



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 08:01 AM GMT

PDB ID : 3CB2  
Title : Crystal structure of human gamma-tubulin bound to GDP  
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Deposited on : 2008-02-21  
Resolution : 2.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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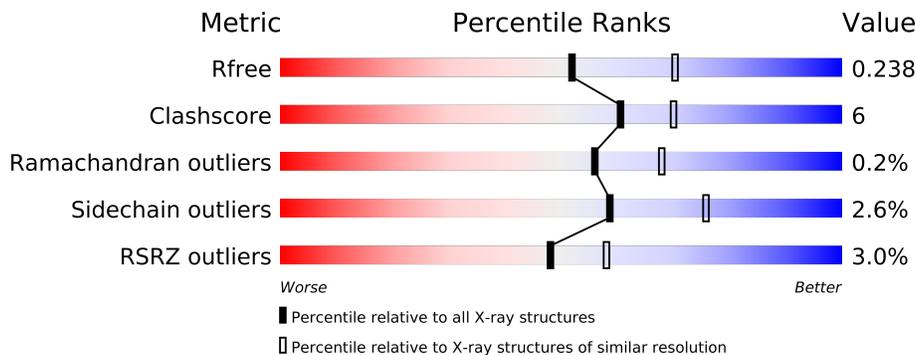
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	475	
1	B	475	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7012 atoms, of which 0 are hydrogen and 0 are deuterium.

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	432	3325	2108	567	634	16	0	0	0
1	B	424	3253	2072	560	605	16	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

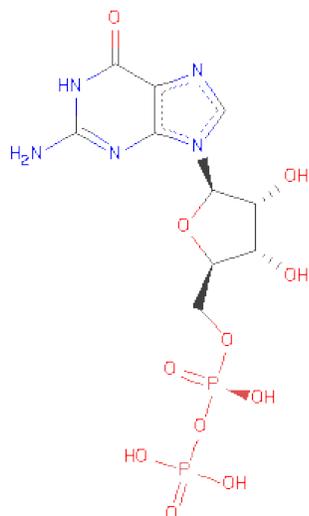
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	ALA	GLY	CONFLICT	UNP P23258
A	202	LEU	VAL	CONFLICT	UNP P23258
A	452	VAL	-	EXPRESSION TAG	UNP P23258
A	453	ASP	-	EXPRESSION TAG	UNP P23258
A	454	VAL	-	EXPRESSION TAG	UNP P23258
A	455	ASP	-	EXPRESSION TAG	UNP P23258
A	456	GLY	-	EXPRESSION TAG	UNP P23258
A	457	GLY	-	EXPRESSION TAG	UNP P23258
A	458	GLN	-	EXPRESSION TAG	UNP P23258
A	459	LYS	-	EXPRESSION TAG	UNP P23258
A	460	LEU	-	EXPRESSION TAG	UNP P23258
A	461	ILE	-	EXPRESSION TAG	UNP P23258
A	462	SER	-	EXPRESSION TAG	UNP P23258
A	463	GLU	-	EXPRESSION TAG	UNP P23258
A	464	GLU	-	EXPRESSION TAG	UNP P23258
A	465	ASP	-	EXPRESSION TAG	UNP P23258
A	466	LEU	-	EXPRESSION TAG	UNP P23258
A	467	LEU	-	EXPRESSION TAG	UNP P23258
A	468	LEU	-	EXPRESSION TAG	UNP P23258
A	469	GLU	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	475	HIS	-	EXPRESSION TAG	UNP P23258
B	35	ALA	GLY	CONFLICT	UNP P23258
B	202	LEU	VAL	CONFLICT	UNP P23258
B	452	VAL	-	EXPRESSION TAG	UNP P23258
B	453	ASP	-	EXPRESSION TAG	UNP P23258
B	454	VAL	-	EXPRESSION TAG	UNP P23258
B	455	ASP	-	EXPRESSION TAG	UNP P23258
B	456	GLY	-	EXPRESSION TAG	UNP P23258
B	457	GLY	-	EXPRESSION TAG	UNP P23258
B	458	GLN	-	EXPRESSION TAG	UNP P23258
B	459	LYS	-	EXPRESSION TAG	UNP P23258
B	460	LEU	-	EXPRESSION TAG	UNP P23258
B	461	ILE	-	EXPRESSION TAG	UNP P23258
B	462	SER	-	EXPRESSION TAG	UNP P23258
B	463	GLU	-	EXPRESSION TAG	UNP P23258
B	464	GLU	-	EXPRESSION TAG	UNP P23258
B	465	ASP	-	EXPRESSION TAG	UNP P23258
B	466	LEU	-	EXPRESSION TAG	UNP P23258
B	467	LEU	-	EXPRESSION TAG	UNP P23258
B	468	LEU	-	EXPRESSION TAG	UNP P23258
B	469	GLU	-	EXPRESSION TAG	UNP P23258
B	470	HIS	-	EXPRESSION TAG	UNP P23258
B	471	HIS	-	EXPRESSION TAG	UNP P23258
B	472	HIS	-	EXPRESSION TAG	UNP P23258
B	473	HIS	-	EXPRESSION TAG	UNP P23258
B	474	HIS	-	EXPRESSION TAG	UNP P23258
B	475	HIS	-	EXPRESSION TAG	UNP P23258

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	226	226	226	0	0
3	B	152	152	152	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.74Å 108.75Å 83.35Å 90.00° 96.33° 90.00°	Depositor
Resolution (Å)	82.76 – 2.30 46.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (82.76-2.30) 98.9 (46.49-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.97 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.187 , 0.238 0.186 , 0.238	Depositor DCC
$R_{free}$ test set	2005 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtrriage
Anisotropy	0.251	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 26.9	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 40156 reflections	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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

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	0.42	0/3393	0.57	2/4618 (0.0%)
1	B	0.39	0/3320	0.55	2/4518 (0.0%)
All	All	0.41	0/6713	0.56	4/9136 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	66	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	124	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	194	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3325	0	3160	36	0
1	B	3253	0	3100	41	0
2	A	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	28	0	12	0	0
3	A	226	0	0	5	0
3	B	152	0	0	1	0
All	All	7012	0	6284	76	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

The worst 5 of 76 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:ALA:HB2	1:A:61:ILE:HD11	1.58	0.84
1:B:202:LEU:HD23	1:B:268:PHE:CE2	2.18	0.78
1:A:90:ASN:OD1	1:A:124:ARG:NH2	2.17	0.77
1:A:35:ALA:HB1	1:A:60:TYR:O	1.87	0.75
1:A:10:LEU:HD11	1:A:153:LEU:HD12	1.69	0.73

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	424/475 (89%)	410 (97%)	14 (3%)	0	100	100
1	B	412/475 (87%)	402 (98%)	8 (2%)	2 (0%)	38	45
All	All	836/950 (88%)	812 (97%)	22 (3%)	2 (0%)	56	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	314	ASN
1	B	35	ALA

### 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	350/422 (83%)	343 (98%)	7 (2%)	68	84
1	B	339/422 (80%)	328 (97%)	11 (3%)	51	67
All	All	689/844 (82%)	671 (97%)	18 (3%)	59	76

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	66	LEU
1	B	139	HIS
1	B	360	LEU
1	A	387	LEU
1	B	43	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	B	115	HIS
1	B	322	ASN

### 5.3.3 RNA [i](#)

There are no RNA chains 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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GDP	A	500	-	30,30,30	1.46	4 (13%)	44,47,47	4.00	9 (20%)
2	GDP	B	501	-	30,30,30	1.51	5 (16%)	44,47,47	2.89	7 (15%)

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
2	GDP	A	500	-	-	0/16/32/32	0/1/3/3
2	GDP	B	501	-	-	0/16/32/32	0/1/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	GDP	C6-C5	4.45	1.48	1.41
2	A	500	GDP	C6-C5	4.44	1.48	1.41
2	B	501	GDP	C5-C4	3.02	1.47	1.40
2	A	500	GDP	C4-N9	-2.94	1.33	1.37
2	A	500	GDP	C5-C4	2.93	1.47	1.40

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	GDP	C6-C5-N7	23.88	137.35	134.14
2	B	501	GDP	C6-C5-N7	14.78	136.13	134.14
2	B	501	GDP	N3-C4-N9	5.58	135.09	126.91
2	B	501	GDP	C5-C4-N3	-5.39	118.14	125.94
2	A	500	GDP	N3-C4-N9	5.17	134.50	126.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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

### 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	432/475 (90%)	0.03	12 (2%) 50 60	10, 20, 38, 44	0
1	B	424/475 (89%)	0.21	14 (3%) 44 54	14, 28, 44, 53	0
All	All	856/950 (90%)	0.12	26 (3%) 48 58	10, 23, 41, 53	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	ASP	4.4
1	B	57	ASP	4.4
1	A	365	PRO	3.9
1	A	285	VAL	3.8
1	A	55	ALA	3.6

### 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

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GDP	B	501	28/28	0.13	0.26	17,20,26,28	0
2	GDP	A	500	28/28	0.09	-0.74	10,12,14,15	0

## 6.5 Other polymers

There are no such residues in this entry.