



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 01:02 PM EDT

PDB ID : 6CE1
Title : Crystal structure of Peptidyl Arginine Deiminase Type III (PADI3)
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Deposited on : 2018-02-10
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

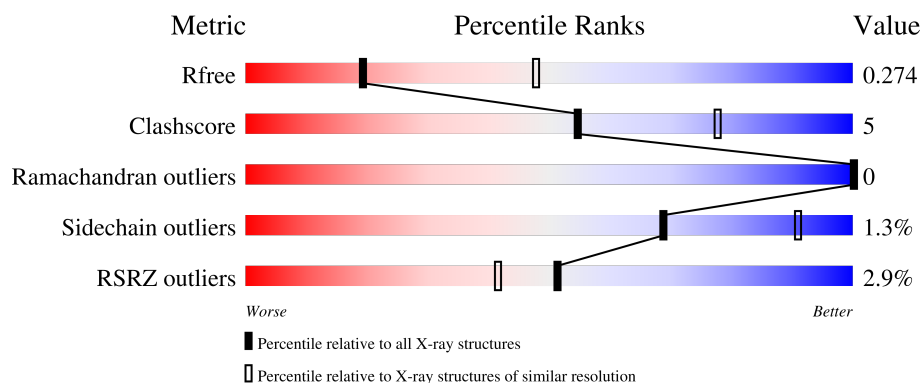
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	686	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4253 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 Protein-arginine deiminase type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	594	4253	2727	724	779	23	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q9ULW8
A	-20	SER	-	expression tag	UNP Q9ULW8
A	-19	TYR	-	expression tag	UNP Q9ULW8
A	-18	TYR	-	expression tag	UNP Q9ULW8
A	-17	HIS	-	expression tag	UNP Q9ULW8
A	-16	HIS	-	expression tag	UNP Q9ULW8
A	-15	HIS	-	expression tag	UNP Q9ULW8
A	-14	HIS	-	expression tag	UNP Q9ULW8
A	-13	HIS	-	expression tag	UNP Q9ULW8
A	-12	HIS	-	expression tag	UNP Q9ULW8
A	-11	LEU	-	expression tag	UNP Q9ULW8
A	-10	GLU	-	expression tag	UNP Q9ULW8
A	-9	SER	-	expression tag	UNP Q9ULW8
A	-8	THR	-	expression tag	UNP Q9ULW8
A	-7	SER	-	expression tag	UNP Q9ULW8
A	-6	LEU	-	expression tag	UNP Q9ULW8
A	-5	TYR	-	expression tag	UNP Q9ULW8
A	-4	LYS	-	expression tag	UNP Q9ULW8
A	-3	LYS	-	expression tag	UNP Q9ULW8
A	-2	ALA	-	expression tag	UNP Q9ULW8
A	-1	GLY	-	expression tag	UNP Q9ULW8
A	0	PHE	-	expression tag	UNP Q9ULW8

- Molecule 1: Protein-arginine deiminase type-3



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	115.02Å 115.02Å 328.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.24 – 2.80 49.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-2.80) 100.0 (49.24-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.81Å)	Xtriage
Refinement program	phenix.refine 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.234 , 0.274 0.234 , 0.274	Depositor DCC
R_{free} test set	1035 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4253	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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](#)

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	0.29	0/4353	0.54	0/5937

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	445	VAL	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	4253	0	3780	42	0
All	All	4253	0	3780	42	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 (42) 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:552:ARG:NH2	1:A:563:GLU:OE2	2.10	0.84
1:A:24:GLU:OE2	1:A:60:ARG:NH1	2.12	0.81
1:A:41:GLU:OE2	1:A:67:ARG:NH2	2.17	0.76
1:A:137:ARG:NH1	1:A:287:ASP:OD1	2.20	0.74
1:A:512:LEU:HB2	1:A:515:GLN:HG3	1.76	0.68
1:A:504:GLN:NE2	1:A:529:ASN:OD1	2.26	0.66
1:A:308:VAL:HG12	1:A:650:VAL:HB	1.78	0.66
1:A:327:ALA:O	1:A:331:GLY:N	2.30	0.63
1:A:49:ASP:HB2	1:A:79:VAL:HG12	1.83	0.61
1:A:276:ASN:HB2	1:A:279:PHE:HB2	1.84	0.58
1:A:183:MET:HB3	1:A:249:PHE:HB2	1.87	0.57
1:A:487:ARG:HG3	1:A:624:LEU:HD21	1.88	0.55
1:A:411:GLU:HB3	1:A:429:LEU:O	2.09	0.53
1:A:441:ARG:NH1	1:A:464:ASP:OD1	2.43	0.52
1:A:258:ASP:H	1:A:261:PHE:HB3	1.75	0.52
1:A:187:THR:HG21	1:A:241:ARG:HD2	1.92	0.51
1:A:228:HIS:CE1	1:A:231:GLY:HA3	2.46	0.51
1:A:215:HIS:NE2	1:A:247:GLU:OE2	2.43	0.49
1:A:139:TRP:CD1	1:A:147:GLY:HA3	2.47	0.49
1:A:358:GLN:HB2	1:A:363:THR:HG22	1.95	0.49
1:A:276:ASN:CB	1:A:279:PHE:HB2	2.42	0.49
1:A:183:MET:O	1:A:249:PHE:N	2.39	0.48
1:A:428:ILE:O	1:A:458:PRO:HA	2.15	0.47
1:A:84:SER:O	1:A:190:PRO:HD3	2.15	0.46
1:A:137:ARG:HG2	1:A:288:THR:O	2.15	0.46
1:A:139:TRP:NE1	1:A:147:GLY:HA3	2.32	0.45
1:A:428:ILE:HD13	1:A:450:LEU:HD23	1.99	0.44
1:A:409:ASN:ND2	1:A:471:VAL:H	2.15	0.44
1:A:592:VAL:O	1:A:652:ARG:NH2	2.26	0.44
1:A:602:PRO:HG2	1:A:611:CYS:SG	2.58	0.44
1:A:104:PRO:HG2	1:A:107:TYR:OH	2.19	0.42
1:A:540:TYR:CZ	1:A:575:THR:HG22	2.54	0.42
1:A:263:GLY:O	1:A:292:ARG:HA	2.20	0.42
1:A:300:PRO:HD2	1:A:303:LEU:HG	2.02	0.42
1:A:457:PRO:HA	1:A:458:PRO:HD3	1.82	0.42
1:A:214:PHE:HD1	1:A:228:HIS:HA	1.84	0.41
1:A:409:ASN:HD21	1:A:471:VAL:H	1.67	0.41
1:A:308:VAL:HA	1:A:650:VAL:HA	2.02	0.41
1:A:71:ASP:HB3	1:A:74:LEU:HD13	2.01	0.41
1:A:210:ARG:HG2	1:A:255:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG22	1:A:63:ALA:HB3	2.03	0.41
1:A:395:GLU:HA	1:A:396:PRO:HD3	1.89	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	578/686 (84%)	539 (93%)	39 (7%)	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	390/608 (64%)	385 (99%)	5 (1%)	69	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	289	VAL
1	A	416	VAL
1	A	515	GLN

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Mol	Chain	Res	Type
1	A	544	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	594/686 (86%)	-0.09	17 (2%) 51 41	41, 70, 117, 184	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	CYS	5.0
1	A	337	CYS	4.3
1	A	312	ARG	4.0
1	A	520	ASP	4.0
1	A	316	ASN	3.3
1	A	225	ALA	3.1
1	A	335	THR	2.7
1	A	646	CYS	2.6
1	A	358	GLN	2.6
1	A	154	CYS	2.4
1	A	647	GLY	2.3
1	A	387	PRO	2.3
1	A	214	PHE	2.3
1	A	313	VAL	2.2
1	A	224	GLU	2.1
1	A	518	VAL	2.1
1	A	389	PHE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.