



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:33 AM GMT

PDB ID : 4AJF  
Title : Identification and structural characterization of PDE10 fragment inhibitors  
Authors : Johansson, P.; Albert, J.S.; Spadola, L.; Akerud, T.; Back, E.; Hillertz, P.;  
Horsefeld, R.; Scott, C.; Spear, N.; Tian, G.; Tigerstrom, A.; Aharony, D.;  
Geschwindner, S.  
Deposited on : 2012-02-16  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

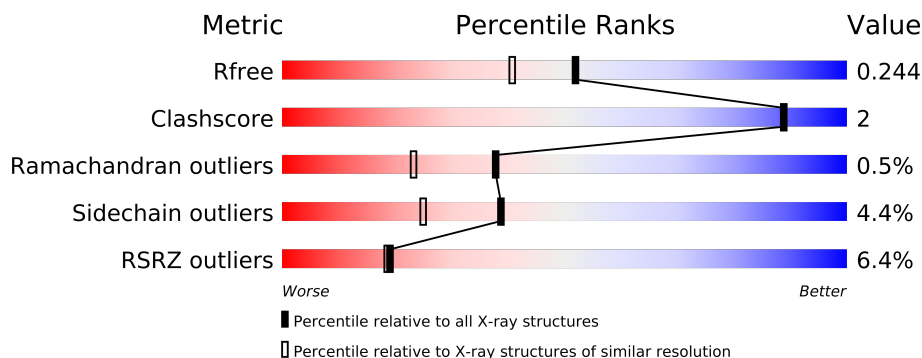
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	328	
1	D	328	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5666 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 CAMP AND CAMP-INHIBITED CGMP 3', 5'-CYCLIC PHOSPHODIESTERASE 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2654	1694	451	485	24			
1	D	324	Total	C	N	O	S	0	0	0
			2624	1674	446	480	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	ASN	-	EXPRESSION TAG	UNP Q9Y233
A	448	ALA	-	EXPRESSION TAG	UNP Q9Y233
D	447	ASN	-	EXPRESSION TAG	UNP Q9Y233
D	448	ALA	-	EXPRESSION TAG	UNP Q9Y233

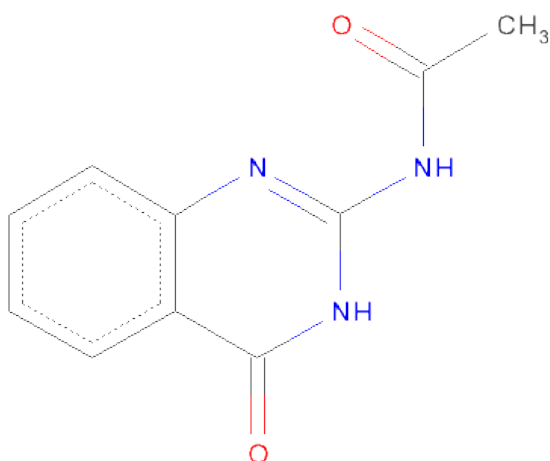
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is N-(4-OXO-3H-QUINAZOLIN-2-YL)ACETAMIDE (three-letter code: F03) (formula: C<sub>10</sub>H<sub>9</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	10	3	2		

- Molecule 5 is water.

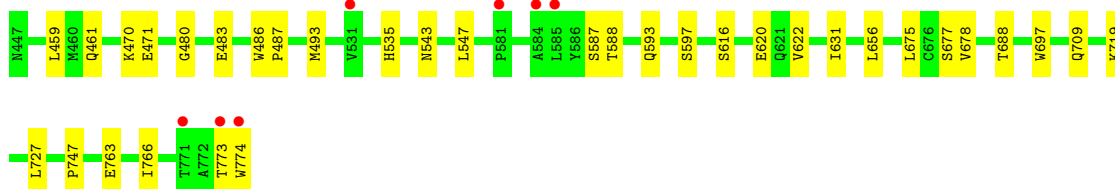
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	217	Total	O	0	0
			217	217		
5	D	152	Total	O	0	0
			152	152		

### 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.

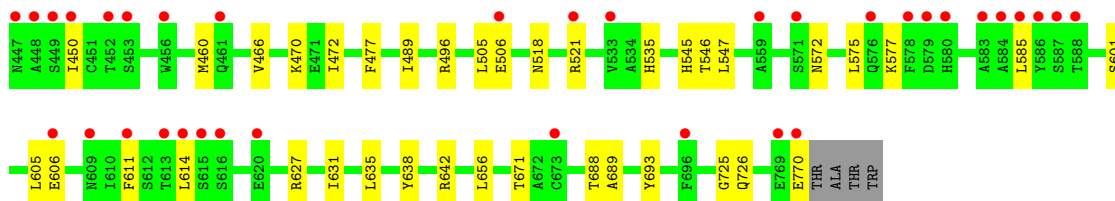
- Molecule 1: CAMP AND CAMP-INHIBITED CGMP 3', 5'-CYCLIC PHOSPHODIESTERASE 10A

Chain A: 



- Molecule 1: CAMP AND CAMP-INHIBITED CGMP 3', 5'-CYCLIC PHOSPHODIESTERASE 10A

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.37Å 81.80Å 156.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.25 – 1.90 29.25 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.25-1.90) 99.5 (29.25-1.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 1.91Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, $R_{free}$	0.213 , 0.248 0.207 , 0.244	Depositor DCC
$R_{free}$ test set	2563 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50627 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: MG, ZN, F03

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	0.52	0/2719	0.62	0/3683
1	D	0.50	0/2688	0.65	0/3640
All	All	0.51	0/5407	0.63	0/7323

There are no bond length outliers.

There are no bond angle outliers.

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	2654	0	2607	12	0
1	D	2624	0	2583	12	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	9	0	0
5	A	217	0	0	0	0
5	D	152	0	0	1	0
All	All	5666	0	5199	24	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 2.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:450:ILE:HG22	1:D:605:LEU:HD13	1.84	0.59
1:D:472:ILE:HD11	1:D:489:ILE:HG23	1.89	0.55
1:A:727:LEU:HD11	1:A:763:GLU:HG3	1.89	0.53
1:D:496:ARG:NH2	5:D:2031:HOH:O	2.34	0.50
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.49	0.48
1:A:459:LEU:HD13	1:A:487:PRO:HB2	1.96	0.48
1:A:727:LEU:HD13	1:A:766:ILE:HD12	1.95	0.47
1:D:506:GLU:H	1:D:506:GLU:CD	2.18	0.47
1:D:693:TYR:OH	1:D:725:GLY:HA3	2.15	0.46
1:D:572:ASN:HA	1:D:575:LEU:HD12	1.98	0.44
1:D:460:MET:HG2	1:D:505:LEU:HG	2.00	0.44
1:D:627:ARG:O	1:D:631:ILE:HG12	2.17	0.44
1:A:697:TRP:CZ2	1:A:719:LYS:HG2	2.53	0.43
1:D:689:ALA:O	1:D:726:GLN:NE2	2.52	0.43
1:A:727:LEU:HD11	1:A:763:GLU:CG	2.49	0.42
1:A:675:LEU:O	1:A:678:VAL:HG22	2.19	0.42
1:D:638:TYR:CD1	1:D:671:THR:HG21	2.54	0.42
1:A:593:GLN:HG2	1:A:631:ILE:HD11	2.03	0.41
1:A:547:LEU:HD22	1:A:656:LEU:HD22	2.02	0.41
1:D:611:PHE:HB3	1:D:614:LEU:HD12	2.03	0.41
1:D:477:PHE:HB3	1:D:535:HIS:CE1	2.55	0.41
1:A:677:SER:OG	1:A:688:THR:HG21	2.22	0.40
1:A:493:MET:SD	1:A:535:HIS:HA	2.61	0.40
1:A:543:ASN:HB3	1:A:747:PRO:HB2	2.04	0.40

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	325/328 (99%)	318 (98%)	6 (2%)	1 (0%)	50 37

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	322/328 (98%)	310 (96%)	10 (3%)	2 (1%)	33	19
All	All	647/656 (99%)	628 (97%)	16 (2%)	3 (0%)	38	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	577	LYS
1	D	518	ASN
1	A	480	GLY

### 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	294/295 (100%)	282 (96%)	12 (4%)	41	28
1	D	292/295 (99%)	278 (95%)	14 (5%)	35	21
All	All	586/590 (99%)	560 (96%)	26 (4%)	39	25

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	470	LYS
1	A	471	GLU
1	A	587	SER
1	A	588	THR
1	A	597	SER
1	A	616	SER
1	A	620	GLU
1	A	622	VAL
1	A	709	GLN
1	A	773	THR
1	A	774	TRP
1	D	466	VAL
1	D	470	LYS
1	D	521	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	545	HIS
1	D	546	THR
1	D	547	LEU
1	D	585	LEU
1	D	601	SER
1	D	606	GLU
1	D	635	LEU
1	D	642	ARG
1	D	656	LEU
1	D	688	THR
1	D	770	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	598	GLN
1	A	743	GLN
1	D	709	GLN
1	D	724	GLN
1	D	743	GLN
1	D	761	GLN

### 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 5 ligands modelled in this entry, 4 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	F03	A	1777	-	16,16,16	1.52	3 (18%)	20,22,22	1.50	4 (20%)

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	F03	A	1777	-	-	0/4/4/4	0/0/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1777	F03	C12-C13	3.51	1.44	1.36
4	A	1777	F03	C9-C14	-2.56	1.39	1.45
4	A	1777	F03	C7-C9	2.54	1.49	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1777	F03	C10-C9-C14	3.65	122.05	118.32
4	A	1777	F03	C1-C2-N4	-2.55	110.75	114.93
4	A	1777	F03	C5-N4-C2	-2.34	126.68	130.39
4	A	1777	F03	O3-C2-N4	2.01	126.44	123.08

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	328/328 (100%)	0.13	7 (2%) 60 62	20, 34, 61, 72	3 (0%)
1	D	324/328 (98%)	0.66	35 (10%) 6 5	22, 43, 73, 93	3 (0%)
All	All	652/656 (99%)	0.39	42 (6%) 19 18	20, 38, 70, 93	6 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	448	ALA	6.5
1	D	450	ILE	5.5
1	D	584	ALA	5.0
1	D	452	THR	4.7
1	A	584	ALA	4.2
1	A	771	THR	3.8
1	D	447	ASN	3.7
1	D	585	LEU	3.7
1	D	616	SER	3.7
1	D	579	ASP	3.6
1	D	456	TRP	3.5
1	D	586	TYR	3.4
1	D	449	SER	3.4
1	A	774	TRP	3.1
1	D	583	ALA	3.0
1	D	521	ARG	2.9
1	D	606	GLU	2.9
1	D	769	GLU	2.8
1	D	559	ALA	2.7
1	D	696	PHE	2.6
1	D	673	CYS	2.5
1	A	581	PRO	2.5
1	D	613	THR	2.4
1	D	587	SER	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	588	THR	2.4
1	D	614	LEU	2.3
1	A	585	LEU	2.3
1	D	576	GLN	2.3
1	D	580	HIS	2.3
1	A	773	THR	2.2
1	D	571	SER	2.2
1	D	453	SER	2.2
1	D	506	GLU	2.1
1	D	611	PHE	2.1
1	D	615	SER	2.1
1	A	531	VAL	2.1
1	D	770	GLU	2.1
1	D	461	GLN	2.1
1	D	609	ASN	2.1
1	D	533	VAL	2.0
1	D	578	PHE	2.0
1	D	620	GLU	2.0

## 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(Å <sup>2</sup> )	Q<0.9
3	MG	A	1776	1/1	0.13	0.22	22,22,22,22	0
4	F03	A	1777	15/15	0.11	-0.46	33,37,39,39	0
3	MG	D	1772	1/1	0.07	-2.42	31,31,31,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	1775	1/1	0.05	-2.75	29,29,29,29	0
2	ZN	D	1771	1/1	0.04	-2.94	35,35,35,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.