wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2023 – 06:27 AM EDT

PDB ID	:	2ZY5
Title	:	R487A mutant of L-aspartate beta-decarboxylase
Authors	:	Chen, H.-J.; Ko, T.-P.; Lee, C.-Y.; Wang, N.-C.; Wang, A.H.-J.
Deposited on	:	2009-01-13
Resolution	:	2.65 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 (i) 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 (1)) were used in the production of this report:

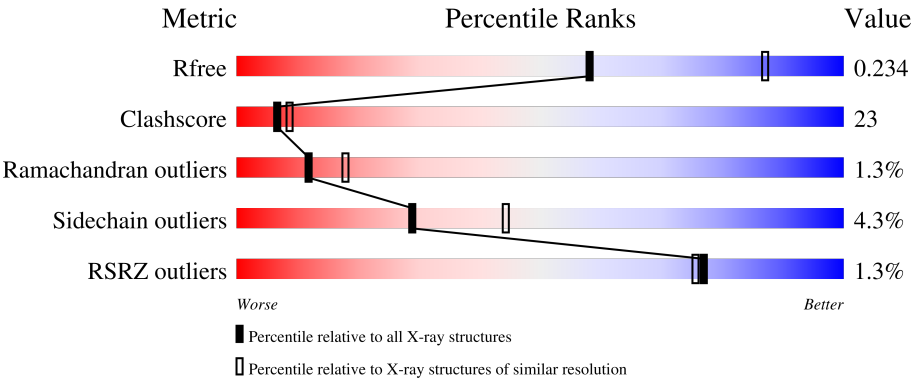
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



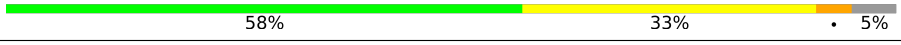
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	546	2% 54% 37% • 7%
1	B	546	% 60% 31% • 6%
1	C	546	% 57% 35% • 6%
1	D	546	% 60% 30% • 6%
1	E	546	2% 54% 37% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	546	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 26213 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 L-aspartate beta-decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4005	2550	681	757	17			
1	B	515	Total	C	N	O	S	0	0	0
			4048	2576	688	767	17			
1	C	515	Total	C	N	O	S	0	0	0
			4048	2576	688	767	17			
1	D	511	Total	C	N	O	S	0	0	0
			4011	2550	685	759	17			
1	E	511	Total	C	N	O	S	0	0	0
			4018	2558	683	760	17			
1	F	521	Total	C	N	O	S	0	0	0
			4094	2605	696	776	17			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	487	ALA	ARG	engineered mutation	UNP Q93QX0
A	534	LYS	-	expression tag	UNP Q93QX0
A	535	LEU	-	expression tag	UNP Q93QX0
A	536	ALA	-	expression tag	UNP Q93QX0
A	537	ALA	-	expression tag	UNP Q93QX0
A	538	ALA	-	expression tag	UNP Q93QX0
A	539	LEU	-	expression tag	UNP Q93QX0
A	540	GLU	-	expression tag	UNP Q93QX0
A	541	HIS	-	expression tag	UNP Q93QX0
A	542	HIS	-	expression tag	UNP Q93QX0
A	543	HIS	-	expression tag	UNP Q93QX0
A	544	HIS	-	expression tag	UNP Q93QX0
A	545	HIS	-	expression tag	UNP Q93QX0
A	546	HIS	-	expression tag	UNP Q93QX0
B	487	ALA	ARG	engineered mutation	UNP Q93QX0
B	534	LYS	-	expression tag	UNP Q93QX0
B	535	LEU	-	expression tag	UNP Q93QX0

Continued on next page...

Continued from previous page...

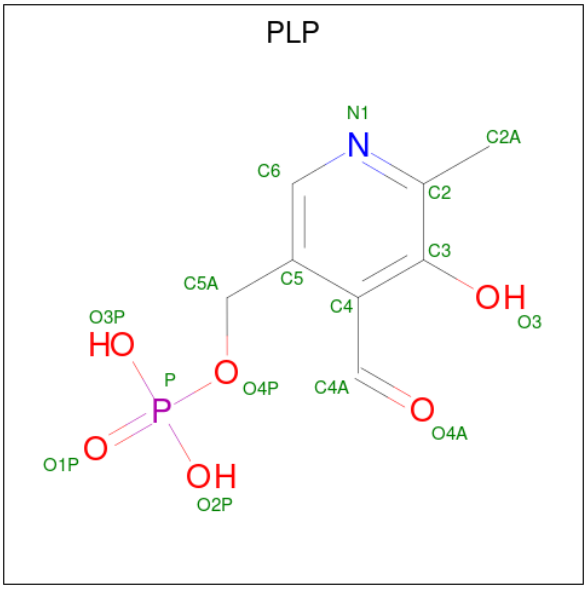
Chain	Residue	Modelled	Actual	Comment	Reference
B	536	ALA	-	expression tag	UNP Q93QX0
B	537	ALA	-	expression tag	UNP Q93QX0
B	538	ALA	-	expression tag	UNP Q93QX0
B	539	LEU	-	expression tag	UNP Q93QX0
B	540	GLU	-	expression tag	UNP Q93QX0
B	541	HIS	-	expression tag	UNP Q93QX0
B	542	HIS	-	expression tag	UNP Q93QX0
B	543	HIS	-	expression tag	UNP Q93QX0
B	544	HIS	-	expression tag	UNP Q93QX0
B	545	HIS	-	expression tag	UNP Q93QX0
B	546	HIS	-	expression tag	UNP Q93QX0
C	487	ALA	ARG	engineered mutation	UNP Q93QX0
C	534	LYS	-	expression tag	UNP Q93QX0
C	535	LEU	-	expression tag	UNP Q93QX0
C	536	ALA	-	expression tag	UNP Q93QX0
C	537	ALA	-	expression tag	UNP Q93QX0
C	538	ALA	-	expression tag	UNP Q93QX0
C	539	LEU	-	expression tag	UNP Q93QX0
C	540	GLU	-	expression tag	UNP Q93QX0
C	541	HIS	-	expression tag	UNP Q93QX0
C	542	HIS	-	expression tag	UNP Q93QX0
C	543	HIS	-	expression tag	UNP Q93QX0
C	544	HIS	-	expression tag	UNP Q93QX0
C	545	HIS	-	expression tag	UNP Q93QX0
C	546	HIS	-	expression tag	UNP Q93QX0
D	487	ALA	ARG	engineered mutation	UNP Q93QX0
D	534	LYS	-	expression tag	UNP Q93QX0
D	535	LEU	-	expression tag	UNP Q93QX0
D	536	ALA	-	expression tag	UNP Q93QX0
D	537	ALA	-	expression tag	UNP Q93QX0
D	538	ALA	-	expression tag	UNP Q93QX0
D	539	LEU	-	expression tag	UNP Q93QX0
D	540	GLU	-	expression tag	UNP Q93QX0
D	541	HIS	-	expression tag	UNP Q93QX0
D	542	HIS	-	expression tag	UNP Q93QX0
D	543	HIS	-	expression tag	UNP Q93QX0
D	544	HIS	-	expression tag	UNP Q93QX0
D	545	HIS	-	expression tag	UNP Q93QX0
D	546	HIS	-	expression tag	UNP Q93QX0
E	487	ALA	ARG	engineered mutation	UNP Q93QX0
E	534	LYS	-	expression tag	UNP Q93QX0
E	535	LEU	-	expression tag	UNP Q93QX0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	536	ALA	-	expression tag	UNP Q93QX0
E	537	ALA	-	expression tag	UNP Q93QX0
E	538	ALA	-	expression tag	UNP Q93QX0
E	539	LEU	-	expression tag	UNP Q93QX0
E	540	GLU	-	expression tag	UNP Q93QX0
E	541	HIS	-	expression tag	UNP Q93QX0
E	542	HIS	-	expression tag	UNP Q93QX0
E	543	HIS	-	expression tag	UNP Q93QX0
E	544	HIS	-	expression tag	UNP Q93QX0
E	545	HIS	-	expression tag	UNP Q93QX0
E	546	HIS	-	expression tag	UNP Q93QX0
F	487	ALA	ARG	engineered mutation	UNP Q93QX0
F	534	LYS	-	expression tag	UNP Q93QX0
F	535	LEU	-	expression tag	UNP Q93QX0
F	536	ALA	-	expression tag	UNP Q93QX0
F	537	ALA	-	expression tag	UNP Q93QX0
F	538	ALA	-	expression tag	UNP Q93QX0
F	539	LEU	-	expression tag	UNP Q93QX0
F	540	GLU	-	expression tag	UNP Q93QX0
F	541	HIS	-	expression tag	UNP Q93QX0
F	542	HIS	-	expression tag	UNP Q93QX0
F	543	HIS	-	expression tag	UNP Q93QX0
F	544	HIS	-	expression tag	UNP Q93QX0
F	545	HIS	-	expression tag	UNP Q93QX0
F	546	HIS	-	expression tag	UNP Q93QX0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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		

- Molecule 3 is water.

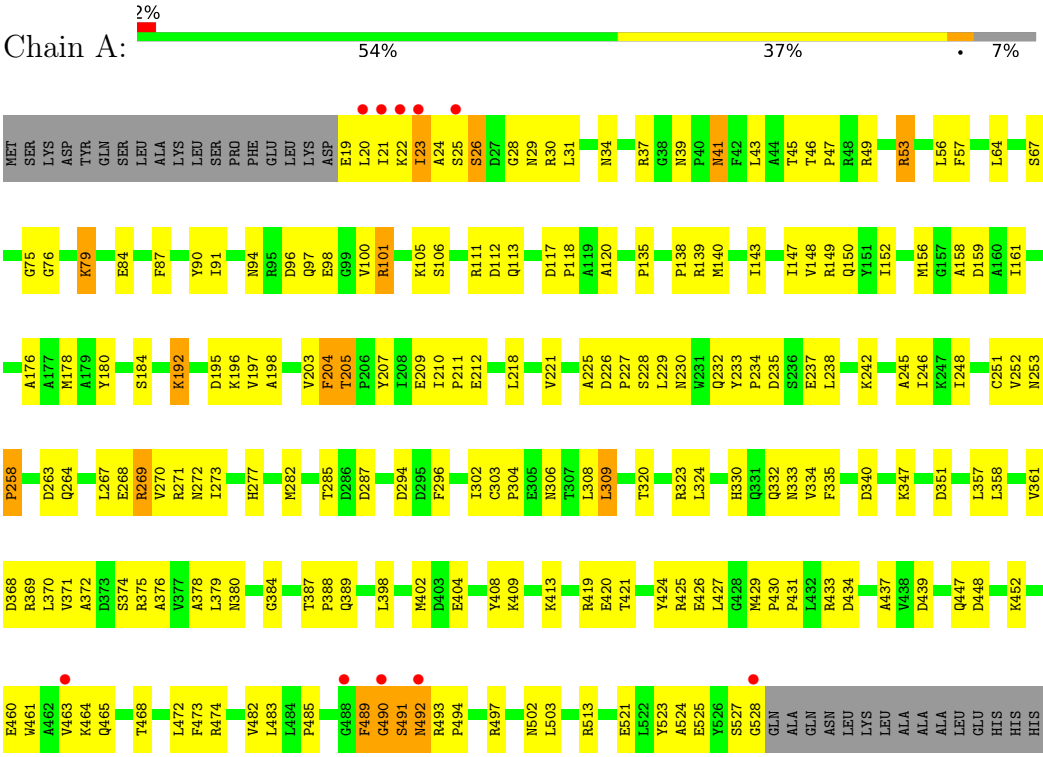
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	318	Total	O	0	0
			318	318		
3	B	355	Total	O	0	0
			355	355		
3	C	337	Total	O	0	0
			337	337		
3	D	342	Total	O	0	0
			342	342		
3	E	282	Total	O	0	0
			282	282		
3	F	265	Total	O	0	0
			265	265		

3 Residue-property plots (i)

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.

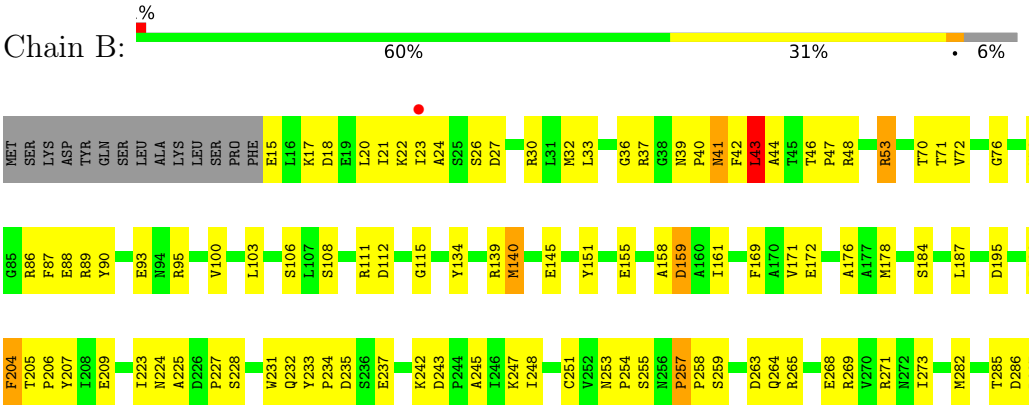
• Molecule 1: L-aspartate beta-decarboxylase

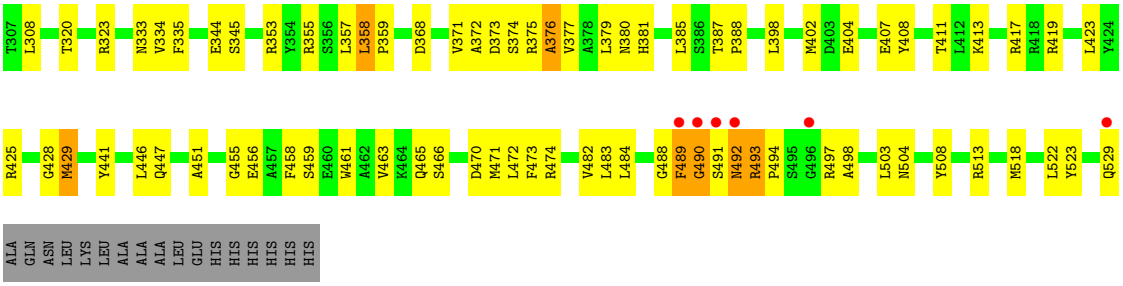
Chain A:



• Molecule 1: L-aspartate beta-decarboxylase

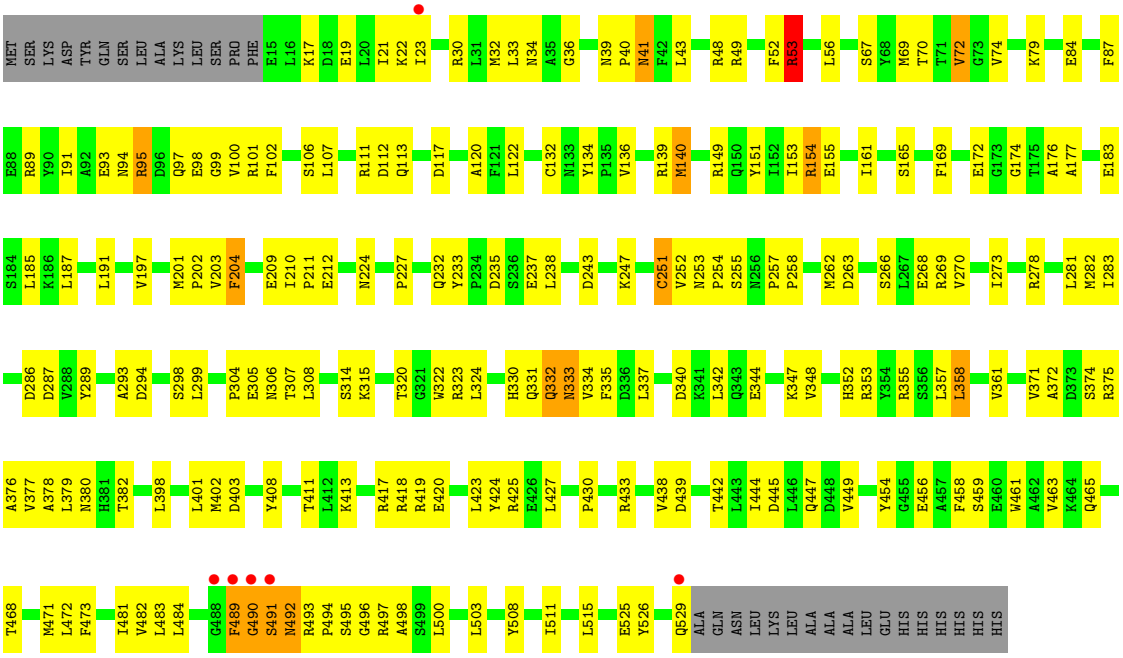
Chain B:





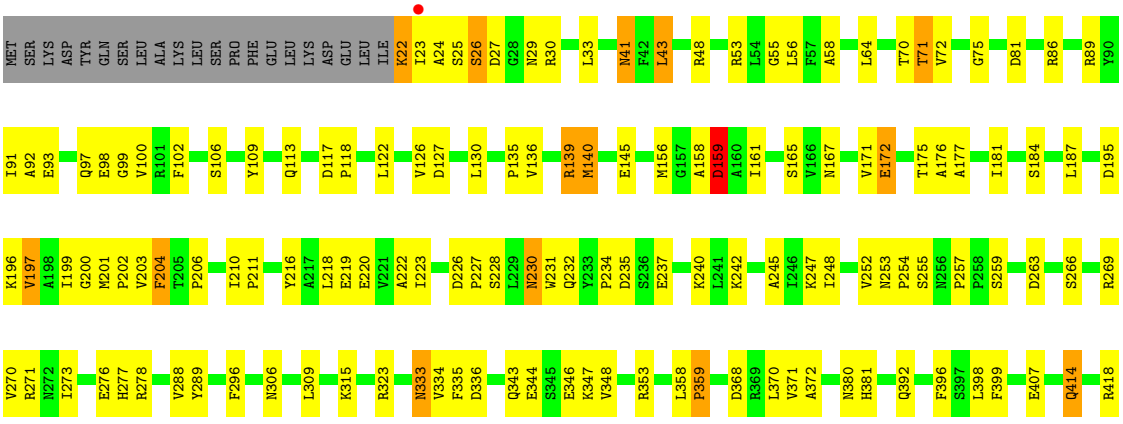
• Molecule 1: L-aspartate beta-decarboxylase

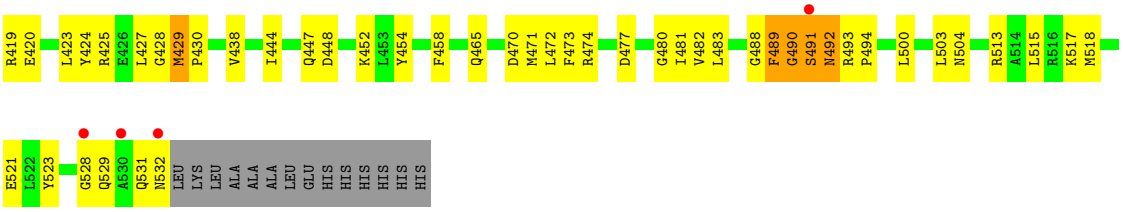
Chain C:



• Molecule 1: L-aspartate beta-decarboxylase

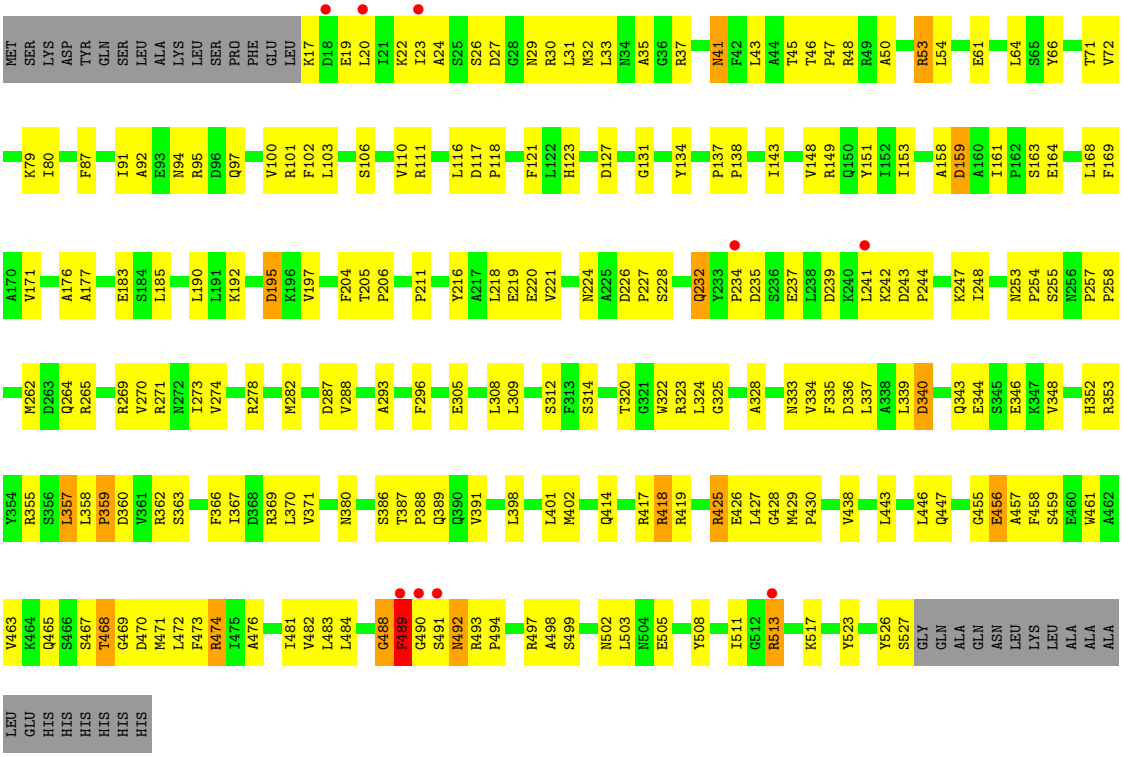
Chain D:





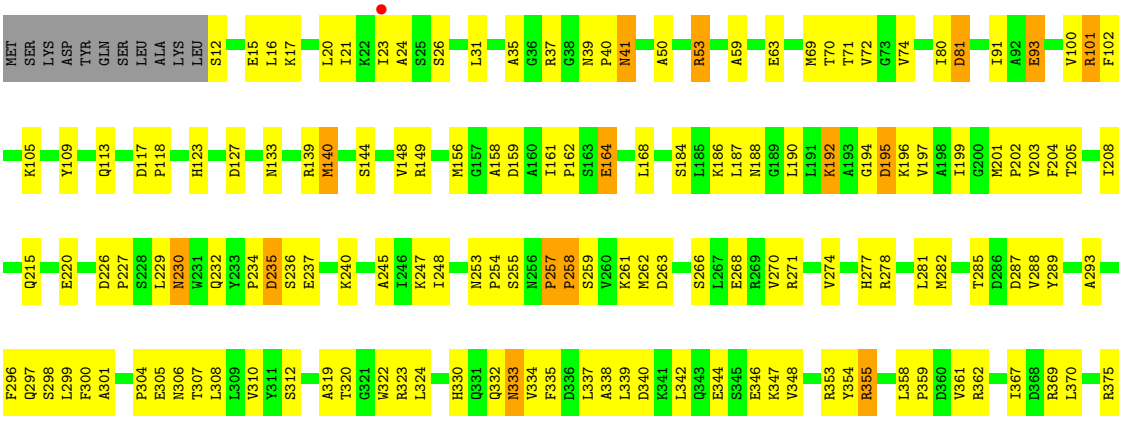
• Molecule 1: L-aspartate beta-decarboxylase

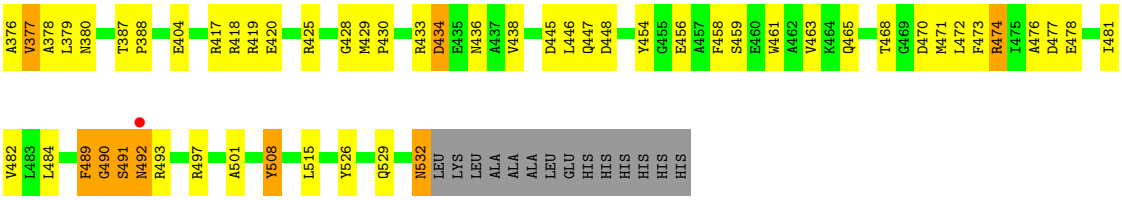
Chain E:



• Molecule 1: L-aspartate beta-decarboxylase

Chain F:




A376 V377 A378 L379 N380 T387 P388 E404 R417 R418 R419 E420 R425 G428 M429 P430 R433 D434 E435 N436 A437 V438 D445 L446 Q447 D448 Y454 G455 E456 A457 F458 S459 E460 W461 A462 V463 K464 Q465 T468 G469 D470 M471 L472 F473 R474 I475 A476 D477 E478 I481
V482 L483 L484 F489 G490 S491 M492 R493 R497 A501 Y508 L515 Y526 Q529 N532 LEU LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	149.95Å 216.22Å 208.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 48.02 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.7 (30.00-2.65) 87.0 (48.02-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.238 0.172 , 0.234	Depositor DCC
R_{free} test set	4320 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26213	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.67	0/4087	0.83	0/5536
1	B	0.69	0/4130	0.86	5/5593 (0.1%)
1	C	0.67	2/4130 (0.0%)	0.86	1/5593 (0.0%)
1	D	0.67	0/4093	0.86	2/5544 (0.0%)
1	E	0.64	0/4100	0.83	1/5553 (0.0%)
1	F	0.69	0/4178	0.85	1/5659 (0.0%)
All	All	0.67	2/24718 (0.0%)	0.85	10/33478 (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	C	0	1
1	D	0	1
1	E	0	2
1	F	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	LYS	CE-NZ	-6.00	1.34	1.49
1	C	251	CYS	CB-SG	-5.50	1.72	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	257	PRO	N-CA-C	7.12	130.61	112.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	488	GLY	O-C-N	6.70	133.42	122.70
1	B	223	ILE	N-CA-C	-5.86	95.17	111.00
1	F	490	GLY	N-CA-C	-5.64	99.00	113.10
1	B	76	GLY	N-CA-C	-5.52	99.30	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	289	TYR	Sidechain
1	D	216	TYR	Sidechain
1	E	134	TYR	Sidechain
1	E	66	TYR	Sidechain
1	F	508	TYR	Sidechain

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	4005	0	3971	218	0
1	B	4048	0	4013	186	0
1	C	4048	0	4013	185	2
1	D	4011	0	3970	184	1
1	E	4018	0	3985	202	0
1	F	4094	0	4052	213	1
2	A	15	0	7	0	0
2	B	15	0	7	1	0
2	C	15	0	7	1	0
2	D	15	0	7	0	0
2	E	15	0	7	0	0
2	F	15	0	6	1	0
3	A	318	0	0	34	0
3	B	355	0	0	22	1
3	C	337	0	0	19	1
3	D	342	0	0	16	0
3	E	282	0	0	19	1
3	F	265	0	0	19	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	26213	0	24045	1136	5

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 23.

The worst 5 of 1136 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:425:ARG:HH12	1:D:159:ASP:CA	1.43	1.31
1:A:21:ILE:HD12	3:A:549:HOH:O	1.32	1.23
1:E:17:LYS:HE3	3:E:1349:HOH:O	1.40	1.21
1:B:425:ARG:NH1	1:D:159:ASP:HA	1.58	1.16
1:D:425:ARG:HH22	1:F:159:ASP:HA	1.01	1.14

All (5) 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:F:1692:HOH:O	3:F:1692:HOH:O[4_566]	1.88	0.32
1:C:529:GLN:NE2	3:B:600:HOH:O[8_456]	1.97	0.23
1:F:72:VAL:O	3:F:856:HOH:O[4_566]	2.04	0.16
1:D:465:GLN:O	3:C:1068:HOH:O[3_756]	2.12	0.08
1:C:425:ARG:NH2	3:E:1465:HOH:O[4_566]	2.14	0.06

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	508/546 (93%)	477 (94%)	26 (5%)	5 (1%)	15 23
1	B	513/546 (94%)	488 (95%)	16 (3%)	9 (2%)	8 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	513/546 (94%)	486 (95%)	22 (4%)	5 (1%)	15 23
1	D	509/546 (93%)	475 (93%)	25 (5%)	9 (2%)	8 12
1	E	509/546 (93%)	451 (89%)	50 (10%)	8 (2%)	9 14
1	F	519/546 (95%)	471 (91%)	43 (8%)	5 (1%)	15 23
All	All	3071/3276 (94%)	2848 (93%)	182 (6%)	41 (1%)	12 18

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	SER
1	B	491	SER
1	C	491	SER
1	C	492	ASN
1	D	491	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	423/454 (93%)	409 (97%)	14 (3%)	38 54
1	B	428/454 (94%)	412 (96%)	16 (4%)	34 50
1	C	428/454 (94%)	409 (96%)	19 (4%)	28 43
1	D	423/454 (93%)	406 (96%)	17 (4%)	31 47
1	E	425/454 (94%)	406 (96%)	19 (4%)	27 42
1	F	433/454 (95%)	408 (94%)	25 (6%)	20 31
All	All	2560/2724 (94%)	2450 (96%)	110 (4%)	29 44

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	172	GLU
1	E	195	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	532	ASN
1	F	236	SER
1	D	204	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	504	ASN
1	F	41	ASN
1	F	447	GLN
1	C	142	ASN
1	C	133	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

6 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	E	900	1	15,15,16	1.81	5 (33%)	20,22,23	1.43	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PLP	C	900	1	15,15,16	2.12	3 (20%)	20,22,23	1.80	4 (20%)
2	PLP	A	900	1	15,15,16	1.78	3 (20%)	20,22,23	2.05	7 (35%)
2	PLP	D	900	1	15,15,16	2.30	7 (46%)	20,22,23	1.99	5 (25%)
2	PLP	B	900	1	15,15,16	2.30	8 (53%)	20,22,23	1.09	2 (10%)
2	PLP	F	900	1	15,15,16	2.02	6 (40%)	20,22,23	1.43	3 (15%)

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	E	900	1	-	1/6/6/8	0/1/1/1
2	PLP	C	900	1	-	0/6/6/8	0/1/1/1
2	PLP	A	900	1	-	3/6/6/8	0/1/1/1
2	PLP	D	900	1	-	1/6/6/8	0/1/1/1
2	PLP	B	900	1	-	2/6/6/8	0/1/1/1
2	PLP	F	900	1	-	0/6/6/8	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	PLP	C3-C2	-5.25	1.35	1.40
2	F	900	PLP	C4A-C4	5.01	1.62	1.51
2	B	900	PLP	C3-C2	4.54	1.45	1.40
2	D	900	PLP	C2-N1	4.35	1.42	1.33
2	C	900	PLP	C4A-C4	4.26	1.60	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	PLP	O4P-P-O1P	-5.21	91.86	106.47
2	D	900	PLP	O4P-C5A-C5	4.88	118.64	109.35
2	C	900	PLP	O2P-P-O4P	-4.67	94.30	106.73
2	F	900	PLP	O4P-C5A-C5	-4.30	101.15	109.35
2	D	900	PLP	O2P-P-O4P	-4.16	95.67	106.73

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	PLP	C5A-O4P-P-O2P
2	B	900	PLP	C5A-O4P-P-O2P
2	B	900	PLP	C5A-O4P-P-O3P
2	E	900	PLP	C5A-O4P-P-O1P
2	A	900	PLP	C5A-O4P-P-O1P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	PLP	1	0
2	B	900	PLP	1	0
2	F	900	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

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, 95^{th} 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	510/546 (93%)	-0.41	10 (1%)	65	60	19, 38, 77, 117	0
1	B	515/546 (94%)	-0.49	7 (1%)	75	73	18, 34, 67, 101	0
1	C	515/546 (94%)	-0.51	6 (1%)	79	77	14, 35, 65, 115	0
1	D	511/546 (93%)	-0.48	5 (0%)	82	81	17, 34, 54, 115	0
1	E	511/546 (93%)	-0.27	9 (1%)	68	65	20, 42, 74, 117	0
1	F	521/546 (95%)	-0.53	2 (0%)	92	93	18, 36, 64, 117	0
All	All	3083/3276 (94%)	-0.45	39 (1%)	77	75	14, 36, 69, 117	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	ILE	5.4
1	A	23	ILE	5.3
1	B	23	ILE	5.2
1	D	491	SER	4.0
1	D	530	ALA	3.8

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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, 95^{th} 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(Å^2)	Q<0.9
2	PLP	A	900	15/16	0.98	0.14	26,30,33,33	0
2	PLP	B	900	15/16	0.98	0.14	22,25,28,29	0
2	PLP	D	900	15/16	0.98	0.12	26,29,33,34	0
2	PLP	E	900	15/16	0.98	0.16	26,36,39,41	0
2	PLP	F	900	15/16	0.98	0.14	26,29,33,33	0
2	PLP	C	900	15/16	0.99	0.12	20,22,24,25	0

6.5 Other polymers (i)

There are no such residues in this entry.