



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:19 AM UTC

PDB ID : 4LM4 / pdb_00004lm4
Title : Crystal structure of PDE10A2 with fragment ZT902
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Deposited on : 2013-07-10
Resolution : 1.48 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

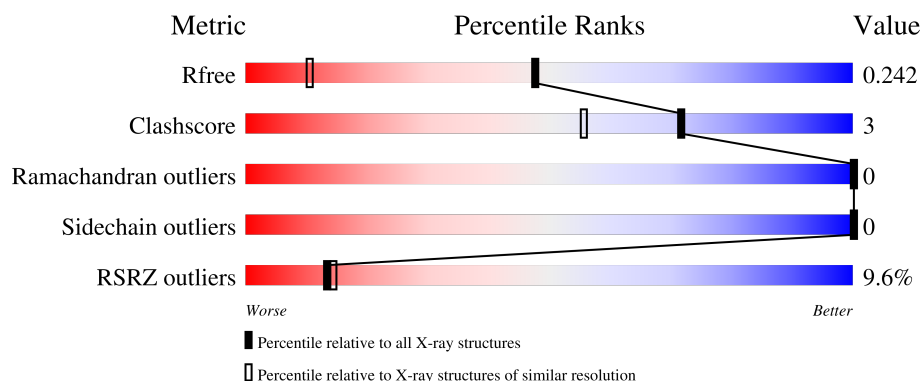
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	345	6% 91% 5%
1	B	345	12% 87% 8% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5700 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.

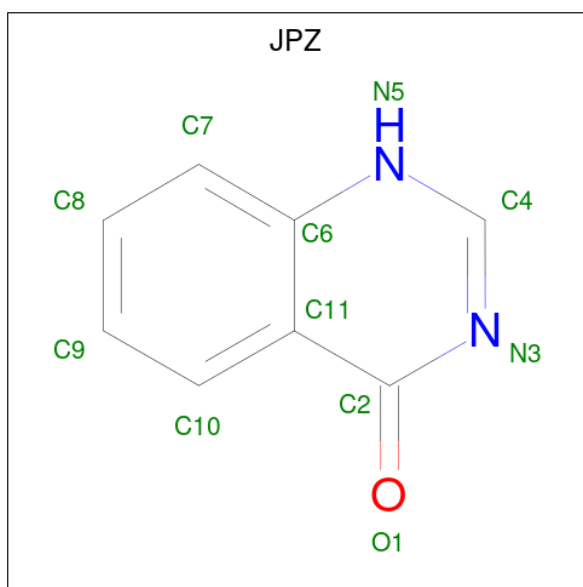
- Molecule 1 is a protein called cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	13	0
			2669	1712	453	480	24			
1	B	327	Total	C	N	O	S	0	8	0
			2635	1689	445	475	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	-	expression tag	UNP Q9Y233
A	446	ALA	-	expression tag	UNP Q9Y233
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	THR	-	expression tag	UNP Q9Y233
B	445	GLY	-	expression tag	UNP Q9Y233
B	446	ALA	-	expression tag	UNP Q9Y233
B	447	GLY	-	expression tag	UNP Q9Y233
B	448	THR	-	expression tag	UNP Q9Y233

- Molecule 2 is quinazolin-4(1H)-one (CCD ID: JPZ) (formula: C₈H₆N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	8	2	1		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ni	0	0
			2	2		
3	B	2	Total	Ni	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	217	Total	O	0	0
			217	217		
4	B	164	Total	O	0	0
			164	164		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.90Å 82.08Å 155.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.25 – 1.48 43.25 – 1.48	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.25-1.48) 99.4 (43.25-1.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.199 , 0.222 (Not available) , 0.242	Depositor DCC
R_{free} test set	5428 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5700	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: NI, JPZ

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	0.69	0/2800	0.81	1/3796 (0.0%)
1	B	0.66	0/2741	0.80	1/3718 (0.0%)
All	All	0.67	0/5541	0.81	2/7514 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	746	PRO	N-CA-C	5.67	117.62	110.70
1	A	746	PRO	N-CA-C	5.16	116.99	110.70

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	2669	0	2630	16	0
1	B	2635	0	2582	21	0
2	A	11	0	6	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	217	0	0	0	0
4	B	164	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5700	0	5218	35	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 3.

All (35) 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:B:699:GLU:HG2	1:B:703[B]:MET:HE2	1.63	0.79
1:B:641:ASN:HD22	1:B:664:ARG:HH11	1.33	0.77
1:A:726:GLN:HE22	2:A:900:JPZ:H4	1.53	0.74
1:B:655:ASN:H	1:B:661:HIS:HD2	1.35	0.71
1:A:641:ASN:HD22	1:A:664:ARG:HH11	1.39	0.71
1:A:727[B]:LEU:HG	1:A:766:ILE:CD1	2.23	0.68
1:B:450:ILE:HG22	1:B:605:LEU:HD13	1.75	0.67
1:B:460:MET:HE3	1:B:505:LEU:HD23	1.76	0.66
1:B:580:HIS:HD2	1:B:582:LEU:H	1.47	0.61
1:B:547[B]:LEU:HD11	1:B:656:LEU:HD12	1.85	0.59
1:B:699:GLU:HG2	1:B:703[B]:MET:CE	2.33	0.58
1:B:700:GLY:HA2	1:B:703[B]:MET:HE3	1.88	0.56
1:A:727[B]:LEU:HG	1:A:766:ILE:HD11	1.90	0.53
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.44	0.53
1:A:464:LEU:HD21	1:A:472[B]:ILE:HD12	1.91	0.52
1:B:483:GLU:HA	1:B:486:TRP:CE2	2.44	0.51
1:A:727[A]:LEU:HD12	1:A:759:LEU:HD11	1.94	0.50
1:B:660:SER:O	1:B:664:ARG:HG3	2.13	0.49
1:B:459[A]:LEU:HD13	1:B:487:PRO:HB2	1.95	0.48
1:B:580:HIS:CD2	1:B:582:LEU:H	2.29	0.48
1:A:771:THR:HA	1:B:713:MET:HB3	1.96	0.47
1:A:472[A]:ILE:CD1	1:A:489:ILE:HG23	2.44	0.47
1:A:726:GLN:HE22	2:A:900:JPZ:C4	2.25	0.47
1:A:472[A]:ILE:HD11	1:A:489:ILE:HG23	1.97	0.46
1:B:655:ASN:ND2	1:B:657:ASN:H	2.15	0.44
1:B:655:ASN:C	1:B:655:ASN:HD22	2.25	0.44
1:A:727[B]:LEU:HG	1:A:766:ILE:HD12	2.00	0.43
1:A:772:ALA:HB3	1:B:693:TYR:CE2	2.54	0.43
1:A:469:CYS:O	1:A:472[A]:ILE:HG22	2.19	0.42
1:B:774:TRP:HD1	4:B:1158:HOH:O	2.02	0.42
1:B:456:TRP:HZ3	1:B:460:MET:SD	2.43	0.42
1:A:724:GLN:HE22	1:A:727[A]:LEU:HD23	1.84	0.41
1:A:726:GLN:NE2	2:A:900:JPZ:H4	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:ASN:HD22	1:B:657:ASN:H	1.69	0.41

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	341/345 (99%)	339 (99%)	2 (1%)	0	100	100
1	B	333/345 (96%)	330 (99%)	3 (1%)	0	100	100
All	All	674/690 (98%)	669 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	296/306 (97%)	296 (100%)	0	100	100
1	B	291/306 (95%)	291 (100%)	0	100	100
All	All	587/612 (96%)	587 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	476	HIS
1	A	641	ASN
1	A	644	GLN
1	A	724	GLN
1	A	726	GLN
1	B	525	HIS
1	B	580	HIS
1	B	593	GLN
1	B	598	GLN
1	B	641	ASN
1	B	655	ASN
1	B	659	GLN
1	B	661	HIS
1	B	761	GLN

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 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	$\# Z > 2$
2	JPZ	A	900	-	12,12,12	2.39	3 (25%)	16,16,16	0.93	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
2	JPZ	A	900	-	-	-	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	JPZ	O1-C2	5.77	1.33	1.23
2	A	900	JPZ	C11-C2	-4.33	1.40	1.48
2	A	900	JPZ	C4-N3	2.87	1.35	1.30

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	JPZ	3	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

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	330/345 (95%)	0.30	20 (6%) 27 29	13, 20, 37, 51	13 (3%)
1	B	327/345 (94%)	0.68	43 (13%) 7 8	14, 24, 42, 48	8 (2%)
All	All	657/690 (95%)	0.49	63 (9%) 13 14	13, 22, 39, 51	21 (3%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	774	TRP	6.5
1	A	775	ILE	6.1
1	A	771	THR	6.0
1	A	772	ALA	5.6
1	A	773	THR	5.0
1	B	584	ALA	5.0
1	B	581	PRO	4.8
1	B	617	SER	4.4
1	B	588	THR	4.2
1	B	585	LEU	4.1
1	B	523	PRO	3.8
1	B	573	SER	3.7
1	A	774	TRP	3.6
1	B	773	THR	3.5
1	B	772	ALA	3.4
1	B	583	ALA	3.4
1	A	502	CYS	3.2
1	A	503	PHE	3.1
1	A	464	LEU	3.1
1	A	446	ALA	3.0
1	B	590	THR	3.0
1	B	502	CYS	3.0
1	A	463	THR	2.9
1	B	579	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	522	VAL	2.8
1	B	605	LEU	2.8
1	B	448	THR	2.7
1	B	569	GLY	2.7
1	B	578	PHE	2.7
1	B	586	TYR	2.7
1	B	453	SER	2.6
1	B	659	GLN	2.6
1	A	708	ILE	2.6
1	B	613	THR	2.5
1	B	574	TYR	2.5
1	B	607	GLY	2.5
1	B	450	ILE	2.5
1	B	524	TYR	2.5
1	B	575	LEU	2.5
1	A	462	PHE	2.5
1	A	770	GLU	2.4
1	B	621	GLN	2.4
1	B	600	VAL	2.3
1	A	500	THR	2.3
1	A	650	GLN	2.3
1	B	577	LYS	2.3
1	B	582	LEU	2.3
1	B	572	ASN	2.2
1	B	580	HIS	2.2
1	A	459	LEU	2.2
1	B	591	MET	2.2
1	B	568	ARG	2.2
1	B	456	TRP	2.2
1	A	466	VAL	2.2
1	B	608	HIS	2.2
1	B	649	TYR	2.1
1	B	587	SER	2.1
1	A	585	LEU	2.1
1	A	450	ILE	2.1
1	B	570	PHE	2.1
1	B	615	SER	2.1
1	A	469	CYS	2.1
1	B	658	ASN	2.1

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
2	JPZ	A	900	11/11	0.78	0.14	46,47,47,47	0
3	NI	A	901	1/1	0.99	0.05	16,16,16,16	0
3	NI	A	902	1/1	0.99	0.15	24,24,24,24	0
3	NI	B	901	1/1	0.99	0.11	24,24,24,24	0
3	NI	B	902	1/1	0.99	0.18	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.