



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:17 AM GMT

PDB ID : 3E22
Title : Tubulin-colchicine-soblidotin: Stathmin-like domain complex
Authors : Cormier, A.; Marchand, M.; Ravelli, R.B.; Knossow, M.; Gigant, B.
Deposited on : 2008-08-05
Resolution : 3.80 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
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 : 1.7 (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

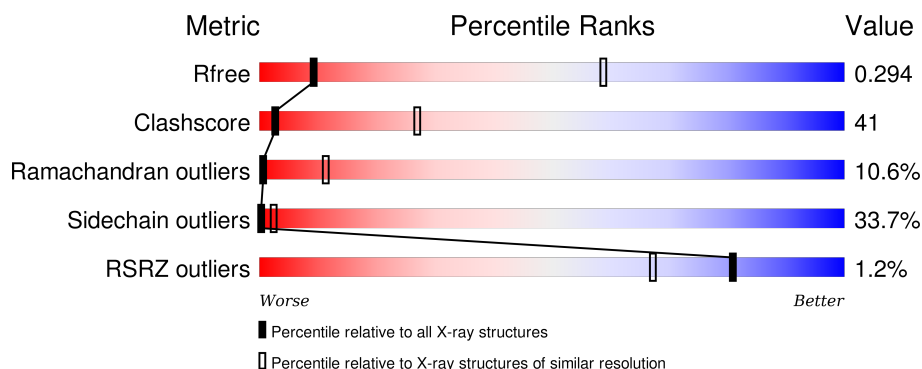
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 ≥ 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	449	<div> <div>31%</div> <div>42%</div> <div>19%</div> <div>• 5%</div> </div>
1	C	449	<div>2%</div> <div>33%</div> <div>41%</div> <div>18%</div> <div>• 6%</div>
2	B	445	<div>30%</div> <div>39%</div> <div>22%</div> <div>• 6%</div>
2	D	445	<div>2%</div> <div>31%</div> <div>40%</div> <div>20%</div> <div>• 6%</div>
3	E	142	<div>36%</div> <div>35%</div> <div>15%</div> <div>• 13%</div>

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
5	MG	A	601	-	-	-	X
8	TZT	B	800	-	-	X	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14154 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-1C chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3290	2089	556	624	21			
1	C	421	Total	C	N	O	S	0	0	0
			3234	2055	547	611	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	TYR	ALA	SEE REMARK 999	UNP Q3ZCJ7
A	442	ASP	GLY	SEE REMARK 999	UNP Q3ZCJ7
A	443	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
A	447	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
C	440	TYR	ALA	SEE REMARK 999	UNP Q3ZCJ7
C	442	ASP	GLY	SEE REMARK 999	UNP Q3ZCJ7
C	443	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7
C	447	GLU	ASP	SEE REMARK 999	UNP Q3ZCJ7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3238	2036	546	632	24			
2	D	419	Total	C	N	O	S	0	0	0
			3246	2041	549	632	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	SER	CYS	SEE REMARK 999	UNP Q6B856
B	318	VAL	ILE	SEE REMARK 999	UNP Q6B856
D	203	SER	CYS	SEE REMARK 999	UNP Q6B856
D	318	VAL	ILE	SEE REMARK 999	UNP Q6B856

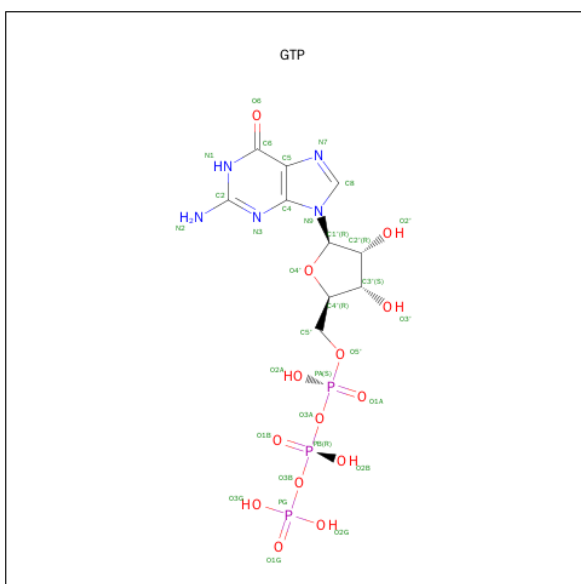
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			916	555	173	183	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043

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



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

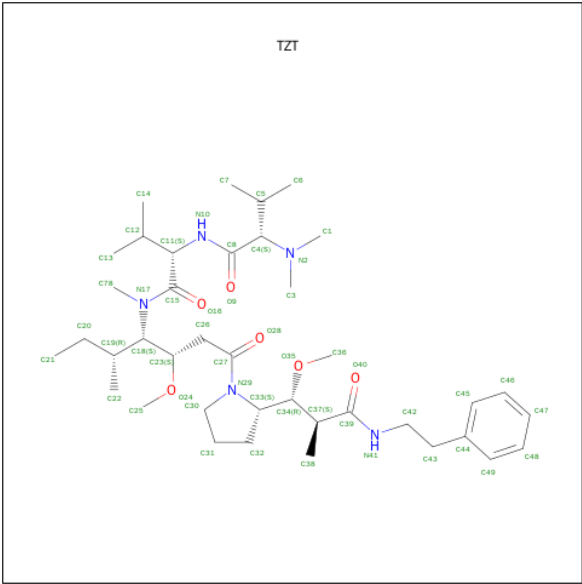
-
- The chemical structure of GDP (Guanosine Diphosphate) is shown. It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is linked to a diphosphate group (two phosphate groups connected 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	
6	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
6	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

-

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			29	22	1	6		
7	D	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 8 is SOBLIDOTIN (three-letter code: TZT) (formula: C₃₉H₆₇N₅O₆).

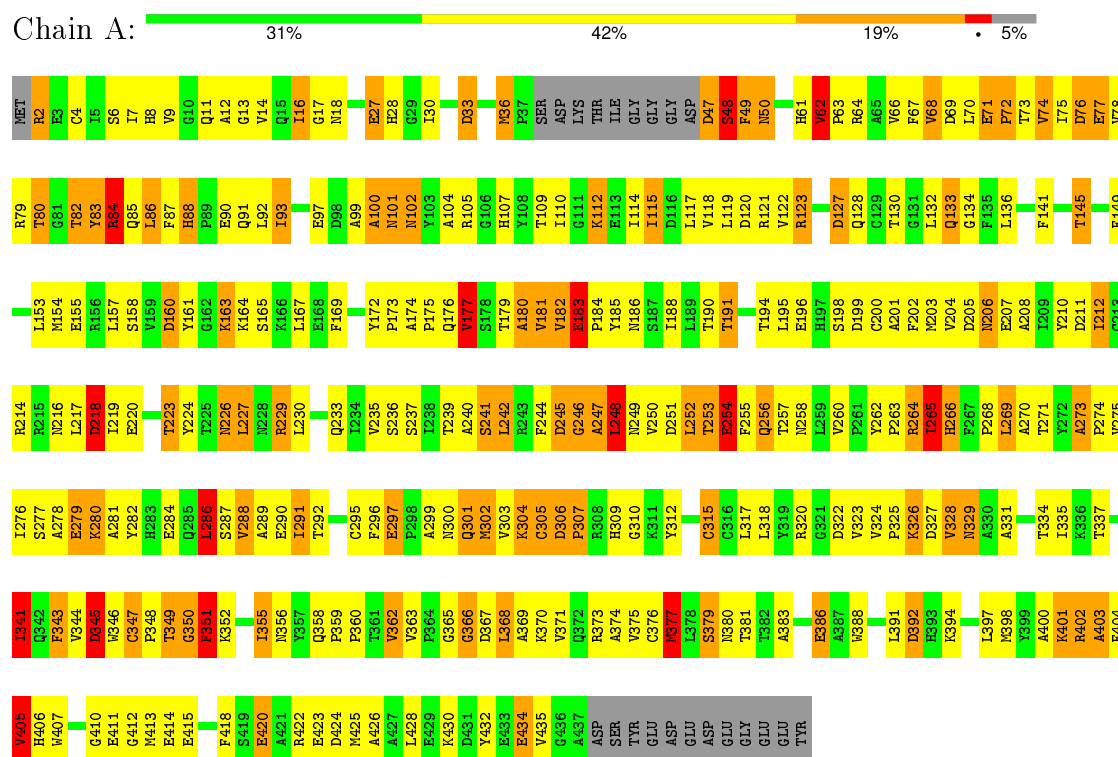


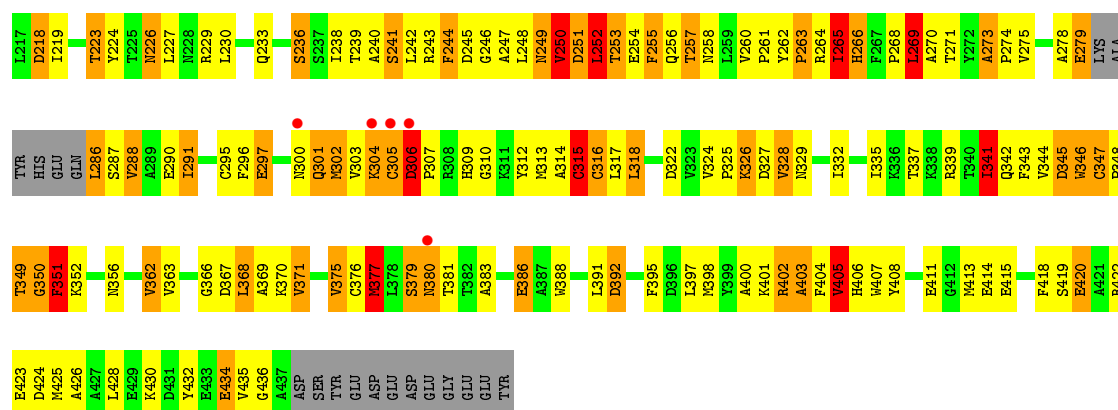
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			50	39	5	6		

3 Residue-property plots

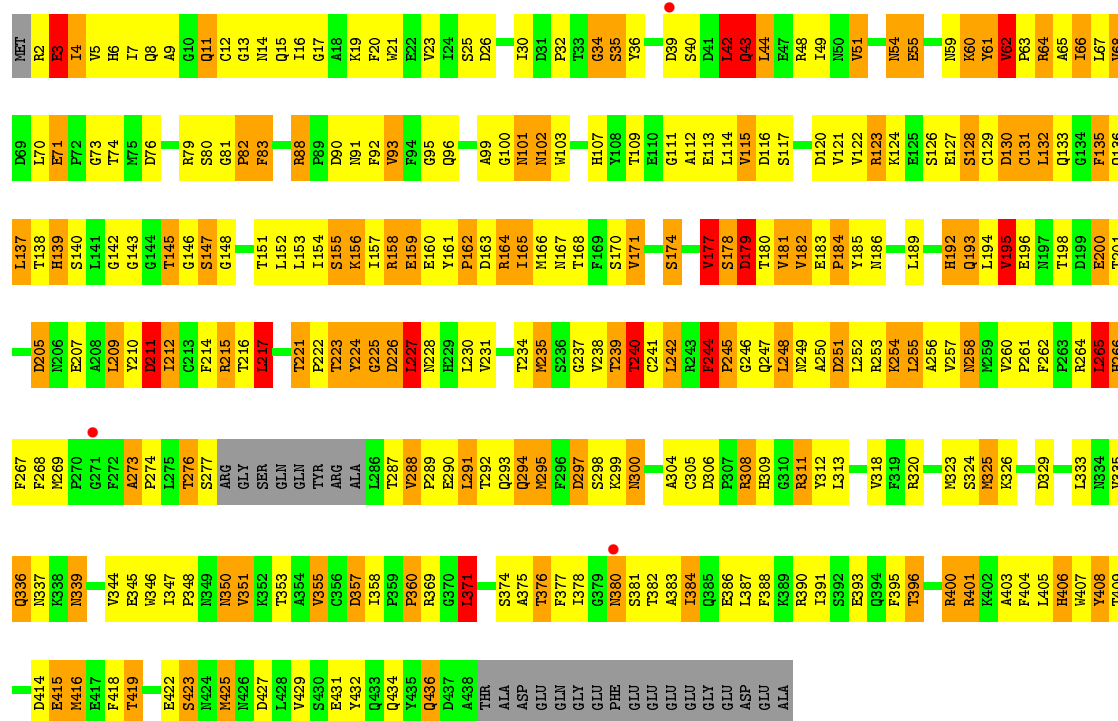
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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-1C chain

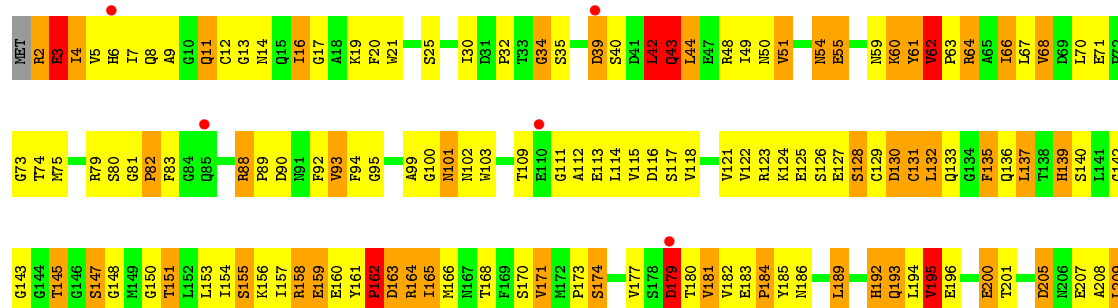


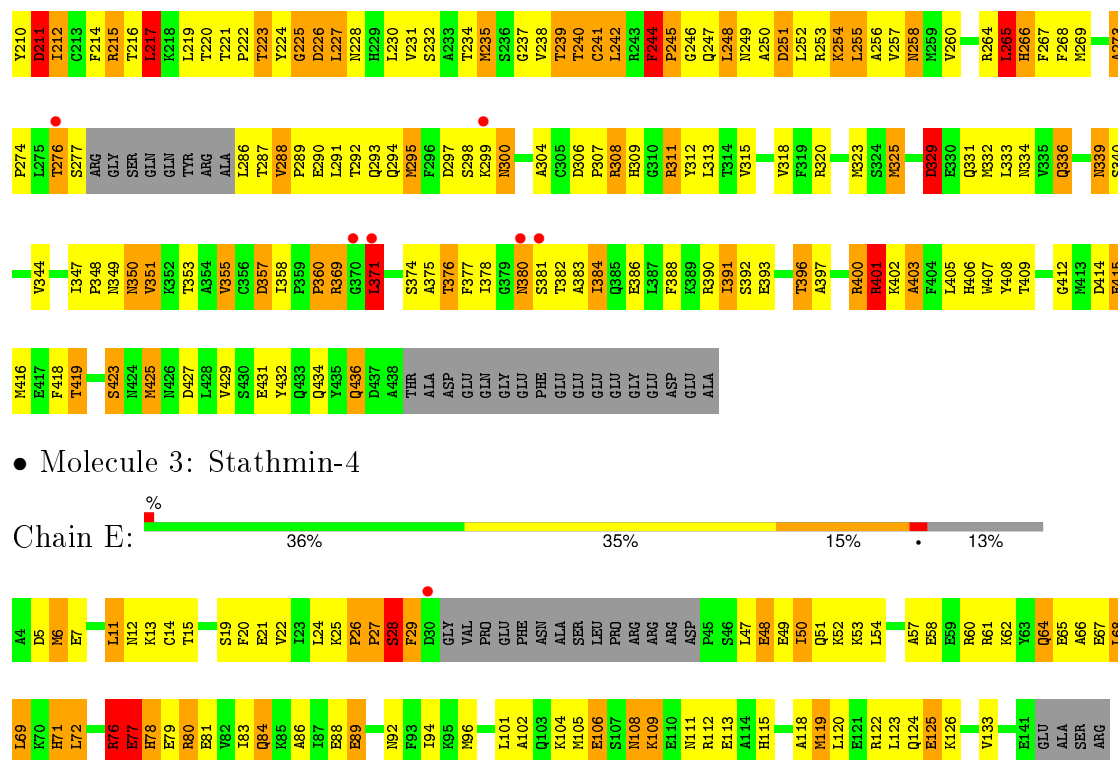


• Molecule 2: Tubulin beta-2B chain



• Molecule 2: Tubulin beta-2B chain





● Molecule 3: Stathmin-4

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	324.09 Å 324.09 Å 53.28 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.80 19.91 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-3.80) 97.6 (19.91-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 3.82 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.295 0.240 , 0.294	Depositor DCC
R_{free} test set	1598 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	140.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 108.5	EDS
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 31414 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14154	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.95	1/3367 (0.0%)	1.09	19/4579 (0.4%)
1	C	0.67	1/3308 (0.0%)	0.96	15/4498 (0.3%)
2	B	0.76	0/3310	0.99	11/4495 (0.2%)
2	D	0.61	0/3318	0.92	13/4505 (0.3%)
3	E	0.72	0/924	0.90	0/1239
All	All	0.76	2/14227 (0.0%)	0.99	58/19316 (0.3%)

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
1	C	0	3
2	B	0	3
2	D	0	2
3	E	0	3
All	All	0	13

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	GLU	CD-OE1	5.64	1.31	1.25
1	C	436	GLY	C-O	-5.23	1.15	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	LEU	CA-CB-CG	7.48	132.51	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	427	ASP	CB-CG-OD2	7.28	124.86	118.30
1	A	33	ASP	CB-CG-OD2	6.95	124.55	118.30
1	A	76	ASP	CB-CG-OD2	6.82	124.43	118.30
1	A	47	ASP	CB-CG-OD2	6.64	124.28	118.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	VAL	Peptide
1	A	265	ILE	Peptide
2	B	162	PRO	Peptide
2	B	244	PHE	Peptide
2	B	265	LEU	Peptide

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	3290	0	3149	276	0
1	C	3234	0	3102	267	0
2	B	3238	0	3049	290	0
2	D	3246	0	3067	253	0
3	E	916	0	799	62	0
4	A	32	0	12	4	0
4	C	32	0	12	6	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	4	0
6	D	28	0	12	1	0
7	B	29	0	23	3	0
7	D	29	0	23	3	0
8	B	50	0	67	30	0
All	All	14154	0	13327	1115	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 41.

The worst 5 of 1115 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:273:ALA:CB	2:B:274:PRO:HD3	1.77	1.14
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.81	1.10
1:C:273:ALA:HB1	1:C:274:PRO:HD3	1.23	1.10
1:A:273:ALA:HB1	1:A:274:PRO:HD3	1.20	1.09
2:B:336:GLN:OE1	2:B:351:VAL:HG11	1.53	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 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	423/449 (94%)	295 (70%)	85 (20%)	43 (10%)	1	13
1	C	415/449 (92%)	300 (72%)	73 (18%)	42 (10%)	1	13
2	B	415/445 (93%)	289 (70%)	81 (20%)	45 (11%)	0	11
2	D	415/445 (93%)	297 (72%)	73 (18%)	45 (11%)	0	11
3	E	120/142 (84%)	71 (59%)	35 (29%)	14 (12%)	0	9
All	All	1788/1930 (93%)	1252 (70%)	347 (19%)	189 (11%)	0	11

5 of 189 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	48	SER
1	A	49	PHE
1	A	62	VAL
1	A	72	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 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	346/378 (92%)	230 (66%)	116 (34%)	0	2
1	C	340/378 (90%)	234 (69%)	106 (31%)	0	3
2	B	347/383 (91%)	229 (66%)	118 (34%)	0	2
2	D	349/383 (91%)	227 (65%)	122 (35%)	0	2
3	E	80/126 (64%)	49 (61%)	31 (39%)	0	1
All	All	1462/1648 (89%)	969 (66%)	493 (34%)	0	2

5 of 493 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	408	TYR
1	C	206	ASN
2	D	419	THR
2	B	425	MET
1	C	102	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	350	ASN
1	C	101	ASN
2	D	380	ASN
2	B	380	ASN
1	C	28	HIS

5.3.3 RNA [i](#)

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
4	GTP	A	600	-	25,34,34	0.98	2 (8%)	34,54,54	1.63	7 (20%)
6	GDP	B	600	-	23,30,30	0.96	1 (4%)	30,47,47	2.06	9 (30%)
7	LOC	B	700	-	29,31,31	3.86	7 (24%)	27,44,44	3.59	9 (33%)
8	TZT	B	800	-	51,51,51	1.83	10 (19%)	56,70,70	2.79	16 (28%)
4	GTP	C	600	-	25,34,34	1.07	2 (8%)	34,54,54	2.01	8 (23%)
6	GDP	D	600	-	23,30,30	1.01	1 (4%)	30,47,47	1.87	7 (23%)
7	LOC	D	700	-	29,31,31	3.56	6 (20%)	27,44,44	3.54	11 (40%)

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
4	GTP	A	600	-	-	0/18/38/38	0/3/3/3
6	GDP	B	600	-	-	0/12/32/32	0/3/3/3
7	LOC	B	700	-	-	0/10/25/25	0/3/3/3
8	TZT	B	800	-	-	0/72/82/82	0/2/2/2
4	GTP	C	600	-	-	0/18/38/38	0/3/3/3
6	GDP	D	600	-	-	0/12/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	LOC	D	700	-	-	0/10/25/25	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	LOC	C20-C21	-12.87	1.20	1.40
7	D	700	LOC	C20-C21	-11.15	1.22	1.40
7	B	700	LOC	C19-C17	-9.93	1.21	1.39
7	D	700	LOC	C19-C17	-9.65	1.22	1.39
7	B	700	LOC	C19-C20	-9.35	1.13	1.40

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	700	LOC	C21-C22-C8	-5.80	114.36	120.63
6	D	600	GDP	N3-C2-N1	-5.56	118.97	127.44
4	C	600	GTP	PA-O3A-PB	-5.13	118.32	132.73
4	C	600	GTP	N3-C2-N1	-5.07	119.72	127.44
6	B	600	GDP	N3-C2-N1	-5.06	119.73	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	4	0
6	B	600	GDP	4	0
7	B	700	LOC	3	0
8	B	800	TZT	30	0
4	C	600	GTP	6	0
6	D	600	GDP	1	0
7	D	700	LOC	3	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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	427/449 (95%)	-0.59	0 100 100	91, 95, 97, 103	0
1	C	421/449 (93%)	-0.31	7 (1%) 73 58	94, 95, 96, 98	1 (0%)
2	B	419/445 (94%)	-0.46	3 (0%) 89 80	94, 95, 96, 97	0
2	D	419/445 (94%)	-0.27	11 (2%) 59 43	94, 95, 96, 96	0
3	E	124/142 (87%)	-0.35	1 (0%) 87 77	91, 95, 97, 99	0
All	All	1810/1930 (93%)	-0.40	22 (1%) 81 67	91, 95, 96, 103	1 (0%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	305	CYS	3.6
1	C	304	LYS	3.5
1	C	306	ASP	3.4
1	C	6	SER	3.3
2	D	299	LYS	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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, 95th 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 ²)	Q<0.9
5	MG	A	601	1/1	0.98	0.26	3.37	93,93,93,93	0
8	TZT	B	800	50/50	0.82	0.33	2.50	92,94,102,102	0
7	LOC	D	700	29/29	0.94	0.32	1.98	94,95,95,95	0
7	LOC	B	700	29/29	0.95	0.27	1.92	95,95,95,95	0
6	GDP	B	600	28/28	0.92	0.23	0.68	94,95,95,96	0
4	GTP	C	600	32/32	0.92	0.20	-0.17	94,95,95,95	0
4	GTP	A	600	32/32	0.94	0.15	-0.35	94,95,95,96	0
6	GDP	D	600	28/28	0.91	0.23	-0.39	95,95,95,95	0
5	MG	C	601	1/1	0.96	0.20	-0.92	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.