



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:38 PM GMT

PDB ID : 4YJ2  
Title : Crystal structure of tubulin bound to MI-181  
Authors : McNamara, D.E.; Torres, J.Z.; Yeates, T.O.  
Deposited on : 2015-03-03  
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

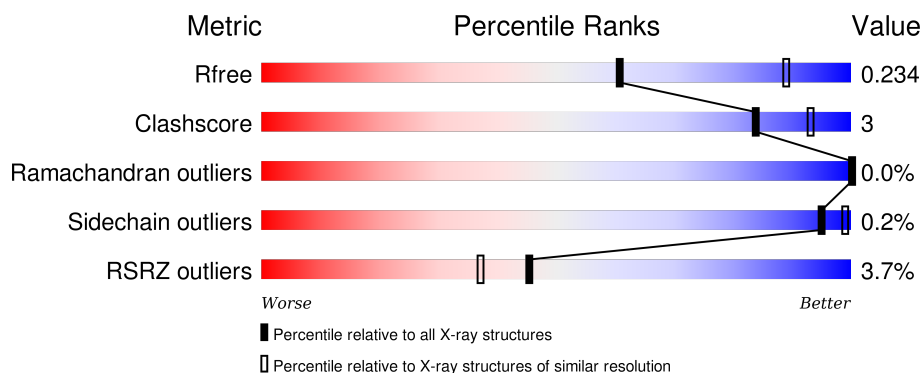
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>90%</div> <div>7%</div> <div>•</div> </div>
1	C	451	<div> <div>92%</div> <div>6%</div> <div>•</div> </div>
2	B	445	<div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
2	D	445	<div> <div>3%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
3	E	143	<div> <div>80%</div> <div>5%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

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
10	4ED	D	503[A]	-	-	-	X
11	MES	B	506	-	-	-	X
12	IMD	C	504	-	-	-	X
8	GOL	A	504	-	-	-	X
8	GOL	A	505	-	-	-	X
8	GOL	C	503	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17335 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	1	0
			3420	2167	581	650	22			
1	C	440	Total	C	N	O	S	0	2	0
			3445	2180	584	658	23			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	2	0
			3336	2098	569	642	27			
2	D	421	Total	C	N	O	S	0	10	0
			3379	2127	572	652	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1003	619	182	197	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

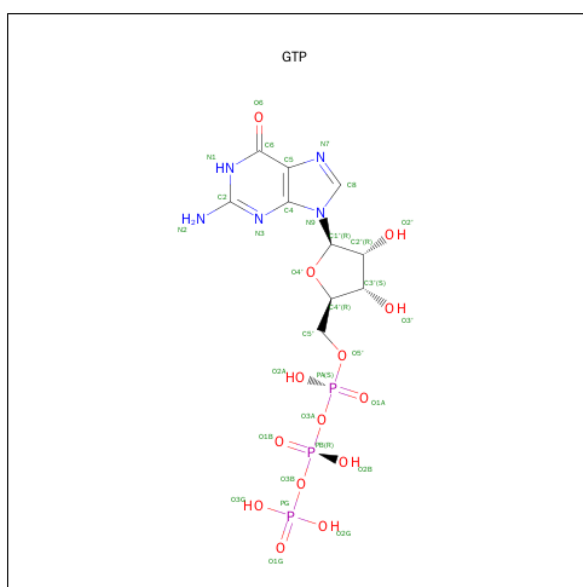
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	296	Total	C	N	O	S	0	0	0
			2417	1564	401	440	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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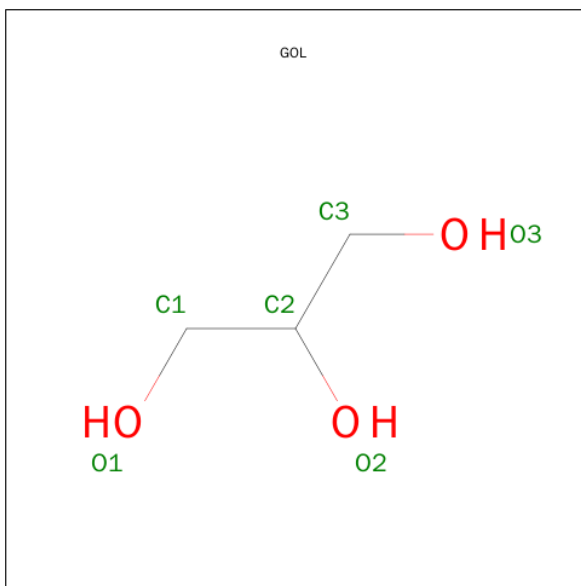
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

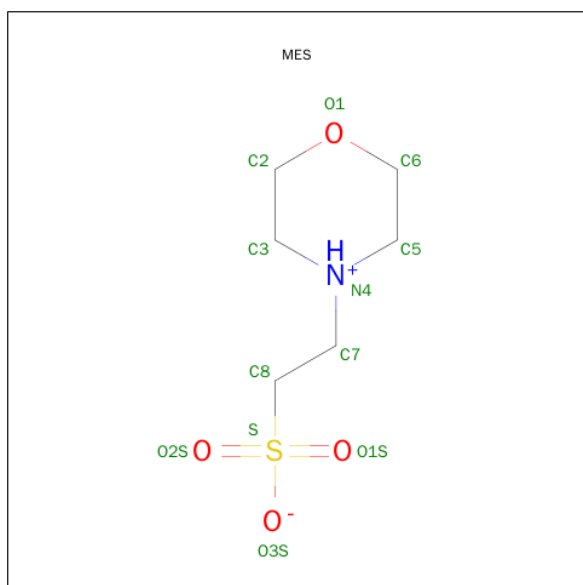
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- The chemical structure of GDP (Guanosine Diphosphate) is shown. It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is linked to a diphosphate group (two phosphate groups connected by an oxygen atom). The atoms are labeled with their respective element symbols and coordinates: N1, N2, N3, N7, N9, O6, O5, O4, O3, O2, O1, O2B, O1B, O3A, O3B, O4', O5', O6', O7', O8', O9', O10', O11', O12', O13', O14', O15', O16', O17', O18', O19', O20', O21', O22', O23', O24', O25', O26', O27', O28', O29', O30', O31', O32', O33', O34', O35', O36', O37', O38', O39', O40', O41', O42', O43', O44', O45', O46', O47', O48', O49', O50', O51', O52', O53', O54', O55', O56', O57', O58', O59', O60', O61', O62', O63', O64', O65', O66', O67', O68', O69', O70', O71', O72', O73', O74', O75', O76', O77', O78', O79', O80', O81', O82', O83', O84', O85', O86', O87', O88', O89', O90', O91', O92', O93', O94', O95', O96', O97', O98', O99', O100', O101', O102', O103', O104', O105', O106', O107', O108', O109', O110', O111', O112', O113', O114', O115', O116', O117', O118', O119', O120', O121', O122', O123', O124', O125', O126', O127', O128', O129', O130', O131', O132', O133', O134', O135', O136', O137', O138', O139', O140', O141', O142', O143', O144', O145', O146', O147', O148', O149', O150', O151', O152', O153', O154', O155', O156', O157', O158', O159', O160', O161', O162', O163', O164', O165', O166', O167', O168', O169', O170', O171', O172', O173', O174', O175', O176', O177', O178', O179', O180', O181', O182', O183', O184', O185', O186', O187', O188', O189', O190', O191', O192', O193', O194', O195', O196', O197', O198', O199', O200', O201', O202', O203', O204', O205', O206', O207', O208', O209', O210', O211', O212', O213', O214', O215', O216', O217', O218', O219', O220', O221', O222', O223', O224', O225', O226', O227', O228', O229', O230', O231', O232', O233', O234', O235', O236', O237', O238', O239', O240', O241', O242', O243', O244', O245', O246', O247', O248', O249', O250', O251', O252', O253', O254', O255', O256', O257', O258', O259', O260', O261', O262', O263', O264', O265', O266', O267', O268', O269', O270', O271', O272', O273', O274', O275', O276', O277', O278', O279', O280', O281', O282', O283', O284', O285', O286', O287', O288', O289', O290', O291', O292', O293', O294', O295', O296', O297', O298', O299', O300', O301', O302', O303', O304', O305', O306', O307', O308', O309', O310', O311', O312', O313', O314', O315', O316', O317', O318', O319', O320', O321', O322', O323', O324', O325', O326', O327', O328', O329', O330', O331', O332', O333', O334', O335', O336', O337', O338', O339', O340', O341', O342', O343', O344', O345', O346', O347', O348', O349', O350', O351', O352', O353', O354', O355', O356', O357', O358', O359', O360', O361', O362', O363', O364', O365', O366', O367', O368', O369', O370', O371', O372', O373', O374', O375', O376', O377', O378', O379', O380', O381', O382', O383', O384', O385', O386', O387', O388', O389', O390', O391', O392', O393', O394', O395', O396', O397', O398', O399', O400', O401', O402', O403', O404', O405', O406', O407', O408', O409', O410', O411', O412', O413', O414', O415', O416', O417', O418', O419', O420', O421', O422', O423', O424', O425', O426', O427', O428', O429', O430', O431', O432', O433', O434', O435', O436', O437', O438', O439', O440', O441', O442', O443', O444', O445', O446', O447', O448', O449', O450', O451', O452', O453', O454', O455', O456', O457', O458', O459', O460', O461', O462', O463', O464', O465', O466', O467', O468', O469', O470', O471', O472', O473', O474', O475', O476', O477', O478', O479', O480', O481', O482', O483', O484', O485', O486', O487', O488', O489', O490', O491', O492', O493', O494', O495', O496', O497', O498', O499', O500', O501', O502', O503', O504', O505', O506', O507', O508', O509', O510', O511', O512', O513', O514', O515', O516', O517', O518', O519', O520', O521', O522', O523', O524', O525', O526', O527', O528', O529', O530', O531', O532', O533', O534', O535', O536', O537', O538', O539', O540', O541', O542', O543', O544', O545', O546', O547', O548', O549', O550', O551', O552', O553', O554', O555', O556', O557', O558', O559', O560', O561', O562', O563', O564', O565', O566', O567', O568', O569', O570', O571', O572', O573', O574', O575', O576', O577', O578', O579', O580', O581', O582', O583', O584', O585', O586', O587', O588', O589', O590', O591', O592', O593', O594', O595', O596', O597', O598', O599', O600', O601', O602', O603', O604', O605', O606', O607', O608', O609', O610', O611', O612', O613', O614', O615', O616', O617', O618', O619', O620', O621', O622', O623', O624', O625', O626', O627', O628', O629', O630', O631', O632', O633', O634', O635', O636', O637', O638', O639', O640', O641', O642', O643', O644', O645', O646', O647', O648', O649', O650', O651', O652', O653', O654', O655', O656', O657', O658', O659', O660', O661', O662', O663', O664', O665', O666', O667', O668', O669', O670', O671', O672', O673', O674', O675', O676', O677', O678', O679', O680', O681', O682', O683', O684', O685', O686', O687', O688', O689', O690', O691', O692', O693', O694', O695', O696', O697', O698', O699', O700', O701', O702', O703', O704', O705', O706', O707', O708', O709', O710', O711', O712', O713', O714', O715', O716', O717', O718', O719', O720', O721', O722', O723', O724', O725', O726', O727', O728', O729', O730', O731', O732', O733', O734', O735', O736', O737', O738', O739', O740', O741', O742', O743', O744', O745', O746', O747', O748', O749', O750', O751', O752', O753', O754', O755', O756', O757', O758', O759', O760', O761', O762', O763', O764', O765', O766', O767', O768', O769', O770', O771', O772', O773', O774', O775', O776', O777', O778', O779', O780', O781', O782', O783', O784', O785', O786', O787', O788', O789', O790', O791', O792', O793', O794', O795', O796', O797', O798', O799', O800', O801', O802', O803', O804', O805', O806', O80

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

- 
- ORTEP diagram of the molecule 4-(4-methylphenyl)-2-((4-methylphenyl)thio)pyridine. The structure shows a central pyridine ring (N13) connected at the 2-position to a thioether group (S15) which is linked to a 4-methylphenyl ring (C01-C06). The pyridine ring is also substituted at the 4-position with a 4-methylphenyl group (C07-C12). Thermal ellipsoids are drawn at the 50% probability level. Displacement ellipsoid coefficients are provided in the table below.
- | Atom | U <sup>11</sup> | U <sup>22</sup> | U <sup>33</sup> | U <sup>12</sup> | U <sup>13</sup> | U <sup>23</sup> |
|------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| C01  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C02  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C03  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C04  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C05  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C06  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C07  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C08  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C09  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C10  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C11  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| C12  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| N05  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| N13  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |
| S15  | 0.025           | 0.025           | 0.025           | 0.000           | 0.000           | 0.000           |

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	S	0	0
			19	16	2	1		
10	D	1	Total	C	N	S	0	1
			19	16	2	1		

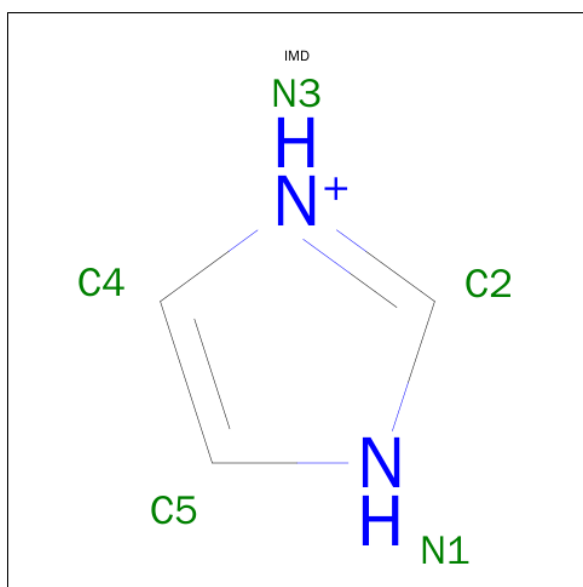
- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
11	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 12 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	N	0	0
			5	3	2		

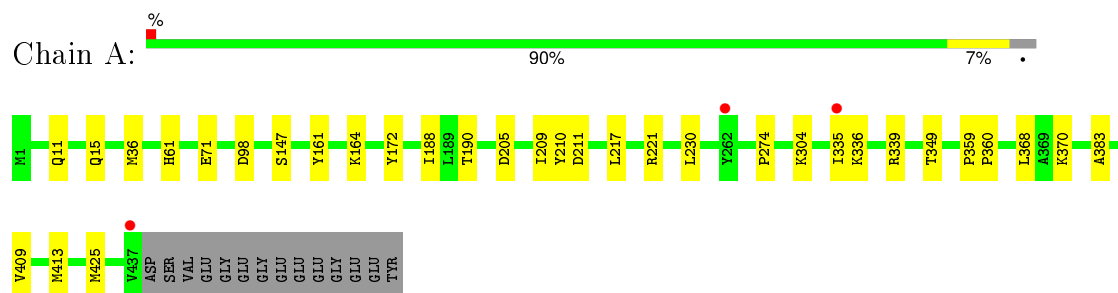
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	23	Total	O	0	0
			23	23		
13	B	30	Total	O	0	0
			30	30		
13	C	47	Total	O	0	0
			47	47		
13	D	9	Total	O	0	1
			9	9		
13	F	2	Total	O	0	0
			2	2		

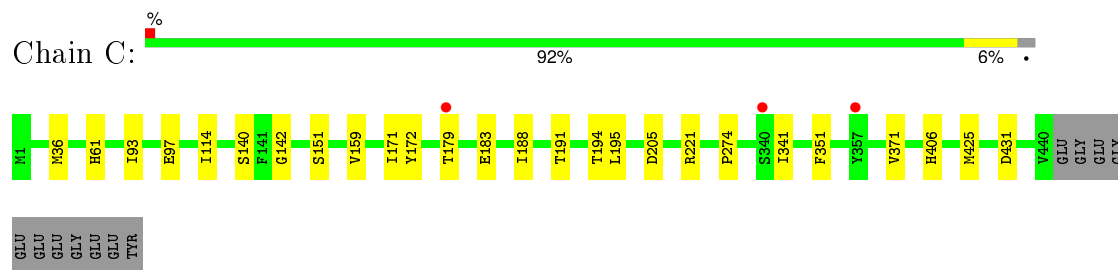
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

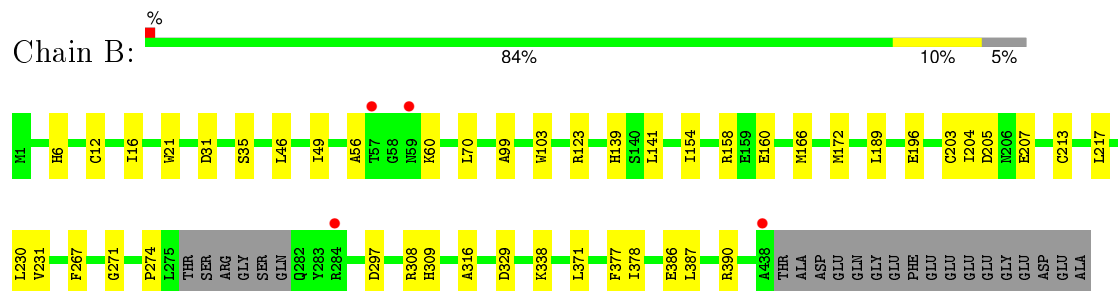
- Molecule 1: Tubulin alpha-1B chain



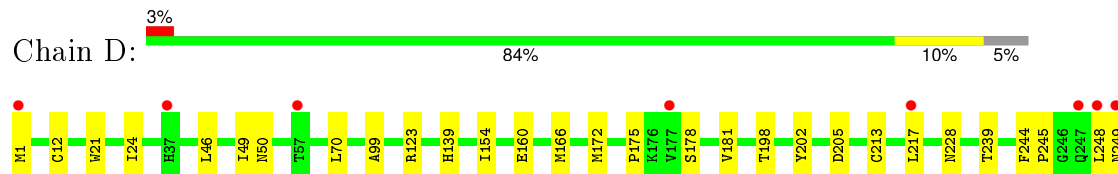
- Molecule 1: Tubulin alpha-1B chain

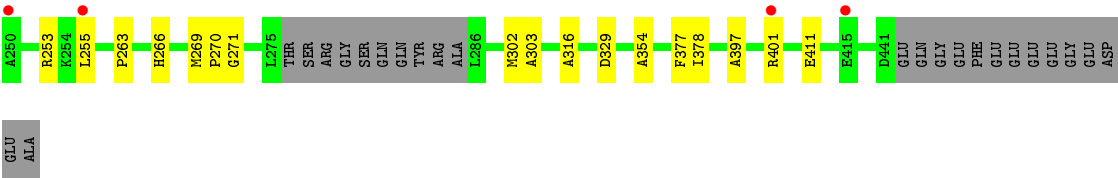


- Molecule 2: Tubulin beta-2B chain

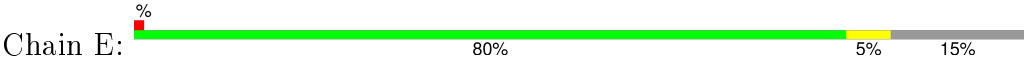


- Molecule 2: Tubulin beta-2B chain

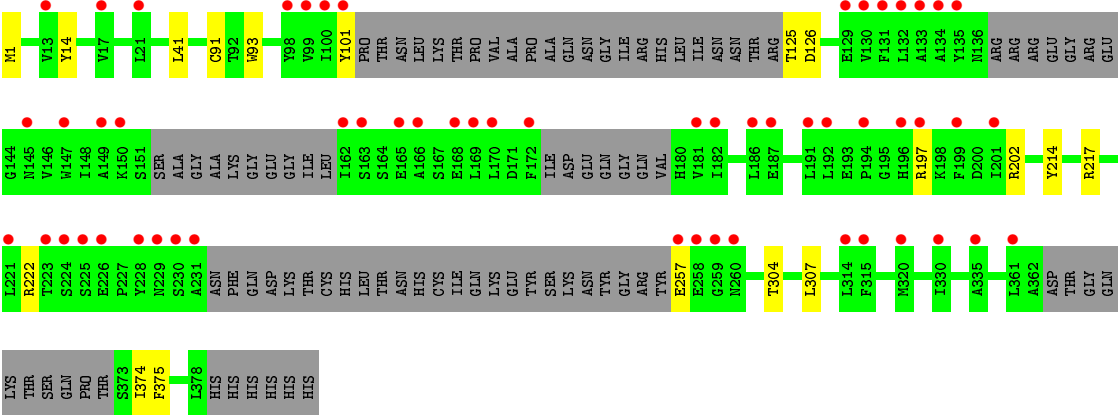




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-tyrosine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.83Å 157.65Å 181.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.72 – 2.60 90.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.72-2.60) 99.8 (90.72-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.188 , 0.231 0.198 , 0.234	Depositor DCC
$R_{free}$ test set	9261 reflections (11.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.9	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 92610 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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, GOL, MG, IMD, CA, 4ED, GTP, MES

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	0.21	0/3501	0.37	0/4753
1	C	0.21	0/3529	0.38	0/4791
2	B	0.22	0/3416	0.36	0/4626
2	D	0.21	0/3460	0.36	0/4688
3	E	0.20	0/1012	0.31	0/1344
4	F	0.21	0/2469	0.35	0/3334
All	All	0.21	0/17387	0.36	0/23536

There are no bond length outliers.

There are no bond angle outliers.

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	3420	0	3339	22	0
1	C	3445	0	3357	16	0
2	B	3336	0	3220	27	0
2	D	3379	0	3261	29	0
3	E	1003	0	1019	5	0
4	F	2417	0	2403	10	0
5	A	32	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	12	0	16	2	0
8	B	6	0	8	0	0
8	C	6	0	8	0	0
8	D	6	0	8	2	0
9	B	28	0	12	1	0
9	D	28	0	12	2	0
10	B	19	0	14	1	0
10	D	19	0	14	3	0
11	B	24	0	24	2	0
12	C	5	0	5	1	0
13	A	23	0	0	0	0
13	B	30	0	0	0	0
13	C	47	0	0	0	0
13	D	9	0	0	0	0
13	F	2	0	0	0	0
All	All	17335	0	16744	101	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 3.

The worst 5 of 101 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:D:253:ARG:HH11	8:D:504:GOL:HO3	1.37	0.70
2:D:253:ARG:NH1	8:D:504:GOL:O3	2.26	0.68
1:C:179:THR:HB	2:D:248[B]:LEU:HD13	1.75	0.67
1:A:383:ALA:HA	8:A:505:GOL:H31	1.78	0.65
4:F:217:ARG:HE	4:F:374:ILE:HA	1.63	0.63

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	436/451 (97%)	421 (97%)	15 (3%)	0	100	100
1	C	440/451 (98%)	430 (98%)	10 (2%)	0	100	100
2	B	420/445 (94%)	408 (97%)	12 (3%)	0	100	100
2	D	427/445 (96%)	416 (97%)	10 (2%)	1 (0%)	52	77
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	282/384 (73%)	268 (95%)	14 (5%)	0	100	100
All	All	2122/2319 (92%)	2059 (97%)	62 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	181	VAL

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	369/379 (97%)	369 (100%)	0	100	100
1	C	373/379 (98%)	373 (100%)	0	100	100
2	B	367/383 (96%)	366 (100%)	1 (0%)	94	99
2	D	372/383 (97%)	371 (100%)	1 (0%)	94	99
3	E	109/127 (86%)	108 (99%)	1 (1%)	84	95
4	F	266/342 (78%)	266 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1856/1993 (93%)	1853 (100%)	3 (0%)	95 99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	139	HIS
2	D	139	HIS
3	E	14	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 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
5	GTP	A	501	6	25,34,34	0.94	1 (4%)	34,54,54	1.75	6 (17%)
8	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.27	0
8	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.26	0
9	GDP	B	501	6	23,30,30	1.19	2 (8%)	30,47,47	1.74	6 (20%)
10	4ED	B	504	-	19,21,21	1.11	1 (5%)	21,29,29	1.22	3 (14%)
11	MES	B	505	-	11,12,12	0.59	0	14,16,16	2.26	7 (50%)
11	MES	B	506	-	11,12,12	0.61	0	14,16,16	2.53	7 (50%)
8	GOL	B	507	-	5,5,5	0.35	0	5,5,5	0.23	0
5	GTP	C	501	6	25,34,34	0.93	1 (4%)	34,54,54	1.61	6 (17%)
8	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.23	0
12	IMD	C	504	-	3,5,5	0.54	0	4,5,5	0.58	0
9	GDP	D	501	6	23,30,30	1.17	2 (8%)	30,47,47	1.84	7 (23%)
10	4ED	D	503[A]	-	19,21,21	1.07	1 (5%)	21,29,29	1.24	3 (14%)
8	GOL	D	504	-	5,5,5	0.36	0	5,5,5	0.22	0

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	GTP	A	501	6	-	0/18/38/38	0/3/3/3
8	GOL	A	504	-	-	0/4/4/4	0/0/0/0
8	GOL	A	505	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	4ED	B	504	-	-	0/3/5/5	0/3/3/3
11	MES	B	505	-	-	0/6/14/14	0/1/1/1
11	MES	B	506	-	-	0/6/14/14	0/1/1/1
8	GOL	B	507	-	-	0/4/4/4	0/0/0/0
5	GTP	C	501	6	-	0/18/38/38	0/3/3/3
8	GOL	C	503	-	-	0/4/4/4	0/0/0/0
12	IMD	C	504	-	-	0/0/0/0	0/1/1/1
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
10	4ED	D	503[A]	-	-	0/3/5/5	0/3/3/3
8	GOL	D	504	-	-	0/4/4/4	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C6-N1	2.90	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C6-N1	2.91	1.38	1.33
9	B	501	GDP	C5-C4	3.00	1.47	1.40
9	D	501	GDP	C5-C4	3.01	1.47	1.40
10	D	503[A]	4ED	C06-S15	3.36	1.78	1.73

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-4.83	120.08	127.44
5	C	501	GTP	N3-C2-N1	-4.72	120.26	127.44
5	A	501	GTP	PA-O3A-PB	-4.34	120.55	132.73
9	D	501	GDP	C5-C6-N1	-4.14	117.92	123.59
9	B	501	GDP	C5-C6-N1	-3.95	118.19	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	3	0
8	A	504	GOL	1	0
8	A	505	GOL	1	0
9	B	501	GDP	1	0
10	B	504	4ED	1	0
11	B	506	MES	2	0
12	C	504	IMD	1	0
9	D	501	GDP	2	0
10	D	503[A]	4ED	3	0
8	D	504	GOL	2	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.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	437/451 (96%)	-0.06	3 (0%) 89 87	47, 70, 104, 124	0
1	C	440/451 (97%)	0.09	3 (0%) 89 87	35, 54, 87, 113	0
2	B	422/445 (94%)	0.06	4 (0%) 85 83	44, 64, 103, 143	0
2	D	421/445 (94%)	0.07	12 (2%) 55 48	49, 80, 120, 137	0
3	E	121/143 (84%)	0.17	2 (1%) 73 68	55, 85, 120, 133	0
4	F	296/384 (77%)	0.94	56 (18%) 2 1	57, 98, 162, 179	0
All	All	2137/2319 (92%)	0.17	80 (3%) 45 37	35, 72, 120, 179	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	8.1
4	F	259	GLY	6.7
4	F	169	LEU	6.3
1	C	179	THR	5.8
4	F	231	ALA	4.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	MES	B	506	12/12	0.75	0.33	7.43	113,119,158,159	0
8	GOL	A	505	6/6	0.81	0.44	5.58	97,101,108,111	0
8	GOL	A	504	6/6	0.86	0.25	2.80	86,87,88,90	0
12	IMD	C	504	5/5	0.93	0.23	2.77	79,79,80,82	0
8	GOL	C	503	6/6	0.90	0.55	2.76	93,100,102,104	0
10	4ED	D	503[A]	19/19	0.83	0.48	2.55	39,51,59,61	19
8	GOL	D	504	6/6	0.89	0.20	1.29	70,72,76,77	0
11	MES	B	505	12/12	0.95	0.17	0.51	56,77,89,90	0
5	GTP	A	501	32/32	0.98	0.16	0.45	44,55,63,76	0
5	GTP	C	501	32/32	0.97	0.19	0.38	42,48,67,76	0
8	GOL	B	507	6/6	0.89	0.20	0.17	88,90,92,92	0
10	4ED	B	504	19/19	0.97	0.18	0.17	47,57,62,64	0
9	GDP	D	501	28/28	0.96	0.17	0.04	63,74,84,135	0
9	GDP	B	501	28/28	0.98	0.18	-0.10	34,46,53,55	0
7	CA	C	502	1/1	0.99	0.13	-0.34	86,86,86,86	0
6	MG	C	505	1/1	0.98	0.14	-0.72	46,46,46,46	0
7	CA	A	503	1/1	0.89	0.09	-1.25	95,95,95,95	0
6	MG	A	502	1/1	0.98	0.10	-2.09	56,56,56,56	0
7	CA	B	503	1/1	0.87	0.20	-	101,101,101,101	0
6	MG	B	502	1/1	0.98	0.14	-	42,42,42,42	0
6	MG	D	502	1/1	0.70	0.10	-	87,87,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.