



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:44 pm GMT

PDB ID : 1J0D
Title : ACC deaminase mutant complexed with ACC
Authors : Ose, T.; Fujino, A.; Yao, M.; Honma, M.; Tanaka, I.
Deposited on : 2002-11-12
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

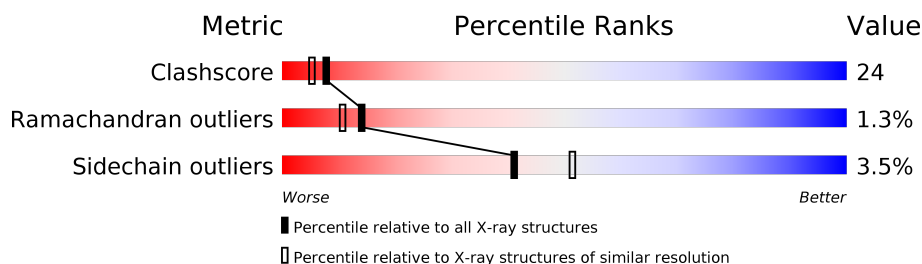
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	341	
1	B	341	
1	C	341	
1	D	341	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5PA	A	1401	-	-	X	-
2	5PA	D	1701	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11443 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 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2605	1653	440	500	12			
1	B	341	Total	C	N	O	S	0	0	0
			2605	1653	440	500	12			
1	C	341	Total	C	N	O	S	0	0	0
			2605	1653	440	500	12			
1	D	341	Total	C	N	O	S	0	0	0
			2605	1653	440	500	12			

There are 8 discrepancies between the modelled and reference sequences:

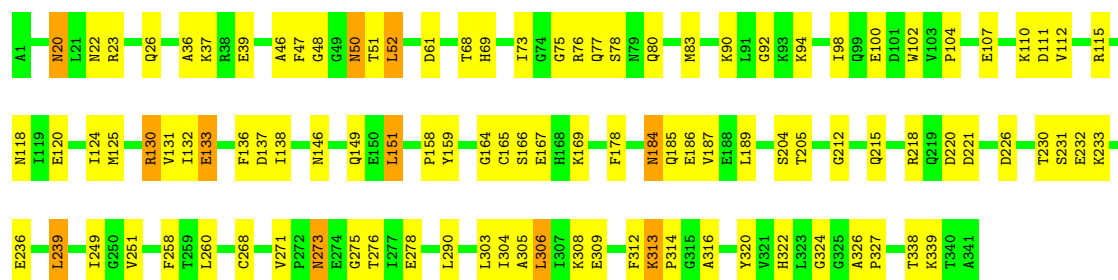
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	SER	ENGINEERED	UNP Q7M523
A	51	THR	LYS	ENGINEERED	UNP Q7M523
B	1	ALA	SER	ENGINEERED	UNP Q7M523
B	51	THR	LYS	ENGINEERED	UNP Q7M523
C	1	ALA	SER	ENGINEERED	UNP Q7M523
C	51	THR	LYS	ENGINEERED	UNP Q7M523
D	1	ALA	SER	ENGINEERED	UNP Q7M523
D	51	THR	LYS	ENGINEERED	UNP Q7M523

- Molecule 2 is N-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-Y-LMETHYL]-1-AMINO-CYCLOPROPANECARBOXYLIC ACID (three-letter code: 5PA) (formula: C₁₂H₁₇N₂O₇P).



- Molecule 3 is water.





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.25Å 267.29Å 187.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	91.1 (10.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.279	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11443	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

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: 5PA

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	0.31	0/2656	0.57	0/3593
1	B	0.31	0/2656	0.56	0/3593
1	C	0.36	0/2656	0.63	1/3593 (0.0%)
1	D	0.40	0/2656	0.63	0/3593
All	All	0.35	0/10624	0.60	1/14372 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	GLY	N-CA-C	5.79	127.57	113.10

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	2605	0	2589	149	0
1	B	2605	0	2589	174	0
1	C	2605	0	2589	89	0
1	D	2605	0	2589	110	1
2	A	22	0	13	8	0
2	B	22	0	13	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	22	0	13	3	0
2	D	22	0	13	16	0
3	A	126	0	0	12	0
3	B	125	0	0	12	0
3	C	366	0	0	22	1
3	D	318	0	0	23	0
All	All	11443	0	10408	500	2

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 24.

The worst 5 of 500 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:77:GLN:HE22	1:B:117:GLY:HA3	1.12	1.07
1:B:116:VAL:HG12	1:B:117:GLY:H	1.17	1.04
1:B:214:ALA:HA	1:B:219:GLN:HE21	1.26	0.99
1:D:164:GLY:HA2	2:D:1701:5PA:H91	1.44	0.98
1:A:116:VAL:HG12	1:A:117:GLY:H	1.28	0.97

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1808:HOH:O	3:C:1808:HOH:O[3_655]	1.49	0.71
1:D:26:GLN:NE2	1:D:26:GLN:NE2[3_655]	2.17	0.03

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	339/341 (99%)	311 (92%)	23 (7%)	5 (2%)	12	9
1	B	339/341 (99%)	286 (84%)	42 (12%)	11 (3%)	5	2
1	C	339/341 (99%)	322 (95%)	16 (5%)	1 (0%)	44	49
1	D	339/341 (99%)	320 (94%)	18 (5%)	1 (0%)	44	49
All	All	1356/1364 (99%)	1239 (91%)	99 (7%)	18 (1%)	14	11

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	ARG
1	B	204	SER
1	B	232	GLU
1	A	2	GLY
1	B	231	SER

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	275/275 (100%)	267 (97%)	8 (3%)	48	60
1	B	275/275 (100%)	268 (98%)	7 (2%)	53	65
1	C	275/275 (100%)	264 (96%)	11 (4%)	36	45
1	D	275/275 (100%)	262 (95%)	13 (5%)	30	37
All	All	1100/1100 (100%)	1061 (96%)	39 (4%)	41	51

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	52	LEU
1	C	236	GLU
1	D	303	LEU
1	C	72	SER
1	C	87	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	219	GLN
1	C	20	ASN
1	D	273	ASN
1	B	273	ASN
1	B	301	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 ⓘ

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	5PA	A	1401	1	19,23,23	2.50	7 (36%)	26,35,35	1.77	6 (23%)
2	5PA	B	1501	1	19,23,23	2.51	7 (36%)	26,35,35	1.77	6 (23%)
2	5PA	C	1601	-	19,23,23	2.50	7 (36%)	26,35,35	1.77	6 (23%)
2	5PA	D	1701	-	19,23,23	2.50	7 (36%)	26,35,35	1.77	6 (23%)

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	5PA	A	1401	1	-	0/9/22/22	0/1/2/2
2	5PA	B	1501	1	-	0/9/22/22	0/1/2/2
2	5PA	C	1601	-	-	0/9/22/22	0/1/2/2
2	5PA	D	1701	-	-	0/9/22/22	0/1/2/2

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1501	5PA	C4A-N	-2.36	1.32	1.45
2	C	1601	5PA	C4A-N	-2.36	1.32	1.45
2	D	1701	5PA	C4A-N	-2.36	1.32	1.45
2	A	1401	5PA	C4A-N	-2.35	1.32	1.45
2	A	1401	5PA	P-O3P	-2.17	1.45	1.54

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1601	5PA	C7-C8-N	-2.71	112.41	116.70
2	D	1701	5PA	C7-C8-N	-2.71	112.41	116.70
2	A	1401	5PA	C7-C8-N	-2.71	112.41	116.70
2	B	1501	5PA	C7-C8-N	-2.70	112.41	116.70
2	C	1601	5PA	C5-C6-N1	-2.43	119.75	123.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1401	5PA	8	0
2	B	1501	5PA	1	0
2	C	1601	5PA	3	0
2	D	1701	5PA	16	0

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 [i](#)

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.