



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3ECM / pdb_00003ecm
Title : Crystal structure of the unliganded PDE8A catalytic domain
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Deposited on : 2008-09-01
Resolution : 1.90 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

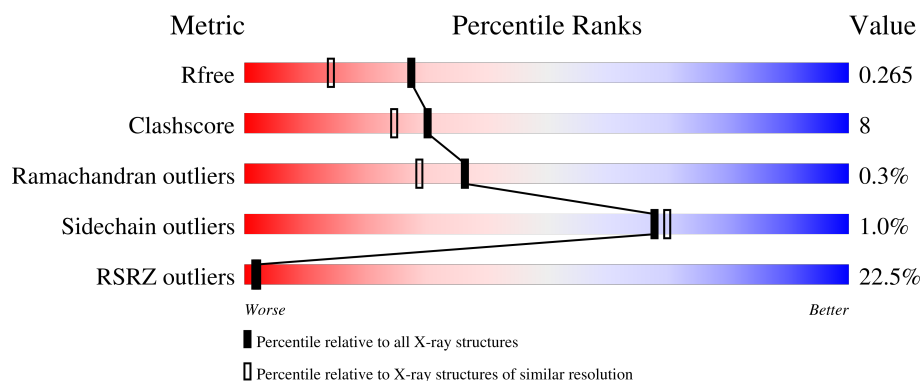
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	338	22% 78% 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2814 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 High affinity cAMP-specific and IBMX-insensitive 3',5'-cyclic phosphodiesterase 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2744	1734	464	527	19			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

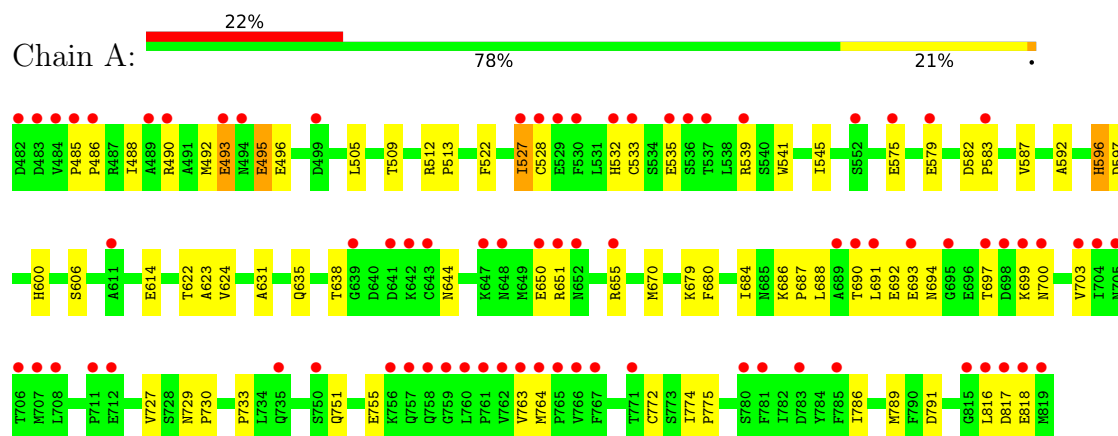
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: High affinity cAMP-specific and IBMX-insensitive 3',5'-cyclic phosphodiesterase 8A



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.26Å 132.66Å 101.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.90) 86.8 (30.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.265 0.235 , 0.265	Depositor DCC
R_{free} test set	3621 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.811	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2814	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.38	0/2809	0.85	8/3811 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	786	ILE	N-CA-C	9.65	119.68	110.42
1	A	624	VAL	N-CA-C	7.71	118.25	110.23
1	A	670	MET	N-CA-C	7.00	119.76	111.71
1	A	596	HIS	N-CA-C	6.64	120.97	112.34
1	A	527	ILE	N-CA-C	6.15	116.93	110.72
1	A	772	CYS	N-CA-C	5.67	118.77	109.76
1	A	493	GLU	N-CA-C	5.19	117.35	111.02
1	A	791	ASP	N-CA-C	-5.17	105.53	111.07

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	2744	0	2631	45	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	68	0	0	2	0
All	All	2814	0	2631	45	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 8.

All (45) 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:694:ASN:HB2	1:A:700:ASN:ND2	2.00	0.76
1:A:680:PHE:CD1	1:A:684:ILE:HD12	2.25	0.71
1:A:697:THR:HG22	1:A:699:LYS:H	1.60	0.67
1:A:492:MET:O	1:A:495:GLU:HG3	1.96	0.66
1:A:763:VAL:HG23	1:A:764:MET:HG3	1.80	0.63
1:A:485:PRO:HG2	1:A:488:ILE:HD12	1.81	0.63
1:A:528:CYS:HB3	1:A:533:CYS:O	2.00	0.61
1:A:686:LYS:HB2	1:A:687:PRO:HD3	1.84	0.60
1:A:690:THR:O	1:A:693:GLU:HG2	2.03	0.59
1:A:575:GLU:O	1:A:579:GLU:HG2	2.02	0.59
1:A:606:SER:HB3	1:A:763:VAL:HG11	1.84	0.58
1:A:490:ARG:HA	1:A:493:GLU:HG3	1.85	0.58
1:A:697:THR:HB	1:A:700:ASN:HB2	1.88	0.56
1:A:688:LEU:O	1:A:692:GLU:HG3	2.05	0.56
1:A:583:PRO:O	1:A:587:VAL:HG23	2.06	0.55
1:A:697:THR:HB	1:A:700:ASN:CB	2.36	0.55
1:A:699:LYS:O	1:A:703:VAL:HG23	2.06	0.54
1:A:694:ASN:HB2	1:A:700:ASN:HD22	1.72	0.54
1:A:751:GLN:O	1:A:755:GLU:HG3	2.07	0.54
1:A:486:PRO:O	1:A:490:ARG:HG3	2.08	0.53
1:A:729:ASN:HB2	1:A:730:PRO:HD3	1.91	0.53
1:A:614:GLU:HG3	4:A:856:HOH:O	2.10	0.52
1:A:631:ALA:O	1:A:635:GLN:HG3	2.11	0.50
1:A:582:ASP:HB3	1:A:583:PRO:HD2	1.94	0.49
1:A:522:PHE:CG	1:A:527:ILE:HD12	2.48	0.48
1:A:528:CYS:O	1:A:532:HIS:N	2.45	0.48
1:A:592:ALA:O	1:A:596:HIS:HB3	2.15	0.46
1:A:774:ILE:N	1:A:775:PRO:HD2	2.30	0.46
1:A:541:TRP:O	1:A:545:ILE:HG12	2.16	0.45
1:A:505:LEU:O	1:A:509:THR:HG23	2.17	0.45
1:A:691:LEU:C	1:A:693:GLU:H	2.24	0.45
1:A:512:ARG:N	1:A:513:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:PRO:CG	1:A:488:ILE:HD12	2.47	0.44
1:A:622:THR:O	1:A:623:ALA:C	2.60	0.44
1:A:535:GLU:O	1:A:539:ARG:HG3	2.17	0.44
1:A:727:VAL:HG21	1:A:789:MET:HE1	2.00	0.43
1:A:486:PRO:HB2	1:A:490:ARG:NH1	2.34	0.42
1:A:755:GLU:OE2	1:A:763:VAL:HG22	2.20	0.42
1:A:650:GLU:O	1:A:651:ARG:C	2.63	0.42
1:A:655:ARG:HD3	1:A:655:ARG:HA	1.87	0.42
1:A:597:ASP:O	1:A:600:HIS:HB2	2.20	0.41
1:A:638:THR:HA	1:A:644:ASN:ND2	2.34	0.41
1:A:575:GLU:HA	1:A:575:GLU:OE1	2.20	0.41
1:A:679:LYS:HG3	4:A:849:HOH:O	2.20	0.40
1:A:816:LEU:O	1:A:817:ASP:C	2.64	0.40

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	336/338 (99%)	314 (94%)	21 (6%)	1 (0%)	36	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	GLU

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	303/303 (100%)	300 (99%)	3 (1%)	68	70

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	495	GLU
1	A	496	GLU
1	A	733	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	700	ASN
1	A	705	ASN
1	A	770	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

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 ⓘ

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	338/338 (100%)	1.17	76 (22%) 2 2	29, 43, 79, 95	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	CYS	6.2
1	A	819	MET	5.9
1	A	816	LEU	5.8
1	A	484	VAL	5.6
1	A	817	ASP	5.3
1	A	533	CYS	5.0
1	A	706	THR	4.5
1	A	697	THR	4.3
1	A	482	ASP	4.3
1	A	483	ASP	4.0
1	A	758	GLN	3.8
1	A	650	GLU	3.8
1	A	765	PRO	3.8
1	A	689	ALA	3.7
1	A	643	CYS	3.7
1	A	767	PHE	3.7
1	A	651	ARG	3.7
1	A	647	LYS	3.6
1	A	750	SER	3.6
1	A	699	LYS	3.5
1	A	785	PHE	3.5
1	A	759	GLY	3.4
1	A	529	GLU	3.4
1	A	703	VAL	3.3
1	A	485	PRO	3.3
1	A	499	ASP	3.2
1	A	527	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	761	PRO	3.2
1	A	642	LYS	3.2
1	A	691	LEU	3.2
1	A	493	GLU	3.2
1	A	695	GLY	3.1
1	A	783	ASP	3.0
1	A	705	ASN	3.0
1	A	536	SER	2.9
1	A	771	THR	2.9
1	A	763	VAL	2.9
1	A	756	LYS	2.9
1	A	780	SER	2.9
1	A	760	LEU	2.9
1	A	490	ARG	2.8
1	A	764	MET	2.8
1	A	757	GLN	2.8
1	A	532	HIS	2.7
1	A	579	GLU	2.7
1	A	707	MET	2.7
1	A	652	ASN	2.7
1	A	700	ASN	2.7
1	A	704	ILE	2.6
1	A	711	PRO	2.6
1	A	712	GLU	2.5
1	A	530	PHE	2.5
1	A	535	GLU	2.4
1	A	690	THR	2.4
1	A	766	VAL	2.4
1	A	539	ARG	2.4
1	A	494	ASN	2.4
1	A	648	ASN	2.3
1	A	693	GLU	2.3
1	A	537	THR	2.3
1	A	489	ALA	2.3
1	A	698	ASP	2.3
1	A	655	ARG	2.2
1	A	641	ASP	2.2
1	A	815	GLY	2.2
1	A	575	GLU	2.2
1	A	708	LEU	2.2
1	A	781	PHE	2.1
1	A	486	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	611	ALA	2.1
1	A	583	PRO	2.1
1	A	735	GLN	2.1
1	A	818	GLU	2.0
1	A	552	SER	2.0
1	A	639	GLY	2.0
1	A	762	VAL	2.0

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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	2	1/1	0.97	0.13	36,36,36,36	0
2	ZN	A	1	1/1	0.99	0.03	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.