



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:15 AM GMT

PDB ID : 3LFV  
Title : crystal structure of unliganded PDE5A GAF domain  
Authors : Wang, H.; Robinson, H.; Ke, H.  
Deposited on : 2010-01-18  
Resolution : 2.80 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](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

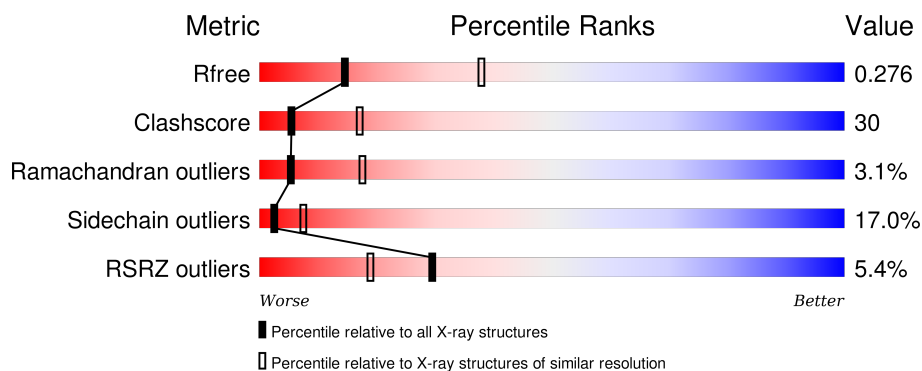
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	431	
1	B	431	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6110 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 cGMP-specific 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3097	1955	524	595	23			
1	B	380	Total	C	N	O	S	0	0	0
			3013	1903	511	576	23			

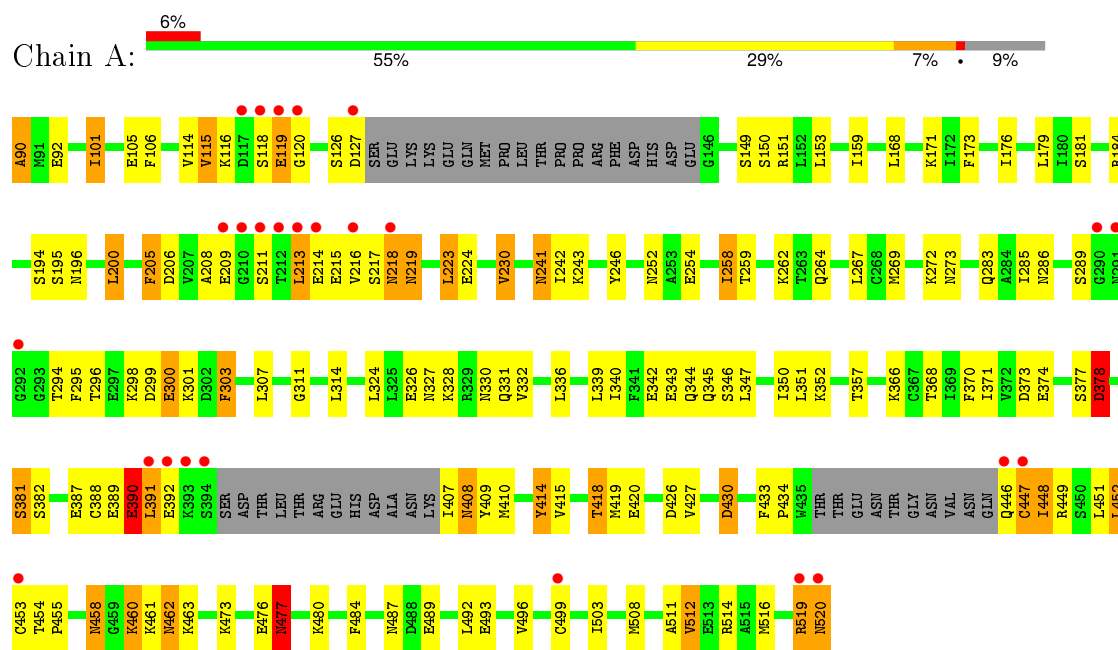
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	ALA	-	expression tag	UNP O76074
A	91	MET	-	expression tag	UNP O76074
A	92	GLU	-	expression tag	UNP O76074
A	93	HIS	-	expression tag	UNP O76074
A	94	MET	-	expression tag	UNP O76074
A	95	ALA	-	expression tag	UNP O76074
A	96	SER	-	expression tag	UNP O76074
A	97	MET	-	expression tag	UNP O76074
A	149	SER	CYS	engineered	UNP O76074
A	519	ARG	-	expression tag	UNP O76074
A	520	ASN	-	expression tag	UNP O76074
B	90	ALA	-	expression tag	UNP O76074
B	91	MET	-	expression tag	UNP O76074
B	92	GLU	-	expression tag	UNP O76074
B	93	HIS	-	expression tag	UNP O76074
B	94	MET	-	expression tag	UNP O76074
B	95	ALA	-	expression tag	UNP O76074
B	96	SER	-	expression tag	UNP O76074
B	97	MET	-	expression tag	UNP O76074
B	149	SER	CYS	engineered	UNP O76074
B	519	ARG	-	expression tag	UNP O76074
B	520	ASN	-	expression tag	UNP O76074

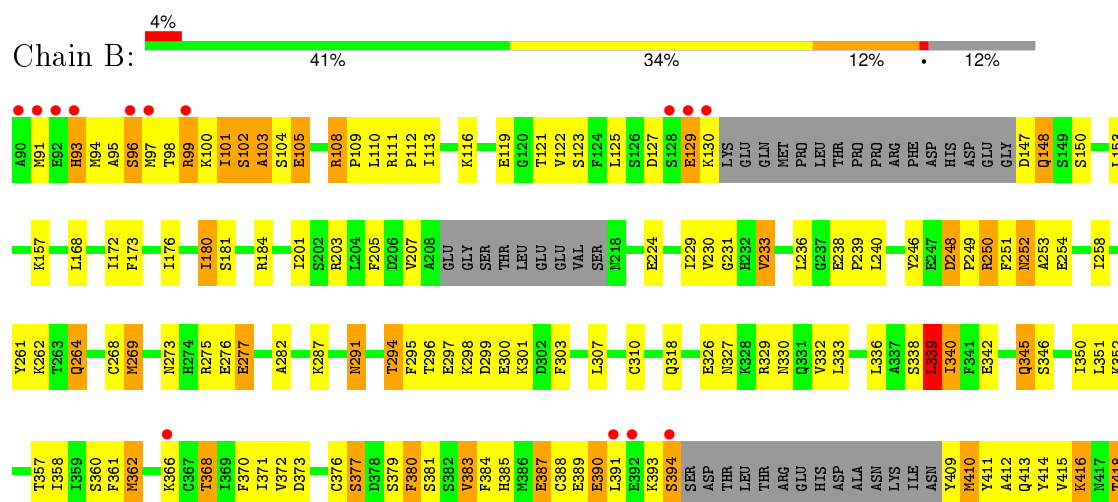
### 3 Residue-property plots

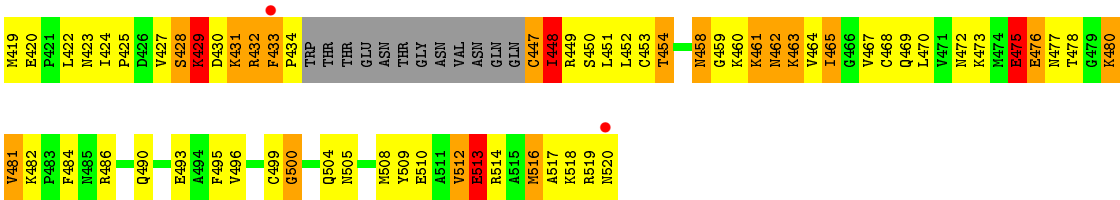
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: cGMP-specific 3',5'-cyclic phosphodiesterase



- Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.19Å 144.19Å 134.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.80) 99.2 (29.67-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.240 , 0.285 0.234 , 0.276	Depositor DCC
$R_{free}$ test set	2034 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.0	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44457 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6110	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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](#)

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	0.32	0/3145	0.42	0/4232
1	B	0.31	0/3058	0.41	0/4110
All	All	0.31	0/6203	0.42	0/8342

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	15
1	B	0	12
All	All	0	27

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	VAL	Peptide
1	A	126	SER	Peptide
1	A	213	LEU	Peptide
1	A	215	GLU	Peptide
1	A	90	ALA	Peptide

### 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	3097	0	3089	158	0
1	B	3013	0	3016	234	0
All	All	6110	0	6105	364	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 364 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:B:103:ALA:HB2	1:B:361:PHE:CE2	1.68	1.27
1:A:414:TYR:CD1	1:A:433:PHE:HZ	1.54	1.24
1:A:414:TYR:HD1	1:A:433:PHE:CZ	1.56	1.22
1:B:475:GLU:O	1:B:475:GLU:HG2	1.44	1.14
1:B:269:MET:HE3	1:B:303:PHE:HB3	1.19	1.12

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	383/431 (89%)	335 (88%)	41 (11%)	7 (2%)	11	34
1	B	370/431 (86%)	303 (82%)	51 (14%)	16 (4%)	3	10
All	All	753/862 (87%)	638 (85%)	92 (12%)	23 (3%)	5	17

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	VAL
1	A	390	GLU

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Mol	Chain	Res	Type
1	A	477	ASN
1	B	103	ALA
1	B	339	LEU

### 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	349/387 (90%)	299 (86%)	50 (14%)	4	12
1	B	340/387 (88%)	273 (80%)	67 (20%)	1	5
All	All	689/774 (89%)	572 (83%)	117 (17%)	2	7

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	GLU
1	B	236	LEU
1	B	475	GLU
1	B	119	GLU
1	B	157	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	505	ASN
1	B	196	ASN
1	B	490	GLN
1	B	148	GLN
1	B	252	ASN

### 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](#)

There are no ligands in this entry.

## 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	391/431 (90%)	0.01	26 (6%)	22 13	43, 77, 123, 156	0
1	B	380/431 (88%)	0.07	16 (4%)	40 28	48, 83, 132, 181	0
All	All	771/862 (89%)	0.04	42 (5%)	29 19	43, 79, 129, 181	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	ALA	10.3
1	B	129	GLU	7.9
1	A	213	LEU	6.5
1	B	391	LEU	6.4
1	A	212	THR	5.1

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.