



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 2, 2025 – 12:35 am BST

PDB ID : 2VYC / pdb_00002vyc
Title : Crystal Structure of Acid Induced Arginine Decarboxylase from E. coli
Authors : Andrell, J.; Hicks, M.G.; Palmer, T.; Carpenter, E.P.; Iwata, S.; Maher, M.J.
Deposited on : 2008-07-22
Resolution : 2.40 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

<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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

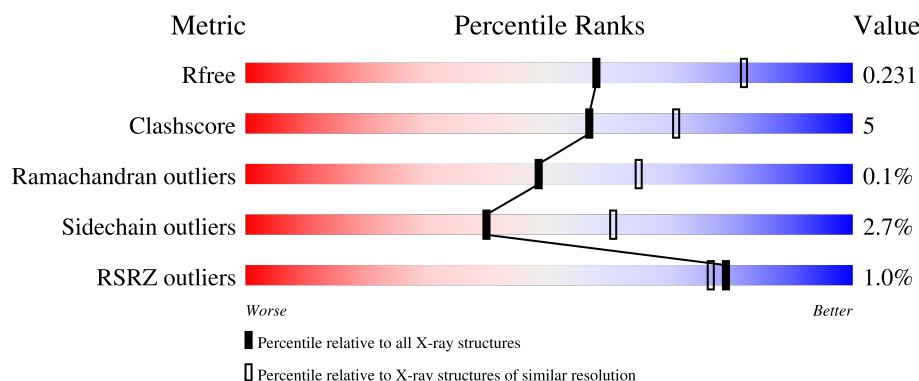
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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	755	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 88%; height: 10px; background-color: green;"></div> <div style="width: 11%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 88% 11% . </div> </div>
1	B	755	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 91% 9% </div> </div>
1	C	755	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: orange;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 87% 13% . </div> </div>
1	D	755	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 90%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 90% 10% . </div> </div>
1	E	755	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> % </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 9%; height: 10px; background-color: yellow;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> 91% 9% </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	755	 87% 12%
1	G	755	 88% 11%
1	H	755	 89% 11%
1	I	755	 89% 11%
1	J	755	 88% 12%

2 Entry composition

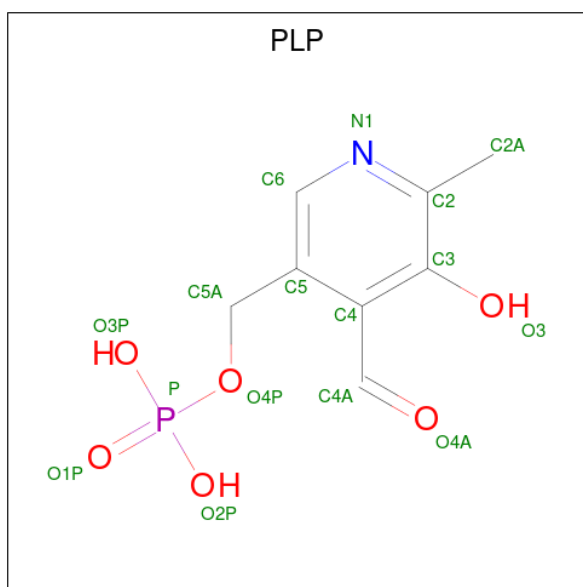
There are 3 unique types of molecules in this entry. The entry contains 62902 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BIODEGRADATIVE ARGININE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	12	0
			6008	3800	1029	1141	38			
1	B	755	Total	C	N	O	S	0	13	0
			6016	3807	1029	1142	38			
1	C	755	Total	C	N	O	S	0	12	0
			6008	3800	1029	1141	38			
1	D	755	Total	C	N	O	S	0	13	0
			6015	3804	1032	1141	38			
1	E	755	Total	C	N	O	S	0	15	0
			6028	3814	1033	1143	38			
1	F	755	Total	C	N	O	S	0	13	0
			6016	3807	1029	1142	38			
1	G	755	Total	C	N	O	S	0	13	0
			6016	3807	1029	1142	38			
1	H	755	Total	C	N	O	S	0	16	0
			6036	3819	1037	1142	38			
1	I	755	Total	C	N	O	S	0	14	0
			6021	3810	1030	1143	38			
1	J	755	Total	C	N	O	S	0	13	0
			6016	3807	1029	1142	38			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	299	Total	O	0	0
			299	299		
3	B	253	Total	O	0	0
			253	253		

Continued on next page...

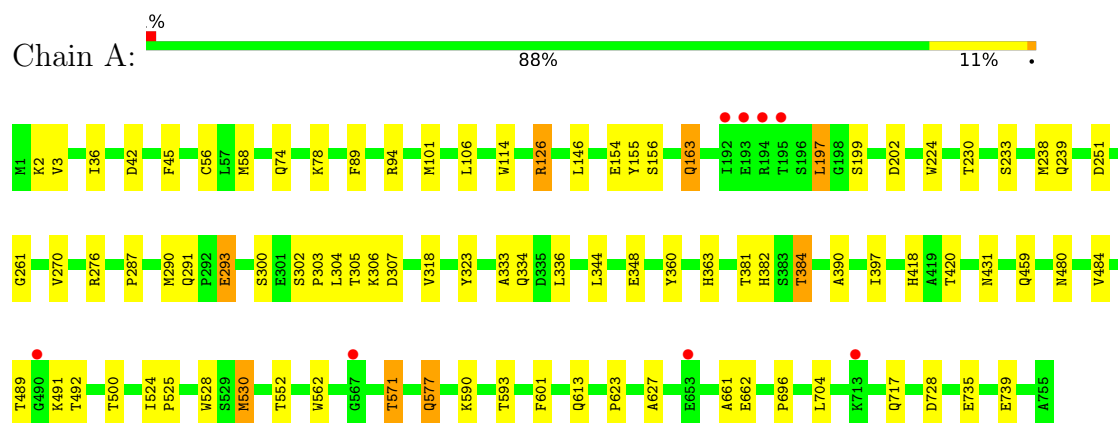
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	219	Total 219	O 219	0	0
3	D	266	Total 266	O 266	0	0
3	E	258	Total 258	O 258	0	0
3	F	268	Total 268	O 268	0	0
3	G	237	Total 237	O 237	0	0
3	H	272	Total 272	O 272	0	0
3	I	262	Total 262	O 262	0	0
3	J	238	Total 238	O 238	0	0

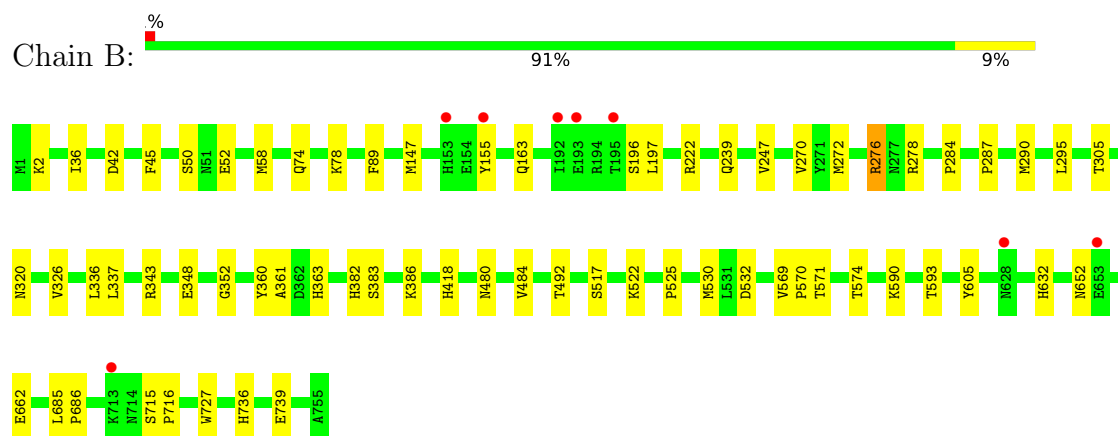
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

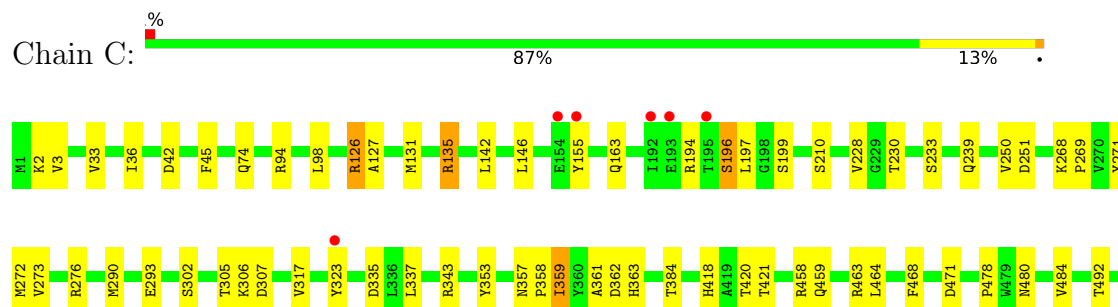
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

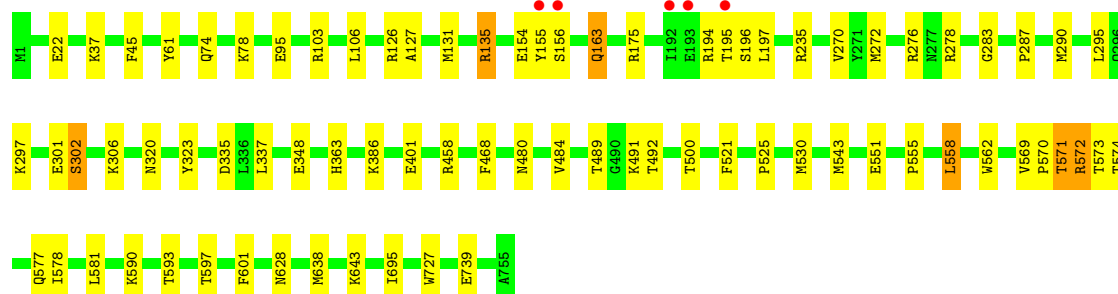


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

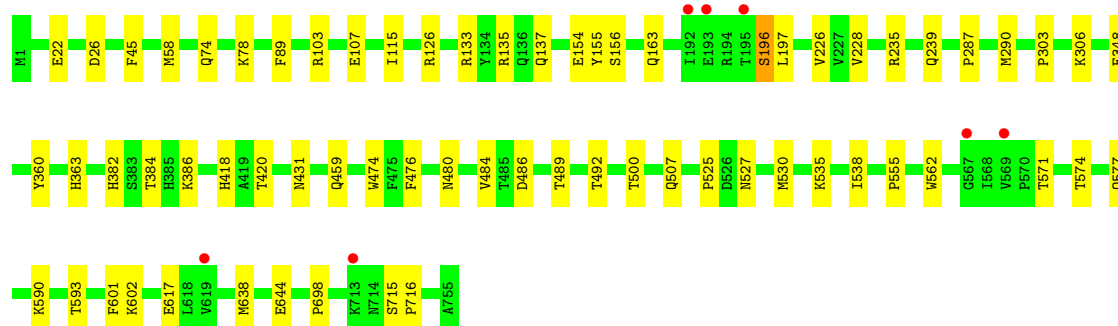




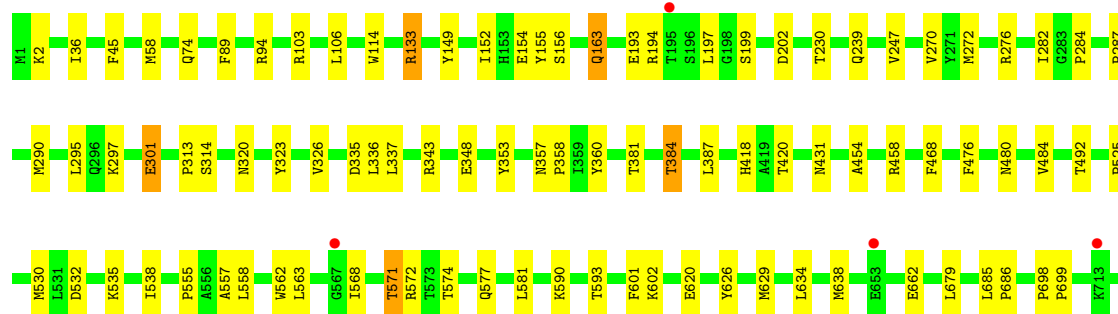
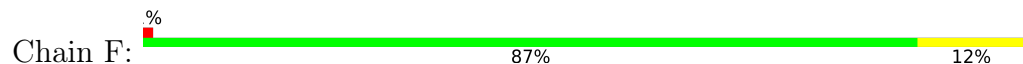
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

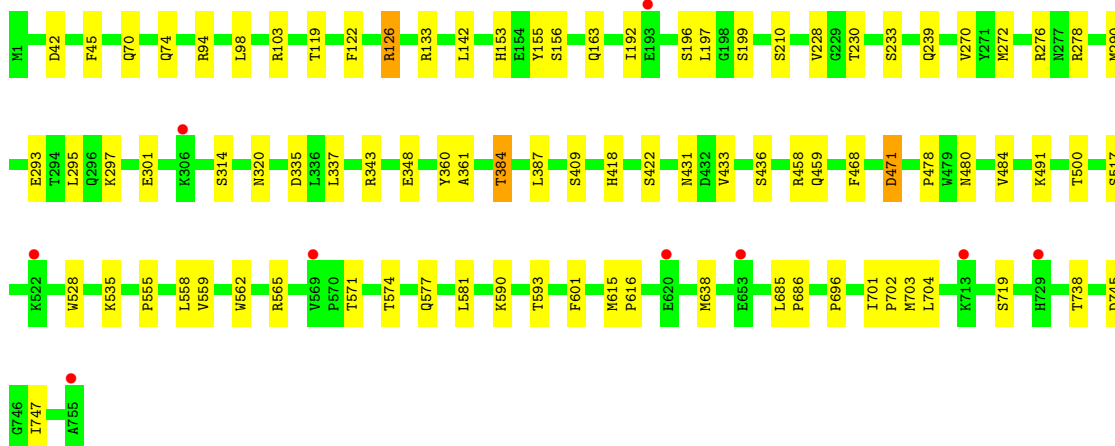
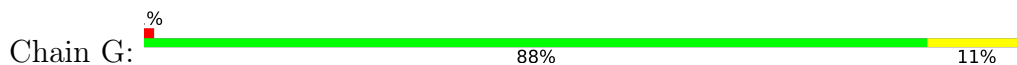


• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE

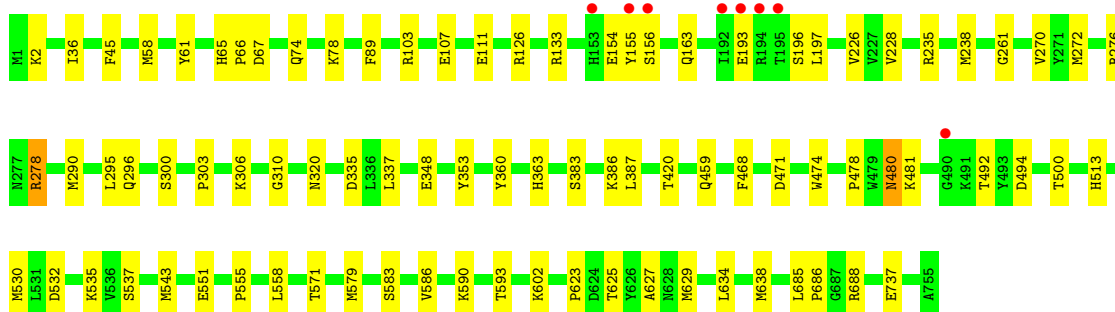
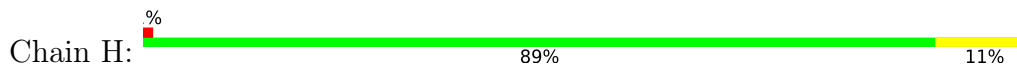




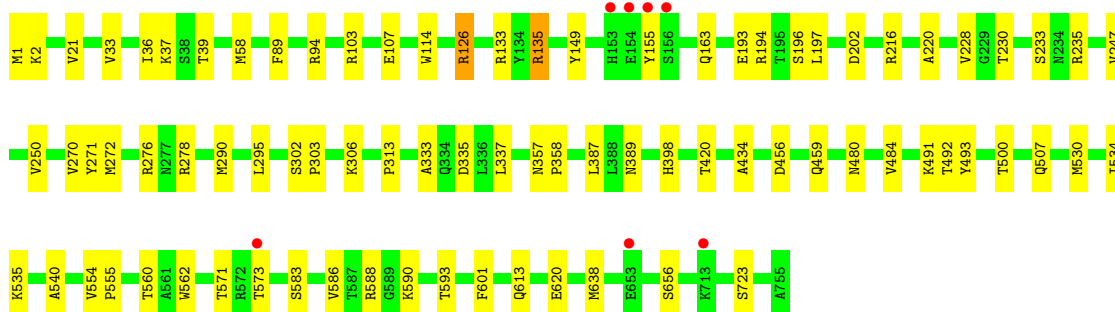
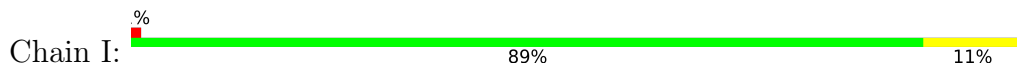
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



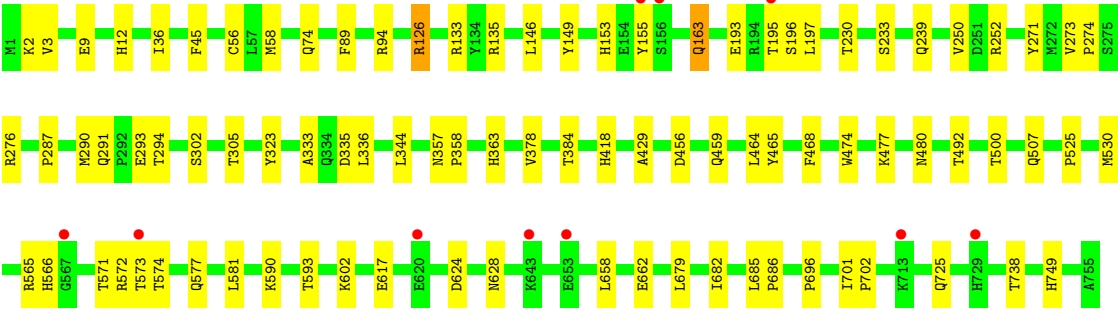
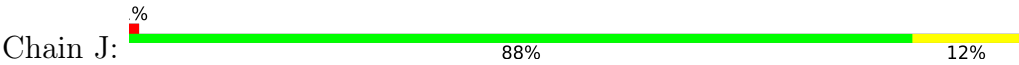
• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



• Molecule 1: BIODEGRADATIVE ARGININE DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	197.65Å 197.65Å 450.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.40) 99.9 (50.00-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.177 , 0.229 0.180 , 0.231	Depositor DCC
R_{free} test set	19417 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	62902	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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

5.1 Standard geometry

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

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	0.61	0/6211	0.67	1/8438 (0.0%)
1	B	0.63	0/6224	0.68	1/8456 (0.0%)
1	C	0.60	0/6211	0.65	3/8438 (0.0%)
1	D	0.65	0/6222	0.69	1/8452 (0.0%)
1	E	0.63	0/6244	0.68	1/8482 (0.0%)
1	F	0.63	0/6224	0.67	0/8456
1	G	0.60	0/6224	0.65	2/8456 (0.0%)
1	H	0.68	0/6257	0.70	3/8499 (0.0%)
1	I	0.65	0/6233	0.70	4/8468 (0.0%)
1	J	0.58	0/6224	0.64	1/8456 (0.0%)
All	All	0.63	0/62274	0.67	17/84601 (0.0%)

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	H	0	1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	235	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	I	235	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	H	235	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	H	688	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	126	ARG	NE-CZ-NH2	-6.70	116.95	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	193	GLU	Peptide

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	6008	0	5762	52	0
1	B	6016	0	5767	41	0
1	C	6008	0	5762	76	0
1	D	6015	0	5771	52	0
1	E	6028	0	5780	40	0
1	F	6016	0	5767	70	0
1	G	6016	0	5767	61	0
1	H	6036	0	5788	64	0
1	I	6021	0	5771	50	0
1	J	6016	0	5767	57	0
2	A	15	0	6	0	0
2	B	15	0	6	1	0
2	C	15	0	6	0	0
2	D	15	0	6	1	0
2	E	15	0	6	1	0
2	F	15	0	6	0	0
2	G	15	0	6	0	0
2	H	15	0	6	1	0
2	I	15	0	6	0	0
2	J	15	0	6	0	0
3	A	299	0	0	3	0
3	B	253	0	0	2	0
3	C	219	0	0	2	0
3	D	266	0	0	5	0
3	E	258	0	0	3	0
3	F	268	0	0	5	0
3	G	237	0	0	2	0
3	H	272	0	0	1	0
3	I	262	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	238	0	0	3	0
All	All	62902	0	57762	535	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.

The worst 5 of 535 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:J:155:TYR:O	1:J:163:GLN:NE2	1.78	1.15
1:C:135[A]:ARG:HG2	1:C:135[A]:ARG:HH11	1.16	1.11
1:I:135[A]:ARG:HH11	1:I:135[A]:ARG:HG2	1.19	1.05
1:E:384:THR:HG21	1:E:431:ASN:OD1	1.63	0.98
1:J:135[B]:ARG:HG2	1:J:135[B]:ARG:HH11	1.29	0.97

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	765/755 (101%)	735 (96%)	30 (4%)	0	100	100
1	B	766/755 (102%)	742 (97%)	22 (3%)	2 (0%)	37	51
1	C	765/755 (101%)	741 (97%)	23 (3%)	1 (0%)	48	65
1	D	766/755 (102%)	747 (98%)	19 (2%)	0	100	100
1	E	768/755 (102%)	745 (97%)	22 (3%)	1 (0%)	48	65
1	F	766/755 (102%)	735 (96%)	31 (4%)	0	100	100
1	G	766/755 (102%)	742 (97%)	24 (3%)	0	100	100
1	H	769/755 (102%)	747 (97%)	22 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	767/755 (102%)	744 (97%)	23 (3%)	0	100	100
1	J	766/755 (102%)	737 (96%)	29 (4%)	0	100	100
All	All	7664/7550 (102%)	7415 (97%)	245 (3%)	4 (0%)	48	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	307	ASP
1	E	196	SER
1	B	196	SER
1	B	361	ALA

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	649/637 (102%)	629 (97%)	20 (3%)	35	56
1	B	650/637 (102%)	637 (98%)	13 (2%)	50	70
1	C	649/637 (102%)	629 (97%)	20 (3%)	35	56
1	D	650/637 (102%)	624 (96%)	26 (4%)	27	45
1	E	652/637 (102%)	639 (98%)	13 (2%)	50	70
1	F	650/637 (102%)	631 (97%)	19 (3%)	37	58
1	G	650/637 (102%)	635 (98%)	15 (2%)	45	66
1	H	653/637 (102%)	631 (97%)	22 (3%)	32	52
1	I	651/637 (102%)	631 (97%)	20 (3%)	35	56
1	J	650/637 (102%)	634 (98%)	16 (2%)	42	63
All	All	6504/6370 (102%)	6320 (97%)	184 (3%)	40	59

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	270	VAL
1	H	558	LEU
1	G	409	SER
1	H	133[B]	ARG
1	I	133[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	19	ASN
1	J	239	GLN
1	G	31	GLN
1	J	163	GLN
1	I	389	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](#)

10 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	PLP	J	1386	1	15,15,16	2.02	4 (26%)	20,22,23	1.75	5 (25%)
2	PLP	D	1386	1	15,15,16	1.90	4 (26%)	20,22,23	1.75	4 (20%)
2	PLP	I	1386	1	15,15,16	2.08	4 (26%)	20,22,23	1.95	4 (20%)
2	PLP	C	1386	1	15,15,16	1.94	3 (20%)	20,22,23	1.72	5 (25%)
2	PLP	A	1386	1	15,15,16	2.05	3 (20%)	20,22,23	1.52	3 (15%)
2	PLP	F	1386	1	15,15,16	1.94	4 (26%)	20,22,23	2.03	7 (35%)
2	PLP	E	1386	1	15,15,16	1.97	4 (26%)	20,22,23	1.65	3 (15%)
2	PLP	B	1386	1	15,15,16	1.91	3 (20%)	20,22,23	1.91	5 (25%)
2	PLP	H	1386	1	15,15,16	1.97	4 (26%)	20,22,23	2.06	4 (20%)
2	PLP	G	1386	1	15,15,16	1.95	4 (26%)	20,22,23	2.01	6 (30%)

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	PLP	J	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	D	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	I	1386	1	-	1/6/6/8	0/1/1/1
2	PLP	C	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	A	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	F	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	E	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	B	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	H	1386	1	-	0/6/6/8	0/1/1/1
2	PLP	G	1386	1	-	0/6/6/8	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1386	PLP	O3-C3	-6.18	1.22	1.37
2	I	1386	PLP	O3-C3	-6.02	1.23	1.37
2	E	1386	PLP	O3-C3	-5.99	1.23	1.37
2	J	1386	PLP	O3-C3	-5.99	1.23	1.37
2	H	1386	PLP	O3-C3	-5.97	1.23	1.37

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1386	PLP	O4P-C5A-C5	6.65	122.03	109.35
2	I	1386	PLP	O4P-C5A-C5	6.16	121.09	109.35
2	G	1386	PLP	O4P-C5A-C5	5.83	120.46	109.35
2	E	1386	PLP	O4P-C5A-C5	5.12	119.11	109.35
2	F	1386	PLP	O4P-C5A-C5	4.97	118.81	109.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1386	PLP	C4-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1386	PLP	1	0
2	E	1386	PLP	1	0
2	B	1386	PLP	1	0
2	H	1386	PLP	1	0

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	755/755 (100%)	-0.49	8 (1%) 77 75	8, 23, 41, 56	16 (2%)
1	B	755/755 (100%)	-0.33	8 (1%) 77 75	10, 22, 40, 55	18 (2%)
1	C	755/755 (100%)	-0.35	10 (1%) 74 71	11, 25, 43, 58	16 (2%)
1	D	755/755 (100%)	-0.62	5 (0%) 84 81	7, 18, 33, 57	16 (2%)
1	E	755/755 (100%)	-0.46	7 (0%) 81 78	8, 20, 38, 54	19 (2%)
1	F	755/755 (100%)	-0.56	4 (0%) 87 85	10, 21, 38, 57	15 (1%)
1	G	755/755 (100%)	-0.35	9 (1%) 76 73	9, 25, 42, 60	20 (2%)
1	H	755/755 (100%)	-0.74	8 (1%) 77 75	6, 15, 31, 59	19 (2%)
1	I	755/755 (100%)	-0.59	7 (0%) 81 78	7, 18, 36, 54	15 (1%)
1	J	755/755 (100%)	-0.31	10 (1%) 74 71	8, 25, 42, 55	17 (2%)
All	All	7550/7550 (100%)	-0.48	76 (1%) 79 76	6, 22, 40, 60	171 (2%)

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	729	HIS	10.9
1	D	193	GLU	8.6
1	C	193	GLU	8.2
1	G	620	GLU	7.6
1	B	628	ASN	7.6

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](#)

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(\AA^2)	Q<0.9
2	PLP	B	1386	15/16	0.94	0.17	2,2,3,5	15
2	PLP	E	1386	15/16	0.95	0.20	2,2,2,4	15
2	PLP	I	1386	15/16	0.95	0.20	2,2,2,4	15
2	PLP	A	1386	15/16	0.96	0.17	2,2,2,4	15
2	PLP	F	1386	15/16	0.96	0.16	2,2,2,3	15
2	PLP	D	1386	15/16	0.96	0.20	2,2,2,2	15
2	PLP	J	1386	15/16	0.96	0.17	2,2,4,6	15
2	PLP	H	1386	15/16	0.97	0.18	2,2,2,2	15
2	PLP	C	1386	15/16	0.97	0.15	2,2,4,6	15
2	PLP	G	1386	15/16	0.97	0.15	2,2,5,8	15

6.5 Other polymers [i](#)

There are no such residues in this entry.