



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6DDX / pdb_00006ddx
Title : Crystal structure of the double mutant (D52N/L375F) of NT5C2-537X in the active state, Northeast Structural Genomics Target
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Deposited on : 2018-05-10
Resolution : 2.90 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
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

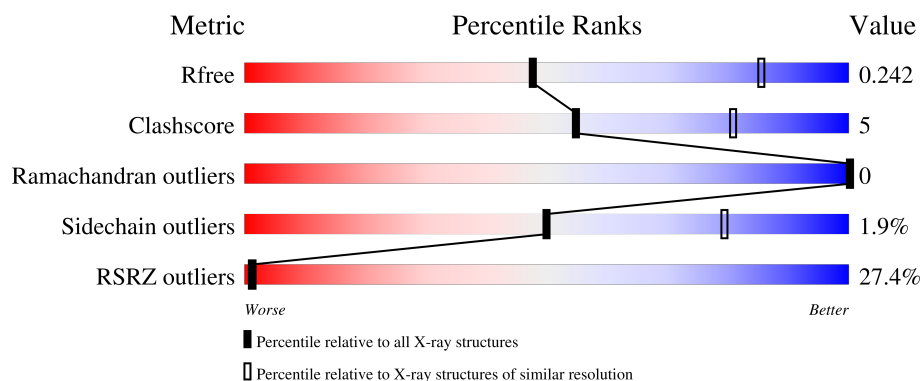
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	554	23% 72% 13% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3881 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	474	Total	C	N	O	S	0	0	0
			3869	2504	642	702	21			

There are 20 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
A	375	PHE	LEU	engineered mutation	UNP P49902

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		

- Molecule 1: Cytosolic purine 5'-nucleotidase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.19Å 127.07Å 130.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.54 – 2.90 45.54 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.1 (45.54-2.90) 99.9 (45.54-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.01 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.205 , 0.274 0.251 , 0.242	Depositor DCC
R_{free} test set	4449 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3881	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% 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	0.33	0/3970	0.52	0/5359

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	PHE	Peptide

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	3869	0	3814	37	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	0	0	0
All	All	3881	0	3814	37	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 5.

All (37) 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:101:VAL:HG22	1:A:152:ILE:HG12	1.65	0.79
1:A:17:ALA:HB1	1:A:19:MET:HE3	1.71	0.73
1:A:219:VAL:HG11	1:A:258:LYS:HD3	1.69	0.73
1:A:186:LYS:NZ	1:A:188:GLY:O	2.32	0.56
1:A:228:LYS:HE3	1:A:262:TYR:O	2.08	0.53
1:A:208:VAL:HG12	1:A:214:LEU:HB2	1.93	0.51
1:A:288:VAL:O	1:A:328:SER:HA	2.11	0.50
1:A:401:GLU:O	1:A:404:LYS:HG3	2.11	0.50
1:A:399:LEU:HD13	1:A:419:ILE:HB	1.94	0.50
1:A:5:TRP:CZ3	1:A:373:PRO:HB3	2.47	0.50
1:A:74:VAL:HG13	1:A:86:LEU:HB3	1.93	0.49
1:A:128:ILE:HG23	1:A:132:GLU:CD	2.37	0.49
1:A:238:ARG:HB3	1:A:473:PHE:CE1	2.46	0.49
1:A:26:LYS:N	1:A:26:LYS:HD3	2.26	0.49
1:A:232:LEU:HD13	1:A:465:PHE:HZ	1.77	0.49
1:A:28:ARG:HD2	1:A:471:TYR:CE1	2.47	0.49
1:A:357:ILE:HG13	1:A:370:LEU:HD13	1.96	0.48
1:A:303:ARG:HB2	1:A:328:SER:HB3	1.95	0.48
1:A:234:LEU:O	1:A:237:SER:OG	2.31	0.47
1:A:449:LEU:O	1:A:453:GLN:HG3	2.15	0.47
1:A:5:TRP:CG	1:A:374:GLU:HA	2.49	0.47
1:A:56:THR:HG23	1:A:371:VAL:HG21	1.97	0.46
1:A:52:ASN:OD1	1:A:350:GLY:HA2	2.17	0.45
1:A:113:ASP:CG	1:A:117:ASN:HB2	2.42	0.45
1:A:197:MET:O	1:A:201:VAL:HG23	2.17	0.45
1:A:266:PHE:C	1:A:268:HIS:H	2.25	0.45
1:A:322:GLN:O	1:A:325:ILE:HG22	2.17	0.44
1:A:95:PHE:HA	1:A:436:MET:HB2	1.99	0.43
1:A:57:LEU:HD13	1:A:260:MET:HE1	2.00	0.42
1:A:165:LEU:O	1:A:169:VAL:HG23	2.20	0.42
1:A:95:PHE:HB3	1:A:96:PRO:HD3	2.02	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HD11	1:A:327:TYR:CD1	2.54	0.41
1:A:375:PHE:HA	1:A:378:GLU:HB2	2.01	0.41
1:A:157:PHE:O	1:A:160:PRO:HD2	2.20	0.41
1:A:358:LEU:HD23	1:A:358:LEU:C	2.47	0.40
1:A:201:VAL:O	1:A:202:ARG:C	2.65	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	470/554 (85%)	450 (96%)	20 (4%)	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	420/496 (85%)	412 (98%)	8 (2%)	50	79

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS

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Mol	Chain	Res	Type
1	A	26	LYS
1	A	79	SER
1	A	144	ARG
1	A	145	ASP
1	A	359	LYS
1	A	404	LYS
1	A	485	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	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](#)

1 ligand is 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	A	601	-	4,4,4	0.99	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	474/554 (85%)	1.51	130 (27%) 1 1	36, 55, 103, 151	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	473	PHE	6.3
1	A	417	SER	5.6
1	A	403	TYR	4.9
1	A	145	ASP	4.9
1	A	210	TYR	4.7
1	A	12	ALA	4.6
1	A	404	LYS	4.4
1	A	114	ALA	4.3
1	A	420	GLN	4.3
1	A	322	GLN	4.3
1	A	324	GLY	4.2
1	A	132	GLU	4.1
1	A	423	ILE	4.1
1	A	16	PRO	4.0
1	A	419	ILE	3.9
1	A	3	THR	3.8
1	A	129	ARG	3.8
1	A	383	THR	3.7
1	A	456	ARG	3.7
1	A	488	SER	3.7
1	A	11	ASN	3.7
1	A	243	GLY	3.6
1	A	398	PHE	3.6
1	A	323	HIS	3.5
1	A	19	MET	3.5
1	A	26	LYS	3.5
1	A	424	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	88	SER	3.4
1	A	18	ASN	3.4
1	A	15	MET	3.4
1	A	186	LYS	3.4
1	A	131	PRO	3.4
1	A	449	LEU	3.4
1	A	402	LEU	3.3
1	A	144	ARG	3.3
1	A	4	SER	3.3
1	A	32	TYR	3.3
1	A	154	ASN	3.3
1	A	387	SER	3.3
1	A	308	LYS	3.2
1	A	396	ASP	3.2
1	A	21	LYS	3.2
1	A	27	TYR	3.1
1	A	216	GLU	3.1
1	A	134	ARG	3.1
1	A	20	ASP	3.0
1	A	242	VAL	3.0
1	A	130	GLY	3.0
1	A	426	VAL	3.0
1	A	5	TRP	2.9
1	A	223	GLU	2.9
1	A	421	ARG	2.9
1	A	211	LYS	2.9
1	A	481	HIS	2.9
1	A	143	GLN	2.8
1	A	474	SER	2.8
1	A	188	GLY	2.8
1	A	428	HIS	2.8
1	A	438	GLY	2.8
1	A	45	LYS	2.7
1	A	192	MET	2.7
1	A	337	ASP	2.7
1	A	50	GLY	2.7
1	A	377	GLN	2.7
1	A	241	GLU	2.7
1	A	17	ALA	2.7
1	A	13	ALA	2.6
1	A	393	GLN	2.6
1	A	346	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	238	ARG	2.6
1	A	24	LEU	2.6
1	A	400	ALA	2.6
1	A	245	VAL	2.5
1	A	325	ILE	2.5
1	A	176	PRO	2.5
1	A	135	GLU	2.5
1	A	29	ARG	2.5
1	A	8	ARG	2.4
1	A	277	ARG	2.4
1	A	477	PHE	2.4
1	A	31	ALA	2.4
1	A	401	GLU	2.4
1	A	386	SER	2.4
1	A	232	LEU	2.4
1	A	10	GLN	2.3
1	A	190	LEU	2.3
1	A	268	HIS	2.3
1	A	472	PRO	2.3
1	A	157	PHE	2.3
1	A	229	ASP	2.3
1	A	75	GLU	2.3
1	A	7	ASP	2.3
1	A	392	LEU	2.3
1	A	22	HIS	2.3
1	A	177	ARG	2.3
1	A	182	GLU	2.2
1	A	425	LYS	2.2
1	A	363	ARG	2.2
1	A	155	THR	2.2
1	A	30	GLU	2.2
1	A	320	PRO	2.2
1	A	44	GLU	2.2
1	A	467	ASN	2.2
1	A	445	SER	2.2
1	A	215	LYS	2.2
1	A	399	LEU	2.2
1	A	23	ALA	2.2
1	A	139	ASN	2.2
1	A	380	HIS	2.2
1	A	384	ASP	2.2
1	A	388	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	443	SER	2.2
1	A	220	GLU	2.2
1	A	335	ILE	2.1
1	A	283	PHE	2.1
1	A	28	ARG	2.1
1	A	444	GLY	2.1
1	A	236	LEU	2.1
1	A	282	TYR	2.1
1	A	463	ALA	2.1
1	A	124	GLY	2.1
1	A	207	TRP	2.1
1	A	148	GLU	2.1
1	A	397	ILE	2.1
1	A	468	LEU	2.1
1	A	319	GLY	2.1
1	A	343	GLY	2.1
1	A	368	THR	2.0
1	A	212	GLY	2.0
1	A	147	THR	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	601	5/5	0.91	0.18	74,76,80,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.