



# wwPDB X-ray Structure Validation Summary Report

Jan 31, 2016 – 11:56 PM GMT

PDB ID : 1Z5V  
Title : Crystal structure of human gamma-tubulin bound to GTPgammaS  
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Deposited on : 2005-03-20  
Resolution : 2.71 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

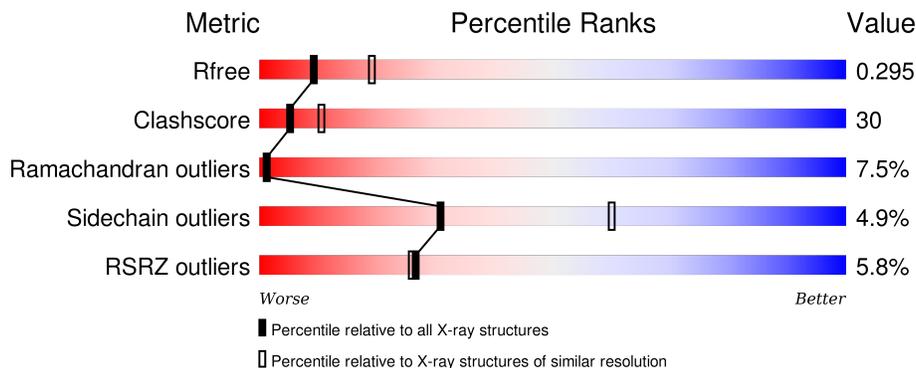
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	474	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3195 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 gamma-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	412	3141	1988	542	597	14	12	0	0

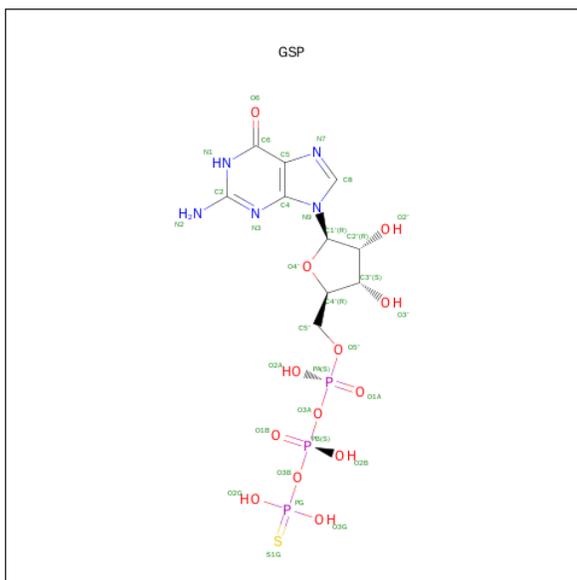
There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	450	VAL	-	CLONING ARTIFACT	UNP P23258
A	451	ASP	-	CLONING ARTIFACT	UNP P23258
A	452	VAL	-	CLONING ARTIFACT	UNP P23258
A	453	ASP	-	CLONING ARTIFACT	UNP P23258
A	454	GLY	-	CLONING ARTIFACT	UNP P23258
A	455	GLY	-	CLONING ARTIFACT	UNP P23258
A	456	GLU	-	CLONING ARTIFACT	UNP P23258
A	457	GLN	-	CLONING ARTIFACT	UNP P23258
A	458	LYS	-	CLONING ARTIFACT	UNP P23258
A	459	LEU	-	CLONING ARTIFACT	UNP P23258
A	460	ILE	-	CLONING ARTIFACT	UNP P23258
A	461	SER	-	CLONING ARTIFACT	UNP P23258
A	462	GLU	-	CLONING ARTIFACT	UNP P23258
A	463	GLU	-	CLONING ARTIFACT	UNP P23258
A	464	ASP	-	CLONING ARTIFACT	UNP P23258
A	465	LEU	-	CLONING ARTIFACT	UNP P23258
A	466	LEU	-	CLONING ARTIFACT	UNP P23258
A	467	LEU	-	CLONING ARTIFACT	UNP P23258
A	468	GLU	-	CLONING ARTIFACT	UNP P23258
A	469	HIS	-	EXPRESSION TAG	UNP P23258
A	470	HIS	-	EXPRESSION TAG	UNP P23258
A	471	HIS	-	EXPRESSION TAG	UNP P23258
A	472	HIS	-	EXPRESSION TAG	UNP P23258
A	473	HIS	-	EXPRESSION TAG	UNP P23258
A	474	HIS	-	EXPRESSION TAG	UNP P23258

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>S).



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

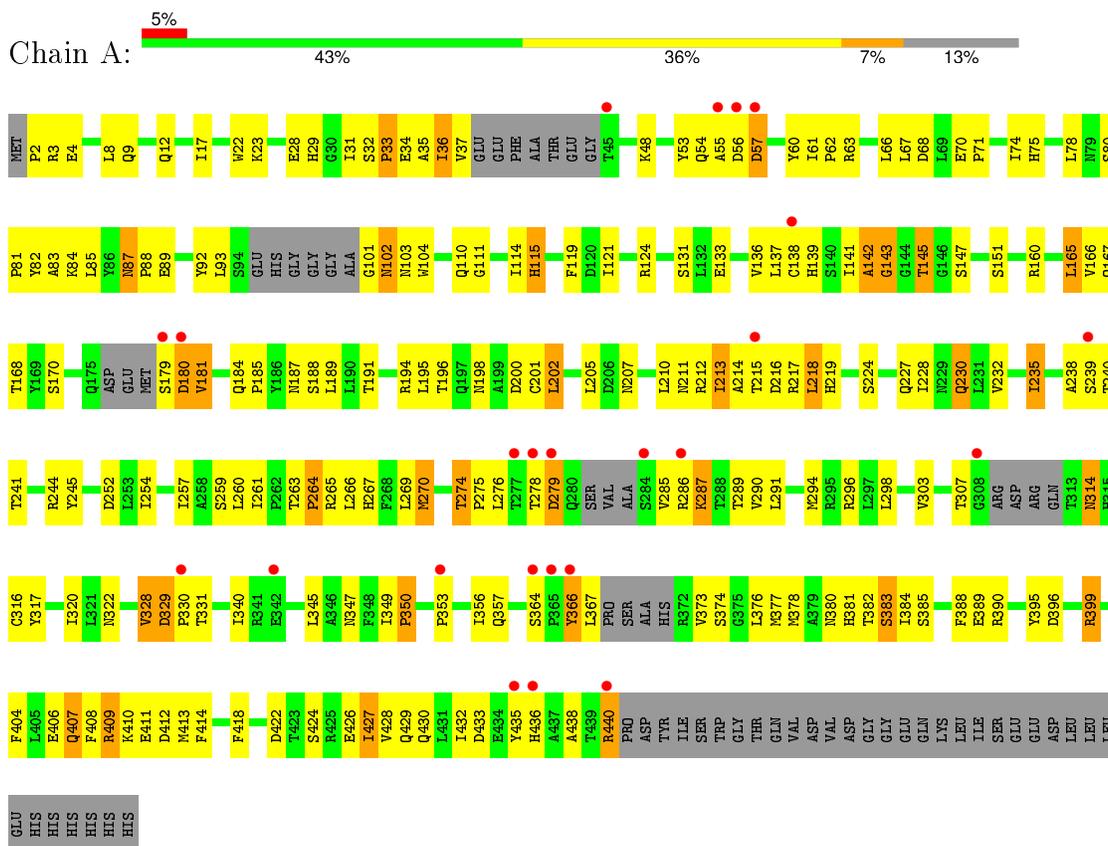
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	21	Total O 21 21	0	0

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 gamma-1 chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.43Å 76.33Å 65.20Å 90.00° 101.93° 90.00°	Depositor
Resolution (Å)	29.04 – 2.71 30.01 – 2.51	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.04-2.71) 91.1 (30.01-2.51)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.293 0.237 , 0.295	Depositor DCC
$R_{free}$ test set	1247 reflections (9.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.9	Xtrriage
Anisotropy	0.619	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 15714 reflections	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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: GSP, MG

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	0.41	0/3197	0.68	2/4347 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ALA	N-CA-C	5.29	125.29	111.00
1	A	2	PRO	N-CA-CB	5.06	109.37	103.30

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	3141	0	2988	187	0
2	A	1	0	0	0	0
3	A	32	0	12	2	0
4	A	21	0	0	2	0
All	All	3195	0	3000	187	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 30.

The worst 5 of 187 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:VAL:HG21	1:A:328:VAL:HG13	1.39	1.05
1:A:238:ALA:HB3	1:A:376:LEU:HD13	1.42	0.99
1:A:84:LYS:HE2	1:A:84:LYS:HA	1.43	0.98
1:A:254:ILE:HA	1:A:257:ILE:CG2	2.03	0.89
1:A:409:ARG:HA	1:A:413:MET:HB3	1.54	0.87

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	398/474 (84%)	329 (83%)	39 (10%)	30 (8%)	<b>1</b> <b>1</b>

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	142	ALA
1	A	180	ASP
1	A	279	ASP
1	A	407	GLN

### 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	329/421 (78%)	313 (95%)	16 (5%)	31 60

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ILE
1	A	263	THR
1	A	380	ASN
1	A	230	GLN
1	A	399	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	322	ASN
1	A	380	ASN
1	A	184	GLN
1	A	357	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GSP	A	2466	2	25,34,34	1.82	7 (28%)	31,54,54	2.89	8 (25%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GSP	A	2466	2	-	0/15/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2466	GSP	C8-N7	-2.05	1.30	1.34
3	A	2466	GSP	C2'-C3'	2.01	1.58	1.53
3	A	2466	GSP	C4-N3	2.16	1.39	1.35
3	A	2466	GSP	C6-C5	2.61	1.46	1.41
3	A	2466	GSP	C2-N1	2.79	1.40	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2466	GSP	C5-C6-N1	-9.94	109.99	123.59
3	A	2466	GSP	N3-C2-N1	-3.24	122.52	127.44
3	A	2466	GSP	C1'-N9-C4	-2.97	122.46	126.94
3	A	2466	GSP	O4'-C1'-N9	-2.93	101.95	108.10
3	A	2466	GSP	PA-O3A-PB	-2.91	124.57	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2466	GSP	2	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, 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	412/474 (86%)	0.21	24 (5%) 26 26	24, 50, 83, 93	3 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	THR	4.9
1	A	365	PRO	4.7
1	A	279	ASP	4.4
1	A	342	GLU	3.4
1	A	366	TYR	3.2

### 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, 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
3	GSP	A	2466	32/32	0.97	0.12	-1.02	27,46,59,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	475	1/1	0.88	0.18	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.