



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:54 AM UTC

PDB ID : 6DDO / pdb_00006ddo
Title : Crystal structure of the single mutant (D52N) of the full-length NT5C2 in the basal state
Authors : Forouhar, F.; Dieck, C.L.; Tzoneva, G.; Carpenter, Z.; Ambesi-Impiombato, A.; Sanchez-Martin, M.; Kirschner-Schwabe, R.; Lew, S.; Seetharaman, J.; Ferrando, A.A.; Tong, L.
Deposited on : 2018-05-10
Resolution : 2.48 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

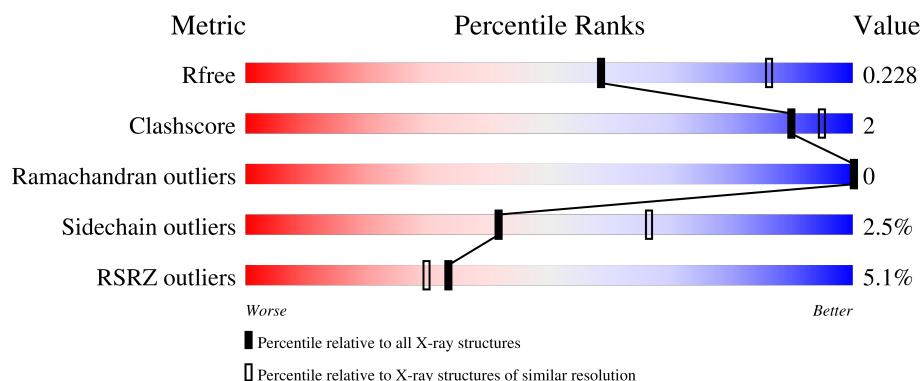
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

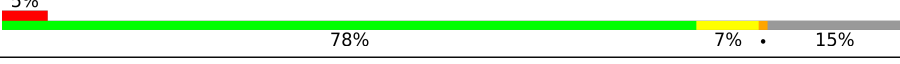
The reported resolution of this entry is 2.48 Å.

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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	579	
1	B	579	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8274 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 Cytosolic purine 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	0	0
			4080	2624	681	754	21			
1	B	490	Total	C	N	O	S	0	0	0
			3997	2575	667	734	21			

There are 38 discrepancies between the modelled and reference sequences:

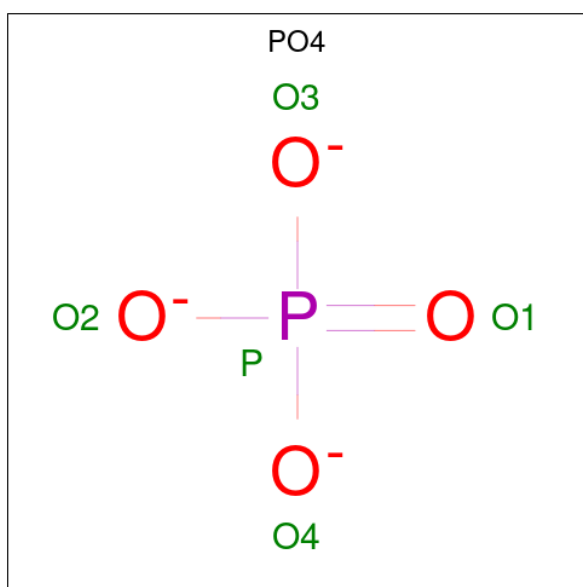
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP P49902
A	-16	SER	-	expression tag	UNP P49902
A	-15	SER	-	expression tag	UNP P49902
A	-14	HIS	-	expression tag	UNP P49902
A	-13	HIS	-	expression tag	UNP P49902
A	-12	HIS	-	expression tag	UNP P49902
A	-11	HIS	-	expression tag	UNP P49902
A	-10	HIS	-	expression tag	UNP P49902
A	-9	HIS	-	expression tag	UNP P49902
A	-8	SER	-	expression tag	UNP P49902
A	-7	SER	-	expression tag	UNP P49902
A	-6	GLY	-	expression tag	UNP P49902
A	-5	LEU	-	expression tag	UNP P49902
A	-4	VAL	-	expression tag	UNP P49902
A	-3	PRO	-	expression tag	UNP P49902
A	-2	ARG	-	expression tag	UNP P49902
A	-1	GLY	-	expression tag	UNP P49902
A	0	SER	-	expression tag	UNP P49902
A	52	ASN	ASP	engineered mutation	UNP P49902
B	-17	GLY	-	expression tag	UNP P49902
B	-16	SER	-	expression tag	UNP P49902
B	-15	SER	-	expression tag	UNP P49902
B	-14	HIS	-	expression tag	UNP P49902
B	-13	HIS	-	expression tag	UNP P49902
B	-12	HIS	-	expression tag	UNP P49902

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP P49902
B	-10	HIS	-	expression tag	UNP P49902
B	-9	HIS	-	expression tag	UNP P49902
B	-8	SER	-	expression tag	UNP P49902
B	-7	SER	-	expression tag	UNP P49902
B	-6	GLY	-	expression tag	UNP P49902
B	-5	LEU	-	expression tag	UNP P49902
B	-4	VAL	-	expression tag	UNP P49902
B	-3	PRO	-	expression tag	UNP P49902
B	-2	ARG	-	expression tag	UNP P49902
B	-1	GLY	-	expression tag	UNP P49902
B	0	SER	-	expression tag	UNP P49902
B	52	ASN	ASP	engineered mutation	UNP P49902

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	56	Total 56	O 56	0	0

- Molecule 1: Cytosolic purine 5'-nucleotidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	122.10Å 173.14Å 123.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.48 48.05 – 2.48	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.05-2.48) 100.0 (48.05-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.188 , 0.227 0.189 , 0.228	Depositor DCC
R_{free} test set	4673 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8274	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: PO4

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	0.10	0/4184	0.28	0/5652
1	B	0.09	0/4097	0.28	0/5530
All	All	0.09	0/8281	0.28	0/11182

There are no bond length outliers.

There are no bond angle outliers.

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	4080	0	3996	14	0
1	B	3997	0	3932	18	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	121	0	0	1	0
3	B	56	0	0	1	0
All	All	8274	0	7928	29	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 2.

All (29) 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:203:ASP:OD2	1:B:291:ARG:NH1	2.25	0.69
1:B:500:MET:N	3:B:701:HOH:O	2.33	0.60
1:B:179:THR:HB	1:B:186:LYS:HB2	1.85	0.59
1:A:298:GLU:HG3	1:B:195:ARG:HG2	1.88	0.56
1:B:453:GLN:OE1	1:B:456:ARG:NH2	2.40	0.54
1:A:48:CYS:HB3	1:A:346:ILE:HG12	1.89	0.54
1:A:100:LEU:HD11	1:A:437:MET:HG3	1.93	0.50
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.94	0.50
1:B:343:GLY:HA3	1:B:364:GLN:HB3	1.94	0.50
1:B:232:LEU:HB3	1:B:233:PRO:HD3	1.94	0.49
1:B:48:CYS:HB2	1:B:346:ILE:HG12	1.96	0.48
1:A:119:LEU:HD13	1:A:443:SER:HB3	1.95	0.47
1:A:315:GLY:HA2	1:B:190:LEU:HD23	1.97	0.47
1:B:303:ARG:HG2	1:B:328:SER:HB3	1.96	0.46
1:B:100:LEU:HD11	1:B:437:MET:HG3	1.97	0.46
1:B:65:TYR:HE2	1:B:157:PHE:HE1	1.64	0.45
1:B:354:PHE:O	1:B:456:ARG:NH1	2.50	0.45
1:A:344:LYS:HB2	1:A:364:GLN:NE2	2.33	0.44
1:B:358:LEU:HD23	1:B:361:LYS:HD3	2.00	0.44
1:A:130:GLY:HA3	1:A:131:PRO:HD3	1.90	0.43
1:A:28:ARG:NH1	3:A:703:HOH:O	2.43	0.42
1:B:145:ASP:O	1:B:147:THR:N	2.51	0.42
1:B:153:LEU:HB3	1:B:158:ASN:HB3	2.01	0.42
1:A:395:LEU:HD11	1:A:422:ARG:HG3	2.02	0.42
1:A:61:LYS:HB3	1:A:61:LYS:NZ	2.35	0.41
1:B:77:LEU:O	1:B:80:ILE:HG22	2.20	0.41
1:A:48:CYS:SG	1:A:339:LEU:HD13	2.60	0.41
1:B:235:LEU:HB2	1:B:469:LEU:HD13	2.02	0.41
1:A:344:LYS:HB2	1:A:364:GLN:CD	2.47	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	496/579 (86%)	484 (98%)	12 (2%)	0	100	100
1	B	482/579 (83%)	471 (98%)	11 (2%)	0	100	100
All	All	978/1158 (84%)	955 (98%)	23 (2%)	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	448/520 (86%)	439 (98%)	9 (2%)	48	72
1	B	439/520 (84%)	426 (97%)	13 (3%)	36	61
All	All	887/1040 (85%)	865 (98%)	22 (2%)	42	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	213	SER
1	A	294	LEU
1	A	311	LYS
1	A	357	ILE
1	A	358	LEU
1	A	363	ARG
1	A	446	ARG
1	A	455	MET
1	B	80	ILE
1	B	135	GLU
1	B	216	GLU
1	B	303	ARG
1	B	308	LYS
1	B	311	LYS

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Mol	Chain	Res	Type
1	B	312	LEU
1	B	344	LYS
1	B	352	HIS
1	B	358	LEU
1	B	424	LYS
1	B	446	ARG
1	B	508	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	428	HIS
1	B	33	HIS
1	B	276	HIS
1	B	428	HIS
1	B	494	HIS

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](#)

4 ligands are modelled in this entry.

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	PO4	B	601	-	4,4,4	0.98	0	6,6,6	0.44	0
2	PO4	A	601	-	4,4,4	1.08	0	6,6,6	0.51	0
2	PO4	B	602	-	4,4,4	0.96	0	6,6,6	0.42	0
2	PO4	A	602	-	4,4,4	0.92	0	6,6,6	0.45	0

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 [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	500/579 (86%)	0.01	21 (4%)	40 36	29, 46, 91, 150	0
1	B	490/579 (84%)	0.28	29 (5%)	28 25	30, 57, 93, 138	1 (0%)
All	All	990/1158 (85%)	0.15	50 (5%)	33 30	29, 51, 92, 150	1 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	539	LEU	6.3
1	A	358	LEU	5.3
1	B	358	LEU	4.9
1	B	357	ILE	4.8
1	A	318	THR	4.3
1	B	495	VAL	4.2
1	A	553	ASP	4.0
1	B	210	TYR	3.9
1	B	189	ASP	3.9
1	A	497	ILE	3.9
1	B	545	THR	3.7
1	A	357	ILE	3.7
1	B	540	ALA	3.6
1	A	510	THR	3.5
1	A	495	VAL	3.5
1	A	320	PRO	3.5
1	B	24	LEU	3.5
1	B	550	GLU	3.4
1	A	323	HIS	3.3
1	B	268	HIS	3.0
1	B	144	ARG	3.0
1	A	24	LEU	3.0
1	B	80	ILE	2.9
1	B	552	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	317	TYR	2.8
1	B	538	PRO	2.8
1	B	541	PRO	2.7
1	B	272	PRO	2.7
1	A	319	GLY	2.7
1	A	210	TYR	2.5
1	B	324	GLY	2.5
1	B	213	SER	2.5
1	B	316	THR	2.5
1	B	32	TYR	2.4
1	B	542	GLN	2.4
1	B	480	ALA	2.4
1	B	185	PHE	2.4
1	A	544	ILE	2.4
1	B	188	GLY	2.3
1	A	25	LYS	2.3
1	B	547	CYS	2.3
1	A	543	GLU	2.2
1	A	500	MET	2.2
1	A	498	ASN	2.2
1	A	551	ASP	2.1
1	A	499	GLU	2.1
1	B	411	ASN	2.1
1	B	356	ASP	2.0
1	A	360	SER	2.0
1	B	129	ARG	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
2	PO4	A	602	5/5	0.80	0.18	61,67,97,105	0
2	PO4	B	602	5/5	0.85	0.15	75,92,101,115	0
2	PO4	B	601	5/5	0.95	0.07	39,44,47,48	0
2	PO4	A	601	5/5	0.99	0.04	23,26,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.