



wwPDB X-ray Structure Validation Summary Report

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PDB ID : 1UDU
Title : Crystal structure of Human Phosphodiesterase 5 complexed with tadalafil(Cialis)
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Deposited on : 2003-05-06
Resolution : 2.83 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the  symbol.

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

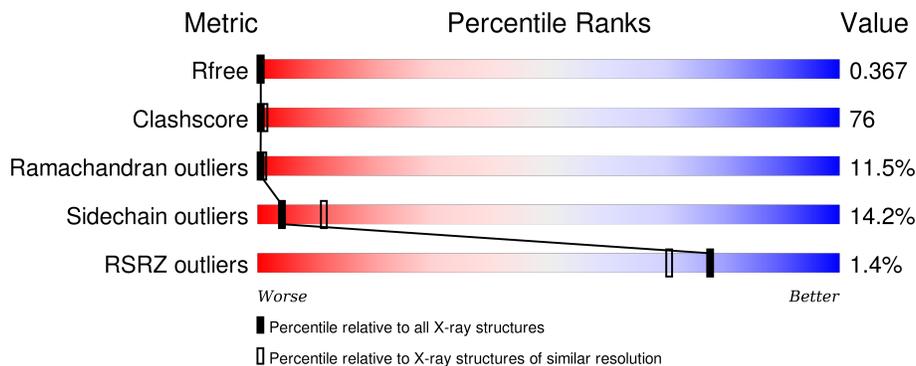
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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 ≥ 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	324	 17% 60% 18% . .
1	B	324	 18% 61% 18% . .

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	1002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5146 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
			Total	C	N	O	S			
1	A	313	2542	1617	442	465	18	0	0	0
1	B	313	2542	1617	442	465	18	0	0	0

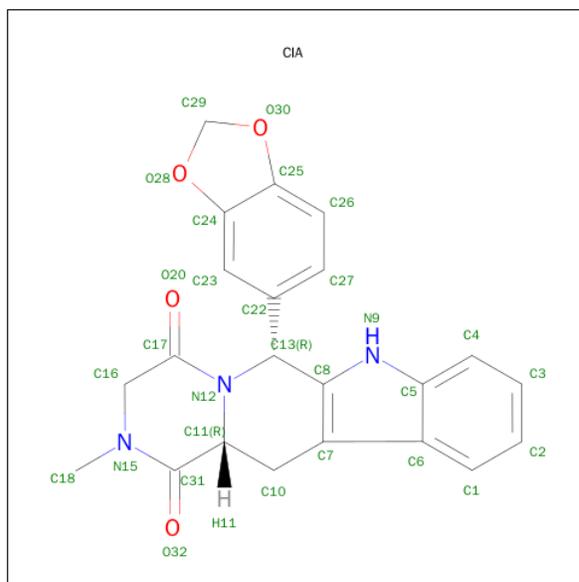
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is 6-BENZO[1,3]DIOXOL-5-YL-2-METHYL-2,3,6,7,12,12A-HEXAHYDRO-PYRAZINO[1',2':1,6]PYRIDO[3,4-B]INDOLE-1,4-DIONE (three-letter code: CIA) (formula: C₂₂H₁₉N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	29	22	3	4	0	0
4	B	1	29	22	3	4	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.35Å 48.56Å 123.86Å 90.00° 117.28° 90.00°	Depositor
Resolution (Å)	19.59 – 2.83 20.13 – 2.83	Depositor EDS
% Data completeness (in resolution range)	71.5 (19.59-2.83) 71.6 (20.13-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.83Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.374 0.260 , 0.367	Depositor DCC
R_{free} test set	624 reflections (5.16%)	DCC
Wilson B-factor (Å ²)	36.6	Xtrriage
Anisotropy	1.008	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.4	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtrriage
Outliers	2 of 13432 reflections (0.015%)	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5146	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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, CIA

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	0/2590	0.74	0/3493
1	B	0.49	0/2590	0.74	0/3493
All	All	0.47	0/5180	0.74	0/6986

There are no bond length outliers.

There are no bond angle outliers.

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	2542	0	2552	395	0
1	B	2542	0	2552	397	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	29	0	19	8	0
4	B	29	0	19	1	0
All	All	5146	0	5142	778	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 76.

The worst 5 of 778 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:653:HIS:HA	1:A:720:ILE:HG23	1.26	1.14
1:B:653:HIS:HA	1:B:720:ILE:HG23	1.26	1.11
1:A:801:PRO:HB2	1:A:806:ASN:HB3	1.34	1.07
1:B:725:LEU:O	1:B:729:ILE:HG13	1.58	1.04
1:B:679:SER:HB3	1:B:682:GLU:HG3	1.39	1.02

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	309/324 (95%)	194 (63%)	78 (25%)	37 (12%)	0	1
1	B	309/324 (95%)	196 (63%)	79 (26%)	34 (11%)	0	1
All	All	618/648 (95%)	390 (63%)	157 (25%)	71 (12%)	0	1

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	549	PRO
1	A	564	PHE
1	A	631	ALA
1	A	693	LEU
1	A	732	ARG

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	279/289 (96%)	239 (86%)	40 (14%)	4	11
1	B	279/289 (96%)	240 (86%)	39 (14%)	4	12
All	All	558/578 (96%)	479 (86%)	79 (14%)	4	11

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	828	LEU
1	B	569	LEU
1	B	822	ASP
1	A	833	THR
1	B	543	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	849	ASN
1	B	587	ASN
1	B	775	GLN
1	B	583	ASN
1	B	592	HIS

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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	CIA	A	1003	-	33,34,34	4.61	21 (63%)	38,52,52	1.49	6 (15%)
4	CIA	B	2003	-	33,34,34	4.22	22 (66%)	38,52,52	1.22	3 (7%)

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	CIA	A	1003	-	-	0/4/42/42	0/6/6/6
4	CIA	B	2003	-	-	0/4/42/42	0/6/6/6

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2003	CIA	O32-C31	2.09	1.26	1.22
4	A	1003	CIA	C6-C5	2.10	1.48	1.42
4	B	2003	CIA	C6-C5	2.10	1.48	1.42
4	B	2003	CIA	C1-C6	2.42	1.47	1.42
4	B	2003	CIA	C16-C17	2.46	1.55	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	CIA	C22-C13-C8	-4.55	104.73	112.62
4	B	2003	CIA	C22-C13-C8	-3.11	107.23	112.62
4	A	1003	CIA	O20-C17-C16	-2.15	114.63	118.70
4	A	1003	CIA	C22-C13-N12	2.30	114.77	112.54
4	A	1003	CIA	O20-C17-N12	2.33	125.57	122.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	CIA	8	0
4	B	2003	CIA	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, 95th 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 ²)	Q<0.9
1	A	313/324 (96%)	-0.23	4 (1%) 79 72	13, 47, 78, 104	0
1	B	313/324 (96%)	-0.19	5 (1%) 74 67	10, 47, 83, 97	0
All	All	626/648 (96%)	-0.21	9 (1%) 78 71	10, 47, 81, 104	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	676	TYR	3.1
1	A	664	TYR	2.9
1	B	608	LYS	2.5
1	B	676	TYR	2.4
1	B	748	ASP	2.3

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, 95th 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(\AA^2)	Q<0.9
3	MG	A	1002	1/1	0.94	0.38	9.15	36,36,36,36	0
4	CIA	B	2003	29/29	0.93	0.19	0.43	9,49,77,105	0
4	CIA	A	1003	29/29	0.93	0.18	-0.13	15,59,81,83	0
3	MG	B	2002	1/1	0.93	0.14	-	15,15,15,15	0
2	ZN	A	1001	1/1	0.93	0.34	-	105,105,105,105	0
2	ZN	B	2001	1/1	0.81	0.30	-	105,105,105,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.