	O1G-PG-O2G	4.24	127.27	110.68
3	A	1700	UTP	O3G-PG-O1G	-4.23	91.47	107.64

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1700	UTP	O4'-C1'-N1-C6
3	A	1700	UTP	C2'-C1'-N1-C6
3	A	1700	UTP	C2'-C1'-N1-C2
3	B	2700	UTP	O4'-C1'-N1-C6
3	A	1700	UTP	O4'-C1'-N1-C2

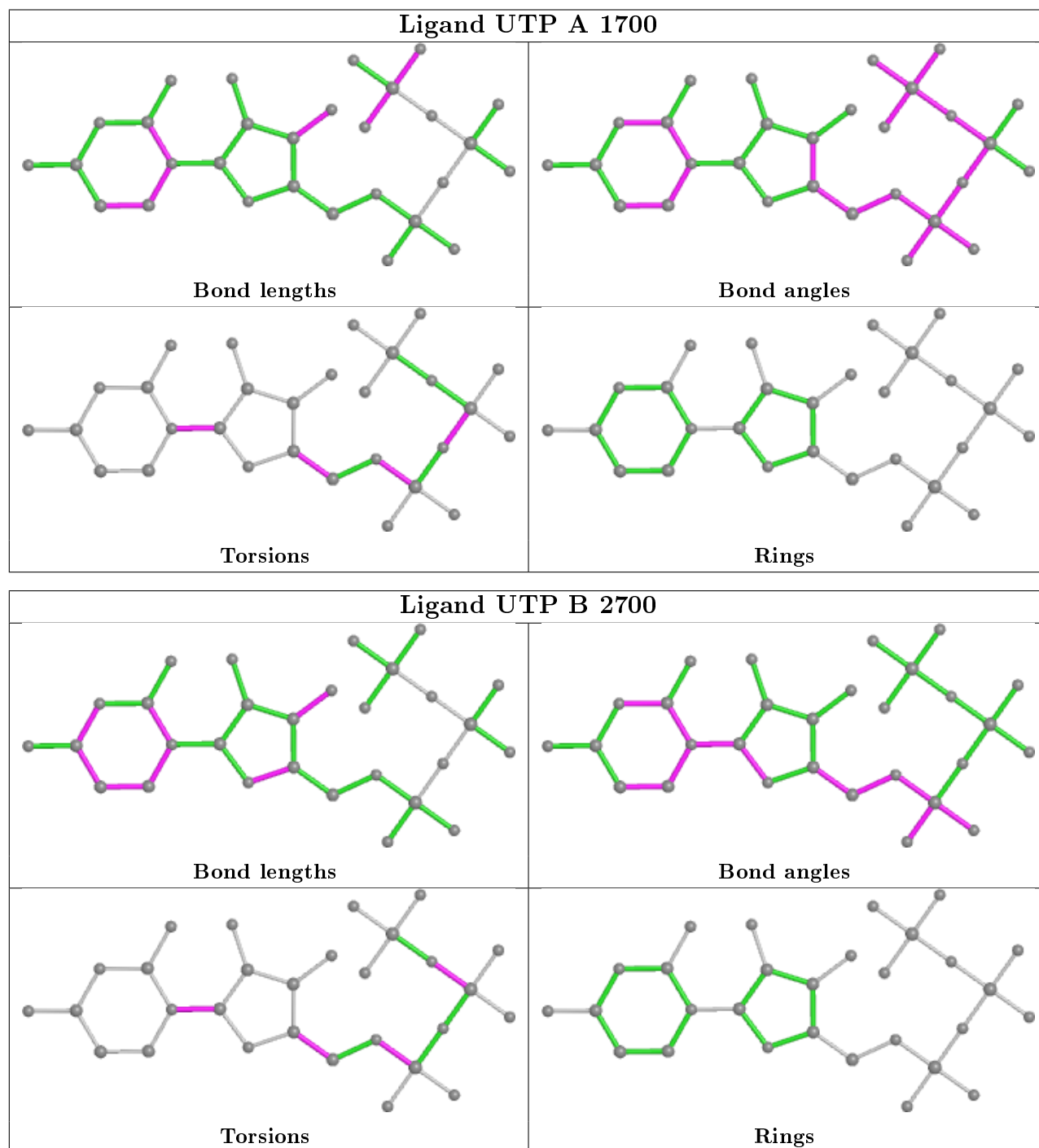
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1700	UTP	2	0
3	B	2700	UTP	2	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.