



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 03:24 am GMT

PDB ID : 3V9I  
Title : Crystal structure of human 1-pyrroline-5-carboxylate dehydrogenase mutant S352L  
Authors : Tanner, J.J.; Singh, R.K.  
Deposited on : 2011-12-27  
Resolution : 2.85 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

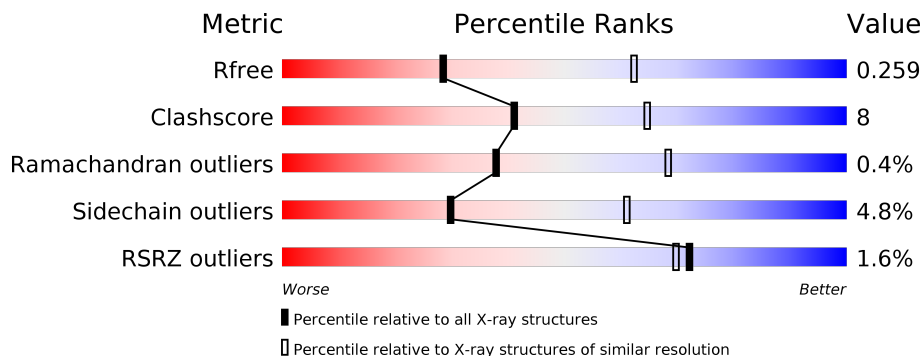
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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  $\geq 3$ , 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	566	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	566	<div> <div></div> <div>72%</div> <div>15%</div> <div>•</div> <div>11%</div> </div>
1	C	566	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	566	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>•</div> <div>15%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13924 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 Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	0	0
			3738	2414	627	682	15			
1	B	502	Total	C	N	O	S	0	0	0
			3587	2324	599	650	14			
1	C	492	Total	C	N	O	S	0	0	0
			3496	2253	588	642	13			
1	D	482	Total	C	N	O	S	0	0	0
			3103	1974	547	571	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P30038
A	-1	GLY	-	EXPRESSION TAG	UNP P30038
A	0	SER	-	EXPRESSION TAG	UNP P30038
A	1	SER	-	EXPRESSION TAG	UNP P30038
A	2	HIS	-	EXPRESSION TAG	UNP P30038
A	3	HIS	-	EXPRESSION TAG	UNP P30038
A	4	HIS	-	EXPRESSION TAG	UNP P30038
A	5	HIS	-	EXPRESSION TAG	UNP P30038
A	6	HIS	-	EXPRESSION TAG	UNP P30038
A	7	HIS	-	EXPRESSION TAG	UNP P30038
A	8	SER	-	EXPRESSION TAG	UNP P30038
A	9	SER	-	EXPRESSION TAG	UNP P30038
A	10	GLY	-	EXPRESSION TAG	UNP P30038
A	11	LEU	-	EXPRESSION TAG	UNP P30038
A	12	VAL	-	EXPRESSION TAG	UNP P30038
A	13	PRO	-	EXPRESSION TAG	UNP P30038
A	14	ARG	-	EXPRESSION TAG	UNP P30038
A	15	GLY	-	EXPRESSION TAG	UNP P30038
A	16	SER	-	EXPRESSION TAG	UNP P30038
A	17	HIS	-	EXPRESSION TAG	UNP P30038
A	352	LEU	SER	ENGINEERED MUTATION	UNP P30038

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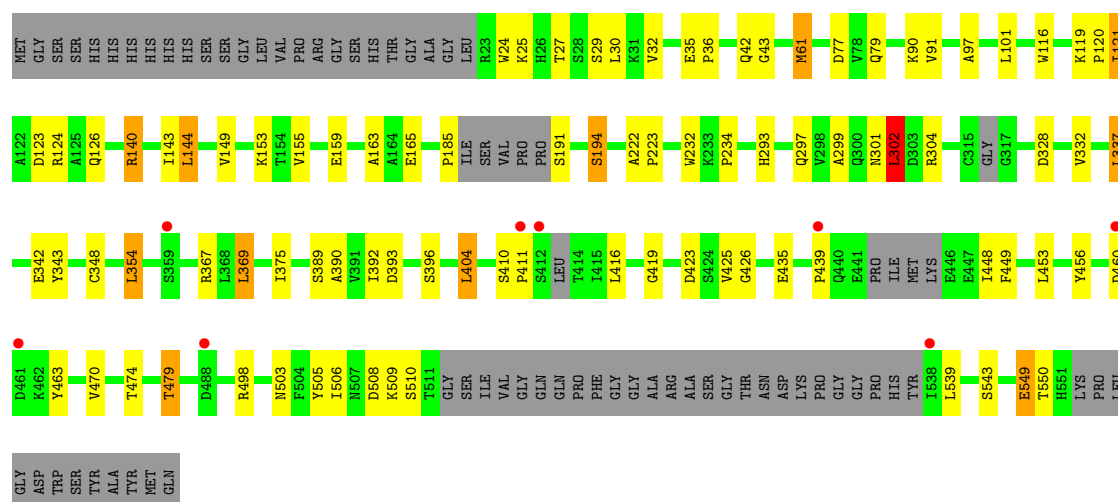
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	EXPRESSION TAG	UNP P30038
B	-1	GLY	-	EXPRESSION TAG	UNP P30038
B	0	SER	-	EXPRESSION TAG	UNP P30038
B	1	SER	-	EXPRESSION TAG	UNP P30038
B	2	HIS	-	EXPRESSION TAG	UNP P30038
B	3	HIS	-	EXPRESSION TAG	UNP P30038
B	4	HIS	-	EXPRESSION TAG	UNP P30038
B	5	HIS	-	EXPRESSION TAG	UNP P30038
B	6	HIS	-	EXPRESSION TAG	UNP P30038
B	7	HIS	-	EXPRESSION TAG	UNP P30038
B	8	SER	-	EXPRESSION TAG	UNP P30038
B	9	SER	-	EXPRESSION TAG	UNP P30038
B	10	GLY	-	EXPRESSION TAG	UNP P30038
B	11	LEU	-	EXPRESSION TAG	UNP P30038
B	12	VAL	-	EXPRESSION TAG	UNP P30038
B	13	PRO	-	EXPRESSION TAG	UNP P30038
B	14	ARG	-	EXPRESSION TAG	UNP P30038
B	15	GLY	-	EXPRESSION TAG	UNP P30038
B	16	SER	-	EXPRESSION TAG	UNP P30038
B	17	HIS	-	EXPRESSION TAG	UNP P30038
B	352	LEU	SER	ENGINEERED MUTATION	UNP P30038
C	-2	MET	-	EXPRESSION TAG	UNP P30038
C	-1	GLY	-	EXPRESSION TAG	UNP P30038
C	0	SER	-	EXPRESSION TAG	UNP P30038
C	1	SER	-	EXPRESSION TAG	UNP P30038
C	2	HIS	-	EXPRESSION TAG	UNP P30038
C	3	HIS	-	EXPRESSION TAG	UNP P30038
C	4	HIS	-	EXPRESSION TAG	UNP P30038
C	5	HIS	-	EXPRESSION TAG	UNP P30038
C	6	HIS	-	EXPRESSION TAG	UNP P30038
C	7	HIS	-	EXPRESSION TAG	UNP P30038
C	8	SER	-	EXPRESSION TAG	UNP P30038
C	9	SER	-	EXPRESSION TAG	UNP P30038
C	10	GLY	-	EXPRESSION TAG	UNP P30038
C	11	LEU	-	EXPRESSION TAG	UNP P30038
C	12	VAL	-	EXPRESSION TAG	UNP P30038
C	13	PRO	-	EXPRESSION TAG	UNP P30038
C	14	ARG	-	EXPRESSION TAG	UNP P30038
C	15	GLY	-	EXPRESSION TAG	UNP P30038
C	16	SER	-	EXPRESSION TAG	UNP P30038
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C	352	LEU	SER	ENGINEERED MUTATION	UNP P30038

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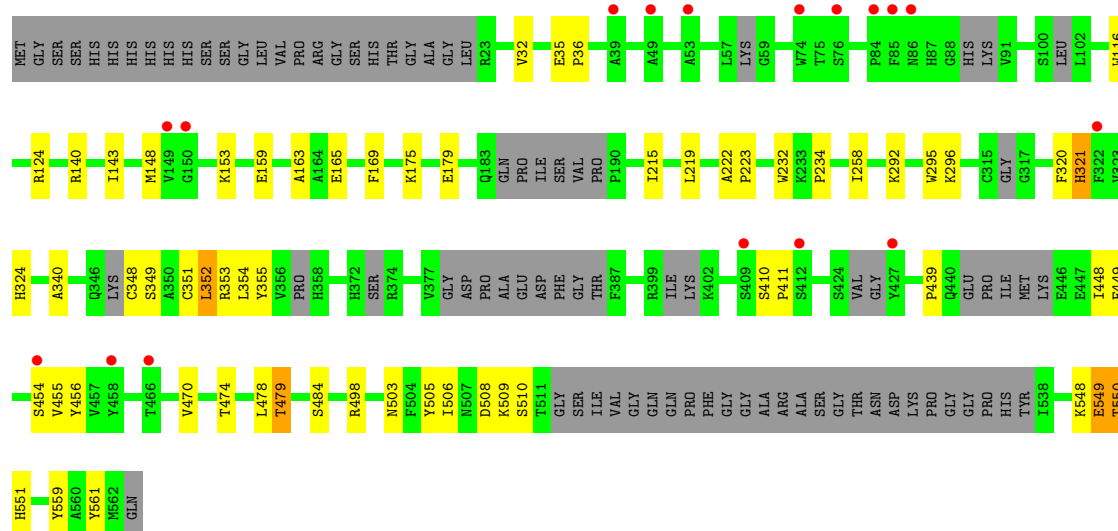
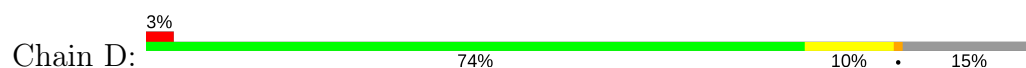
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	EXPRESSION TAG	UNP P30038
D	-1	GLY	-	EXPRESSION TAG	UNP P30038
D	0	SER	-	EXPRESSION TAG	UNP P30038
D	1	SER	-	EXPRESSION TAG	UNP P30038
D	2	HIS	-	EXPRESSION TAG	UNP P30038
D	3	HIS	-	EXPRESSION TAG	UNP P30038
D	4	HIS	-	EXPRESSION TAG	UNP P30038
D	5	HIS	-	EXPRESSION TAG	UNP P30038
D	6	HIS	-	EXPRESSION TAG	UNP P30038
D	7	HIS	-	EXPRESSION TAG	UNP P30038
D	8	SER	-	EXPRESSION TAG	UNP P30038
D	9	SER	-	EXPRESSION TAG	UNP P30038
D	10	GLY	-	EXPRESSION TAG	UNP P30038
D	11	LEU	-	EXPRESSION TAG	UNP P30038
D	12	VAL	-	EXPRESSION TAG	UNP P30038
D	13	PRO	-	EXPRESSION TAG	UNP P30038
D	14	ARG	-	EXPRESSION TAG	UNP P30038
D	15	GLY	-	EXPRESSION TAG	UNP P30038
D	16	SER	-	EXPRESSION TAG	UNP P30038
D	17	HIS	-	EXPRESSION TAG	UNP P30038
D	352	LEU	SER	ENGINEERED MUTATION	UNP P30038





● Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.38Å 150.38Å 192.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.83 – 2.85 45.71 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.83-2.85) 97.1 (45.71-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.209 , 0.264 0.204 , 0.259	Depositor DCC
$R_{free}$ test set	1340 reflections (2.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 67.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.58	1/3834 (0.0%)	0.82	15/5239 (0.3%)
1	B	0.59	3/3677 (0.1%)	0.73	10/5038 (0.2%)
1	C	0.50	0/3579	0.71	9/4898 (0.2%)
1	D	0.42	0/3164	0.67	6/4343 (0.1%)
All	All	0.53	4/14254 (0.0%)	0.74	40/19518 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	GLU	CD-OE1	8.75	1.35	1.25
1	B	371	GLU	CD-OE2	7.46	1.33	1.25
1	B	371	GLU	CG-CD	6.95	1.62	1.51
1	A	425	VAL	CB-CG2	-5.05	1.42	1.52

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH2	-15.99	112.30	120.30
1	A	140	ARG	NE-CZ-NH1	14.29	127.44	120.30
1	B	498	ARG	NE-CZ-NH1	-13.28	113.66	120.30
1	D	140	ARG	NE-CZ-NH1	13.24	126.92	120.30
1	A	304	ARG	NE-CZ-NH1	-12.97	113.81	120.30

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	3738	0	3492	67	0
1	B	3587	0	3236	60	0
1	C	3496	0	3151	58	0
1	D	3103	0	2428	42	0
All	All	13924	0	12307	212	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 8.

The worst 5 of 212 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:C:506:ILE:HB	1:D:549:GLU:HG3	1.52	0.91
1:B:439:PRO:HB3	1:B:469:LEU:HD11	1.58	0.86
1:D:354:LEU:HD22	1:D:455:VAL:HG13	1.59	0.82
1:C:299:ALA:HA	1:C:302:LEU:HD12	1.62	0.82
1:C:470:VAL:O	1:C:474:THR:HG23	1.82	0.79

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	498/566 (88%)	477 (96%)	20 (4%)	1 (0%)	51	80
1	B	492/566 (87%)	462 (94%)	25 (5%)	5 (1%)	18	46
1	C	480/566 (85%)	459 (96%)	20 (4%)	1 (0%)	51	80
1	D	454/566 (80%)	431 (95%)	22 (5%)	1 (0%)	51	80
All	All	1924/2264 (85%)	1829 (95%)	87 (4%)	8 (0%)	38	68

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	HIS
1	D	352	LEU
1	B	408	ARG
1	B	405	GLU
1	B	164	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	357/464 (77%)	340 (95%)	17 (5%)	30	61
1	B	315/464 (68%)	301 (96%)	14 (4%)	33	64
1	C	311/464 (67%)	292 (94%)	19 (6%)	22	49
1	D	201/464 (43%)	194 (96%)	7 (4%)	41	73
All	All	1184/1856 (64%)	1127 (95%)	57 (5%)	30	61

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	460	ASP
1	C	27	THR
1	D	321	HIS
1	B	463	TYR
1	B	469	LEU

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

### 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 [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	506/566 (89%)	-0.07	5 (0%) 82 81	26, 47, 77, 115	0
1	B	502/566 (88%)	-0.12	2 (0%) 92 92	25, 52, 81, 117	0
1	C	492/566 (86%)	-0.13	8 (1%) 72 70	28, 56, 82, 113	0
1	D	482/566 (85%)	0.10	17 (3%) 44 38	24, 67, 104, 136	0
All	All	1982/2264 (87%)	-0.06	32 (1%) 72 70	24, 55, 90, 136	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	ALA	4.6
1	D	409	SER	4.4
1	D	149	VAL	4.2
1	D	427	TYR	4.1
1	D	84	PRO	3.4

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.