



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:33 PM GMT

PDB ID : 3IBJ
Title : X-ray structure of PDE2A
Authors : Pandit, J.
Deposited on : 2009-07-16
Resolution : 3.02 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>

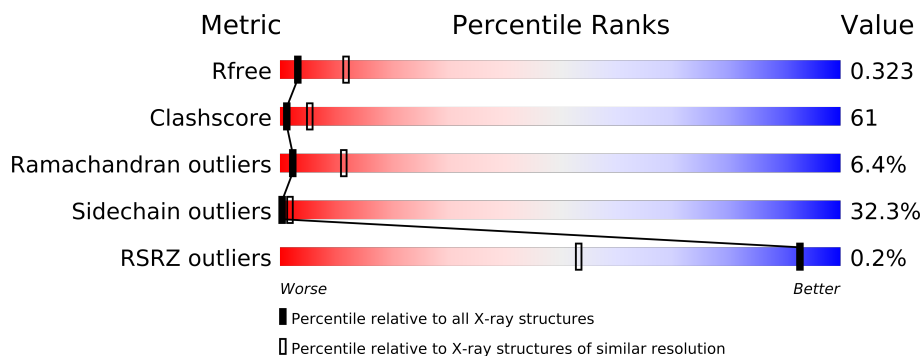
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.02 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	1332 (3.04-3.00)
Clashscore	79885	1732 (3.04-3.00)
Ramachandran outliers	78287	1669 (3.04-3.00)
Sidechain outliers	78261	1672 (3.04-3.00)
RSRZ outliers	66119	1333 (3.04-3.00)

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	691	
1	B	691	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	905	-	X
3	MG	B	905	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10650 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-dependent 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	0	0
			5291	3360	890	1000	41			
1	B	643	Total	C	N	O	S	0	0	0
			5164	3278	874	970	42			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MET	-	INITIATING METHIONINE	UNP O00408
A	901	LEU	-	EXPRESSION TAG	UNP O00408
A	902	VAL	-	EXPRESSION TAG	UNP O00408
A	903	PRO	-	EXPRESSION TAG	UNP O00408
A	904	ARG	-	EXPRESSION TAG	UNP O00408
B	214	MET	-	INITIATING METHIONINE	UNP O00408
B	901	LEU	-	EXPRESSION TAG	UNP O00408
B	902	VAL	-	EXPRESSION TAG	UNP O00408
B	903	PRO	-	EXPRESSION TAG	UNP O00408
B	904	ARG	-	EXPRESSION TAG	UNP O00408

- 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		

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total 96	O 96	0	0
4	B	95	Total 95	O 95	0	0

M848	M849	D849	G787	V766	S724	H656	V693	P527	G464	K401	R338	S275	MET
R850	D850	Y788	Y788	G787	V725	H657	I596	W528	I465	M402	A339	C276	GLU
E851	D851	Y789	Y789	G789	E727	W528	D597	F529	A466	L403	T340	K277	ASP
K852	R852	R790	S663	S663	R728	S663	S598	S598	H468	H406	Q341	V278	GLN
Y854	A854	R791	H666	F600	H729	H666	F600	K531	A469	D408	V343	Q280	GLY
I855	P855	H792	F667	S602	H730	F667	A601	F532	A470	D409	V344	D281	GLY
P856	P856	F731	G668	E534	F731	G668	E534	D533	A471	V410	A346	K282	ALA
									I472	I472	I472	V283	ALA
Q859	I860	I735	Y669	F603	A736	Y669	F603	D535	G473	S411	A349	E287	Y223
I860	S861	I737	L670	Y605	A737	L670	Y605	E537	G474	I413	F350	V288	T224
S861	F862	L738	L671	T606	A738	L671	T606		Q474	L414	F350	V288	D225
F862	M863	L739	K673	P607	A739	K673	P607	F540	I476	I414	R351	S289	R226
M863	E864	I740	M674	R608	A740	M674	R608	S541	I477	Q415	K352	F290	D227
			L675	S609	A741	L675	S609		I478	E416	L353	P291	R228
H865	I866	G742	E676	P611	G743	E676	P611	I546	A481	I418	G355	T293	K230
I866	A867	C743	E677	P612	G744	E677	P612	I547	A482		D356	T293	L230
A867	M868	N744	T678	E612	A745	T678	E612	I548	Y482	A421	L357	L286	Q232
M868	P869	I745	H679	D613	I745	H679	D613	H550	ALA	R422	F358	G287	L233
I870	D808	F746	D614	D614			D614		HIS	M423	T358	Q298	C234
Y871	L809	D747	T615	T615			T615	L553	PRO	L424	D360	V299	G235
K872	S810	H749	D683	M617			D683	Y554	LEU	S425	E361	V300	E236
L873	D811	S750	I684	A618			I684	K555	PHE	N426	D362	E301	L237
L874	Q812	R751	E685	T619			E685	K556	THR	A427	E363	D302	Y238
Q875	R752	K752	F686	L620			F686	V557	ARG	E428	R366	K303	
D876	D753	F754	F687	L621			F687	N558	GLY	I429	V365	K304	D241
L877	Y754	Q755	A688	M622			A688	E559	VAL	V432	I366	S305	A242
	K817	Q756	L689	N622			L689	A560	ASP	F433	Q307	I306	S243
	T818	R756		Q624				Q561	SER	L434	C369	K308	S244
A882	T819	M757	C685	Q624				Y562	THR	L435	F370	K309	L245
	R820	L758	H696	D625				H565	GLY	D436	H371	L246	Q246
E885	R821	D759	D697	M626				L566	PHE	I437	D310	L247	
R887	I822	L760	L698	N627				A567		Q437	L311	K248	Y249
V888	A823	M761	D699	F628					R498	T372	T312	V249	
A889	E824	R762	H700	I629					T499	S374	S314	L250	
S890	L825	D763	R701	N630				M570	R500	E439	E314	Q251	
N891	I826	I764	G702	N631				M571	N501	L440	T375	Q251	
E893	R828	L765	K633	T632				M572	L502	V441	V376	Y252	
H894	K828	L766	I634	I634				Y573	C504	A442	L377	L253	
H895	F830	A767	D635	D635				H574	F505	V444		Q254	
T896	P831	D768	P637	P637				M575	P506	PHE	L381	Q255	
K897	S832	L770	T638	T638				K576	ASP	GLY	A382	T257	
V898	Q833	A771	L639	L639				V577	GLU	GLY	M322	P258	
S899	G834	H772	A640	A640				S578	VAL	VAL	L323	S260	
H900	D835	H773	R641	R641				D579	VAL	Q387	G324	R261	
L901	L836	L774	F642	F642				D580	ASP	K388	C325	C262	
Y902	E837	R775	S713	S713				E581	ASP	L389	E326	C263	
R904	K838	I776	S714	S714				Y582	GLU	K390	L327	L264	
	MET	F777	L715	L715				T583	S484	C391	Q328	L265	
	GLY	K778	L716	L716				K584	Y485	A329	L266	L266	
	ASN	D779	A717	A717				L585	E456	M300	V267	V267	
	PRO	L780	L718	L718				D586	Q516	L331	S268	S268	
	ARG	Q781	Y719	Y719				H587	I457	C332	C332	C332	
	MET	K782	S720	S720				E519	R458	A395	C269	D270	
	GLU	A784	P653	P653				D588	I459	V333	V333	D270	
	MET	E785	E722	E722				G589	P460	L397	P334	V271	
	MET		P654	P654				I590	A461	Q398	V335	L272	
			G723	G723				Q591	D462	Q273	I336	L272	
								P592	Q463		S337	L274	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.23Å 89.70Å 264.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.26 – 3.02 18.17 – 3.02	Depositor EDS
% Data completeness (in resolution range)	99.5 (18.26-3.02) 99.6 (18.17-3.02)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.03Å)	Xtriage
Refinement program	BUSTER-TNT 2.1.1	Depositor
R, R_{free}	0.210 , 0.311 0.218 , 0.323	Depositor DCC
R_{free} test set	1598 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 64.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 31511 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10650	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: ZN, 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	0.66	0/5394	0.86	4/7292 (0.1%)
1	B	0.68	1/5260 (0.0%)	0.88	7/7105 (0.1%)
All	All	0.67	1/10654 (0.0%)	0.87	11/14397 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	722	GLU	CG-CD	5.25	1.59	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	855	ILE	C-N-CD	-8.18	102.61	120.60
1	A	478	ILE	C-N-CD	-7.99	103.03	120.60
1	B	902	VAL	C-N-CD	-7.13	104.91	120.60
1	B	478	ILE	C-N-CD	-6.90	105.43	120.60
1	B	723	GLY	N-CA-C	-6.66	96.44	113.10

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	5291	0	5225	671	0
1	B	5164	0	5128	656	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	96	0	0	10	0
4	B	95	0	0	7	0
All	All	10650	0	10353	1263	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 61.

The worst 5 of 1263 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:704:ASN:ND2	1:A:705:ASN:H	1.41	1.17
1:B:312:THR:HG22	1:B:314:GLU:H	1.06	1.14
1:A:774:LEU:HD12	1:B:838:LYS:HG3	1.27	1.14
1:B:320:GLN:HG2	1:B:327:LEU:HD13	1.14	1.14
1:B:460:PRO:HG2	1:B:463:GLN:HB3	1.30	1.12

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	655/691 (95%)	512 (78%)	95 (14%)	48 (7%)	2	8
1	B	633/691 (92%)	514 (81%)	84 (13%)	35 (6%)	3	16
All	All	1288/1382 (93%)	1026 (80%)	179 (14%)	83 (6%)	2	11

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	GLU

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Mol	Chain	Res	Type
1	A	293	THR
1	A	354	GLU
1	A	356	ASP
1	A	371	HIS

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	590/614 (96%)	393 (67%)	197 (33%)	0	1
1	B	577/614 (94%)	397 (69%)	180 (31%)	0	2
All	All	1167/1228 (95%)	790 (68%)	377 (32%)	0	2

5 of 377 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	789	ASP
1	B	263	CYS
1	B	776	ILE
1	A	810	SER
1	A	877	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	859	GLN
1	B	273	GLN
1	B	748	HIS
1	A	875	GLN
1	A	900	HIS

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, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	661/691 (95%)	-0.27	2 (0%) 91 47	43, 79, 109, 128	0
1	B	643/691 (93%)	-0.29	0 100 100	46, 74, 107, 125	0
All	All	1304/1382 (94%)	-0.28	2 (0%) 93 53	43, 76, 108, 128	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	588	ASP	2.5
1	A	452	ASP	2.3

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
3	MG	A	905	1/1	0.88	22.92	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	B	905	1/1	0.72	16.63	44,44,44,44	0
2	ZN	B	2	1/1	0.14	-0.47	67,67,67,67	0
2	ZN	A	1	1/1	0.16	-0.63	73,73,73,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.