



wwPDB EM Model Validation Summary Report ⓘ

May 17, 2020 – 11:57 pm BST

PDB ID : 1TUB
Title : TUBULIN ALPHA-BETA DIMER, ELECTRON DIFFRACTION
Authors : Nogales, E.; Downing, K.H.
Deposited on : 1997-09-23
Resolution : 3.70 Å(reported)

This is a wwPDB EM Model 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 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) : 2.11

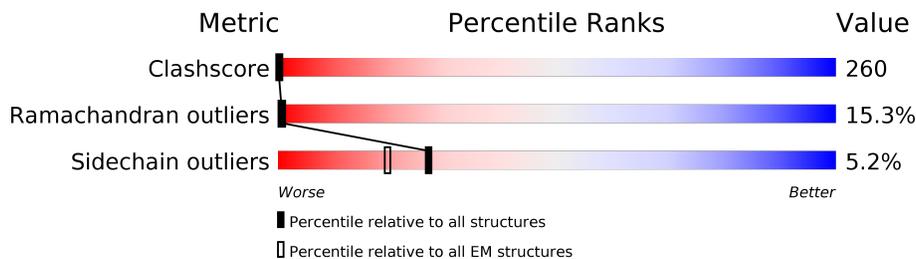
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.70 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 on 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	440	8% 50% 27% 15%
2	B	427	5% 49% 29% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GTP	A	500	-	-	X	-
4	GDP	B	500	-	-	X	-
5	TXL	B	501	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6907 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	440	3430	2168	583	657	22	0	0

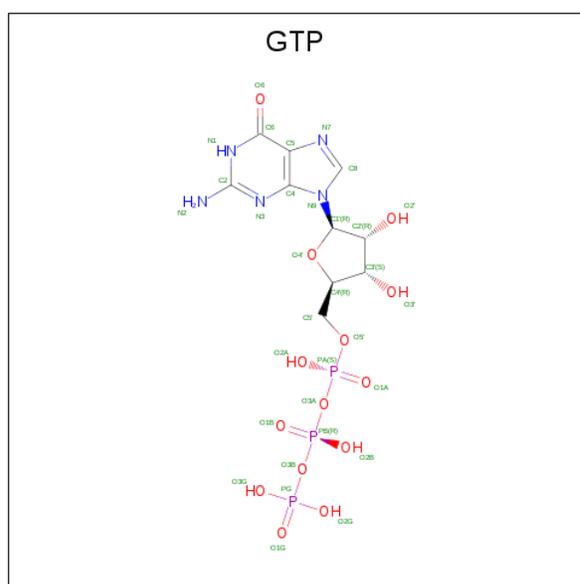
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	CONFLICT	UNP P02550

- Molecule 2 is a protein called TUBULIN.

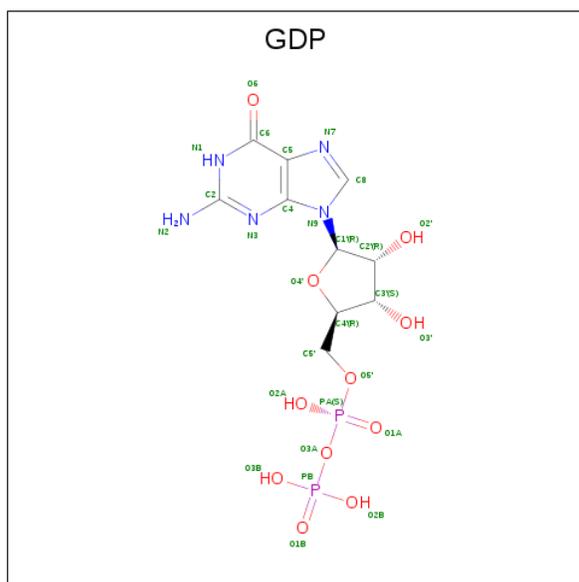
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	427	3359	2110	576	647	26	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



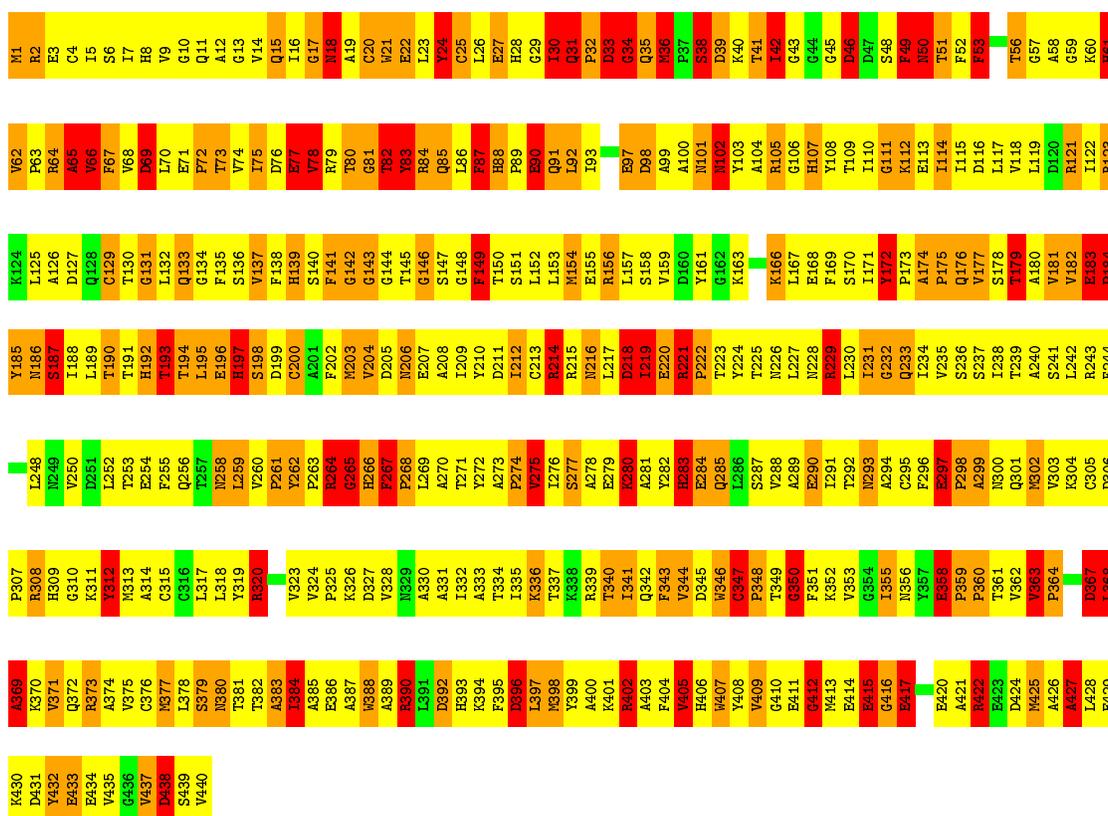
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	B	1	58	43	1	14	0

3 Residue-property plots

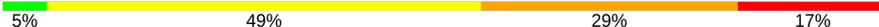
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

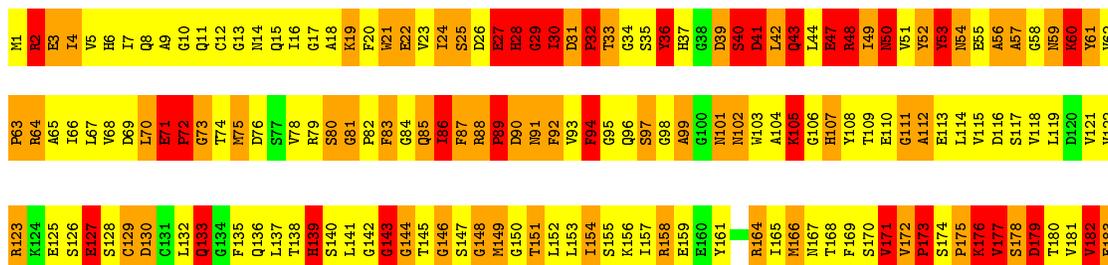
- Molecule 1: TUBULIN

Chain A: 



- Molecule 2: TUBULIN

Chain B: 



Y432	K372	A304	F244	P184
Q433	M373	C305	F245	Y185
Q434	S374	D306	Q246	M186
Y435	A375	P307	Q247	A187
Q436	T376	R308	L248	T188
D437	F377	H309	M249	L189
	I378	G310	A250	S190
	G379	R311	D251	V191
	M380	Y312	L252	R192
	S381	L313	R253	Q193
	T382	T314	K254	L194
	A383	V315	L255	V195
	I384	A316	A256	E196
	Q385	A317	V257	M197
	E386	F318	M258	T198
	F388	R320	M259	D199
	K389	G321	V260	E200
	R390	R322	F262	T201
	I391	M323	F263	Y202
	S392	S324	F264	G203
	E393	M325	L265	L204
	Q394	K326	H266	D205
	F395	E327	F267	N206
	T396	V328	F268	E207
	A397	E329	M269	A208
	M398	E330	F270	L209
	F399	Q331	G271	Y210
	R400	M332	F272	D211
	R401	L333	A273	I212
	K402	N334	P274	C213
	A403	V335	L275	F214
	F404	Q336	L276	R215
	L405	N337	S277	T216
	H406	K338	R278	L217
	W407	M339	G279	K218
	Y408	S340	S280	L219
	T409	S341	Q281	T220
	G410	Y342	Q282	T221
	E411	F343	Y283	P222
	G412	V344	R284	T223
	M413	E345	A285	Y224
	D414	W346	L286	G225
	E415	I347	T287	D226
	M416	F348	V288	L227
	E417	N349	P289	M228
	F418	N350	E290	H229
	T419	V351	L291	L230
	E420	K352	T292	V231
	A421	T353	Q293	S232
	E422	A354	Q294	A233
	S423	V355	M295	T234
	N424	C356	F296	M235
	M425	D357	D297	S236
	N426	I358	A298	G237
	D427	P359	K299	V238
	L428	P360	M300	T239
	V429	R369	M301	T240
	S430	G370	M302	C241
	E431	L371	A303	L242

4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 4000, JEOL 4000	Depositor
Voltage (kV)	400, 400	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GENERIC FILM	Depositor

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, GTP, TXL

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	2.34	110/3508 (3.1%)	2.76	214/4762 (4.5%)
2	B	2.47	111/3434 (3.2%)	3.07	266/4652 (5.7%)
All	All	2.41	221/6942 (3.2%)	2.92	480/9414 (5.1%)

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	56
2	B	0	59
All	All	0	115

The worst 5 of 221 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	278	ARG	CA-CB	34.96	2.30	1.53
2	B	105	LYS	C-N	-29.38	0.80	1.33
2	B	73	GLY	C-N	-28.00	0.69	1.34
1	A	38	SER	C-N	-27.48	0.70	1.34
1	A	347	CYS	C-N	-23.43	0.89	1.34

The worst 5 of 480 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	LEU	O-C-N	-54.19	36.00	122.70
1	A	363	VAL	C-N-CD	-48.68	13.51	120.60
2	B	273	ALA	C-N-CD	-46.48	18.35	120.60
2	B	105	LYS	O-C-N	-44.51	47.53	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	88	ARG	C-N-CD	-44.07	23.65	120.60

There are no chirality outliers.

5 of 115 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	ASN	Mainchain
1	A	24	TYR	Mainchain,Peptide
1	A	30	ILE	Mainchain,Peptide
1	A	34	GLY	Peptide
1	A	36	MET	Mainchain

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	3430	0	3257	1656	34
2	B	3359	0	3172	1914	15
3	A	32	0	11	29	0
4	B	28	0	12	14	0
5	B	58	0	51	55	0
All	All	6907	0	6503	3472	35

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 260.

The worst 5 of 3472 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:229:HIS:CE1	5:B:501:TXL:H343	1.28	1.68
2:B:346:TRP:CE3	2:B:347:ILE:HG13	1.25	1.66
1:A:212:ILE:HD11	1:A:230:LEU:CD2	1.25	1.65
2:B:151:THR:CB	2:B:192:HIS:CD2	1.75	1.62
1:A:115:ILE:CD1	1:A:152:LEU:HG	1.15	1.62

The worst 5 of 35 symmetry-related close contacts are listed below. The label for Atom-2 includes

the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:CG	1:A:420:GLU:CD[2_444]	0.73	1.47
1:A:1:MET:CE	2:B:72:PRO:CG[1_655]	1.00	1.20
1:A:283:HIS:CG	1:A:420:GLU:OE1[2_444]	1.01	1.19
1:A:283:HIS:ND1	1:A:420:GLU:CD[2_444]	1.11	1.09
1:A:283:HIS:CD2	1:A:420:GLU:CA[2_444]	1.18	1.02

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	438/440 (100%)	323 (74%)	62 (14%)	53 (12%)	0 4
2	B	425/427 (100%)	297 (70%)	49 (12%)	79 (19%)	0 1
All	All	863/867 (100%)	620 (72%)	111 (13%)	132 (15%)	0 3

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	33	ASP
1	A	35	GLN
1	A	39	ASP
1	A	42	ILE

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	369/369 (100%)	351 (95%)	18 (5%)	25	56
2	B	368/368 (100%)	348 (95%)	20 (5%)	22	54
All	All	737/737 (100%)	699 (95%)	38 (5%)	27	55

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	432	TYR
2	B	101	ASN
2	B	426	ASN
2	B	30	ILE
2	B	139	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	28	HIS
2	B	102	ASN
2	B	350	ASN
2	B	59	ASN
1	A	192	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](#)

3 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
3	GTP	A	500	1	26,34,34	1.75	6 (23%)	33,54,54	2.46	8 (24%)
4	GDP	B	500	2	24,30,30	1.87	6 (25%)	31,47,47	2.30	7 (22%)
5	TXL	B	501	2	63,63,63	4.25	46 (73%)	100,100,100	3.30	53 (53%)

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	GTP	A	500	1	-	0/18/38/38	0/3/3/3
4	GDP	B	500	2	-	4/12/32/32	0/3/3/3
5	TXL	B	501	2	-	0/38/124/124	0/6/6/6

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	TXL	O3-C4	-9.59	1.26	1.46
5	B	501	TXL	C41-C36	8.34	1.53	1.39
5	B	501	TXL	C8-C3	-7.74	1.38	1.57
5	B	501	TXL	C37-C36	-7.66	1.26	1.39
5	B	501	TXL	O6-C9	-7.61	1.08	1.21

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	TXL	C15-C1-C2	10.94	123.89	111.91
3	A	500	GTP	C5-C6-N1	-9.38	110.61	123.43
5	B	501	TXL	C39-C38-C37	8.99	133.89	120.19
4	B	500	GDP	C5-C6-N1	-8.95	111.19	123.43
5	B	501	TXL	C38-C37-C36	-8.08	110.78	120.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

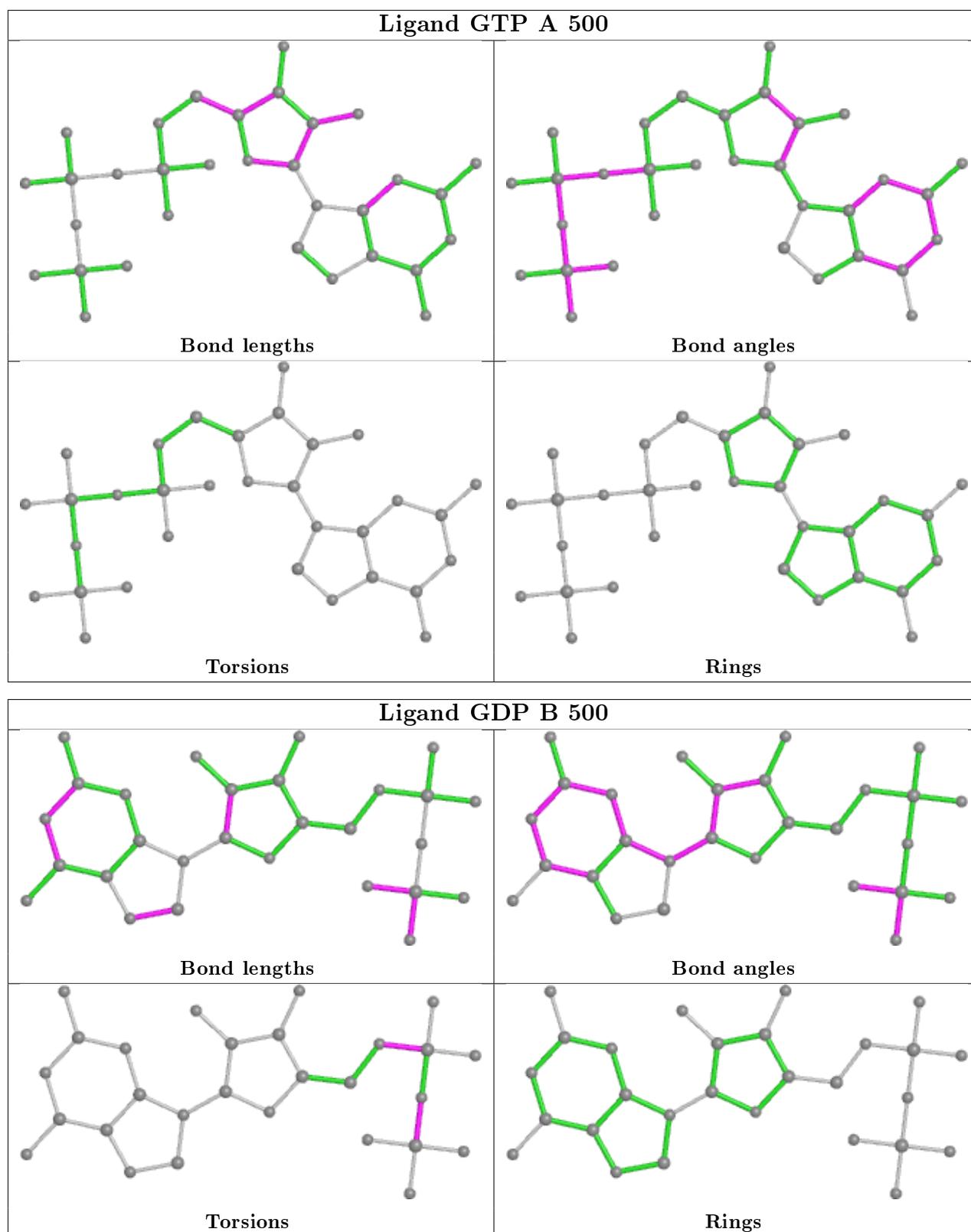
Mol	Chain	Res	Type	Atoms
4	B	500	GDP	PA-O3A-PB-O2B
4	B	500	GDP	PA-O3A-PB-O1B
4	B	500	GDP	PA-O3A-PB-O3B
4	B	500	GDP	C5'-O5'-PA-O1A

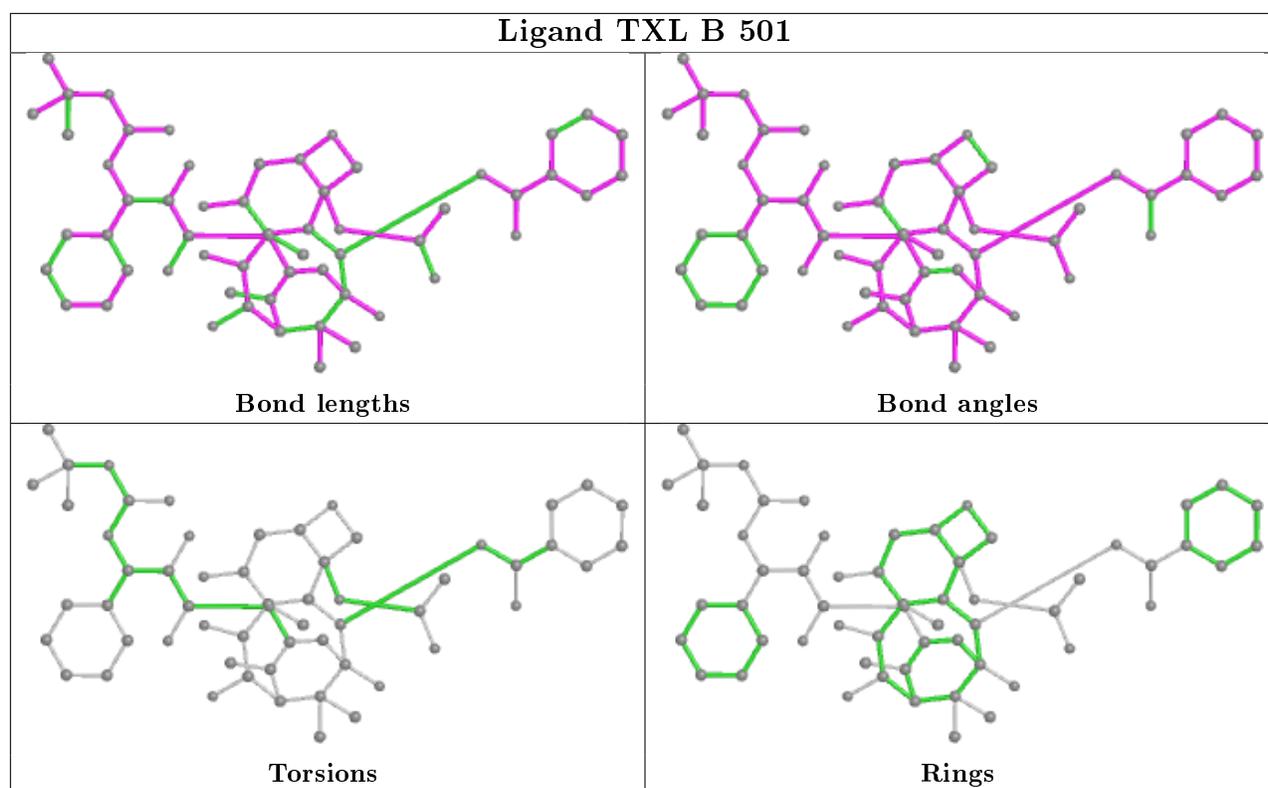
There are no ring outliers.

3 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	GTP	29	0
4	B	500	GDP	14	0
5	B	501	TXL	55	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	52
1	A	41

The worst 5 of 93 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	387:LEU	C	388:PHE	N	1.63
1	A	283:HIS	C	284:GLU	N	1.20
1	A	380:ASN	C	381:THR	N	1.20
1	A	437:VAL	C	438:ASP	N	1.20
1	B	52:TYR	C	53:TYR	N	1.20