



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:32 PM GMT

PDB ID : 1XP0  
Title : Catalytic Domain Of Human Phosphodiesterase 5A In Complex With Vardenafil  
Authors : Card, G.L.; England, B.P.; Suzuki, Y.; Fong, D.; Powell, B.; Lee, B.; Luu, C.; Tabrizizad, M.; Gillette, S.; Ibrahim, P.N.; Artis, D.R.; Bollag, G.; Milburn, M.V.; Kim, S.-H.; Schlessinger, J.; Zhang, K.Y.J.  
Deposited on : 2004-10-07  
Resolution : 1.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

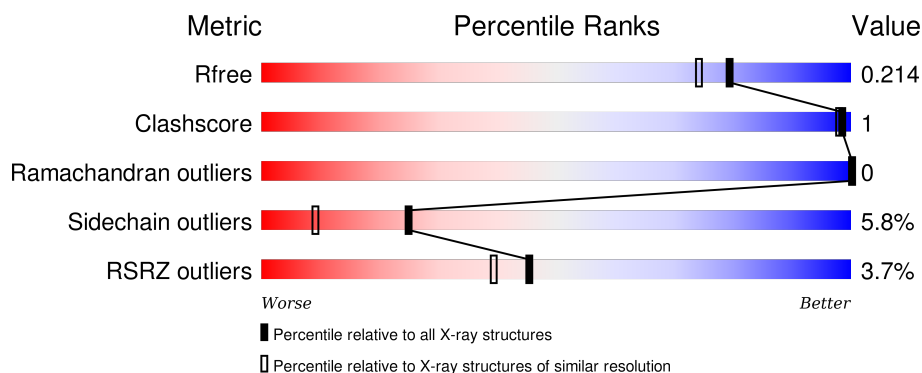
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	364	

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
3	MG	A	2	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2829 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	326	Total	C	N	O	S	0	0	0
			2637	1678	451	491	17			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	513	MET	-	INITIATING METHIONINE	UNP O76074
A	514	GLY	-	CLONING ARTIFACT	UNP O76074
A	515	SER	-	CLONING ARTIFACT	UNP O76074
A	516	SER	-	CLONING ARTIFACT	UNP O76074
A	517	HIS	-	EXPRESSION TAG	UNP O76074
A	518	HIS	-	EXPRESSION TAG	UNP O76074
A	519	HIS	-	EXPRESSION TAG	UNP O76074
A	520	HIS	-	EXPRESSION TAG	UNP O76074
A	521	HIS	-	EXPRESSION TAG	UNP O76074
A	522	HIS	-	EXPRESSION TAG	UNP O76074
A	523	SER	-	CLONING ARTIFACT	UNP O76074
A	524	SER	-	CLONING ARTIFACT	UNP O76074
A	525	GLY	-	CLONING ARTIFACT	UNP O76074
A	526	LEU	-	CLONING ARTIFACT	UNP O76074
A	527	VAL	-	CLONING ARTIFACT	UNP O76074
A	528	PRO	-	CLONING ARTIFACT	UNP O76074
A	529	ARG	-	CLONING ARTIFACT	UNP O76074
A	530	GLY	-	CLONING ARTIFACT	UNP O76074
A	531	SER	-	CLONING ARTIFACT	UNP O76074
A	532	HIS	-	CLONING ARTIFACT	UNP O76074
A	533	MET	-	CLONING ARTIFACT	UNP O76074
A	658	PRO	ARG	ENGINEERED	UNP O76074
A	661	SER	ASN	ENGINEERED	UNP O76074
A	663	GLN	ASN	ENGINEERED	UNP O76074
A	647	LEU	SER	ENGINEERED	UNP O76074
A	648	ILE	TYR	ENGINEERED	UNP O76074
A	667	ASN	ARG	ENGINEERED	UNP O76074

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Chain	Residue	Modelled	Actual	Comment	Reference
A	668	THR	SER	ENGINEERED	UNP O76074
A	669	ASN	GLU	ENGINEERED	UNP O76074
A	670	SER	HIS	ENGINEERED	UNP O76074
A	671	GLU	PRO	ENGINEERED	UNP O76074
A	674	LEU	GLN	ENGINEERED	UNP O76074
A	675	MET	LEU	ENGINEERED	UNP O76074
A	676A	ASN	CYS	ENGINEERED	UNP O76074
A	677	ASP	-	ENGINEERED	UNP O76074
A	678	GLU	HIS	ENGINEERED	UNP O76074
A	680	VAL	ILE	ENGINEERED	UNP O76074
A	681	LEU	MET	ENGINEERED	UNP O76074

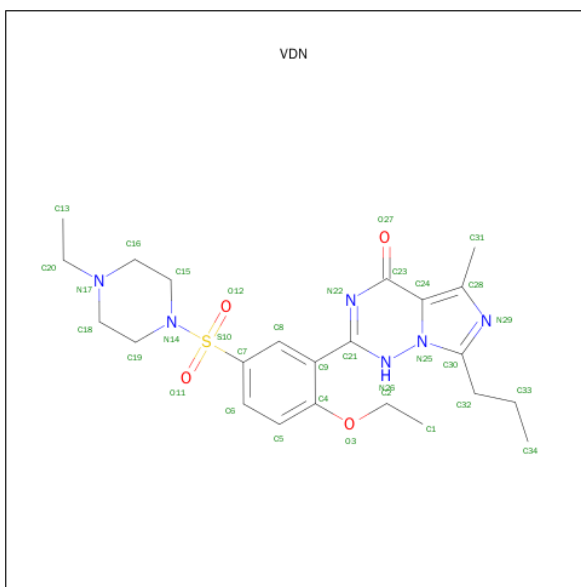
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 2-{2-ETHOXY-5-[(4-ETHYLPIPERAZIN-1-YL)SULFONYL]PHENYL}-5-METHYL-7-PROPYLIMIDAZO[5,1-F][1,2,4]TRIAZIN-4(1H)-ONE (three-letter code: VDN) (formula: C<sub>23</sub>H<sub>32</sub>N<sub>6</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	23	6	4	1		

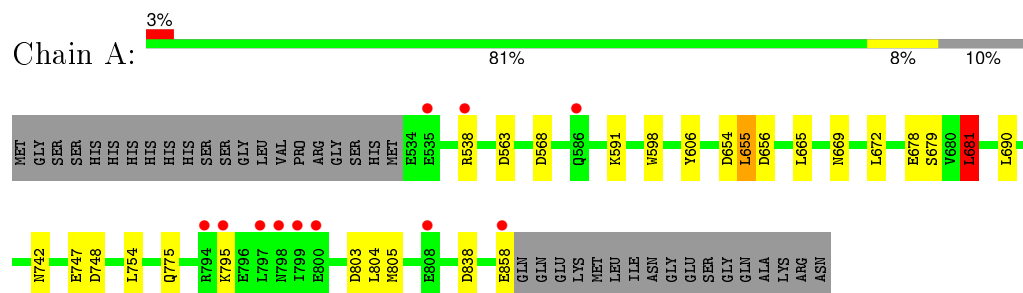
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	156	Total	O	0	0
			156	156		

### 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 ( $\text{RSRZ} > 2$ ). 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.66 Å 89.66 Å 222.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.70 – 1.79 73.30 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.2 (76.70-1.79) 95.7 (73.30-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.193 , 0.208 0.202 , 0.214	Depositor DCC
$R_{free}$ test set	2521 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 56382 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: ZN, MG, VDN

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	0.46	0/2686	0.74	8/3629 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	656	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	563	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	568	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	748	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	681	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	838	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	654	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	803	ASP	CB-CG-OD2	5.04	122.84	118.30

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	2637	0	2643	5	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	34	0	32	0	0
5	A	156	0	0	0	0
All	All	2829	0	2675	5	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 1.

All (5) 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:598:TRP:HA	1:A:698:ASN:HD22	1.74	0.52
1:A:665:LEU:HD11	1:A:681:LEU:HD13	1.92	0.50
1:A:678:GLU:O	1:A:679:SER:C	2.53	0.47
1:A:606:TYR:CE1	1:A:655:LEU:HD13	2.50	0.47
1:A:665:LEU:CD1	1:A:681:LEU:HD13	2.50	0.42

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	324/364 (89%)	320 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	291/323 (90%)	274 (94%)	17 (6%)	25 9

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	ARG
1	A	591	LYS
1	A	655	LEU
1	A	669	ASN
1	A	672	LEU
1	A	681	LEU
1	A	690	LEU
1	A	704	LEU
1	A	707	GLU
1	A	742	ASN
1	A	747	GLU
1	A	754	LEU
1	A	775	GLN
1	A	795	LYS
1	A	804	LEU
1	A	805	MET
1	A	858	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	635	GLN
1	A	694	ASN
1	A	698	ASN
1	A	718	GLN
1	A	811	ASN
1	A	817	GLN

### 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 3 ligands modelled in this entry, 2 are 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$
4	VDN	A	201	-	31,37,37	2.48	4 (12%)	36,54,54	3.64	16 (44%)

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	VDN	A	201	-	-	0/24/34/34	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	201	VDN	C7-S10	-10.44	1.61	1.76
4	A	201	VDN	S10-N14	-6.62	1.53	1.63
4	A	201	VDN	C23-C24	3.35	1.48	1.41
4	A	201	VDN	C21-N22	4.54	1.44	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	201	VDN	N26-C21-N22	-10.09	116.23	125.14
4	A	201	VDN	C24-C23-N22	-6.45	114.77	123.59
4	A	201	VDN	O12-S10-O11	-5.63	109.75	119.47
4	A	201	VDN	C15-C16-N17	-2.63	105.92	110.63
4	A	201	VDN	C16-N17-C20	2.20	115.97	110.83
4	A	201	VDN	O12-S10-N14	2.24	108.90	106.69
4	A	201	VDN	C30-N29-C28	2.27	109.95	104.88
4	A	201	VDN	C8-C9-C4	2.45	120.98	118.00
4	A	201	VDN	C2-O3-C4	2.68	123.02	118.01
4	A	201	VDN	O11-S10-C7	3.02	111.92	108.00
4	A	201	VDN	C18-N17-C20	3.16	118.21	110.83
4	A	201	VDN	C7-S10-N14	3.76	111.95	107.32
4	A	201	VDN	C16-C15-N14	4.28	112.49	109.02
4	A	201	VDN	C18-C19-N14	6.22	114.07	109.02
4	A	201	VDN	C23-N22-C21	7.34	123.45	116.23
4	A	201	VDN	C19-N14-C15	10.14	124.52	112.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	326/364 (89%)	0.08	12 (3%) 45 39	13, 20, 36, 47	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	795	LYS	3.9
1	A	808	GLU	3.7
1	A	799	ILE	3.3
1	A	538	ARG	3.0
1	A	858	GLU	2.9
1	A	800	GLU	2.8
1	A	798	ASN	2.8
1	A	535	GLU	2.8
1	A	794	ARG	2.5
1	A	707	GLU	2.1
1	A	797	LEU	2.1
1	A	586	GLN	2.1

### 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](#)

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	MG	A	2	1/1	0.95	0.17	6.02	24,24,24,24	0
4	VDN	A	201	34/34	0.95	0.11	0.86	32,40,57,60	0
2	ZN	A	1	1/1	0.98	0.07	-1.86	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.