



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 02:14 AM UTC

PDB ID : 1JFF / pdb_00001jff
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

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>.

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)
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

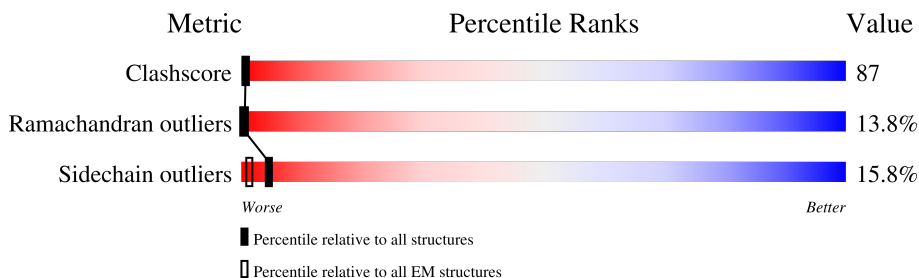
1 Overall quality at a glance i

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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 ≥ 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 [i](#)

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
			Total	C	N	O	S		
1	A	412	3227	2043	551	613	20	0	0

- Molecule 2 is a protein called tubulin beta chain.

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

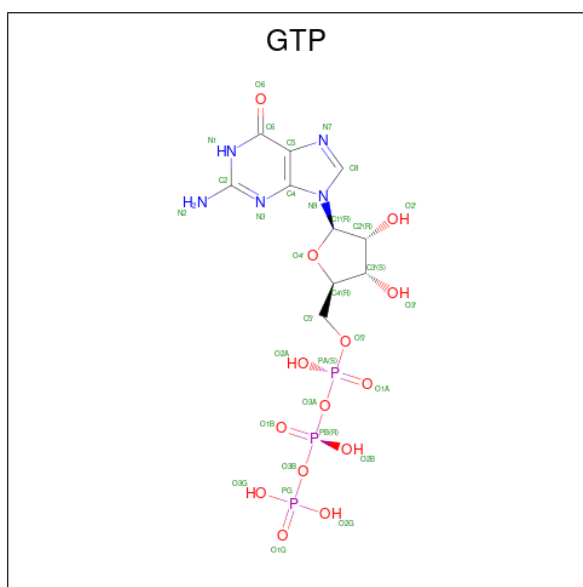
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

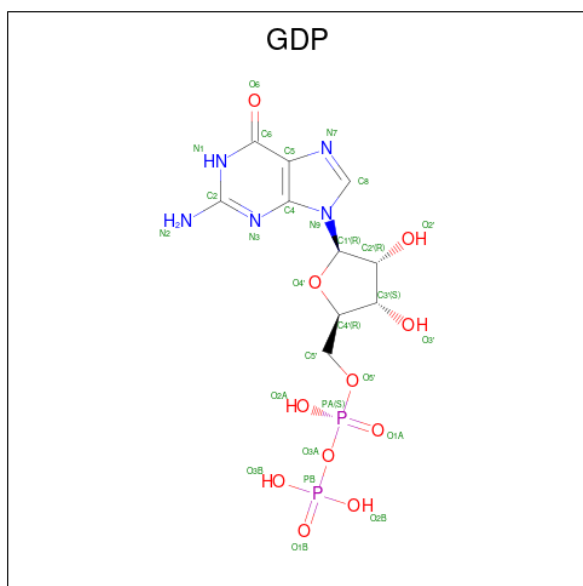
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



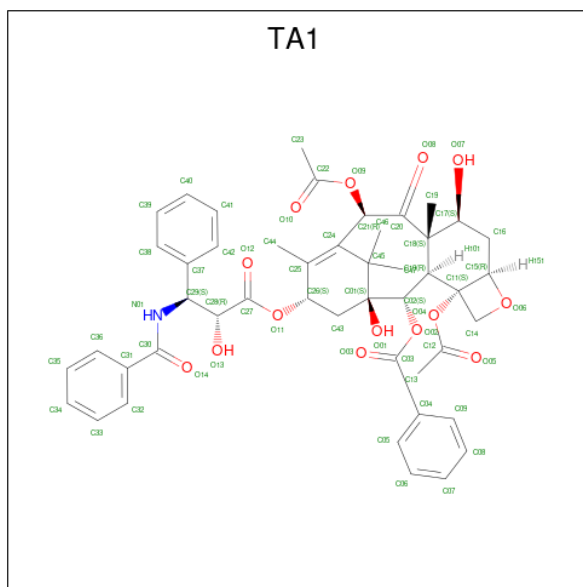
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	32	10	5	14	3	0

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



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

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



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

GLU	L387	V315	L255	H192	L132
GLU	F388	V318	A256	Q193	Q133
ASP	K389	F319	N257	L194	G134
GLU	R390	R320	N258	V195	F135
ALA	I391	G321	V260	M197	Q136
	F395	R322	P261	T198	L137
	T396	M323	F262	D199	T138
	F399	S324	P263	E200	H139
	R400	N325	R264	T201	S140
	R401	K326	L265	Y202	L141
	K402	E327	H266	C203	G142
	A403	V328	F267	L204	G143
	F404	D329	F268	D205	G144
	L405	E330	M269	N206	T145
	W406	Q331	P270	E207	G146
	Y408	L333	F272	A208	S147
	T409	N334	A273	L209	G148
	G410	V335	P274	Y210	M149
	E411	Q336	L275	D211	G150
	G412	N337	T276	L212	T151
	M413	Y342	S277	F214	L152
	D414	F343	R278	L153	L153
		V344	G279	I154	I154
		E345	S280	S155	S155
		W346	Q281	K156	K156
		I347	Q282	L157	L157
		E420	Y283	R158	R158
		A421	R284	E159	E159
		E422	A285	E160	E160
		S423	L286	Y161	Y161
		M424	T287	P162	P162
		N425	V288	D163	D163
		N426	P289	R164	R164
		D427	E290	I165	I165
		L428	E291	M166	M166
		Y429	L291	N167	N167
		S430	T292	T168	T168
		E431	Q293	V171	V171
		Y432	Q294	V172	V172
		Q433	M295	P173	P173
		Q434	F296	M235	M235
		Y435	D297	G237	G237
		Q436	A298	G337	G337
		D437	K299	V238	V238
		ALA	M300	V238	V238
		THR	M301	T239	T239
		ALA	M302	T240	T240
		ALA	S374	C241	C241
		ASP	A375	L242	L242
		GLU	T376	R243	R243
		GLN	F377	F244	F244
		GLY	I378	Q247	Q247
		GLY	G379	L248	L248
		GLY	N380	Y185	Y185
		GLY	S381	N249	N249
		PHE	T382	A250	A250
		GLU	A883	D251	D251
		GLU	I384	L252	L252
		GLU	Q385	R253	R253
		GLY	E386	K254	K254

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, α , β , γ	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 ²)	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, TA1, ZN, GTP, MG

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	0.62	1/3300 (0.0%)	1.09	22/4482 (0.5%)
2	B	0.63	0/3426	1.11	22/4642 (0.5%)
All	All	0.62	1/6726 (0.0%)	1.10	44/9124 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	TYR	CA-C	-5.50	1.48	1.53

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	CA-C-N	10.67	133.18	119.84
1	A	172	TYR	C-N-CA	10.67	133.18	119.84
2	B	262	PHE	CA-C-N	9.98	132.32	119.84
2	B	262	PHE	C-N-CA	9.98	132.32	119.84
1	A	283	HIS	N-CA-C	-8.23	101.27	113.61

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	578	0
2	B	3351	0	3229	595	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
All	All	6702	0	6447	1146	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 87.

The worst 5 of 1146 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 3
All	All	832/896 (93%)	539 (65%)	178 (21%)	115 (14%)	0 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
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%)	294 (85%)	53 (15%)	3	16
2	B	367/381 (96%)	307 (84%)	60 (16%)	2	14
All	All	714/758 (94%)	601 (84%)	113 (16%)	4	15

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	67	LEU
2	B	431	GLU
2	B	163	ASP
2	B	427	ASP
2	B	331	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	349	ASN
2	B	380	ASN
2	B	436	GLN
1	A	309	HIS
1	A	301	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](#)

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
6	GDP	B	600	-	29,30,30	2.86	11 (37%)	45,47,47	3.48	16 (35%)
5	GTP	A	500	4	33,34,34	1.89	3 (9%)	50,54,54	0.91	3 (6%)
7	TA1	B	601	-	68,68,68	2.20	26 (38%)	105,105,105	1.50	13 (12%)

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
6	GDP	B	600	-	-	4/16/32/32	0/3/3/3
5	GTP	A	500	4	-	4/22/38/38	0/3/3/3
7	TA1	B	601	-	-	9/41/127/127	0/7/7/7

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	GDP	PA-O3A	7.55	1.67	1.59
7	B	601	TA1	C06-C05	6.50	1.50	1.38
5	A	500	GTP	PA-O3A	-6.00	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	GDP	O6-C6	5.96	1.34	1.23
6	B	600	GDP	C8-N9	5.87	1.50	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	GDP	N9-C8-N7	-10.76	93.44	113.40
6	B	600	GDP	C8-N7-C5	9.22	120.69	104.26
6	B	600	GDP	C6-C5-N7	8.59	145.92	130.29
6	B	600	GDP	N2-C2-N3	6.28	131.94	119.67
6	B	600	GDP	C6-C5-C4	-6.19	109.52	118.83

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

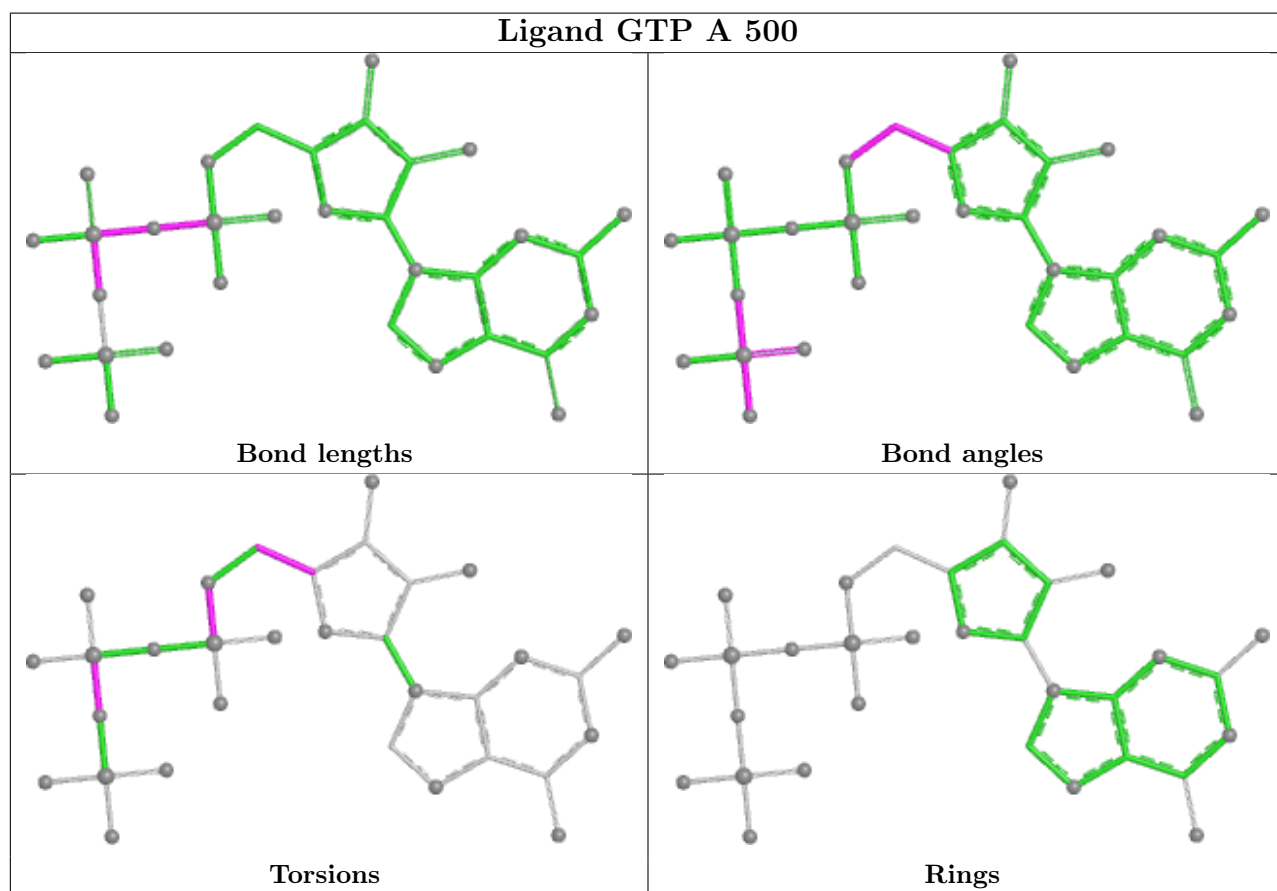
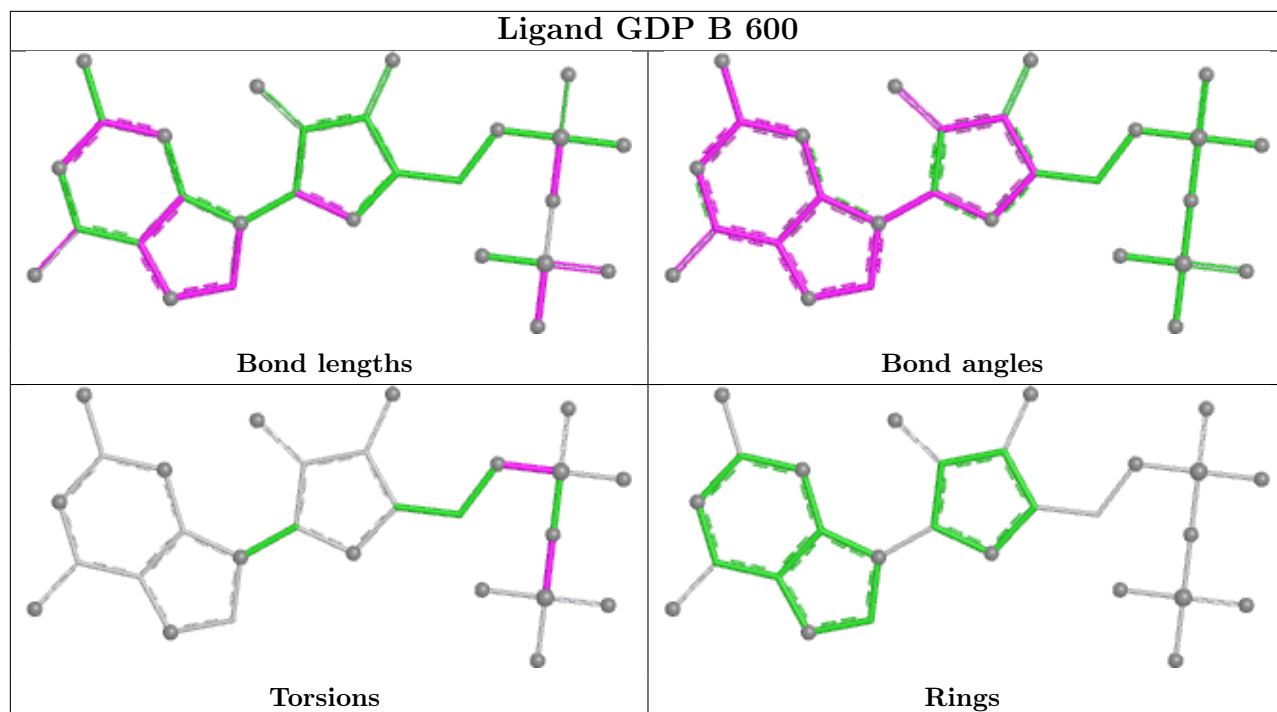
Mol	Chain	Res	Type	Atoms
6	B	600	GDP	PA-O3A-PB-O2B
6	B	600	GDP	C5'-O5'-PA-O3A
6	B	600	GDP	C5'-O5'-PA-O1A
7	B	601	TA1	O02-C03-C04-C05
7	B	601	TA1	O02-C03-C04-C09

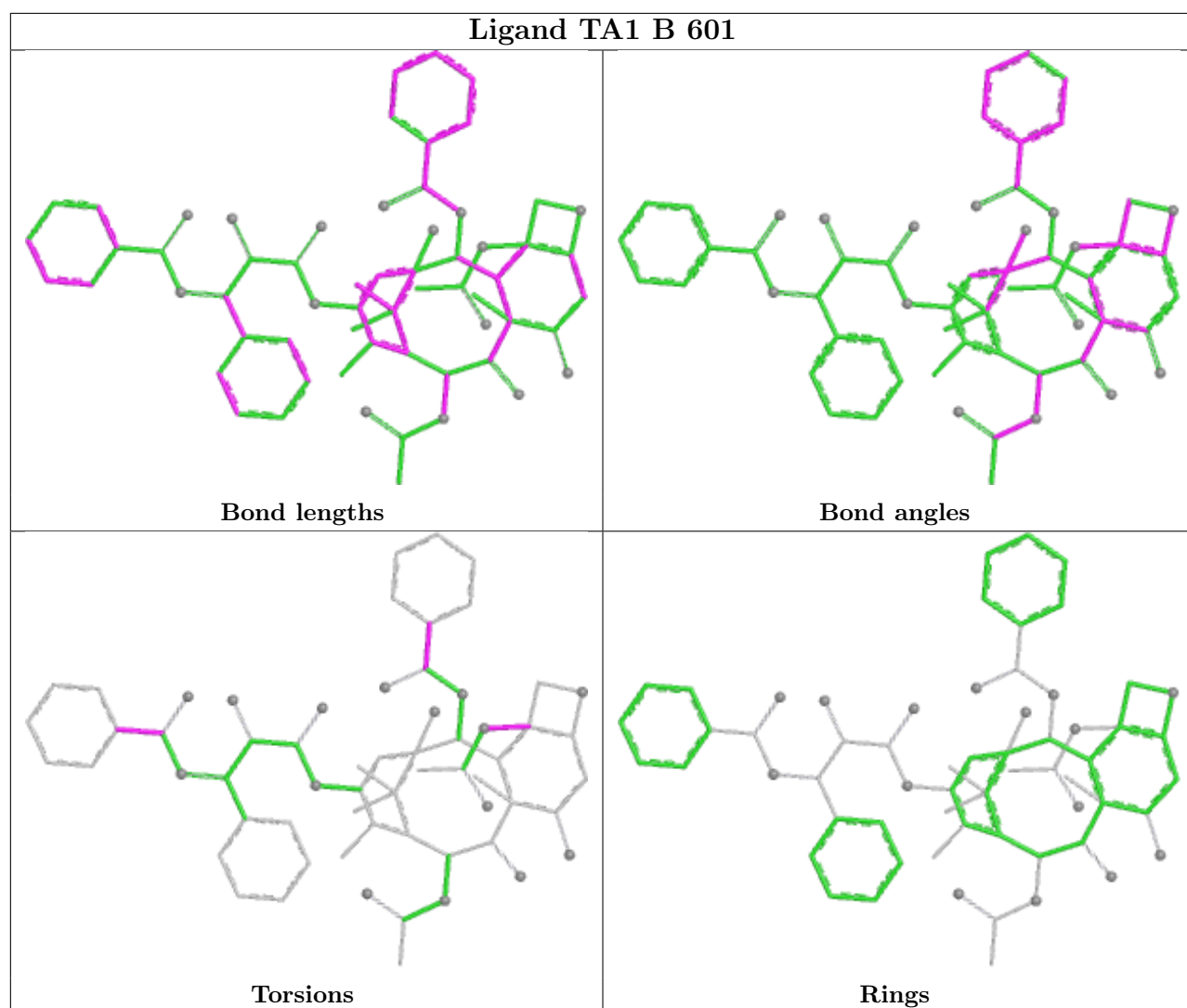
There are no ring outliers.

3 monomers are involved in 11 short contacts:

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