wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:02 PM BST

PDB ID	:	4ABO
EMDB ID:	:	EMD-2005
Title	:	Mal3 CH domain homology model and mammalian tubulin (2XRP) docked into the 8.6-Angstrom cryo-EM map of Mal3-GTPgammaS-microtubules
Authors	:	Maurer, S.P.; Fourniol, F.J.; Bohner, G.; Moores, C.A.; Surrey, T.
Deposited on	:	2011-12-09
Resolution	:	8.60 Å(reported)
Based on PDB ID	:	2XRP

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

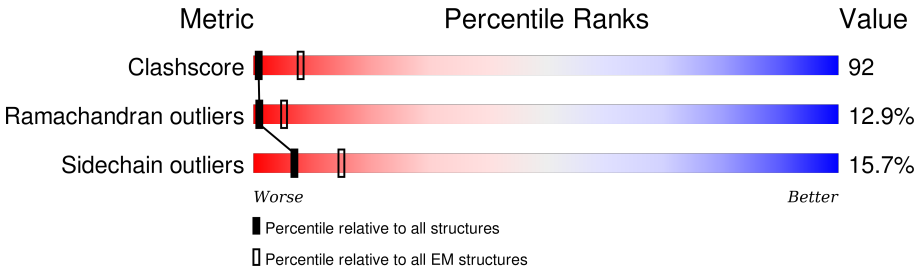
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.60 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	445	20% 55% 18% • •
1	C	445	19% 56% 18% • •
1	E	445	21% 55% 18% • •
1	G	445	20% 56% 18% • •
2	B	451	16% 59% 19% • 5%
2	D	451	17% 58% 19% • 5%
2	F	451	17% 59% 18% • 5%
2	H	451	18% 58% 18% • 5%
3	I	145	22% 58% • 19%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27996 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 BETA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	426	Total	C	N	O	S	0	0
			3350	2105	574	646	25		
1	C	426	Total	C	N	O	S	0	0
			3350	2105	574	646	25		
1	E	426	Total	C	N	O	S	0	0
			3350	2105	574	646	25		
1	G	426	Total	C	N	O	S	0	0
			3350	2105	574	646	25		

- Molecule 2 is a protein called TUBULIN ALPHA-1A CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	429	Total	C	N	O	S	0	0
			3333	2114	568	630	21		
2	D	429	Total	C	N	O	S	0	0
			3333	2114	568	630	21		
2	F	430	Total	C	N	O	S	0	1
			3357	2125	571	640	21		
2	H	429	Total	C	N	O	S	0	0
			3333	2114	568	630	21		

- Molecule 3 is a protein called MICROTUBULE INTEGRITY PROTEIN MAL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	118	Total	C	N	O	S	0	1
			984	628	173	178	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-2	GLY	-	EXPRESSION TAG	UNP Q10113
I	-1	ALA	-	EXPRESSION TAG	UNP Q10113
I	0	MET	-	EXPRESSION TAG	UNP Q10113

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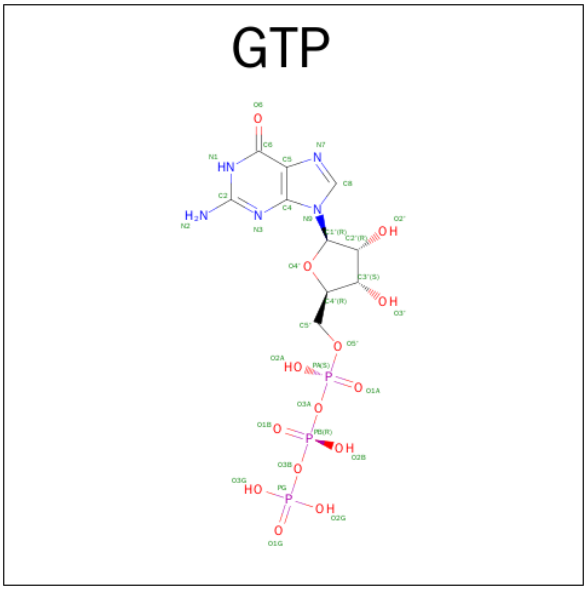
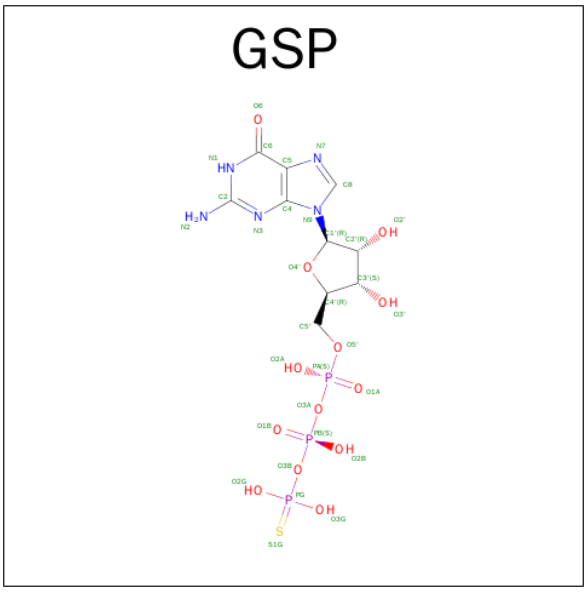
Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	EXPRESSION TAG	UNP Q10113

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
4	H	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



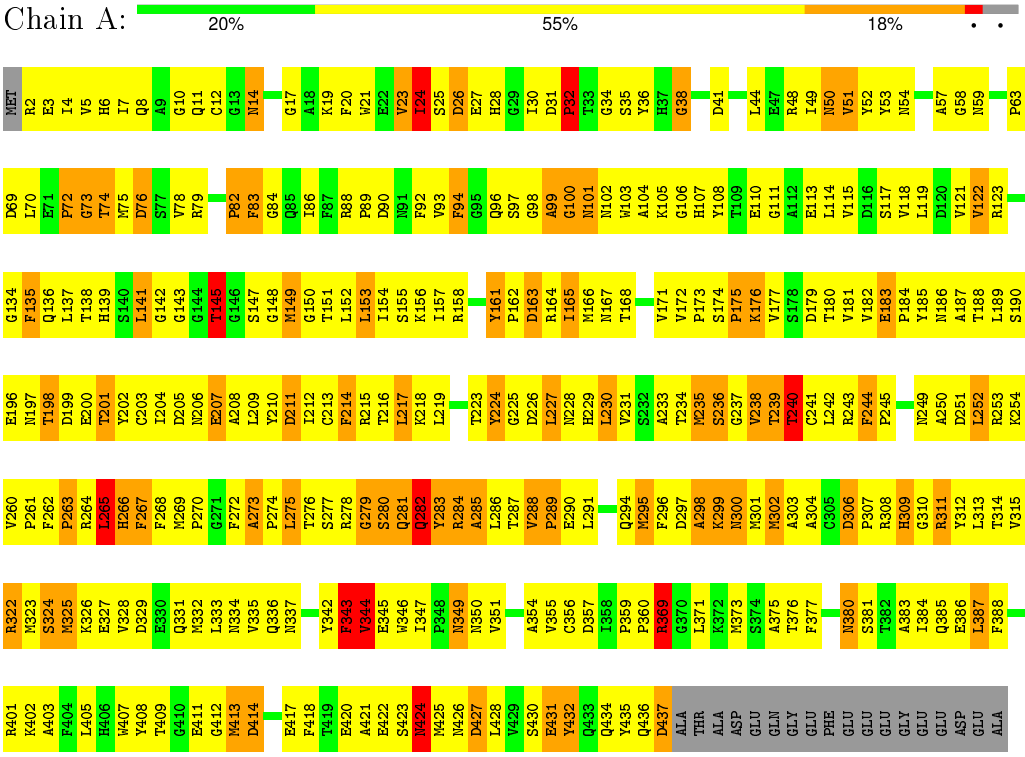
Mol	Chain	Residues	Atoms						AltConf
5	C	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
5	A	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
5	E	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	
5	G	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

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 errors 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.

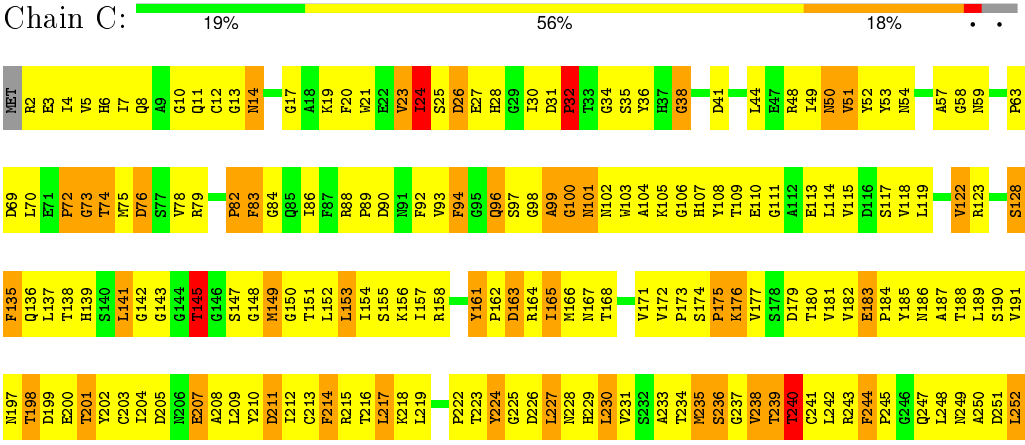
- Molecule 1: TUBULIN BETA CHAIN

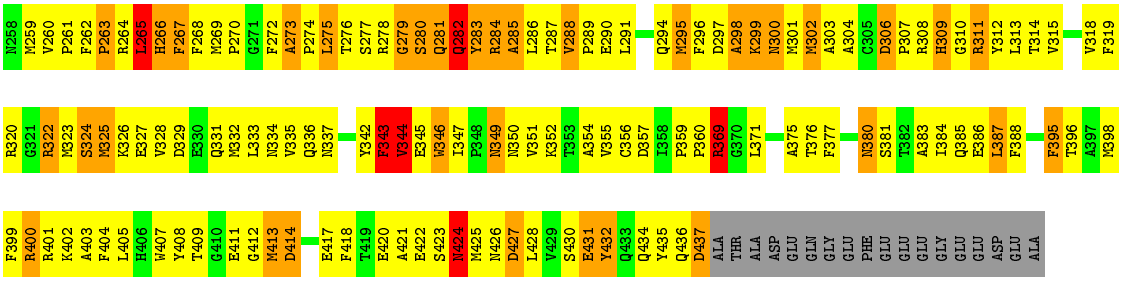
Chain A:



- Molecule 1: TUBULIN BETA CHAIN

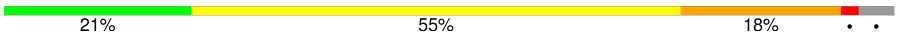
Chain C:

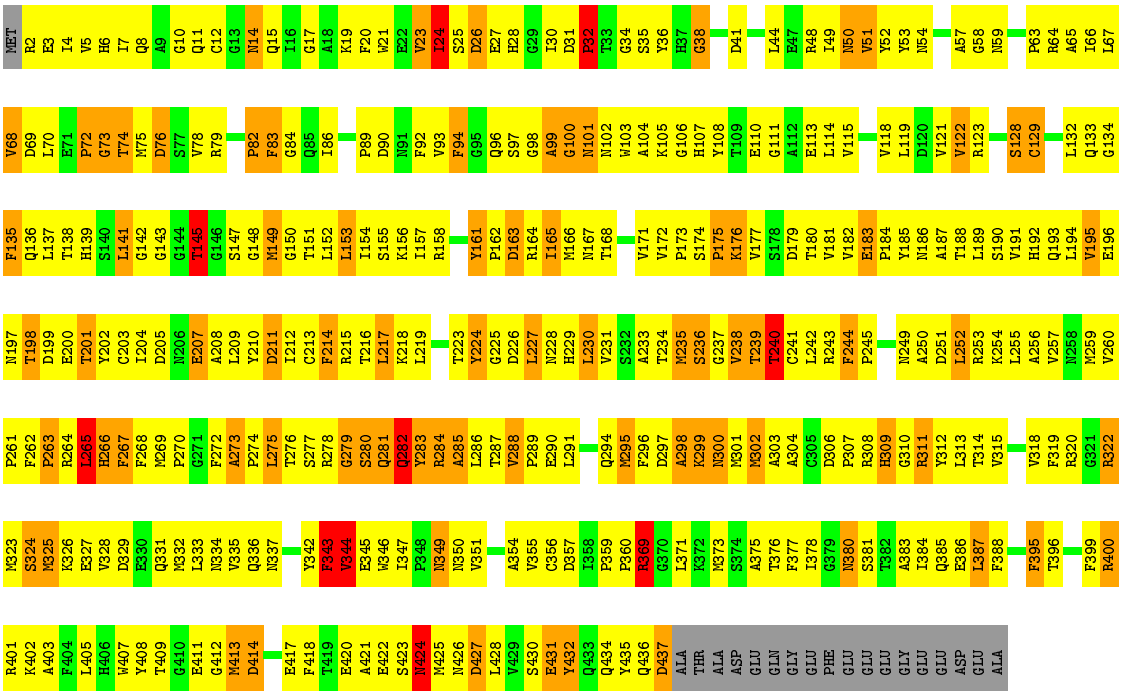




• Molecule 1: TUBULIN BETA CHAIN

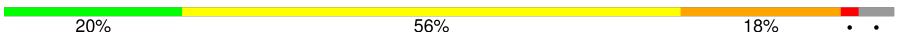
Chain E:

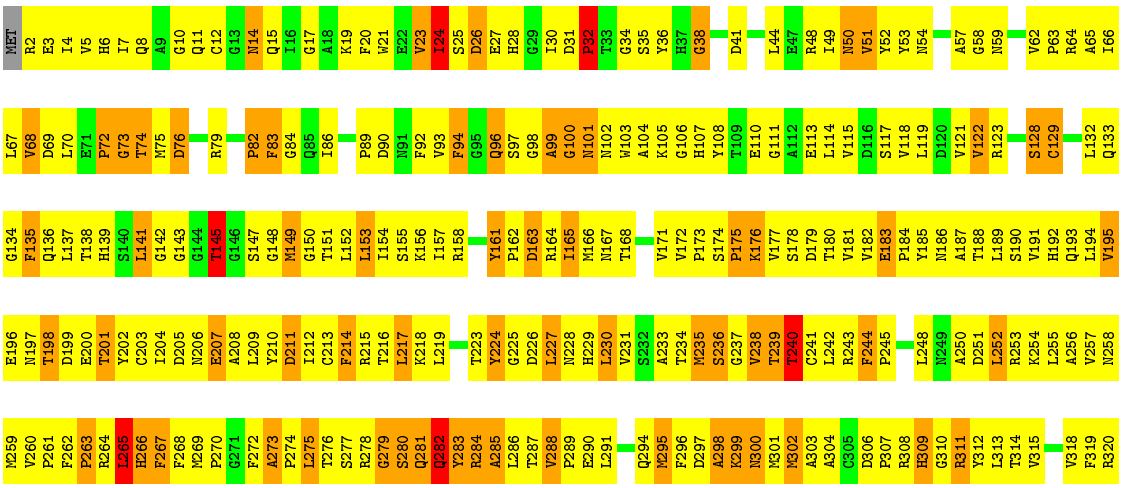


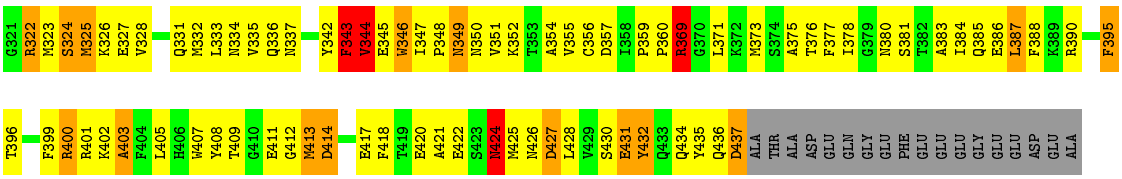


• Molecule 1: TUBULIN BETA CHAIN

Chain G:

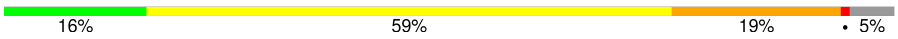


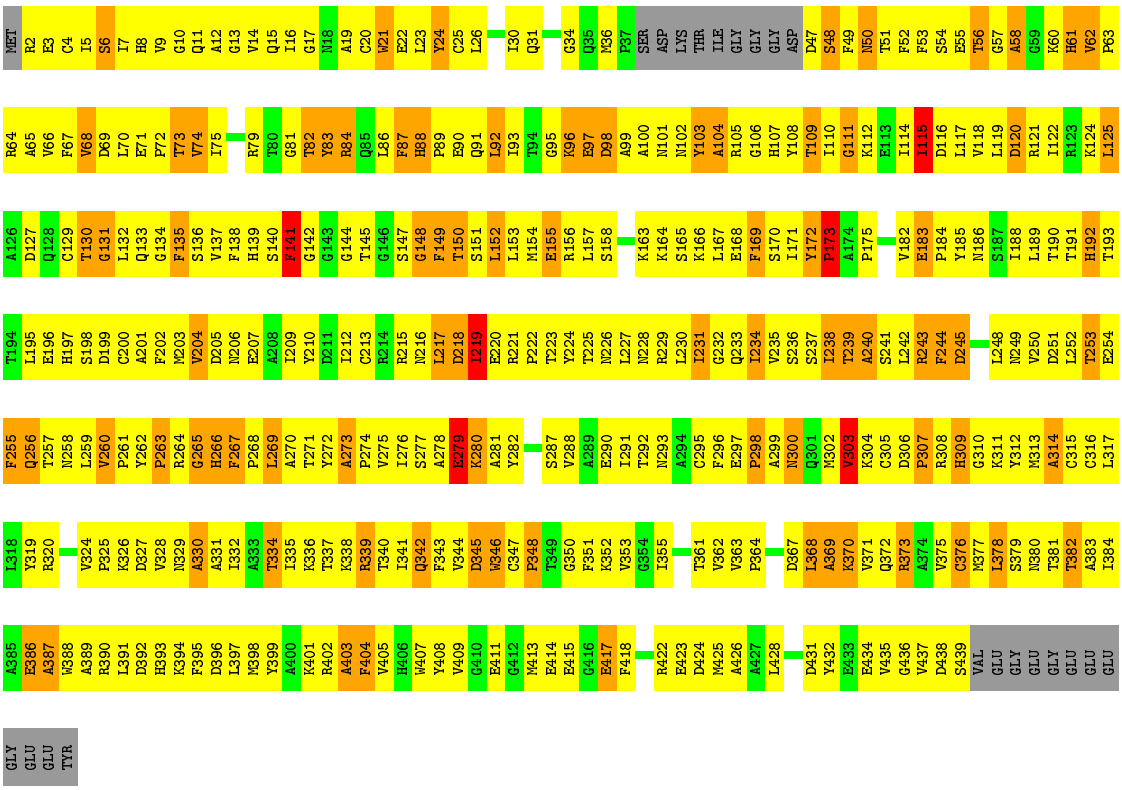




- Molecule 2: TUBULIN ALPHA-1A CHAIN

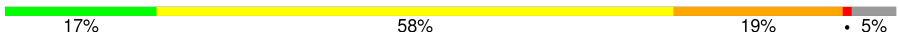
Chain B:

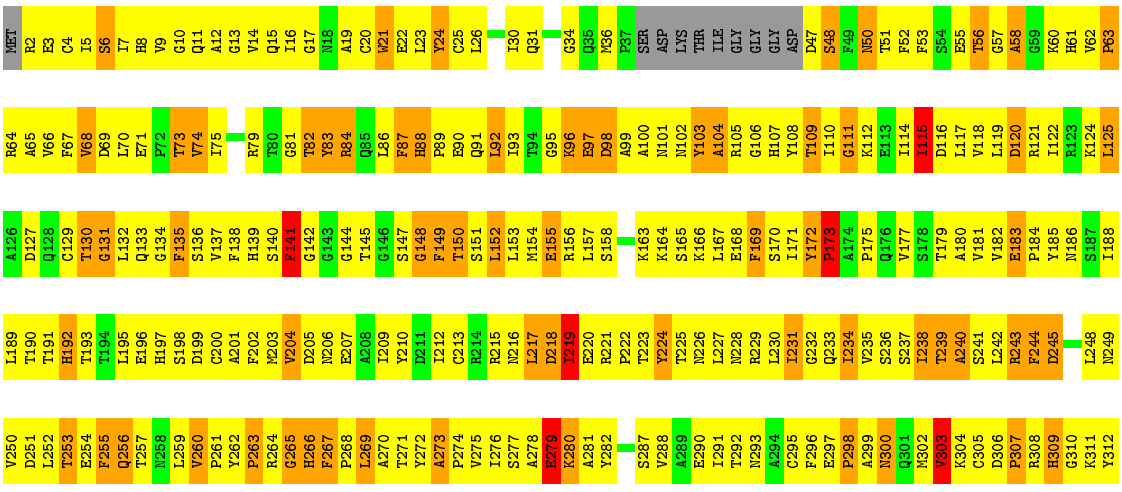


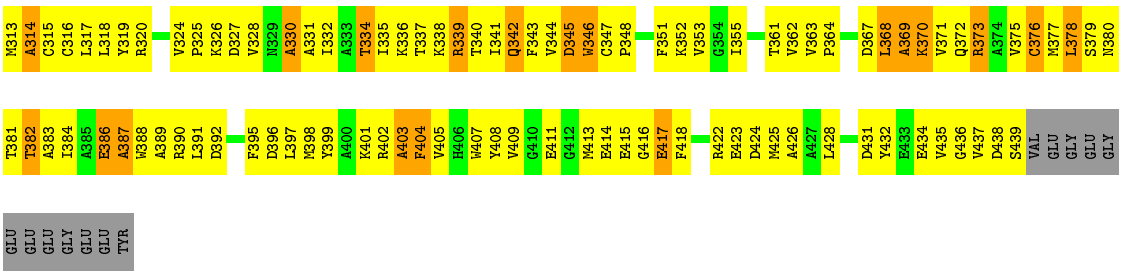


- Molecule 2: TUBULIN ALPHA-1A CHAIN

Chain D:

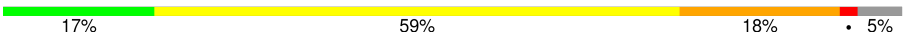


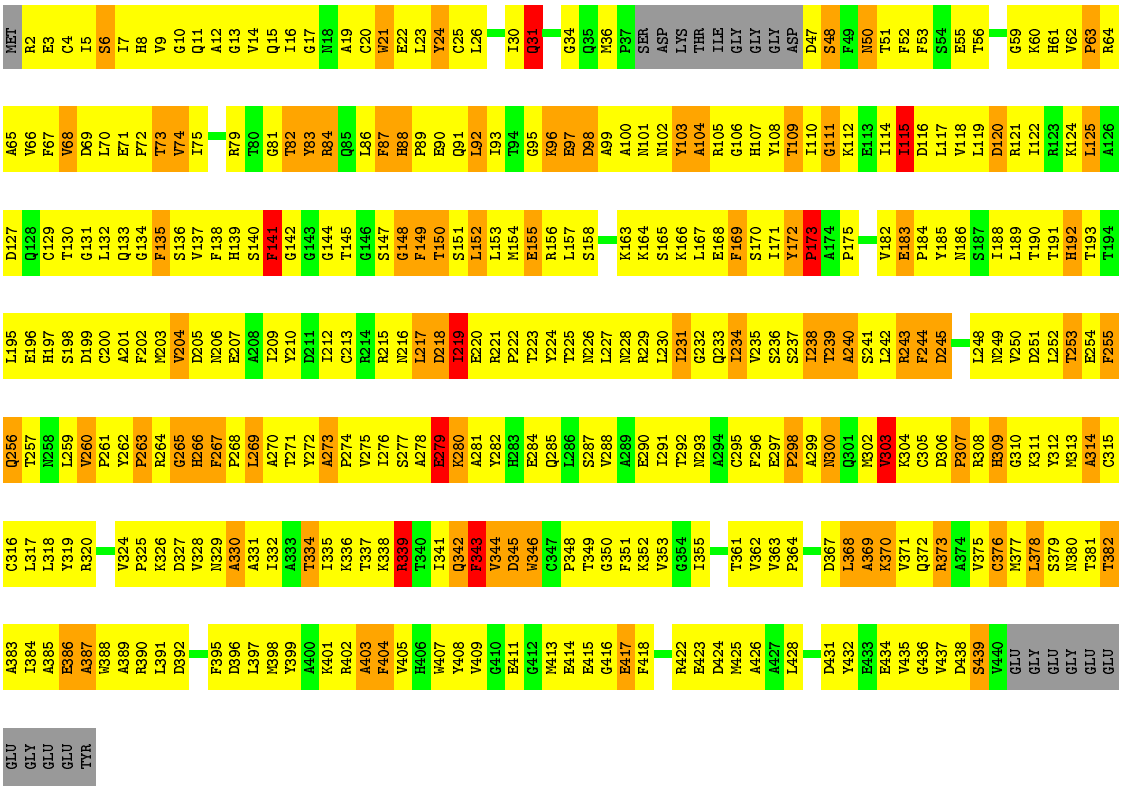




• Molecule 2: TUBULIN ALPHA-1A CHAIN

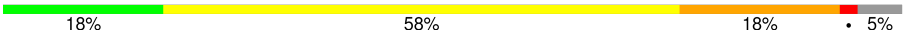
Chain F:

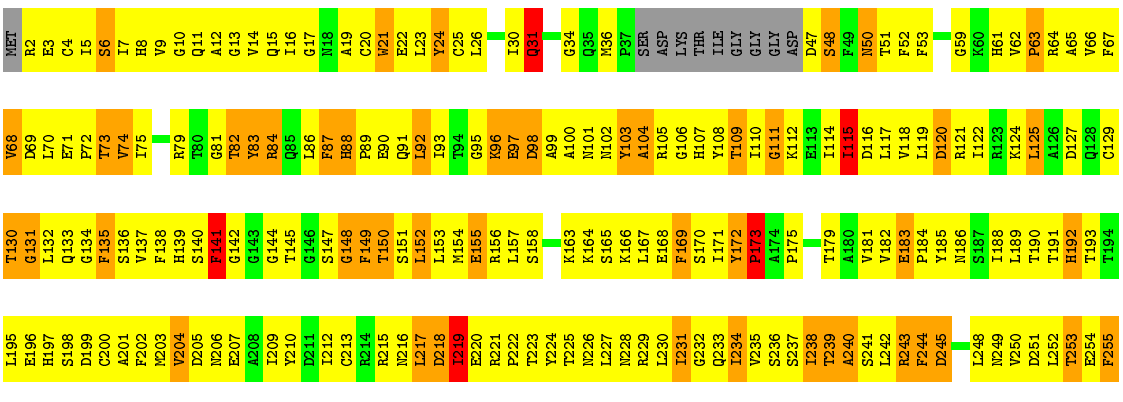


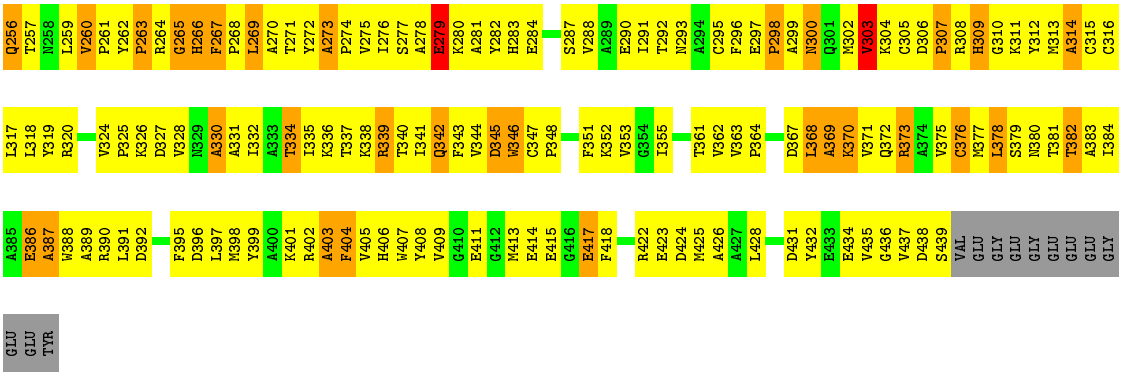


• Molecule 2: TUBULIN ALPHA-1A CHAIN

Chain H:

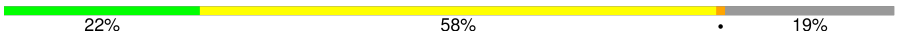


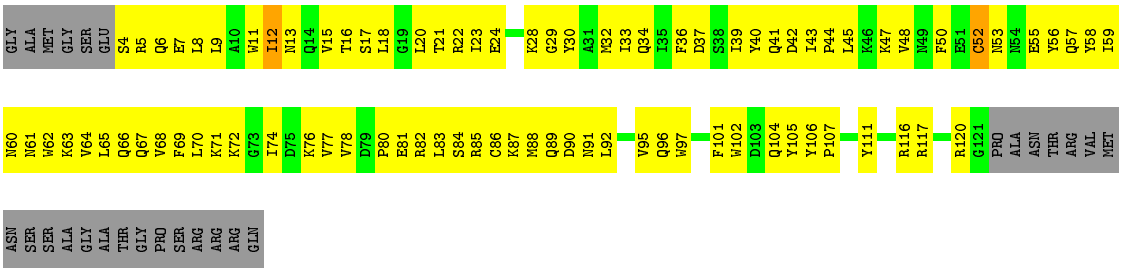




- Molecule 3: MICROTUBULE INTEGRITY PROTEIN MAL3

Chain I:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FREALIGN	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	17	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	68000	Depositor
Image detector	GATAN ULTRASCAN 4000 4K CCD CAMERA	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.51	0/3425	0.76	2/4640 (0.0%)
1	C	0.51	0/3425	0.76	2/4640 (0.0%)
1	E	0.51	0/3425	0.76	2/4640 (0.0%)
1	G	0.51	0/3425	0.76	2/4640 (0.0%)
2	B	0.82	3/3409 (0.1%)	0.77	3/4627 (0.1%)
2	D	0.82	3/3409 (0.1%)	0.78	3/4627 (0.1%)
2	F	0.87	4/3433 (0.1%)	1.55	24/4659 (0.5%)
2	H	0.82	3/3409 (0.1%)	0.78	3/4627 (0.1%)
3	I	0.93	0/1006	1.08	0/1357
All	All	0.70	13/28366 (0.0%)	0.91	41/38457 (0.1%)

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
2	F	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	92	LEU	C-N	28.00	1.98	1.34
2	H	92	LEU	C-N	27.98	1.98	1.34
2	B	92	LEU	C-N	27.95	1.98	1.34
2	F	92	LEU	C-N	27.91	1.98	1.34
2	F	298	PRO	C-N	17.31	1.73	1.34

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	439	SER	O-C-N	-56.45	32.38	122.70
2	F	346	TRP	CD2-CE2-CZ2	-48.00	64.70	122.30
2	F	346	TRP	CZ3-CH2-CZ2	-31.44	83.87	121.60
2	F	346	TRP	CH2-CZ2-CE2	16.26	133.66	117.40
2	F	346	TRP	CE3-CZ3-CH2	-15.77	103.85	121.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	342	GLN	Peptide
2	F	345	ASP	Peptide
2	F	439	SER	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	3350	0	3228	537	0
1	C	3350	0	3228	595	0
1	E	3350	0	3228	537	0
1	G	3350	0	3228	667	0
2	B	3333	0	3222	646	0
2	D	3333	0	3222	680	0
2	F	3357	0	3254	655	0
2	H	3333	0	3222	725	0
3	I	984	0	963	242	0
4	B	32	0	12	6	0
4	D	32	0	12	4	0
4	F	32	0	12	5	0
4	H	32	0	12	4	0
5	A	32	0	12	3	0
5	C	32	0	12	1	0
5	E	32	0	12	3	0
5	G	32	0	12	6	0
All	All	27996	0	26891	5033	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 92.

The worst 5 of 5033 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:G:257:VAL:HG21	2:H:407:TRP:CG	1.28	1.66
2:B:296:PHE:CE1	2:B:341:ILE:HD11	1.32	1.62
2:H:296:PHE:CE1	2:H:341:ILE:HD11	1.32	1.61
2:D:296:PHE:CE1	2:D:341:ILE:HD11	1.32	1.59
2:D:57:GLY:N	2:H:284:GLU:HG3	1.27	1.50

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	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0 7
1	C	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0 7
1	E	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0 7
1	G	424/445 (95%)	274 (65%)	94 (22%)	56 (13%)	0 7
2	B	423/451 (94%)	279 (66%)	87 (21%)	57 (14%)	0 7
2	D	423/451 (94%)	281 (66%)	85 (20%)	57 (14%)	0 7
2	F	424/451 (94%)	283 (67%)	86 (20%)	55 (13%)	0 7
2	H	423/451 (94%)	278 (66%)	88 (21%)	57 (14%)	0 7
3	I	116/145 (80%)	112 (97%)	3 (3%)	1 (1%)	21 67
All	All	3505/3729 (94%)	2328 (66%)	726 (21%)	451 (13%)	1 7

5 of 451 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	24	ILE
1	A	32	PRO
1	A	50	ASN
1	A	82	PRO

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	366/381 (96%)	306 (84%)	60 (16%)	3 19
1	C	366/381 (96%)	307 (84%)	59 (16%)	3 20
1	E	366/381 (96%)	307 (84%)	59 (16%)	3 20
1	G	366/381 (96%)	307 (84%)	59 (16%)	3 20
2	B	353/377 (94%)	294 (83%)	59 (17%)	3 19
2	D	353/377 (94%)	295 (84%)	58 (16%)	3 19
2	F	360/377 (96%)	302 (84%)	58 (16%)	3 20
2	H	353/377 (94%)	297 (84%)	56 (16%)	3 21
3	I	105/124 (85%)	104 (99%)	1 (1%)	82 92
All	All	2988/3156 (95%)	2519 (84%)	469 (16%)	7 21

5 of 469 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	234	ILE
1	E	214	PHE
2	H	150	THR
2	D	269	LEU
1	E	26	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 128 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	226	ASN
1	E	334	ASN
2	H	197	HIS
2	D	309	HIS
1	E	107	HIS

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

8 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	$\#\|Z\| > 2$
5	GSP	A	1438	-	26,34,34	1.92	9 (34%)	27,54,54	3.29	7 (25%)
4	GTP	B	500	-	26,34,34	1.61	4 (15%)	29,54,54	2.40	7 (24%)
5	GSP	C	1438	-	26,34,34	1.92	10 (38%)	27,54,54	3.30	7 (25%)
4	GTP	D	500	-	26,34,34	1.38	3 (11%)	29,54,54	2.31	4 (13%)
5	GSP	E	1438	-	26,34,34	1.92	9 (34%)	27,54,54	3.29	7 (25%)
4	GTP	F	500	-	26,34,34	1.39	3 (11%)	29,54,54	2.31	4 (13%)
5	GSP	G	1438	-	26,34,34	1.91	9 (34%)	27,54,54	3.29	7 (25%)
4	GTP	H	500	-	26,34,34	1.39	3 (11%)	29,54,54	2.32	4 (13%)

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
5	GSP	A	1438	-	-	0/17/38/38	0/3/3/3
4	GTP	B	500	-	-	0/18/38/38	0/3/3/3
5	GSP	C	1438	-	-	0/17/38/38	0/3/3/3
4	GTP	D	500	-	-	0/18/38/38	0/3/3/3
5	GSP	E	1438	-	-	0/17/38/38	0/3/3/3
4	GTP	F	500	-	-	0/18/38/38	0/3/3/3
5	GSP	G	1438	-	-	0/17/38/38	0/3/3/3
4	GTP	H	500	-	-	0/18/38/38	0/3/3/3

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1438	GSP	PG-O2G	-2.41	1.48	1.55
5	C	1438	GSP	PG-O2G	-2.39	1.48	1.55
5	E	1438	GSP	PG-O2G	-2.39	1.48	1.55
5	G	1438	GSP	PG-O2G	-2.38	1.48	1.55
4	D	500	GTP	PB-O2B	-2.18	1.45	1.55

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1438	GSP	C5-C6-N1	-10.35	109.99	123.52
5	C	1438	GSP	C5-C6-N1	-10.35	109.99	123.52
5	G	1438	GSP	C5-C6-N1	-10.35	110.00	123.52
5	E	1438	GSP	C5-C6-N1	-10.33	110.02	123.52
4	H	500	GTP	C5-C6-N1	-7.84	113.27	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1438	GSP	3	0
4	B	500	GTP	6	0
5	C	1438	GSP	1	0
4	D	500	GTP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1438	GSP	3	0
4	F	500	GTP	5	0
5	G	1438	GSP	6	0
4	H	500	GTP	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.