



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:17 AM GMT

PDB ID : 1TBF
Title : Catalytic Domain Of Human Phosphodiesterase 5A in Complex with Sildenafil
Authors : Zhang, K.Y.J.; Card, G.L.; Suzuki, Y.; Artis, D.R.; Fong, D.; Gillette, S.;
Hsieh, D.; Neiman, J.; West, B.L.; Zhang, C.; Milburn, M.V.; Kim, S.-H.;
Schlessinger, J.; Bollag, G.
Deposited on : 2004-05-20
Resolution : 1.30 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

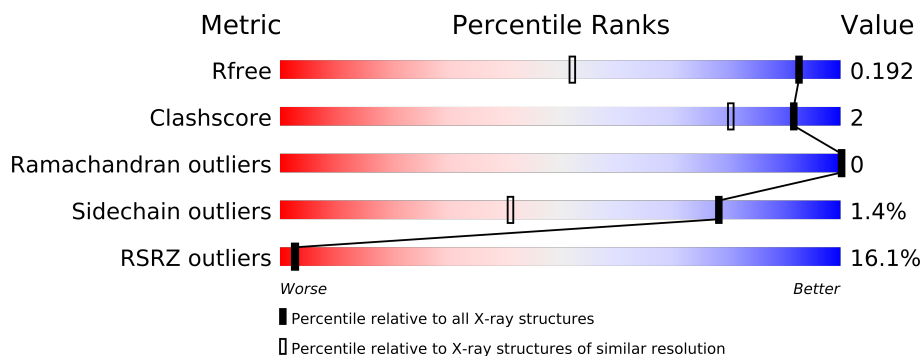
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.30 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	1025 (1.34-1.26)
Clashscore	79885	1140 (1.34-1.26)
Ramachandran outliers	78287	1093 (1.34-1.26)
Sidechain outliers	78261	1092 (1.34-1.26)
RSRZ outliers	66119	1025 (1.34-1.26)

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. 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	347	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3021 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 cGMP-specific 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	7	0
			2657	1689	455	493	20			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	513	MET	-	EXPRESSION TAG	UNP O76074
A	514	GLY	-	EXPRESSION TAG	UNP O76074
A	515	SER	-	EXPRESSION TAG	UNP O76074
A	516	SER	-	EXPRESSION TAG	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	-	EXPRESSION TAG	UNP O76074
A	524	SER	-	EXPRESSION TAG	UNP O76074
A	525	GLY	-	EXPRESSION TAG	UNP O76074
A	526	LEU	-	EXPRESSION TAG	UNP O76074
A	527	VAL	-	EXPRESSION TAG	UNP O76074
A	528	PRO	-	EXPRESSION TAG	UNP O76074
A	529	ARG	-	EXPRESSION TAG	UNP O76074
A	530	GLY	-	EXPRESSION TAG	UNP O76074
A	531	SER	-	EXPRESSION TAG	UNP O76074
A	532	HIS	-	EXPRESSION TAG	UNP O76074
A	533	MET	-	EXPRESSION TAG	UNP O76074
A	658	PRO	ARG	ENGINEERED	UNP O76074
A	661	SER	ASN	ENGINEERED	UNP O76074
A	663	GLN	SER	ENGINEERED	UNP O76074
A	664	PHE	TYR	ENGINEERED	UNP O76074
A	665	LEU	ILE	ENGINEERED	UNP O76074
A	666	ILE	GLN	ENGINEERED	UNP O76074

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Chain	Residue	Modelled	Actual	Comment	Reference
A	667	ASN	ARG	ENGINEERED	UNP O76074
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

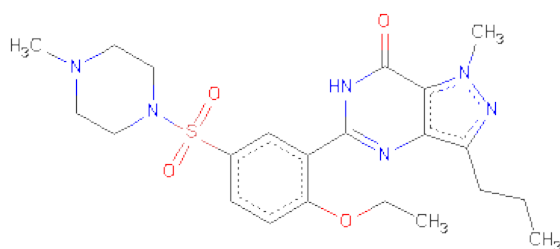
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

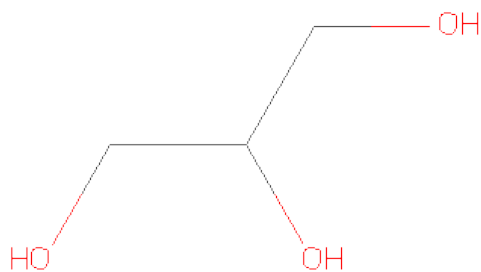
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is 5-{2-ETHOXY-5-[(4-METHYLPIPERAZIN-1-YL)SULFONYL]PHENYL}-1-METHYL-3-PROPYL-1H,6H,7H-PYRAZOLO[4,3-D]PYRIMIDIN-7-ONE (three-letter code: VIA) (formula: C₂₂H₃₀N₆O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	33	22	6	4	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	6	3	3	0	0

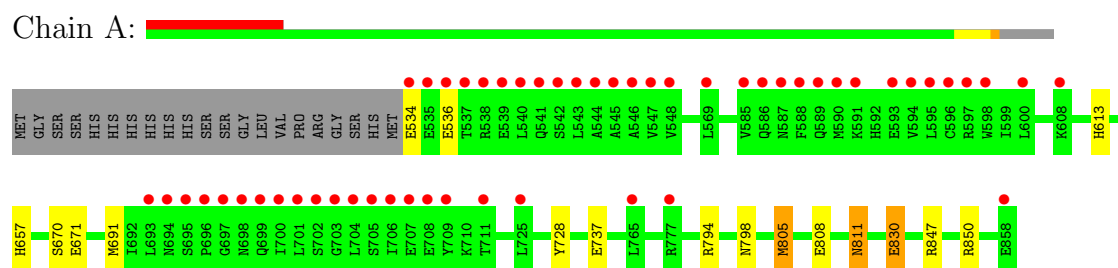
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	323	Total 323	O 323	0	0

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.10Å 76.10Å 99.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.94 – 1.30 65.90 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (65.94-1.30) 99.2 (65.90-1.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.157 , 0.185 0.170 , 0.192	Depositor DCC
R_{free} test set	4089 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 40.2	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 81465 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3021	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, VIA, 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	1.08	7/2743 (0.3%)	1.03	4/3703 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	830	GLU	CD-OE2	-6.99	1.18	1.25
1	A	670[A]	SER	CB-OG	-6.59	1.33	1.42
1	A	670[B]	SER	CB-OG	-6.59	1.33	1.42
1	A	798	ASN	CB-CG	-6.30	1.36	1.51
1	A	728	TYR	CE1-CZ	-5.88	1.30	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	805[A]	MET	CA-CB-CG	8.65	128.01	113.30
1	A	805[B]	MET	CA-CB-CG	8.65	128.01	113.30
1	A	850	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	A	794	ARG	CB-CA-C	5.64	121.68	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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	2657	0	0	5	2
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	33	0	0	0	0
5	A	6	0	0	0	0
6	A	323	0	0	3	3
All	All	3021	0	0	5	3

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 2.

All (5) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:671:GLU:OE1	6:A:1122:HOH:O	1.91	0.86
1:A:830:GLU:OE1	6:A:900:HOH:O	2.05	0.75
1:A:534:GLU:OE2	1:A:536:GLU:OE2	2.09	0.68
1:A:811:ASN:ND2	6:A:913:HOH:O	2.39	0.56
1:A:613:HIS:CB	1:A:657:HIS:CD2	2.99	0.46

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:847[A]:ARG:NH2	6:A:908:HOH:O[2_655]	1.13	1.07
6:A:908:HOH:O	6:A:984:HOH:O[3_664]	2.00	0.20
1:A:847[A]:ARG:CZ	6:A:908:HOH:O[2_655]	2.01	0.19

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	331/347 (95%)	329 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	298/309 (96%)	292 (98%)	6 (2%)	68 23

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	737	GLU
1	A	811	ASN
1	A	805[A]	MET
1	A	691[B]	MET
1	A	805[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 4 ligands modelled in this entry, 2 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	VIA	A	501	-	36,36,36	1.76	9 (25%)	49,53,53	2.45	18 (36%)
5	GOL	A	502	-	5,5,5	0.32	0	5,5,5	0.54	0

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	VIA	A	501	-	-	0/22/32/32	0/2/4/4
5	GOL	A	502	-	-	0/4/4/4	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	VIA	O11-S10	-5.19	1.37	1.43
4	A	501	VIA	C15-N14	-3.31	1.44	1.47
4	A	501	VIA	C19-N14	-2.80	1.44	1.47
4	A	501	VIA	C21-N22	2.76	1.39	1.34
4	A	501	VIA	O12-S10	-2.73	1.40	1.43

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	VIA	C30-N29-N28	7.44	110.90	104.48
4	A	501	VIA	C18-C19-N14	6.00	113.77	109.02
4	A	501	VIA	C19-N14-S10	4.00	124.28	117.00
4	A	501	VIA	N22-C21-N26	3.96	127.03	122.70
4	A	501	VIA	C21-N26-C25	-3.82	112.21	116.33

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, 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	326/347 (93%)	1.08	53 (16%) 2 3	4, 10, 19, 33	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	LEU	8.9
1	A	541	GLN	8.8
1	A	538	ARG	7.8
1	A	545	ALA	6.9
1	A	535	GLU	6.8

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	VIA	A	501	33/33	0.17	-	12,17,40,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	502	6/6	0.15	-	19,24,25,30	0
3	MG	A	2	1/1	0.21	-	11,11,11,11	0
2	ZN	A	1	1/1	0.17	-	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.