



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:38 am GMT

PDB ID : 4ZHQ  
Title : Crystal structure of Tubulin-Stathmin-TTL-MMAE Complex  
Authors : Wang, Y.; Zhang, R.  
Deposited on : 2015-04-26  
Resolution : 2.55 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

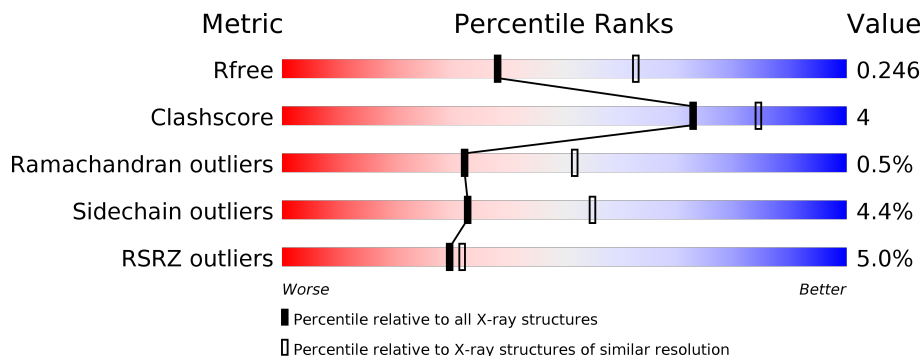
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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  $\geq 3$ , 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 89%, green 89%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>89%</span> <span>8%</span> <span>.</span> </div> </div>
1	C	451	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, yellow 89%, green 89%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>89%</span> <span>8%</span> <span>.</span> </div> </div>
2	B	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 83%, green 83%, grey 12%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>12%</span> <span>.</span> </div> </div>
2	D	445	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 6%, yellow 79%, green 79%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>6%</span> <span>79%</span> <span>15%</span> <span>• 5%</span> </div> </div>
3	E	143	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 7%, orange 7%, yellow 77%, green 77%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>7%</span> <span>77%</span> <span>8%</span> <span>• 14%</span> </div> </div>
4	F	384	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 16%, yellow 74%, green 74%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>16%</span> <span>74%</span> <span>14%</span> <span>• 10%</span> </div> </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
8	GOL	A	505	-	-	-	X
8	GOL	A	506	-	-	-	X
8	GOL	B	506	-	-	-	X
8	GOL	C	503	-	-	-	X
8	GOL	C	506	-	-	X	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17988 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	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	1	0
			3446	2180	585	659	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3360	2111	576	647	26			
2	D	422	Total	C	N	O	S	0	0	0
			3311	2082	563	640	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

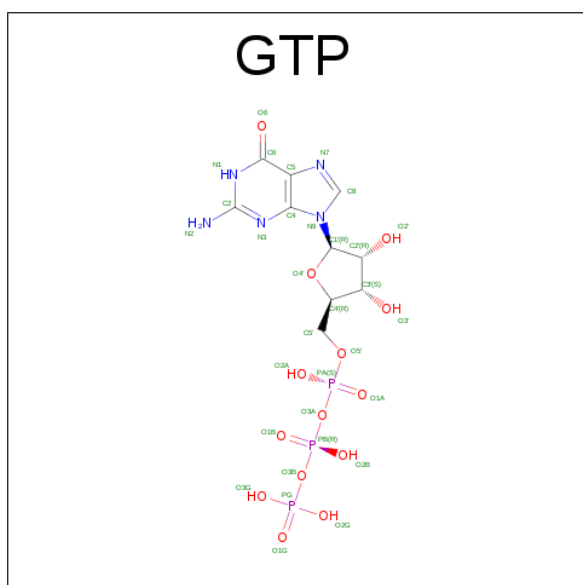
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	0	0
			2849	1825	492	518	14			

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		

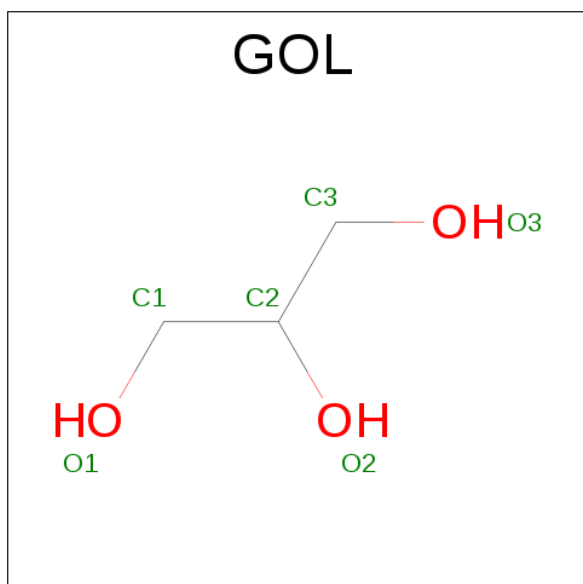
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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		
6	C	1	Total	Mg	0	0
			1	1		

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

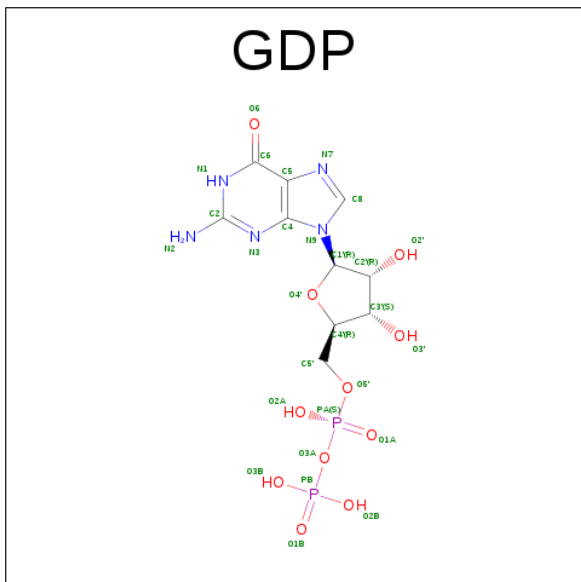
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



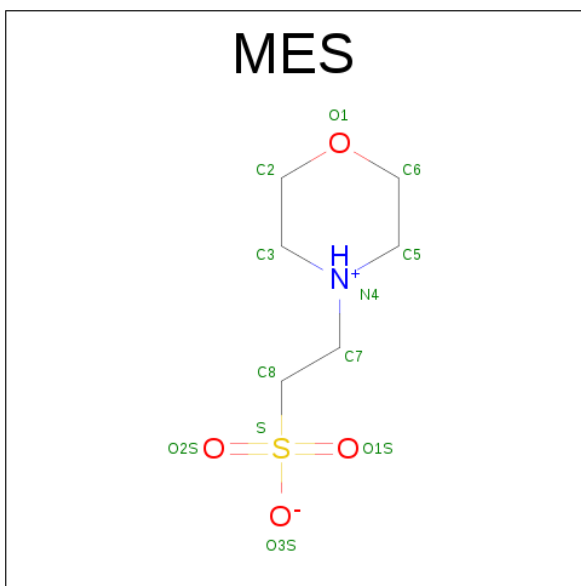
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



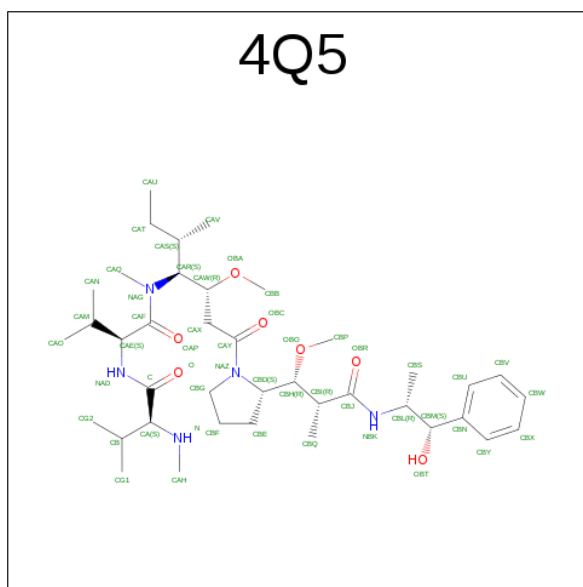
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

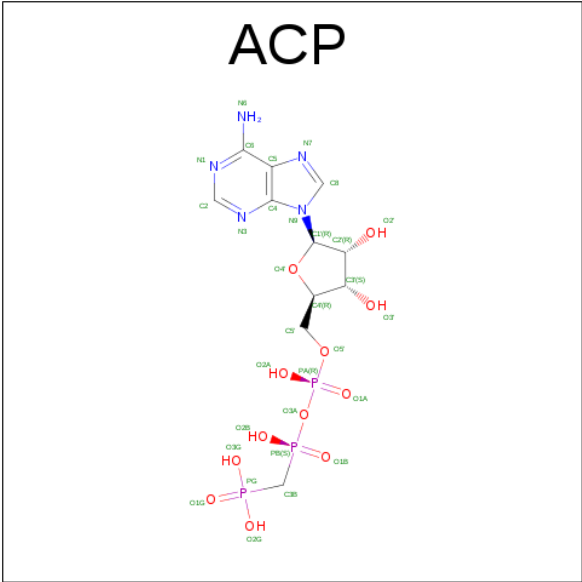
- Molecule 11 is N-methyl-L-valyl-N-[(3R,4S,5S)-1-{(2S)-2-[(1R,2R)-3-{[(1S,2R)-1-hydroxy-1-phenylpropan-2-yl]amino}-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl}-3-methoxy-5-methyl-1-oxoheptan-4-yl]-N-methyl-L-valinamide (three-letter code: 4Q5) (formula: C<sub>39</sub>H<sub>67</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			51	39	5	7		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

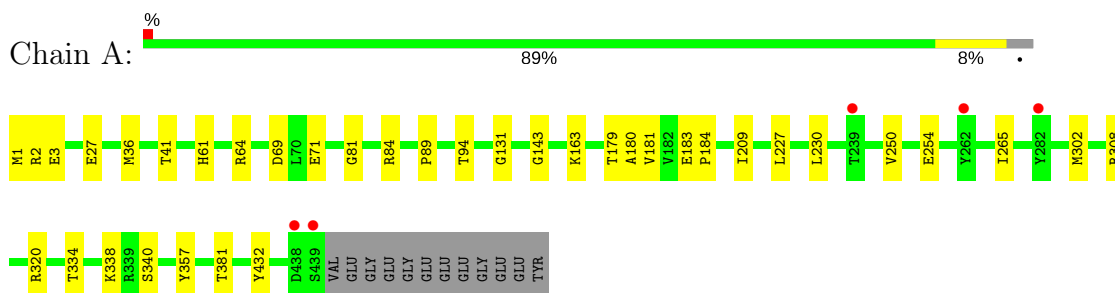
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	63	Total	O	0	0
			63	63		
13	B	66	Total	O	0	0
			66	66		
13	C	110	Total	O	0	0
			110	110		
13	D	19	Total	O	0	0
			19	19		
13	E	2	Total	O	0	0
			2	2		
13	F	37	Total	O	0	0
			37	37		

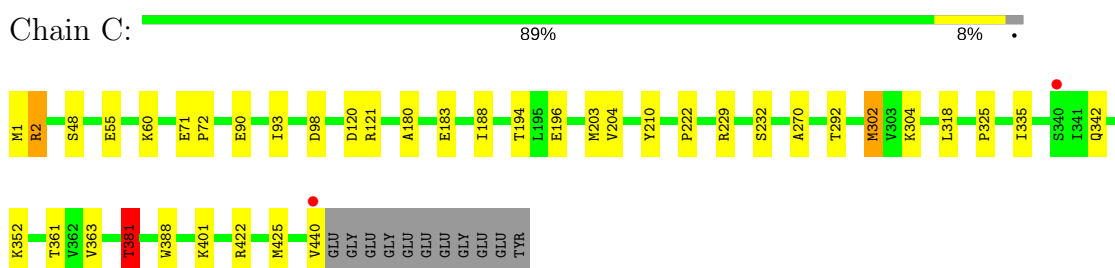
### 3 Residue-property plots [i](#)

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 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.

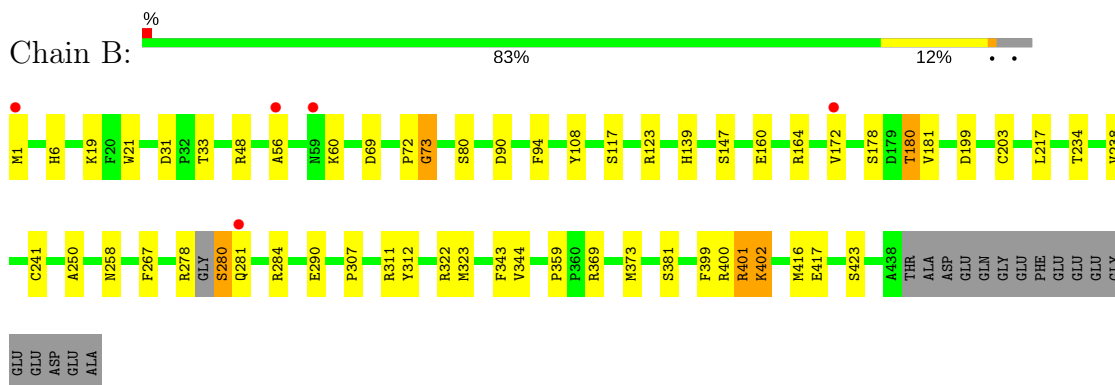
- Molecule 1: Tubulin alpha-1B chain



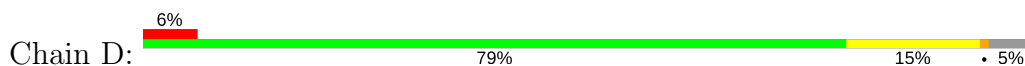
- Molecule 1: Tubulin alpha-1B chain

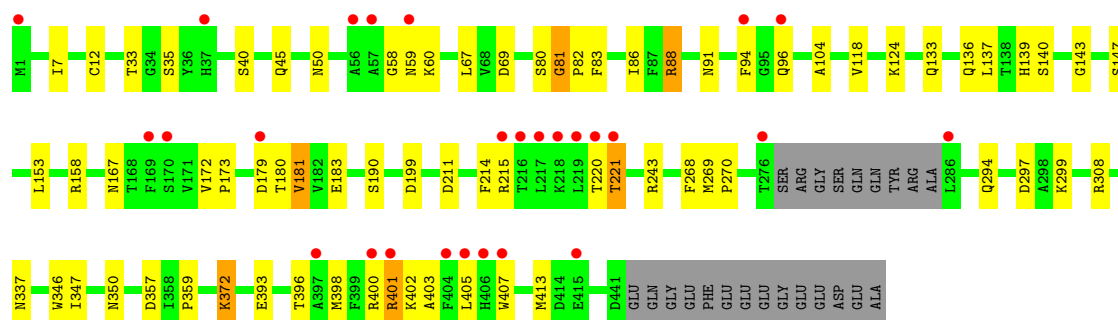


- Molecule 2: Tubulin beta chain

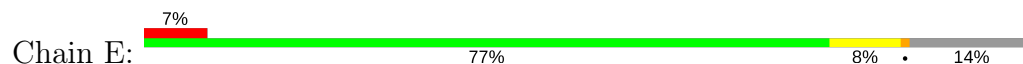


- Molecule 2: Tubulin beta chain

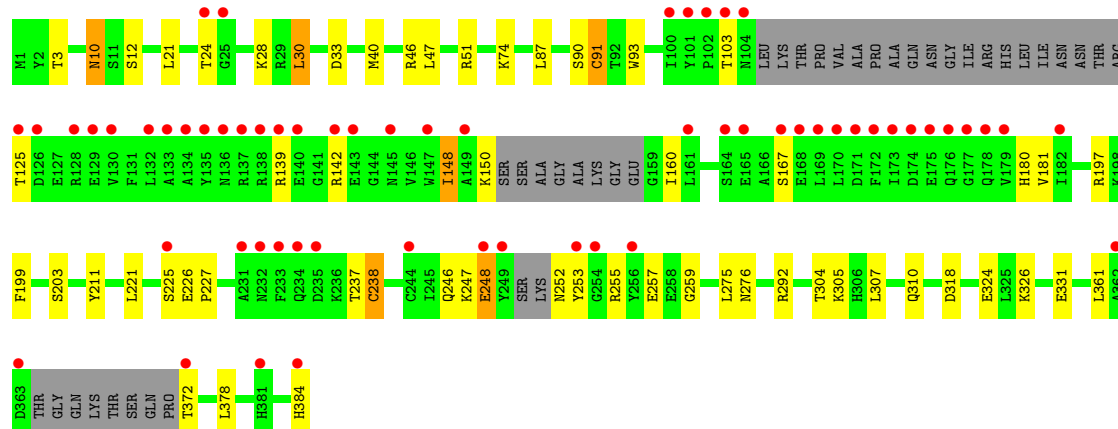




• Molecule 3: Stathmin-4



• 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, $\alpha$ , $\beta$ , $\gamma$	104.94Å 156.81Å 182.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.34 – 2.55 39.34 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.34-2.55) 99.7 (39.34-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.190 , 0.245 0.192 , 0.246	Depositor DCC
$R_{free}$ test set	4896 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, CA, GTP, 4Q5, ACP, 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	0.70	0/3508	0.83	1/4762 (0.0%)
1	C	0.79	0/3524	0.88	3/4785 (0.1%)
2	B	0.78	0/3434	0.84	5/4651 (0.1%)
2	D	0.67	1/3384 (0.0%)	0.80	4/4586 (0.1%)
3	E	0.73	0/1022	0.81	0/1356
4	F	0.58	0/2916	0.76	2/3940 (0.1%)
All	All	0.71	1/17788 (0.0%)	0.83	15/24080 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	173	PRO	N-CD	5.17	1.55	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	221	THR	N-CA-C	-8.78	87.29	111.00
1	C	381	THR	CB-CA-C	-6.49	94.09	111.60
1	C	422	ARG	NE-CZ-NH2	-6.28	117.16	120.30
4	F	51	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	D	243	ARG	NE-CZ-NH1	6.08	123.34	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	MET	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	3430	0	3340	17	0
1	C	3446	0	3354	35	0
2	B	3360	0	3242	29	0
2	D	3311	0	3192	32	1
3	E	1014	0	1029	5	0
4	F	2849	0	2796	22	1
5	A	32	0	12	1	0
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	18	0	24	1	0
8	B	6	0	8	3	0
8	C	24	0	32	9	0
9	B	28	0	12	0	0
9	D	28	0	12	0	0
10	B	24	0	26	2	0
11	B	51	0	0	0	0
12	F	31	0	14	1	0
13	A	63	0	0	1	0
13	B	66	0	0	1	0
13	C	110	0	0	2	0
13	D	19	0	0	0	0
13	E	2	0	0	0	0
13	F	37	0	0	1	0
All	All	17988	0	17105	137	1

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 137 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:C:229:ARG:HG2	8:C:506:GOL:O2	1.50	1.09
1:C:204:VAL:HG22	1:C:302:MET:CE	1.99	0.91
1:C:204:VAL:HG22	1:C:302:MET:HE2	1.51	0.90
1:C:363:VAL:HG21	8:C:506:GOL:H2	1.62	0.80
2:D:33:THR:OG1	2:D:60:LYS:NZ	2.16	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:ASN:OD1	4:F:384:HIS:NE2[3_555]	2.17	0.03

## 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	437/451 (97%)	419 (96%)	17 (4%)	1 (0%)	51 71
1	C	439/451 (97%)	424 (97%)	14 (3%)	1 (0%)	51 71
2	B	423/445 (95%)	409 (97%)	13 (3%)	1 (0%)	51 71
2	D	418/445 (94%)	401 (96%)	14 (3%)	3 (1%)	25 42
3	E	119/143 (83%)	112 (94%)	6 (5%)	1 (1%)	22 38
4	F	336/384 (88%)	308 (92%)	24 (7%)	4 (1%)	15 26
All	All	2172/2319 (94%)	2073 (95%)	88 (4%)	11 (0%)	32 52

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	402	LYS
3	E	27	PRO
4	F	91	CYS
4	F	142	ARG
2	B	73	GLY

### 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	370/379 (98%)	361 (98%)	9 (2%)	54	78
1	C	372/379 (98%)	363 (98%)	9 (2%)	54	78
2	B	368/381 (97%)	350 (95%)	18 (5%)	29	50
2	D	363/381 (95%)	346 (95%)	17 (5%)	30	52
3	E	110/127 (87%)	103 (94%)	7 (6%)	20	36
4	F	312/342 (91%)	289 (93%)	23 (7%)	16	28
All	All	1895/1989 (95%)	1812 (96%)	83 (4%)	33	55

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	88	ARG
2	D	299	LYS
4	F	255	ARG
2	D	96	GLN
2	D	179	ASP

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

Mol	Chain	Res	Type
4	F	383	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 ⓘ

Of 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 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	27,34,34	1.04	2 (7%)	27,54,54	1.93	8 (29%)
8	GOL	A	504	-	5,5,5	0.45	0	5,5,5	0.52	0
8	GOL	A	505	-	5,5,5	0.43	0	5,5,5	1.03	0
8	GOL	A	506	-	5,5,5	0.51	0	5,5,5	0.32	0
9	GDP	B	501	6	25,30,30	1.23	3 (12%)	26,47,47	1.93	6 (23%)
10	MES	B	504	-	12,12,12	1.97	3 (25%)	14,16,16	7.89	8 (57%)
10	MES	B	505	-	12,12,12	2.19	2 (16%)	14,16,16	2.74	4 (28%)
8	GOL	B	506	-	5,5,5	0.85	0	5,5,5	0.84	0
11	4Q5	B	507	-	51,52,52	1.36	5 (9%)	53,72,72	1.67	11 (20%)
5	GTP	C	501	6	27,34,34	1.10	1 (3%)	27,54,54	2.17	8 (29%)
8	GOL	C	503	-	5,5,5	0.55	0	5,5,5	0.84	0
8	GOL	C	505	-	5,5,5	0.64	0	5,5,5	0.85	0
8	GOL	C	506	-	5,5,5	0.63	0	5,5,5	0.91	0
8	GOL	C	507	-	5,5,5	0.35	0	5,5,5	0.69	0
9	GDP	D	501	6	25,30,30	1.13	2 (8%)	26,47,47	2.17	7 (26%)
12	ACP	F	401	-	27,33,33	2.14	8 (29%)	30,52,52	1.43	2 (6%)

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
8	GOL	A	506	-	-	0/4/4/4	0/0/0/0
9	GDP	B	501	6	-	0/12/32/32	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	MES	B	505	-	-	0/6/14/14	0/1/1/1
8	GOL	B	506	-	-	0/4/4/4	0/0/0/0
11	4Q5	B	507	-	-	0/76/86/86	0/2/2/2
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
8	GOL	C	505	-	-	0/4/4/4	0/0/0/0
8	GOL	C	506	-	-	0/4/4/4	0/0/0/0
8	GOL	C	507	-	-	0/4/4/4	0/0/0/0
9	GDP	D	501	6	-	0/12/32/32	0/3/3/3
12	ACP	F	401	-	-	0/15/38/38	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	MES	C8-S	-6.98	1.67	1.77
10	B	504	MES	C8-S	-5.53	1.69	1.77
11	B	507	4Q5	CBN-CBM	-5.16	1.44	1.51
9	B	501	GDP	C2'-C1'	-3.57	1.48	1.53
5	A	501	GTP	C2'-C1'	-2.52	1.49	1.53

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O3S-S-C8	-13.07	89.98	106.06
10	B	504	MES	O3S-S-O2S	-12.49	82.73	111.37
10	B	504	MES	O3S-S-O1S	-11.71	84.53	111.37
12	F	401	ACP	N3-C2-N1	-5.57	124.01	128.86
11	B	507	4Q5	CB-CA-C	-5.55	97.65	111.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
8	A	504	GOL	1	0
10	B	504	MES	2	0
8	B	506	GOL	3	0
8	C	505	GOL	1	0
8	C	506	GOL	7	0
8	C	507	GOL	1	0
12	F	401	ACP	1	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 [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, 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	439/451 (97%)	-0.17	5 (1%) 80 82	18, 35, 61, 98	0
1	C	440/451 (97%)	-0.49	2 (0%) 90 91	16, 28, 51, 79	0
2	B	427/445 (95%)	-0.26	5 (1%) 79 81	16, 30, 61, 101	0
2	D	422/445 (94%)	0.17	27 (6%) 20 21	25, 47, 80, 93	0
3	E	123/143 (86%)	0.32	10 (8%) 13 13	29, 51, 85, 109	0
4	F	346/384 (90%)	0.53	60 (17%) 2 1	27, 59, 116, 135	0
All	All	2197/2319 (94%)	-0.05	109 (4%) 30 32	16, 39, 85, 135	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	372	THR	6.8
4	F	133	ALA	6.2
4	F	101	TYR	5.2
4	F	235	ASP	4.7
1	A	439	SER	4.5

### 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

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
8	GOL	C	506	6/6	0.73	0.53	22.48	50,68,69,82	0
8	GOL	A	505	6/6	0.91	0.20	5.06	46,59,60,67	0
8	GOL	B	506	6/6	0.84	0.26	3.34	49,51,54,55	0
8	GOL	A	506	6/6	0.82	0.22	3.26	54,61,65,67	0
8	GOL	C	503	6/6	0.88	0.27	3.24	54,69,72,77	0
10	MES	B	505	12/12	0.96	0.17	1.66	49,52,53,55	0
8	GOL	C	507	6/6	0.97	0.15	1.44	45,51,53,55	0
8	GOL	A	504	6/6	0.85	0.19	0.69	63,69,72,81	0
11	4Q5	B	507	51/51	0.97	0.11	0.08	18,22,25,25	0
9	GDP	B	501	28/28	0.99	0.13	-0.10	15,18,19,20	0
10	MES	B	504	12/12	0.95	0.13	-0.26	45,49,56,60	0
5	GTP	C	501	32/32	0.99	0.12	-0.28	17,20,23,23	0
5	GTP	A	501	32/32	0.99	0.14	-0.55	18,22,25,26	0
12	ACP	F	401	31/31	0.90	0.17	-0.66	66,83,96,109	0
9	GDP	D	501	28/28	0.97	0.12	-1.12	34,38,48,60	0
6	MG	A	502	1/1	0.97	0.05	-2.49	25,25,25,25	0
7	CA	A	503	1/1	0.90	0.04	-2.57	57,57,57,57	0
7	CA	C	504	1/1	0.98	0.03	-3.37	35,35,35,35	0
6	MG	C	502	1/1	0.98	0.07	-3.83	23,23,23,23	0
7	CA	B	503	1/1	0.84	0.15	-	82,82,82,82	0
6	MG	B	502	1/1	0.96	0.08	-	63,63,63,63	0
6	MG	D	502	1/1	0.92	0.08	-	46,46,46,46	0
8	GOL	C	505	6/6	0.90	0.34	-	44,53,55,63	0

## 6.5 Other polymers

There are no such residues in this entry.