



wwPDB EM Validation Summary Report ⓘ

Dec 13, 2022 – 12:15 AM EST

PDB ID : 1TVK
Title : The binding mode of epothilone A on α,β -tubulin by electron crystallography
Authors : Nettles, J.H.; Li, H.; Cornett, B.; Krahn, J.M.; Snyder, J.P.; Downing, K.H.
Deposited on : 2004-06-29
Resolution : 2.89 Å (reported)
Based on initial model : 1JFF

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 : 4.02b-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)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

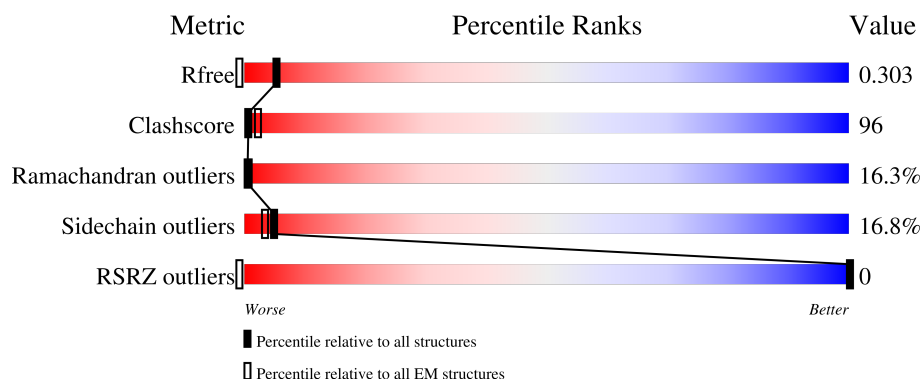
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 2.89 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)
R_{free}	130704	0
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RSRZ outliers	127900	0

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	440	<div> <div>9%</div> <div>61%</div> <div>22%</div> <div>• 6%</div> </div>
2	B	427	<div> <div>14%</div> <div>61%</div> <div>23%</div> <div>•</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6672 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

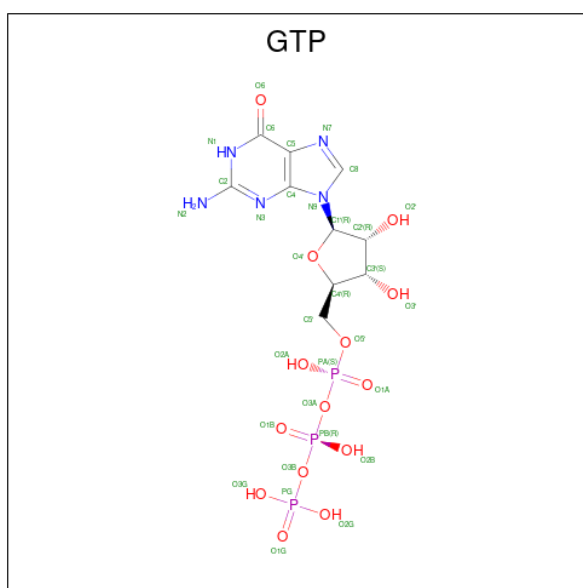
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called Tubulin beta chain.

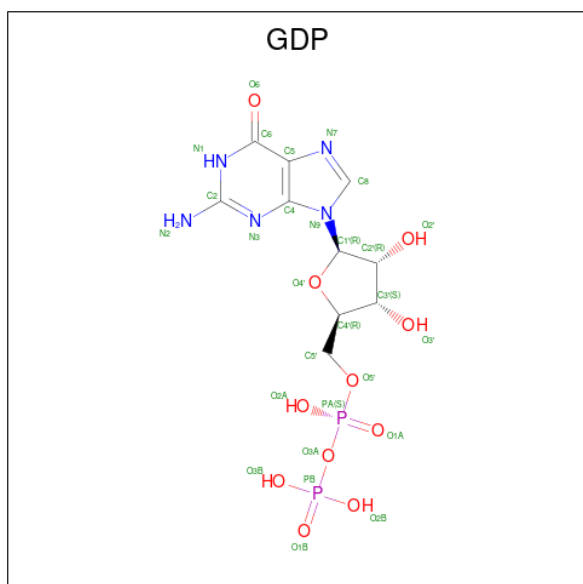
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3351	2105	575	646	25	0	0

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



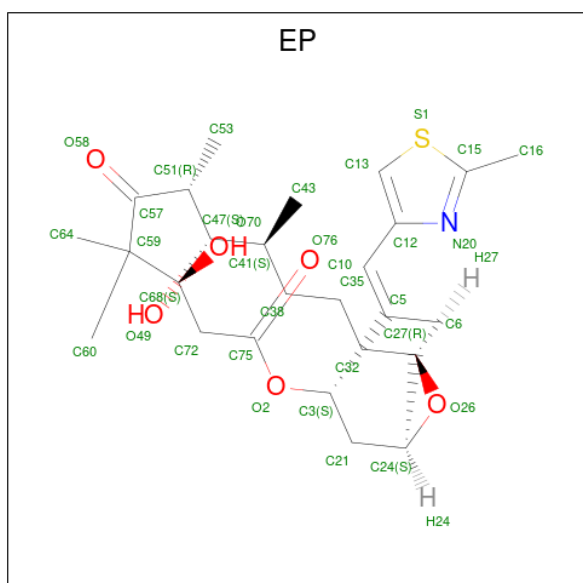
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



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

- Molecule 5 is EPOTHILONE A (three-letter code: EP) (formula: $C_{26}H_{39}NO_6S$).

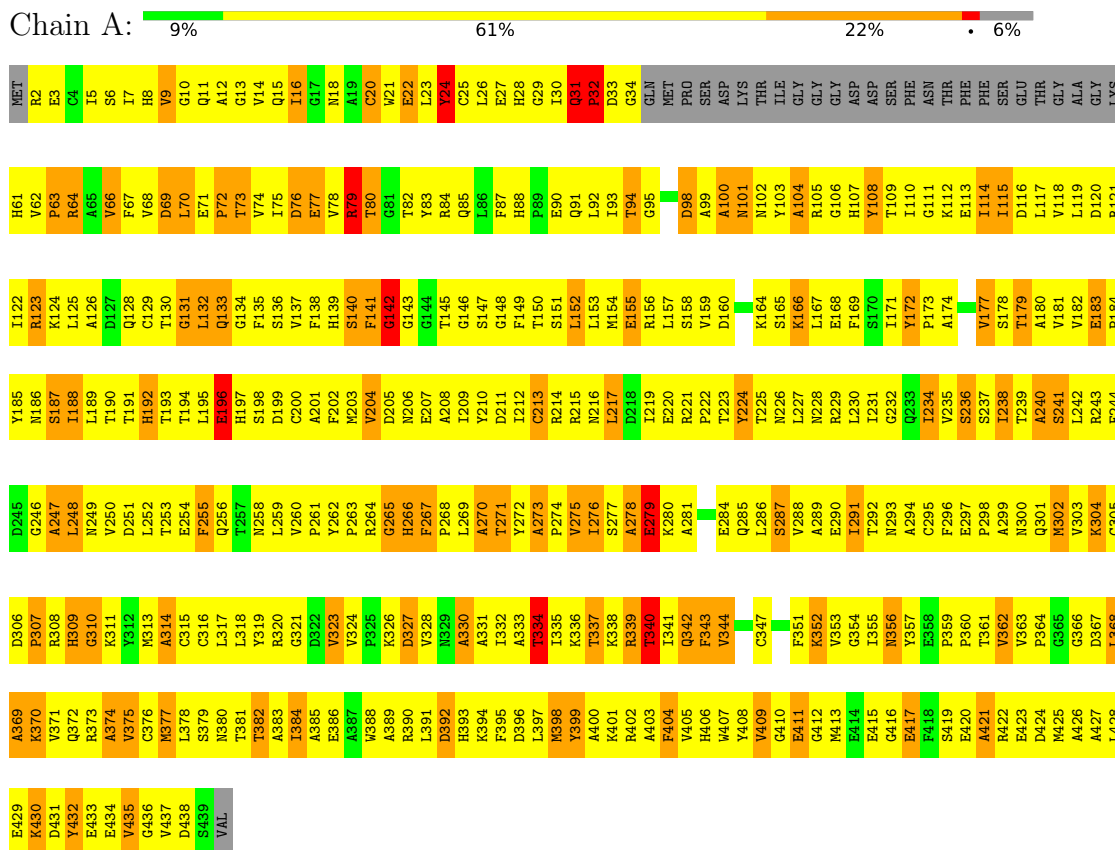


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	B	1	34	26	1	6	1	0

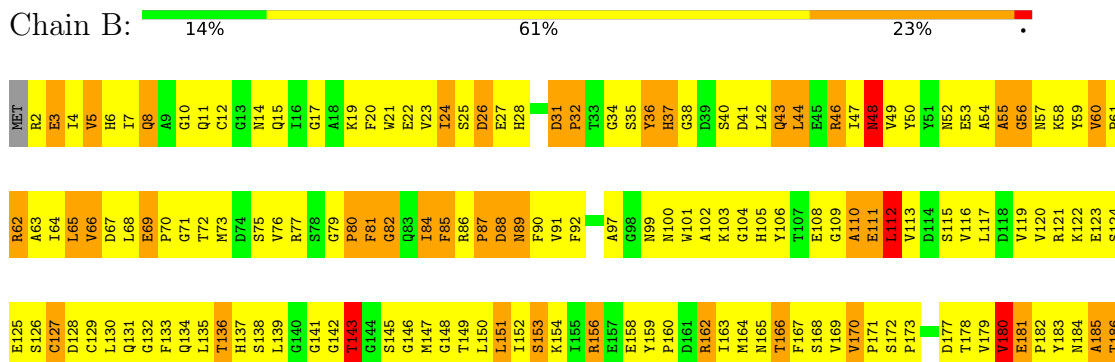
3 Residue-property plots

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



N370	S371	T372	A373	I374	Q375	E376	L377	F378	K379	R380	I381	S382	E383	Q384	F385	T386	A387	M388	F389	R390	R391	K392	A393	F394	L395	Y398	T399	G400	E401	G402	M403	D404	M406	E407	F408	T409	E410	A411	E412	S413	N414	M415	N416	D417	L418	V419	S420	E421	Y422	Y425	Q426	D427						
R309	Y310	L311	T312	V313	A314	A315	R318	G319	R320	M321	S322	M323	K324	E325	V326	D327	E328	Q329	M330	L331	N332	V333	G334	N335	K336	N337	S338	S339	Y340	F341	V342	W344	I345	P346	N347	N348	V349	K350	T351	A352	V353	C354	D355	I356	P357	P358	R359	G360	L361	K362	M363	S364	A365	E366	F367	I368	G369	
A248	D249	L250	R251	K252	L253	A254	V255	N256	M257	V258	P259	F260	P261	R262	L263	H264	F265	F266	M267	P268	G269	F270	A271	P272	L273	T274	S275	R276	Q279	Q280	Y281	R282	A283	L284	T285	V286	P287	E288	L289	T290	Q291	Q292	M293	F294	D295	A296	K297	N298	M299	M300	A301	A302	C303	D304	P305	R306	H307	G308
L187	S188	V189	H190	Q191	L192	V193	E194	N195	T196	D197	E198	T199	Y200	C201	I202	D203	N204	E205	A206	L207	Y208	D209	I210	C211	F212	R213	T214	L215	K216	L217	P220	T221	Y222	G223	D224	L225	N226	H227	L228	V229	S230	A231	T232	M233	S234	G235	V236	T237	L238	C239	L240	R241	F242	P243	G244	Q245	L246	N247

4 Data and refinement statistics

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)	91.29 – 2.89 23.84 – 2.89	Depositor EDS
% Data completeness (in resolution range)	67.0 (91.29-2.89) 63.9 (23.84-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 2.89Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.333 , 0.321 0.314 , 0.303	Depositor DCC
R_{free} test set	967 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.096 for -h,-l,-k 0.070 for -h,l,k 0.118 for h,-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8280e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EP, GTP, GDP

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	0.48	0/3300	0.71	2/4482 (0.0%)
2	B	0.51	0/3426	0.76	3/4642 (0.1%)
All	All	0.50	0/6726	0.73	5/9124 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	LEU	CA-CB-CG	6.52	130.30	115.30
2	B	282	ARG	CG-CD-NE	-6.12	98.96	111.80
1	A	142	GLY	N-CA-C	5.35	126.46	113.10
2	B	227	HIS	CG-CD2-NE2	-5.22	99.27	109.20
2	B	282	ARG	N-CA-CB	-5.22	101.20	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	668	0
2	B	3351	0	3229	620	0
3	A	32	0	12	4	0
4	B	28	0	12	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	34	0	39	4	0
All	All	6672	0	6435	1260	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 96.

The worst 5 of 1260 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:A:11:GLN:HG2	1:A:15:GLN:HE21	1.04	1.12
2:B:172:SER:HB3	2:B:205:GLU:HG2	1.16	1.10
2:B:286:VAL:H	2:B:287:PRO:HD2	1.11	1.09
1:A:229:ARG:HD3	1:A:363:VAL:HG21	1.33	1.08
2:B:285:THR:HB	2:B:287:PRO:HD2	1.31	1.07

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	408/440 (93%)	223 (55%)	113 (28%)	72 (18%)	0	0
2	B	424/427 (99%)	251 (59%)	109 (26%)	64 (15%)	0	0
All	All	832/867 (96%)	474 (57%)	222 (27%)	136 (16%)	0	0

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	72	PRO
1	A	73	THR

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Mol	Chain	Res	Type
1	A	100	ALA
1	A	101	ASN

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	347/369 (94%)	291 (84%)	56 (16%)	2	7
2	B	367/368 (100%)	303 (83%)	64 (17%)	2	6
All	All	714/737 (97%)	594 (83%)	120 (17%)	5	6

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	5	VAL
2	B	364	SER
2	B	85	PHE
2	B	358	PRO
2	B	416	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
2	B	347	ASN
2	B	226	ASN
2	B	298	ASN
2	B	414	ASN

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](#)

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	9500	-	26,34,34	1.10	2 (7%)	32,54,54	0.95	3 (9%)
4	GDP	B	1500	-	24,30,30	1.03	2 (8%)	30,47,47	1.00	3 (10%)
5	EP	B	1001	-	32,36,36	2.15	7 (21%)	39,53,53	2.76	7 (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	GTP	A	9500	-	-	2/18/38/38	0/3/3/3
4	GDP	B	1500	-	-	2/12/32/32	0/3/3/3
5	EP	B	1001	-	-	13/49/55/55	0/2/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	EP	C27-C24	7.79	1.60	1.46
5	B	1001	EP	C13-S1	5.88	1.79	1.70
3	A	9500	GTP	C5-C6	-2.98	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	EP	C72-C68	2.76	1.56	1.53
3	A	9500	GTP	C8-N7	-2.44	1.30	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	EP	C27-O26-C24	12.26	69.53	60.69
5	B	1001	EP	O26-C27-C24	-7.05	55.15	59.65
5	B	1001	EP	O26-C24-C27	-6.77	55.32	59.65
3	A	9500	GTP	PB-O3B-PG	-2.77	123.33	132.83
5	B	1001	EP	O2-C75-C72	2.54	116.13	111.46

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

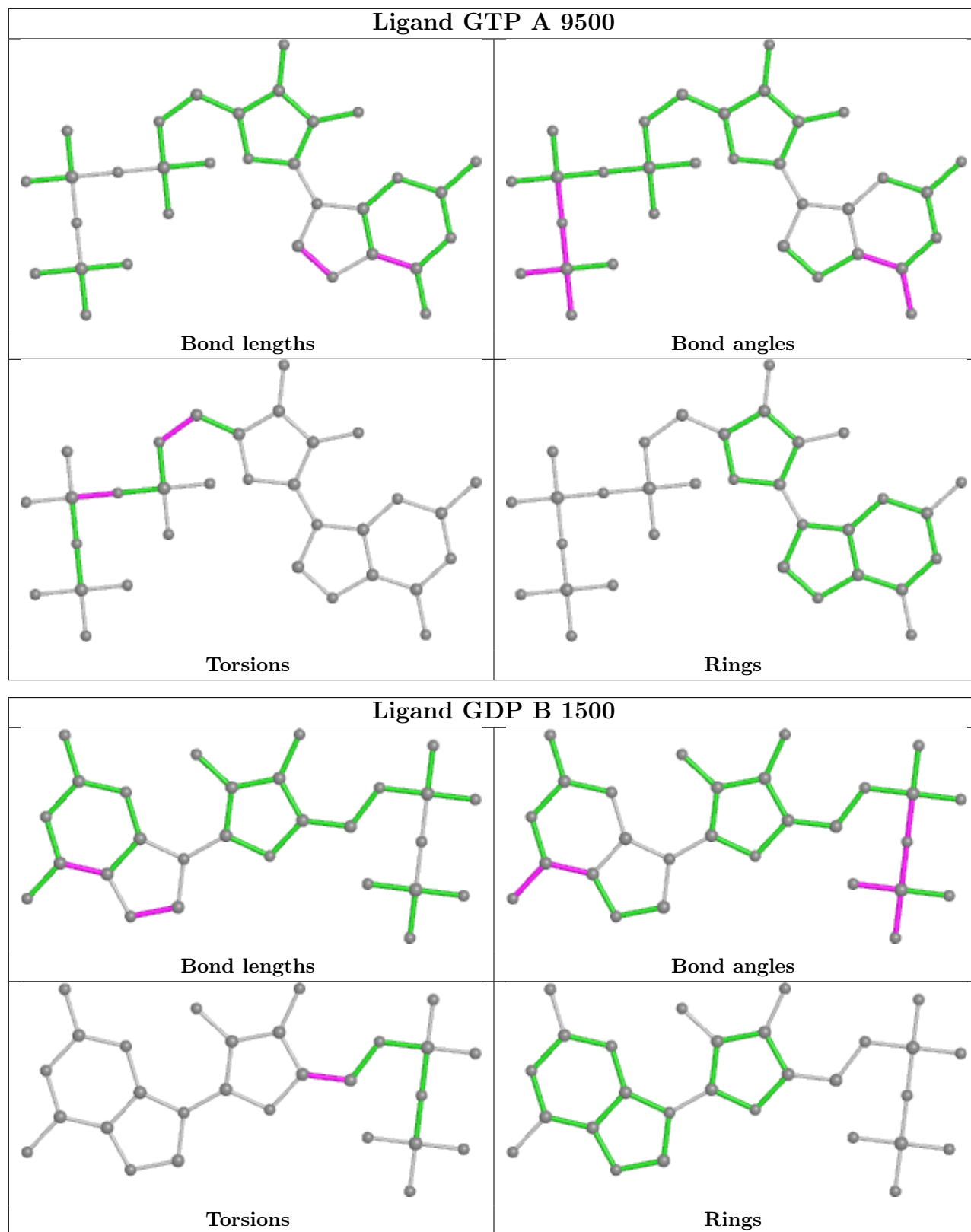
Mol	Chain	Res	Type	Atoms
5	B	1001	EP	C5-C10-C12-N20
5	B	1001	EP	C59-C68-C72-C75
5	B	1001	EP	O70-C68-C72-C75
5	B	1001	EP	C41-C47-C51-C53
5	B	1001	EP	O49-C47-C51-C57

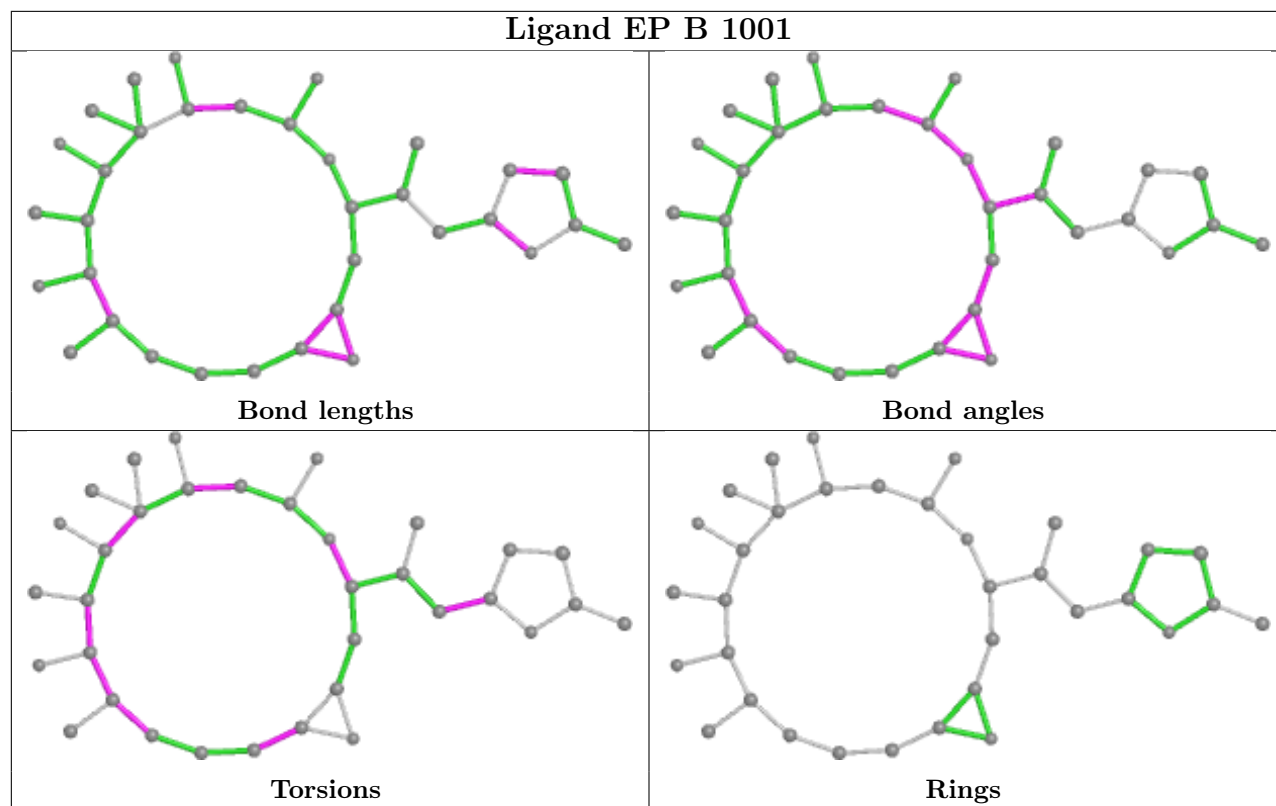
There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	9500	GTP	4	0
4	B	1500	GDP	8	0
5	B	1001	EP	4	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.