



## wwPDB EM Validation Summary Report ⓘ

Dec 13, 2022 – 12:03 AM EST

PDB ID : 1JFF  
Title : Refined structure of alpha-beta tubulin from zinc-induced sheets stabilized with taxol  
Authors : Lowe, J.; Li, H.; Downing, K.H.; Nogales, E.  
Deposited on : 2001-06-20  
Resolution : 3.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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>.

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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)  
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) : 2.31.2

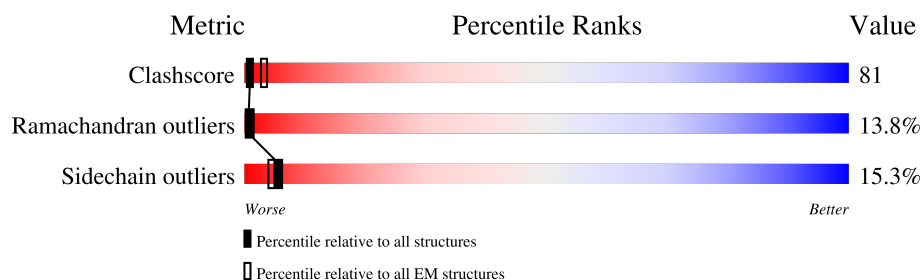
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON CRYSTALLOGRAPHY*

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	451	
2	B	445	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6702 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

- Molecule 2 is a protein called tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

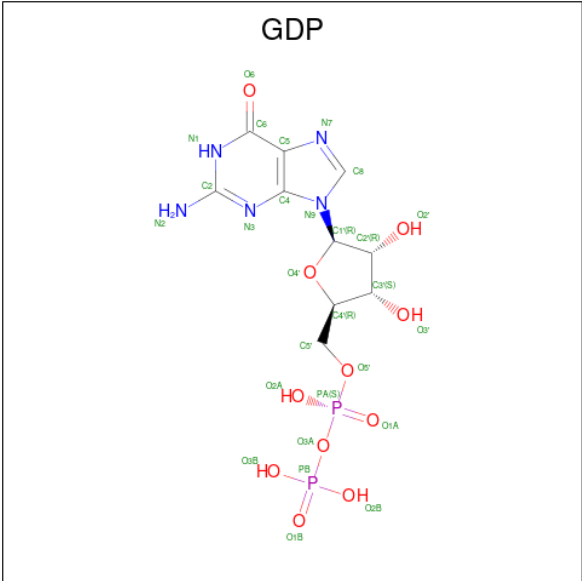
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



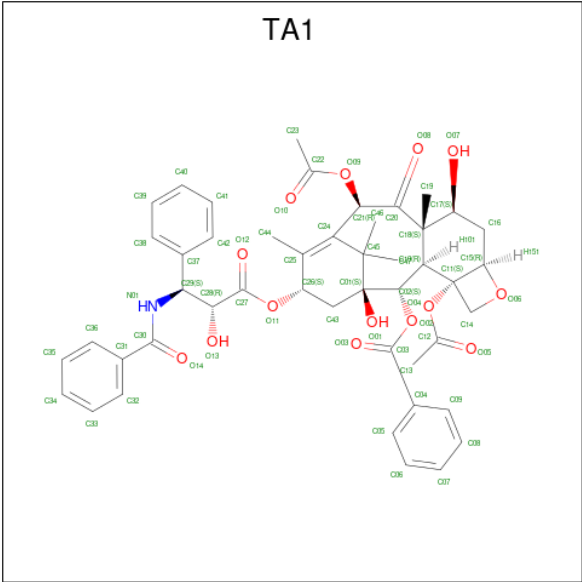
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 7 is TAXOL (three-letter code: TA1) (formula:  $C_{47}H_{51}NO_{14}$ ).

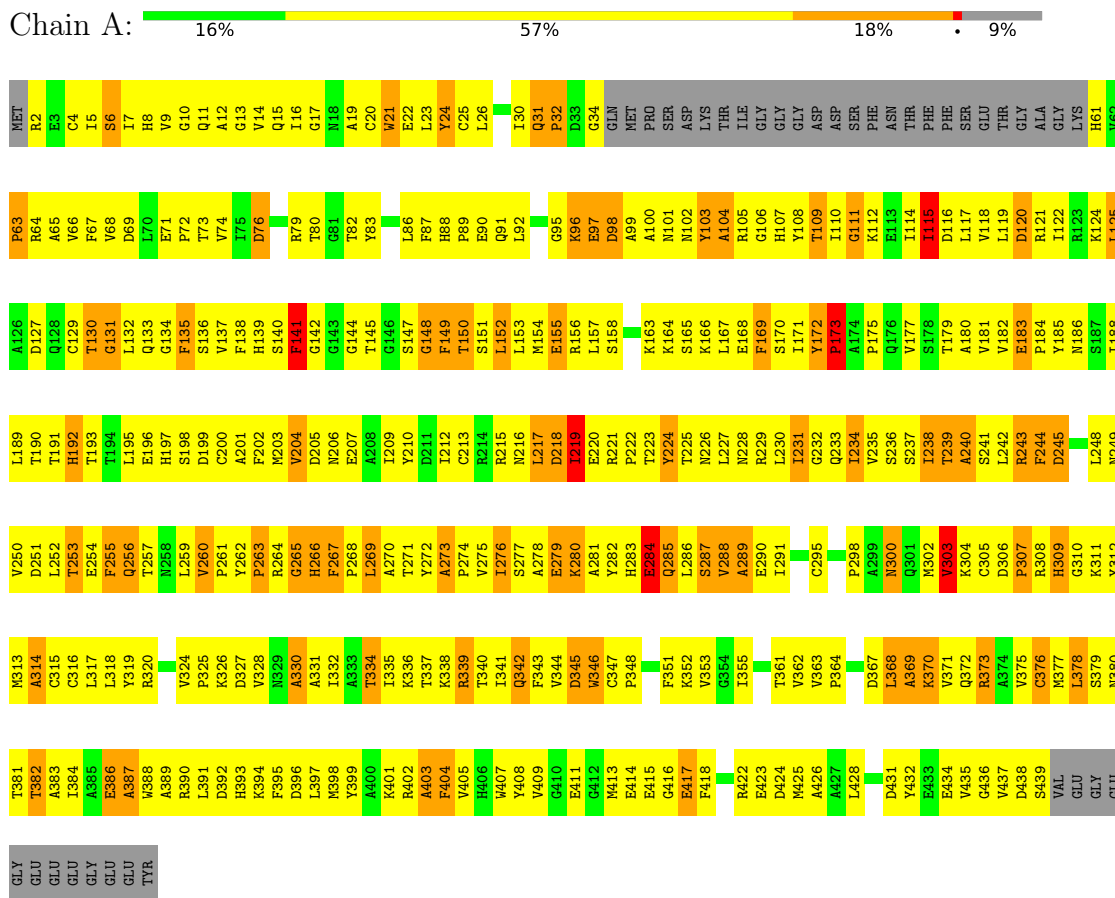


Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			62	47	1	14	

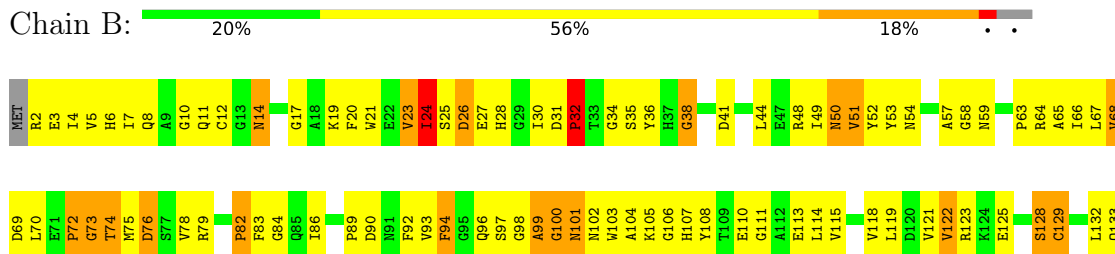
### 3 Residue-property plots

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.

- Molecule 1: tubulin alpha chain



- Molecule 2: tubulin beta chain



	G134	F135	Q136	L137	T138	H139	S140	L141	G142	G143	G144	T145	G146	S147	G148	M149	G150	T151	L152	L153	I154	S155	K156	I157	R158		Y161	P162	D163	R164	I165	M166	M167	T168		V171	V172	P173	S174	P175	K176	V177	S178	D179	T180	V181	V182	E183	P184	Y185	M186	A187	T188	L189	S190	V191	H192	Q193	L194	V195	
	E196	N197	T198	D199	E200	T201	Y202	C203	I204	D205	N206	E207	A208	L209	Y210	D211	I212	C213	F214	R215	T216	L217	K218	L219		T223	Y224	G225	D226	L227	N228	H229	L230	V231	S232	A233	T234	M235	S236	G237	V238	T239	T240	C241	L242	R243	F244		Q247	L248	N249	A250	D251	L252	R253	K254	L255	A256	V257	N258	
	M259	V260	P261	F262	P263	R264	L265	H266	F267	M268	M269	P270	G271	F272	A273	P274	L275	T276	S277	R278	G279	S280	Q281	Q282	Y283	R284	R284	A285	L286	T287	V288	P289	E290	L291		Q294	M295	F296	D297	A298	K299	N300	M301	M302	A303	A304	C305	D306	P307	R308	H309	G310	R311	Y312	L313	T314	V315		V318	F319	R320
	G321	R322	M323	S324	M325	K326	E327	V328	D329	E330	Q331	M332	L333	N334	V335	Q336	N337		Y342	F343	Y344	E345	W346	I347	P348	N349	N350	V351	K352	T353	A354	V355	C356	D357	I358	P359	P360	E369	G370	L371	R372	M373	S374	A375	T376	F377	I378	G379	N380	S381	T382	A383	I384	Q385	E386	L387	F388		F395	T396	
	F399	R400	R401	A402	A403	F404	L405	H406	W407	Y408	T409	G410	E411	G412	M413	D414		E417	F418	T419	E420	A421	E422	S423	M424	N425	N426	D427	L428	W429	S430	E431	Y432	Q433	Q434	Y435	Q436	D437	ALA	THR	ALA	ASP	GLU	GLN	GLY	GLU	PHE	GLU	GLU	GLY	GLU	ASP	GLU	ALA							

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.20Å 93.50Å 90.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.50)	Depositor
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.232 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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: GDP, MG, ZN, GTP, TA1

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	0.50	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
All	All	0.51	0/6726	0.75	2/9124 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	235	MET	CG-SD-CE	6.09	109.95	100.20
2	B	217	LEU	N-CA-C	-5.37	96.51	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3227	0	3143	542	0
2	B	3351	0	3229	553	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	32	0	12	5	0
6	B	28	0	12	1	0
7	B	62	0	51	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6702	0	6447	1068	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 81.

The worst 5 of 1068 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)
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.15
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.12
2:B:93:VAL:HG11	2:B:118:VAL:HG22	1.30	1.10
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.37	1.06
2:B:299:LYS:H	2:B:299:LYS:HD3	1.24	1.03

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 PDB entries followed by that with respect to all EM entries.

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	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0	3
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0	4
All	All	832/896 (93%)	539 (65%)	178 (21%)	115 (14%)	1	3

5 of 115 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	97	GLU
1	A	108	TYR
1	A	109	THR

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Mol	Chain	Res	Type
1	A	141	PHE

### 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 PDB entries followed by that with respect to all EM entries.

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	347/377 (92%)	298 (86%)	49 (14%)	3	19
2	B	367/381 (96%)	307 (84%)	60 (16%)	2	13
All	All	714/758 (94%)	605 (85%)	109 (15%)	6	17

5 of 109 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	94	PHE
2	B	201	THR
2	B	369	ARG
2	B	122	VAL
2	B	153	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	101	ASN
2	B	436	GLN
2	B	136	GLN
2	B	349	ASN
2	B	107	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 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	$\# Z  > 2$
7	TA1	B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
5	GTP	A	500	4	26,34,34	1.29	4 (15%)	32,54,54	1.10	3 (9%)
6	GDP	B	600	-	24,30,30	2.60	9 (37%)	30,47,47	2.93	8 (26%)

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
7	TA1	B	601	-	-	9/41/127/127	0/7/7/7
5	GTP	A	500	4	-	3/18/38/38	0/3/3/3
6	GDP	B	600	-	-	4/12/32/32	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	GDP	O4'-C1'	6.24	1.49	1.41
6	B	600	GDP	O6-C6	5.69	1.34	1.23
7	B	601	TA1	C06-C05	5.28	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	TA1	C18-C10	5.11	1.69	1.57
6	B	600	GDP	C2-N1	4.66	1.49	1.37

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	C8-N7-C5	9.29	120.69	102.99
6	B	600	GDP	N2-C2-N3	6.27	131.94	119.74
6	B	600	GDP	C5-C6-N1	6.10	124.72	113.95
7	B	601	TA1	C06-C05-C04	-4.85	114.61	120.34
7	B	601	TA1	C07-C08-C09	4.70	127.35	120.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	600	GDP	PA-O3A-PB-O2B
6	B	600	GDP	C5'-O5'-PA-O3A
6	B	600	GDP	C5'-O5'-PA-O1A
7	B	601	TA1	O02-C03-C04-C05
7	B	601	TA1	O02-C03-C04-C09

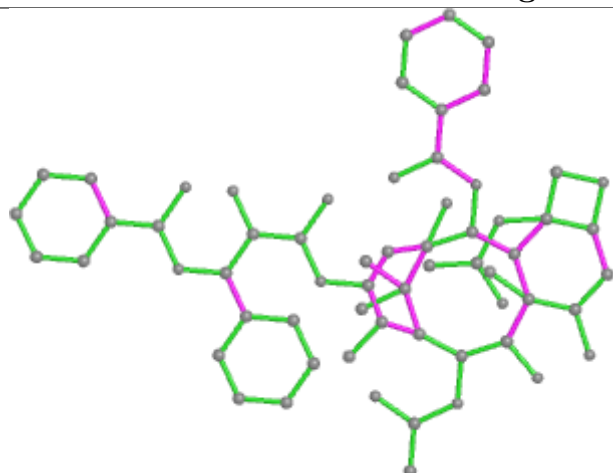
There are no ring outliers.

3 monomers are involved in 11 short contacts:

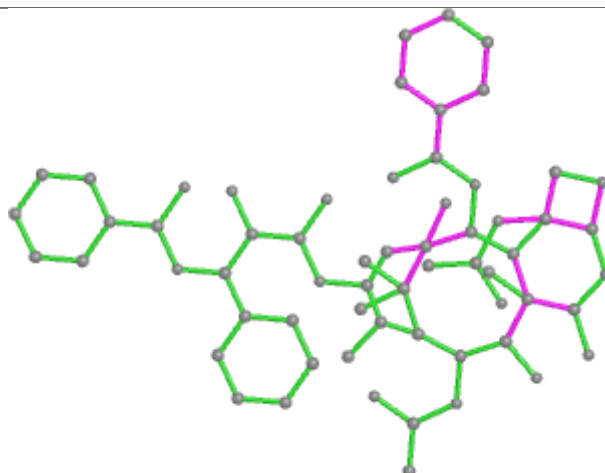
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	601	TA1	5	0
5	A	500	GTP	5	0
6	B	600	GDP	1	0

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.

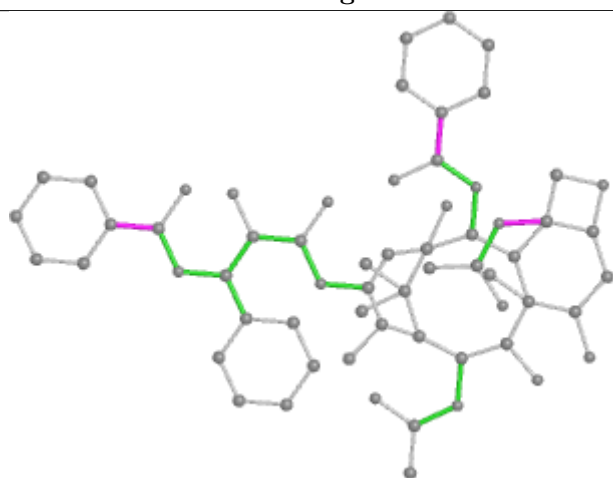
## Ligand TA1 B 601



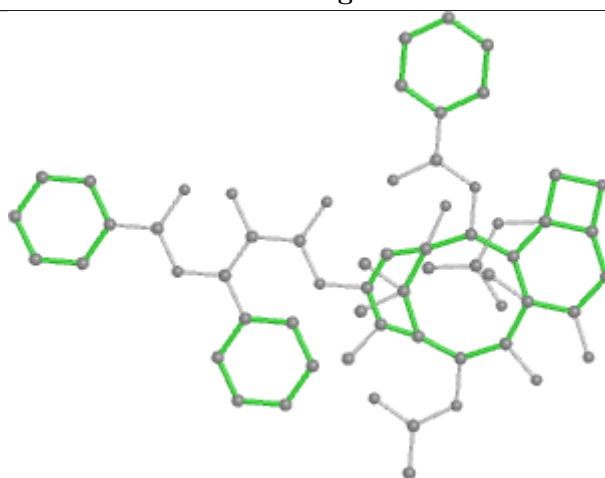
Bond lengths



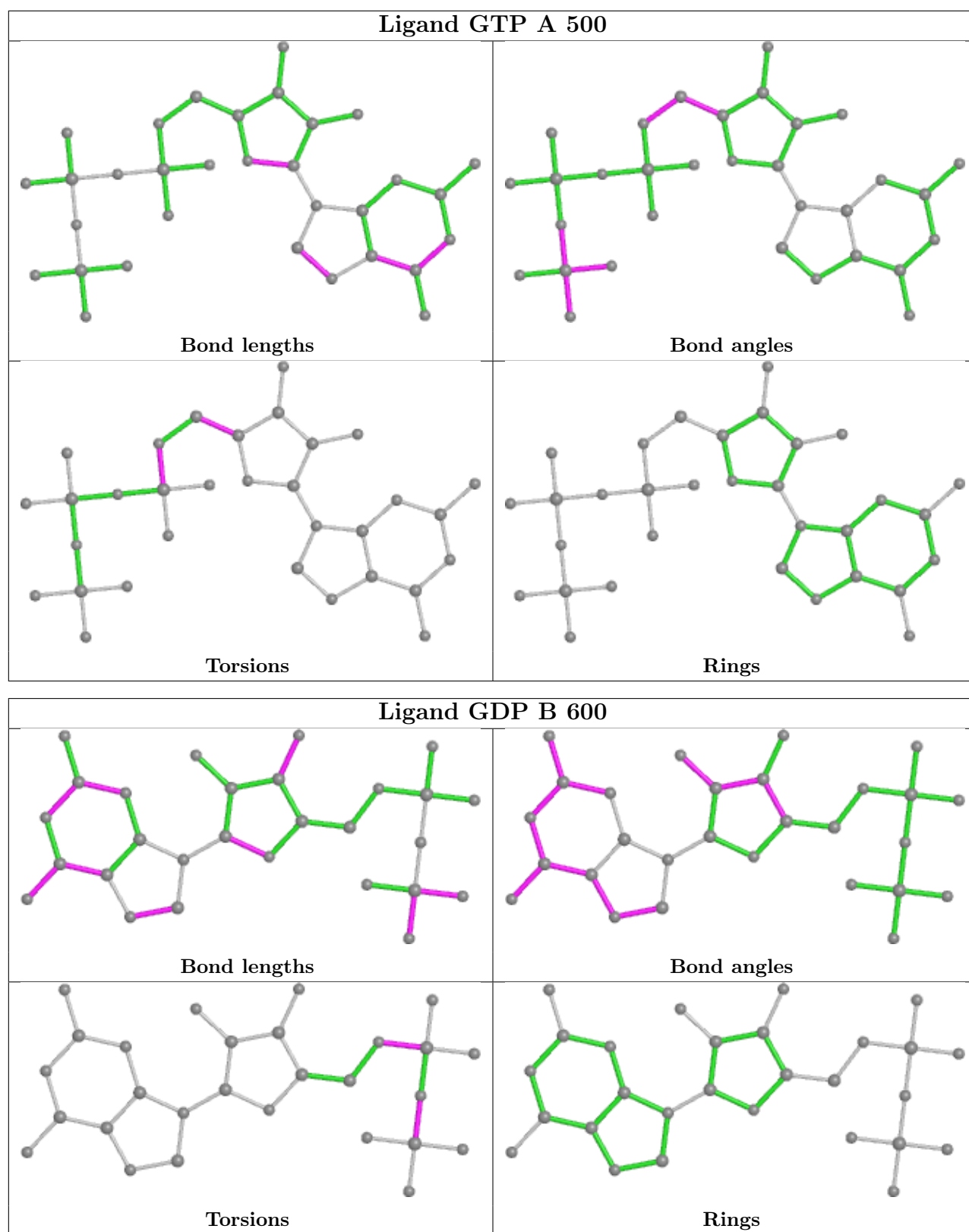
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.