



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 11, 2017 – 02:34 AM EDT

PDB ID : 5W3H
EMDB ID: : EMD-8756
Title : Yeast microtubule stabilized with epothilone
Authors : Howes, S.C.; Geyer, E.A.; LaFrance, B.; Zhang, R.; Kellogg, E.H.; Westermann, S.; Rice, L.M.; Nogales, E.
Deposited on : unknown
Resolution : 4.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

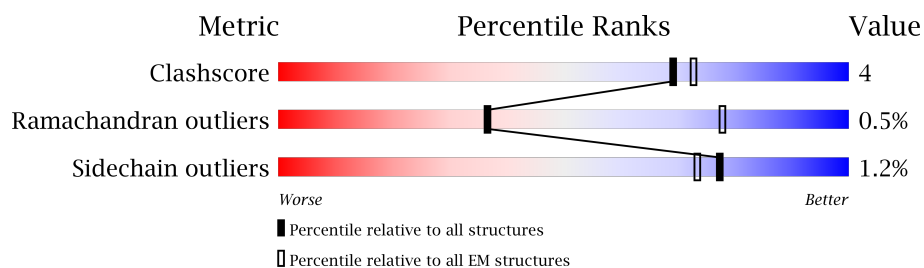
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. 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. 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	447	
2	B	457	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6876 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.

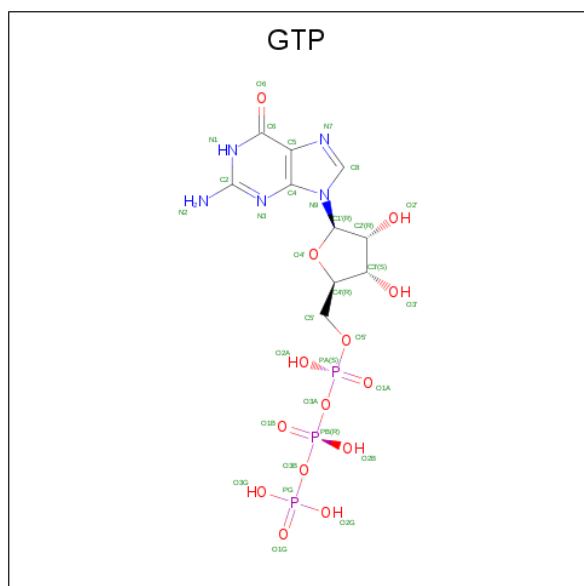
- Molecule 1 is a protein called Tubulin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	440	3438	2167	585	667	19	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	427	3343	2098	571	653	21	0	0

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

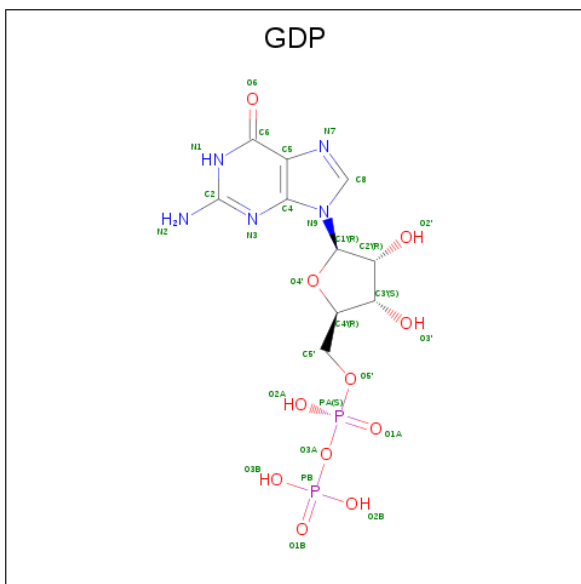


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	32	10	5	14	3	0

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

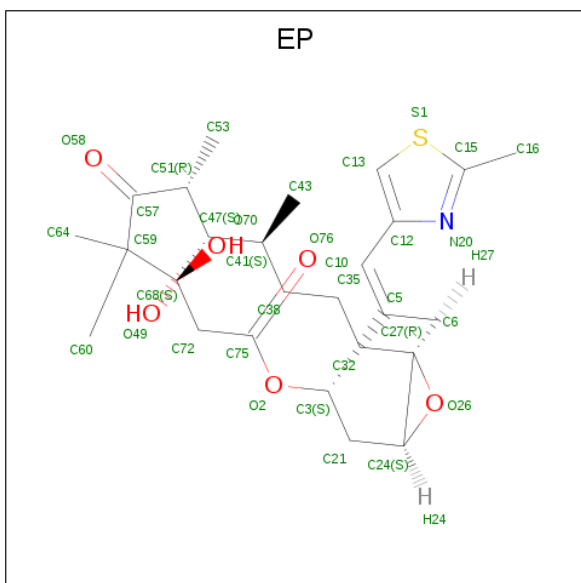
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	

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



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

- Molecule 6 is EPOTHILONE A (three-letter code: EP) (formula: $C_{26}H_{39}NO_6S$).

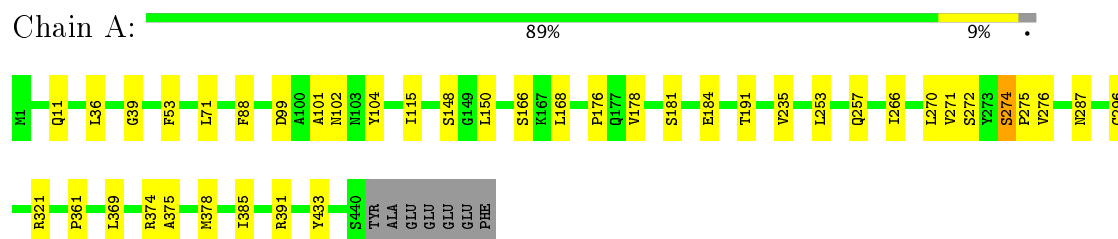


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
6	B	1	34	26	1	6	1	0

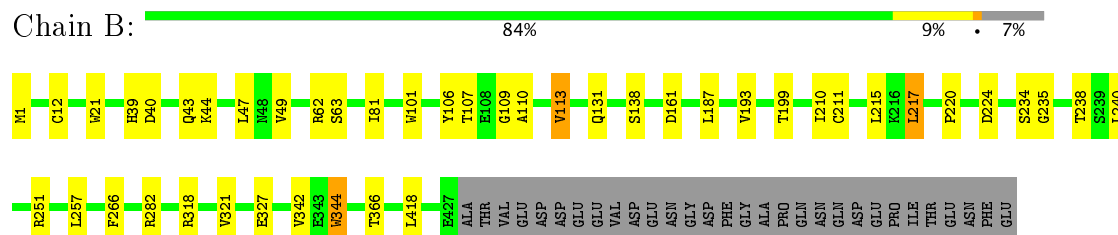
3 Residue-property plots [i](#)

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 alpha-1 chain



- Molecule 2: Tubulin beta chain



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-29.87°, rise=10.43 Å, axial sym=C1	Depositor
Number of segments used	27829	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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, MG, EP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.29	1/3514 (0.0%)	0.46	0/4766
2	B	0.26	0/3416	0.45	0/4627
All	All	0.28	1/6930 (0.0%)	0.46	0/9393

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	SER	C-N	7.71	1.49	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ALA	Peptide
1	A	39	GLY	Peptide

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	3438	0	3339	24	0
2	B	3343	0	3208	34	0
3	A	32	0	12	1	0
4	A	1	0	0	0	0
5	B	28	0	12	1	0
6	B	34	0	37	9	0
All	All	6876	0	6608	58	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 4.

The worst 5 of 58 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:274:SER:OG	1:A:296:CYS:SG	2.43	0.76
2:B:215:LEU:HD13	6:B:502:EP:H721	1.73	0.70
2:B:211:CYS:HA	2:B:215:LEU:HD12	1.76	0.66
2:B:12:CYS:SG	2:B:138:SER:OG	2.55	0.64
2:B:49:VAL:O	2:B:62:ARG:NH2	2.31	0.63

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	438/447 (98%)	418 (95%)	19 (4%)	1 (0%)	51	84
2	B	425/457 (93%)	408 (96%)	14 (3%)	3 (1%)	25	68
All	All	863/904 (96%)	826 (96%)	33 (4%)	4 (0%)	37	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	81	ILE
2	B	113	VAL
1	A	53	PHE
2	B	107	THR

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 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	375/381 (98%)	372 (99%)	3 (1%)	85	93
2	B	366/392 (93%)	360 (98%)	6 (2%)	68	86
All	All	741/773 (96%)	732 (99%)	9 (1%)	77	89

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	106	TYR
2	B	344	TRP
2	B	217	LEU
1	A	104	TYR
2	B	199	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	381	ASN
2	B	39	HIS
2	B	131	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is 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	$\# Z > 2$
3	GTP	A	500	-	27,34,34	1.11	2 (7%)	27,54,54	2.30	4 (14%)
5	GDP	B	501	-	25,30,30	1.20	2 (8%)	26,47,47	2.33	4 (15%)
6	EP	B	502	-	32,36,36	0.49	0	39,53,53	0.98	2 (5%)

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	-	-	0/18/38/38	0/3/3/3
5	GDP	B	501	-	-	0/12/32/32	0/3/3/3
6	EP	B	502	-	-	1/49/55/55	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	GTP	PG-O3B	-3.00	1.55	1.60
5	B	501	GDP	PB-O3A	-2.99	1.55	1.60
3	A	500	GTP	C6-N1	3.75	1.39	1.33
5	B	501	GDP	C6-N1	3.77	1.39	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	GTP	C5-C6-N1	-8.52	111.35	123.48
5	B	501	GDP	C5-C6-N1	-8.49	111.39	123.48
6	B	502	EP	C35-C32-C27	-3.03	105.56	113.60
3	A	500	GTP	N3-C2-N1	-2.68	123.54	127.46
5	B	501	GDP	N3-C2-N1	-2.65	123.59	127.46

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	502	EP	C5-C10-C12-N20

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	GTP	1	0
5	B	501	GDP	1	0
6	B	502	EP	9	0

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.