



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:49 PM GMT

PDB ID : 1HD7
Title : A SECOND DIVALENT METAL ION IN THE ACTIVE SITE OF A NEW CRYSTAL FORM OF HUMAN APURINIC/APYRIDINIMIC EN-DONUCLEASE, APE1, AND ITS IMPLICATIONS FOR THE CATALYTIC MECHANISM
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Deposited on : 2000-11-09
Resolution : 1.95 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

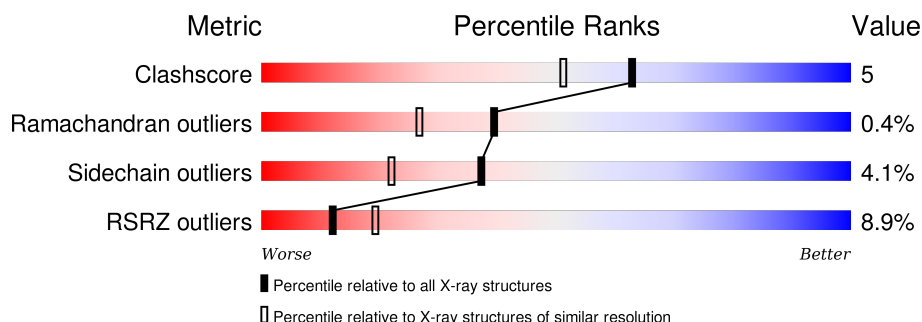
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	318	<div> <div>7%</div> <div>61%</div> <div>17%</div> <div>•</div> <div>19%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2359 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 DNA-(APURINIC OR APYRIMIDINIC SITE) LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2070	1325	359	377	9			

- Molecule 2 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

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

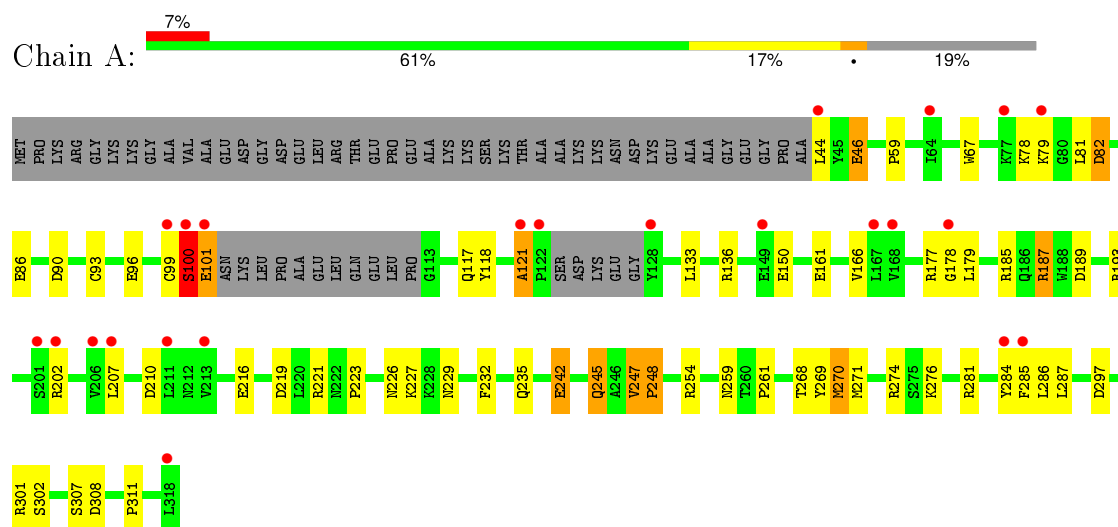
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	288	Total	O	0	0
			288	288		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DNA-(APURINIC OR APYRIMIDINIC SITE) LYASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.39Å 44.85Å 78.14Å 90.00° 124.54° 90.00°	Depositor
Resolution (Å)	25.00 – 1.95 24.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.2 (25.00-1.95) 98.8 (24.97-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.255 0.204 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 62.6	EDS
Estimated twinning fraction	0.019 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33834 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2359	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PB

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	0.85	1/2124 (0.0%)	1.70	45/2876 (1.6%)

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	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	GLY	N-CA	5.07	1.53	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-12.37	114.12	120.30
1	A	136	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	281	ARG	NE-CZ-NH2	-10.77	114.91	120.30
1	A	247	VAL	CA-C-O	-10.37	98.31	120.10
1	A	187	ARG	NE-CZ-NH1	-10.05	115.28	120.30
1	A	281	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	221	ARG	NE-CZ-NH2	8.59	124.59	120.30
1	A	248	PRO	CA-N-CD	-8.51	99.59	111.50
1	A	269	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	A	177	ARG	NH1-CZ-NH2	8.05	128.25	119.40
1	A	96	GLU	OE1-CD-OE2	7.94	132.83	123.30
1	A	185	ARG	NE-CZ-NH1	-7.88	116.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	202	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	A	270	MET	CA-CB-CG	7.32	125.74	113.30
1	A	187	ARG	NH1-CZ-NH2	6.76	126.83	119.40
1	A	136	ARG	NH1-CZ-NH2	-6.39	112.37	119.40
1	A	221	ARG	NH1-CZ-NH2	-6.31	112.45	119.40
1	A	297	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	301	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	99	CYS	CA-C-O	6.11	132.94	120.10
1	A	242	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	A	177	ARG	CG-CD-NE	5.98	124.37	111.80
1	A	90	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	A	287	LEU	CB-CA-C	-5.87	99.05	110.20
1	A	216	GLU	OE1-CD-OE2	-5.86	116.26	123.30
1	A	121	ALA	CB-CA-C	-5.85	101.33	110.10
1	A	101	GLU	N-CA-CB	5.84	121.12	110.60
1	A	235	GLN	CA-CB-CG	5.80	126.17	113.40
1	A	210	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	46	GLU	OE1-CD-OE2	5.59	130.01	123.30
1	A	307	SER	N-CA-CB	-5.58	102.13	110.50
1	A	219	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	232	PHE	CB-CG-CD1	5.43	124.60	120.80
1	A	177	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	285	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	A	189	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	284	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	A	82	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	221	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	78	LYS	O-C-N	-5.27	114.27	122.70
1	A	235	GLN	CG-CD-OE1	5.20	132.00	121.60
1	A	193	ARG	CB-CG-CD	5.20	125.11	111.60
1	A	308	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	96	GLU	CG-CD-OE1	-5.01	108.27	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	GLN	Mainchain
1	A	118	TYR	Mainchain
1	A	179	LEU	Mainchain
1	A	247	VAL	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	A	93	CYS	Mainchain

5.2 Too-close contacts ⓘ

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	2070	0	2045	22	0
2	A	1	0	0	0	0
3	A	288	0	0	4	0
All	All	2359	0	2045	22	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 (22) 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:100:SER:HB3	1:A:121:ALA:HB2	1.61	0.83
1:A:100:SER:CB	1:A:121:ALA:HB2	2.11	0.81
1:A:59:PRO:HD2	3:A:2020:HOH:O	1.90	0.72
1:A:270:MET:HG3	3:A:2251:HOH:O	1.95	0.67
1:A:226:ASN:HD22	1:A:229:ASN:HD22	1.44	0.66
1:A:226:ASN:ND2	1:A:229:ASN:HD22	1.98	0.61
1:A:81:LEU:HB2	3:A:2046:HOH:O	2.03	0.57
1:A:271:MET:HE3	3:A:2137:HOH:O	2.08	0.54
1:A:161:GLU:HG3	1:A:166:VAL:HG22	1.93	0.51
1:A:268:THR:HG23	1:A:270:MET:O	2.11	0.51
1:A:133:LEU:HD23	1:A:133:LEU:C	2.38	0.44
1:A:254:ARG:HD3	1:A:254:ARG:HA	1.85	0.44
1:A:100:SER:HB2	1:A:121:ALA:HB2	1.92	0.44
1:A:223:PRO:O	1:A:227:LYS:HG3	2.17	0.44
1:A:187:ARG:HH11	1:A:187:ARG:HD2	1.49	0.44
1:A:67:TRP:CD2	1:A:311:PRO:HG3	2.54	0.43
1:A:245:GLN:HB3	1:A:245:GLN:HE21	1.50	0.42
1:A:259:ASN:O	1:A:261:PRO:HD3	2.20	0.42
1:A:207:LEU:HD23	1:A:286:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:CD	1:A:187:ARG:HH12	2.23	0.41
1:A:86:GLU:OE1	1:A:86:GLU:HA	2.21	0.41
1:A:79:LYS:O	1:A:82:ASP:HB2	2.21	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	253/318 (80%)	247 (98%)	5 (2%)	1 (0%)	39 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	SER

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	222/266 (84%)	213 (96%)	9 (4%)	37 22

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	46	GLU
1	A	100	SER
1	A	101	GLU
1	A	242	GLU
1	A	245	GLN
1	A	248	PRO
1	A	276	LYS
1	A	302	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	ASN
1	A	245	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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	259/318 (81%)	0.26	23 (8%) 12 19	20, 33, 52, 73	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	SER	7.2
1	A	44	LEU	6.2
1	A	99	CYS	4.1
1	A	211	LEU	3.4
1	A	101	GLU	3.4
1	A	167	LEU	3.2
1	A	202	ARG	3.1
1	A	168	VAL	2.7
1	A	128	TYR	2.6
1	A	213	VAL	2.6
1	A	201	SER	2.6
1	A	64	ILE	2.6
1	A	318	LEU	2.5
1	A	121	ALA	2.5
1	A	207	LEU	2.5
1	A	79	LYS	2.4
1	A	285	PHE	2.3
1	A	206	VAL	2.3
1	A	122	PRO	2.2
1	A	149	GLU	2.2
1	A	77	LYS	2.1
1	A	284	TYR	2.0
1	A	178	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	PB	A	1319	1/1	0.98	0.16	-	84,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.