



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 01:01 am BST

PDB ID : 3RJL  
Title : Crystal structure of 1-pyrroline-5-carboxylate dehydrogenase from *Bacillus licheniformis* (Target NYSGRC-000337)  
Authors : Patskovsky, Y.; Toro, R.; Foti, R.; Seidel, R.D.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRC)  
Deposited on : 2011-04-15  
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](mailto: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.

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

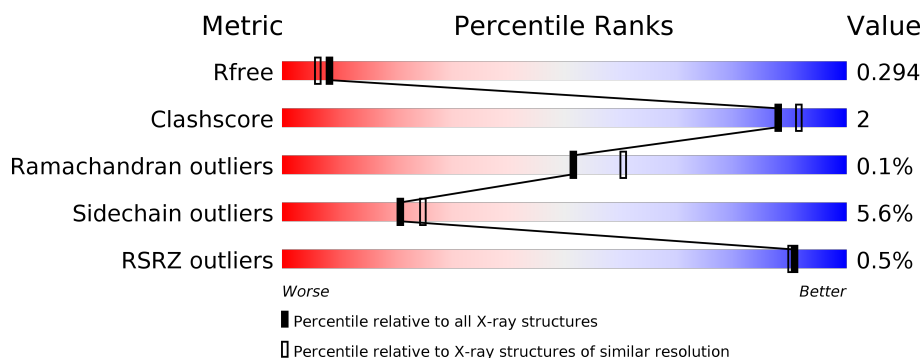
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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  $\geq 3$ , 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	538	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	538	<div> <div>85%</div> <div>10%</div> <div></div> </div>
1	C	538	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
1	D	538	<div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	E	538	<div> <div>87%</div> <div>8%</div> <div>5%</div> </div>
1	F	538	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	538	 87% 8% 5%
1	H	538	 88% 7% 5%

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
3	ACT	A	548	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32569 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-pyrroline-5-carboxylate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	3	0
			3984	2532	671	767	14			
1	B	514	Total	C	N	O	S	0	2	0
			3983	2531	671	768	13			
1	C	513	Total	C	N	O	S	0	2	0
			3983	2531	671	768	13			
1	D	513	Total	C	N	O	S	0	3	0
			3987	2534	670	770	13			
1	E	513	Total	C	N	O	S	0	1	0
			3975	2526	670	766	13			
1	F	513	Total	C	N	O	S	0	1	0
			3975	2526	670	766	13			
1	G	513	Total	C	N	O	S	0	0	0
			3965	2519	667	766	13			
1	H	513	Total	C	N	O	S	0	1	0
			3965	2521	667	764	13			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	517	ALA	-	EXPRESSION TAG	UNP Q65NN2
A	518	GLU	-	EXPRESSION TAG	UNP Q65NN2
A	519	ASN	-	EXPRESSION TAG	UNP Q65NN2
A	520	LEU	-	EXPRESSION TAG	UNP Q65NN2
A	521	TYR	-	EXPRESSION TAG	UNP Q65NN2
A	522	PHE	-	EXPRESSION TAG	UNP Q65NN2
A	523	GLN	-	EXPRESSION TAG	UNP Q65NN2
A	524	SER	-	EXPRESSION TAG	UNP Q65NN2
A	525	HIS	-	EXPRESSION TAG	UNP Q65NN2
A	526	HIS	-	EXPRESSION TAG	UNP Q65NN2
A	527	HIS	-	EXPRESSION TAG	UNP Q65NN2
A	528	HIS	-	EXPRESSION TAG	UNP Q65NN2
A	529	HIS	-	EXPRESSION TAG	UNP Q65NN2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	530	HIS	-	EXPRESSION TAG	UNP Q65NN2
A	531	TRP	-	EXPRESSION TAG	UNP Q65NN2
A	532	SER	-	EXPRESSION TAG	UNP Q65NN2
A	533	HIS	-	EXPRESSION TAG	UNP Q65NN2
A	534	PRO	-	EXPRESSION TAG	UNP Q65NN2
A	535	GLN	-	EXPRESSION TAG	UNP Q65NN2
A	536	PHE	-	EXPRESSION TAG	UNP Q65NN2
A	537	GLU	-	EXPRESSION TAG	UNP Q65NN2
A	538	LYS	-	EXPRESSION TAG	UNP Q65NN2
B	517	ALA	-	EXPRESSION TAG	UNP Q65NN2
B	518	GLU	-	EXPRESSION TAG	UNP Q65NN2
B	519	ASN	-	EXPRESSION TAG	UNP Q65NN2
B	520	LEU	-	EXPRESSION TAG	UNP Q65NN2
B	521	TYR	-	EXPRESSION TAG	UNP Q65NN2
B	522	PHE	-	EXPRESSION TAG	UNP Q65NN2
B	523	GLN	-	EXPRESSION TAG	UNP Q65NN2
B	524	SER	-	EXPRESSION TAG	UNP Q65NN2
B	525	HIS	-	EXPRESSION TAG	UNP Q65NN2
B	526	HIS	-	EXPRESSION TAG	UNP Q65NN2
B	527	HIS	-	EXPRESSION TAG	UNP Q65NN2
B	528	HIS	-	EXPRESSION TAG	UNP Q65NN2
B	529	HIS	-	EXPRESSION TAG	UNP Q65NN2
B	530	HIS	-	EXPRESSION TAG	UNP Q65NN2
B	531	TRP	-	EXPRESSION TAG	UNP Q65NN2
B	532	SER	-	EXPRESSION TAG	UNP Q65NN2
B	533	HIS	-	EXPRESSION TAG	UNP Q65NN2
B	534	PRO	-	EXPRESSION TAG	UNP Q65NN2
B	535	GLN	-	EXPRESSION TAG	UNP Q65NN2
B	536	PHE	-	EXPRESSION TAG	UNP Q65NN2
B	537	GLU	-	EXPRESSION TAG	UNP Q65NN2
B	538	LYS	-	EXPRESSION TAG	UNP Q65NN2
C	517	ALA	-	EXPRESSION TAG	UNP Q65NN2
C	518	GLU	-	EXPRESSION TAG	UNP Q65NN2
C	519	ASN	-	EXPRESSION TAG	UNP Q65NN2
C	520	LEU	-	EXPRESSION TAG	UNP Q65NN2
C	521	TYR	-	EXPRESSION TAG	UNP Q65NN2
C	522	PHE	-	EXPRESSION TAG	UNP Q65NN2
C	523	GLN	-	EXPRESSION TAG	UNP Q65NN2
C	524	SER	-	EXPRESSION TAG	UNP Q65NN2
C	525	HIS	-	EXPRESSION TAG	UNP Q65NN2
C	526	HIS	-	EXPRESSION TAG	UNP Q65NN2
C	527	HIS	-	EXPRESSION TAG	UNP Q65NN2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	528	HIS	-	EXPRESSION TAG	UNP Q65NN2
C	529	HIS	-	EXPRESSION TAG	UNP Q65NN2
C	530	HIS	-	EXPRESSION TAG	UNP Q65NN2
C	531	TRP	-	EXPRESSION TAG	UNP Q65NN2
C	532	SER	-	EXPRESSION TAG	UNP Q65NN2
C	533	HIS	-	EXPRESSION TAG	UNP Q65NN2
C	534	PRO	-	EXPRESSION TAG	UNP Q65NN2
C	535	GLN	-	EXPRESSION TAG	UNP Q65NN2
C	536	PHE	-	EXPRESSION TAG	UNP Q65NN2
C	537	GLU	-	EXPRESSION TAG	UNP Q65NN2
C	538	LYS	-	EXPRESSION TAG	UNP Q65NN2
D	517	ALA	-	EXPRESSION TAG	UNP Q65NN2
D	518	GLU	-	EXPRESSION TAG	UNP Q65NN2
D	519	ASN	-	EXPRESSION TAG	UNP Q65NN2
D	520	LEU	-	EXPRESSION TAG	UNP Q65NN2
D	521	TYR	-	EXPRESSION TAG	UNP Q65NN2
D	522	PHE	-	EXPRESSION TAG	UNP Q65NN2
D	523	GLN	-	EXPRESSION TAG	UNP Q65NN2
D	524	SER	-	EXPRESSION TAG	UNP Q65NN2
D	525	HIS	-	EXPRESSION TAG	UNP Q65NN2
D	526	HIS	-	EXPRESSION TAG	UNP Q65NN2
D	527	HIS	-	EXPRESSION TAG	UNP Q65NN2
D	528	HIS	-	EXPRESSION TAG	UNP Q65NN2
D	529	HIS	-	EXPRESSION TAG	UNP Q65NN2
D	530	HIS	-	EXPRESSION TAG	UNP Q65NN2
D	531	TRP	-	EXPRESSION TAG	UNP Q65NN2
D	532	SER	-	EXPRESSION TAG	UNP Q65NN2
D	533	HIS	-	EXPRESSION TAG	UNP Q65NN2
D	534	PRO	-	EXPRESSION TAG	UNP Q65NN2
D	535	GLN	-	EXPRESSION TAG	UNP Q65NN2
D	536	PHE	-	EXPRESSION TAG	UNP Q65NN2
D	537	GLU	-	EXPRESSION TAG	UNP Q65NN2
D	538	LYS	-	EXPRESSION TAG	UNP Q65NN2
E	517	ALA	-	EXPRESSION TAG	UNP Q65NN2
E	518	GLU	-	EXPRESSION TAG	UNP Q65NN2
E	519	ASN	-	EXPRESSION TAG	UNP Q65NN2
E	520	LEU	-	EXPRESSION TAG	UNP Q65NN2
E	521	TYR	-	EXPRESSION TAG	UNP Q65NN2
E	522	PHE	-	EXPRESSION TAG	UNP Q65NN2
E	523	GLN	-	EXPRESSION TAG	UNP Q65NN2
E	524	SER	-	EXPRESSION TAG	UNP Q65NN2
E	525	HIS	-	EXPRESSION TAG	UNP Q65NN2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	526	HIS	-	EXPRESSION TAG	UNP Q65NN2
E	527	HIS	-	EXPRESSION TAG	UNP Q65NN2
E	528	HIS	-	EXPRESSION TAG	UNP Q65NN2
E	529	HIS	-	EXPRESSION TAG	UNP Q65NN2
E	530	HIS	-	EXPRESSION TAG	UNP Q65NN2
E	531	TRP	-	EXPRESSION TAG	UNP Q65NN2
E	532	SER	-	EXPRESSION TAG	UNP Q65NN2
E	533	HIS	-	EXPRESSION TAG	UNP Q65NN2
E	534	PRO	-	EXPRESSION TAG	UNP Q65NN2
E	535	GLN	-	EXPRESSION TAG	UNP Q65NN2
E	536	PHE	-	EXPRESSION TAG	UNP Q65NN2
E	537	GLU	-	EXPRESSION TAG	UNP Q65NN2
E	538	LYS	-	EXPRESSION TAG	UNP Q65NN2
F	517	ALA	-	EXPRESSION TAG	UNP Q65NN2
F	518	GLU	-	EXPRESSION TAG	UNP Q65NN2
F	519	ASN	-	EXPRESSION TAG	UNP Q65NN2
F	520	LEU	-	EXPRESSION TAG	UNP Q65NN2
F	521	TYR	-	EXPRESSION TAG	UNP Q65NN2
F	522	PHE	-	EXPRESSION TAG	UNP Q65NN2
F	523	GLN	-	EXPRESSION TAG	UNP Q65NN2
F	524	SER	-	EXPRESSION TAG	UNP Q65NN2
F	525	HIS	-	EXPRESSION TAG	UNP Q65NN2
F	526	HIS	-	EXPRESSION TAG	UNP Q65NN2
F	527	HIS	-	EXPRESSION TAG	UNP Q65NN2
F	528	HIS	-	EXPRESSION TAG	UNP Q65NN2
F	529	HIS	-	EXPRESSION TAG	UNP Q65NN2
F	530	HIS	-	EXPRESSION TAG	UNP Q65NN2
F	531	TRP	-	EXPRESSION TAG	UNP Q65NN2
F	532	SER	-	EXPRESSION TAG	UNP Q65NN2
F	533	HIS	-	EXPRESSION TAG	UNP Q65NN2
F	534	PRO	-	EXPRESSION TAG	UNP Q65NN2
F	535	GLN	-	EXPRESSION TAG	UNP Q65NN2
F	536	PHE	-	EXPRESSION TAG	UNP Q65NN2
F	537	GLU	-	EXPRESSION TAG	UNP Q65NN2
F	538	LYS	-	EXPRESSION TAG	UNP Q65NN2
G	517	ALA	-	EXPRESSION TAG	UNP Q65NN2
G	518	GLU	-	EXPRESSION TAG	UNP Q65NN2
G	519	ASN	-	EXPRESSION TAG	UNP Q65NN2
G	520	LEU	-	EXPRESSION TAG	UNP Q65NN2
G	521	TYR	-	EXPRESSION TAG	UNP Q65NN2
G	522	PHE	-	EXPRESSION TAG	UNP Q65NN2
G	523	GLN	-	EXPRESSION TAG	UNP Q65NN2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	524	SER	-	EXPRESSION TAG	UNP Q65NN2
G	525	HIS	-	EXPRESSION TAG	UNP Q65NN2
G	526	HIS	-	EXPRESSION TAG	UNP Q65NN2
G	527	HIS	-	EXPRESSION TAG	UNP Q65NN2
G	528	HIS	-	EXPRESSION TAG	UNP Q65NN2
G	529	HIS	-	EXPRESSION TAG	UNP Q65NN2
G	530	HIS	-	EXPRESSION TAG	UNP Q65NN2
G	531	TRP	-	EXPRESSION TAG	UNP Q65NN2
G	532	SER	-	EXPRESSION TAG	UNP Q65NN2
G	533	HIS	-	EXPRESSION TAG	UNP Q65NN2
G	534	PRO	-	EXPRESSION TAG	UNP Q65NN2
G	535	GLN	-	EXPRESSION TAG	UNP Q65NN2
G	536	PHE	-	EXPRESSION TAG	UNP Q65NN2
G	537	GLU	-	EXPRESSION TAG	UNP Q65NN2
G	538	LYS	-	EXPRESSION TAG	UNP Q65NN2
H	517	ALA	-	EXPRESSION TAG	UNP Q65NN2
H	518	GLU	-	EXPRESSION TAG	UNP Q65NN2
H	519	ASN	-	EXPRESSION TAG	UNP Q65NN2
H	520	LEU	-	EXPRESSION TAG	UNP Q65NN2
H	521	TYR	-	EXPRESSION TAG	UNP Q65NN2
H	522	PHE	-	EXPRESSION TAG	UNP Q65NN2
H	523	GLN	-	EXPRESSION TAG	UNP Q65NN2
H	524	SER	-	EXPRESSION TAG	UNP Q65NN2
H	525	HIS	-	EXPRESSION TAG	UNP Q65NN2
H	526	HIS	-	EXPRESSION TAG	UNP Q65NN2
H	527	HIS	-	EXPRESSION TAG	UNP Q65NN2
H	528	HIS	-	EXPRESSION TAG	UNP Q65NN2
H	529	HIS	-	EXPRESSION TAG	UNP Q65NN2
H	530	HIS	-	EXPRESSION TAG	UNP Q65NN2
H	531	TRP	-	EXPRESSION TAG	UNP Q65NN2
H	532	SER	-	EXPRESSION TAG	UNP Q65NN2
H	533	HIS	-	EXPRESSION TAG	UNP Q65NN2
H	534	PRO	-	EXPRESSION TAG	UNP Q65NN2
H	535	GLN	-	EXPRESSION TAG	UNP Q65NN2
H	536	PHE	-	EXPRESSION TAG	UNP Q65NN2
H	537	GLU	-	EXPRESSION TAG	UNP Q65NN2
H	538	LYS	-	EXPRESSION TAG	UNP Q65NN2

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

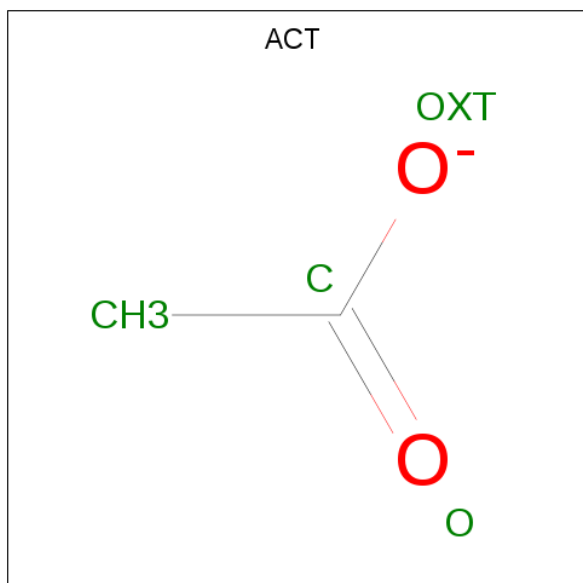
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	6	Total Cd 6 6	0	0
2	D	5	Total Cd 5 5	0	0
2	E	5	Total Cd 5 5	0	0
2	H	3	Total Cd 3 3	0	0
2	B	4	Total Cd 4 4	0	0
2	C	11	Total Cd 11 11	0	0
2	A	9	Total Cd 9 9	0	0
2	F	4	Total Cd 4 4	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	E	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

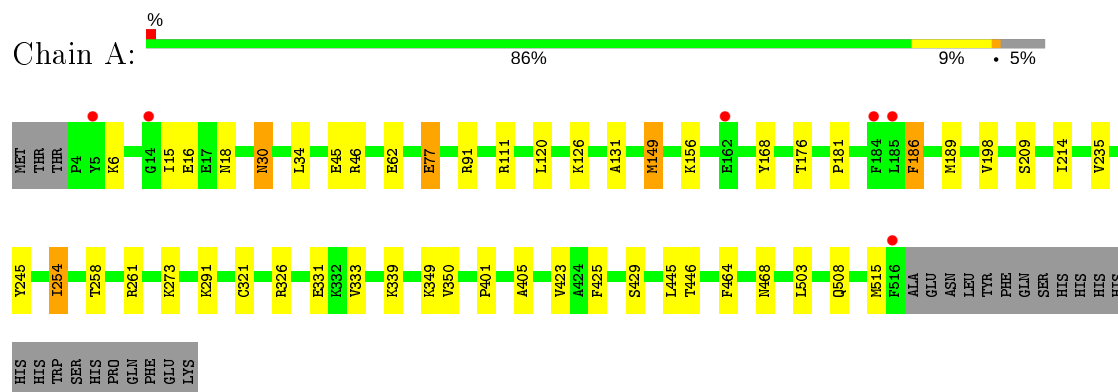
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	89	Total O 89 89	0	0
4	B	102	Total O 102 102	0	0
4	C	104	Total O 104 104	0	0
4	D	83	Total O 83 83	0	0
4	E	76	Total O 76 76	0	0
4	F	67	Total O 67 67	0	0
4	G	79	Total O 79 79	0	0
4	H	73	Total O 73 73	0	0

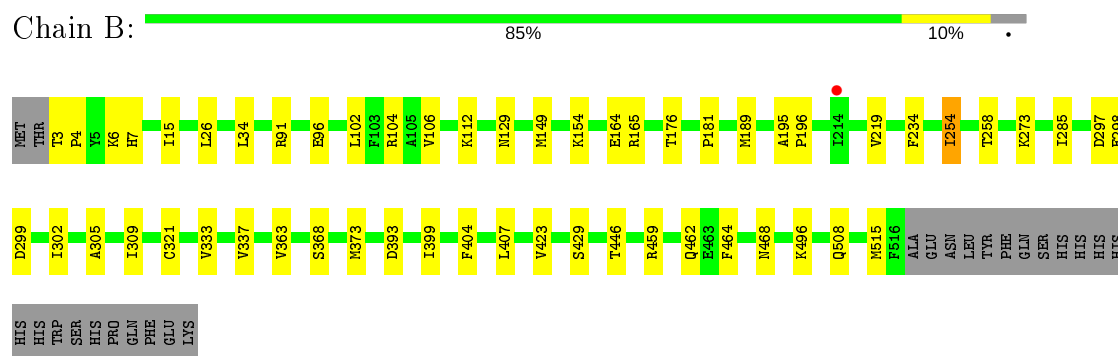
### 3 Residue-property plots [i](#)

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

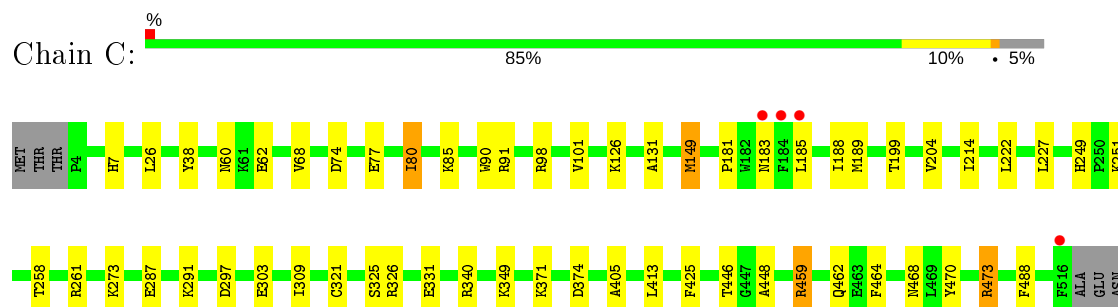
- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase



- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase




- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase



LEU  
TYR  
PHE  
GLN  
SER  
HIS  
HIS  
HIS  
HIS  
HIS  
TRP  
SER  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS


- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain D:  87% 8% 5%

MET THR THR P4 E8 P9 R19 S37 Y38 N80 T67 V68 R91 D94 L102 F103 R104 A105 V106 A124 K154 E164 P181 L185 F186 M189 S209 E224 V235 S238 T258 K273 K291 I302 C321 R326

V329 Y334 T345 S355 P401 V423 V428 A434 T446 R459 Q462 E463 F464 N468 G486 F516 ALA GLU ASN LEU TYR PHE GLN SER HIS HIS HIS HIS TRP SER PRO GLN GLU LYS


- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain E:  87% 8% 5%

MET THR THR P4 H7 E8 E23 L26 N30 S37 N60 V61 E62 E77 I80 F87 R91 L102 V106 E143 M149 I150 E151 K154 E162 V175 T176 P181 L185 M189 L205 S209 A210 K211 V219

F234 Y245 I254 T258 K273 D297 E298 D299 T302 C321 K373 L413 E436 T446 Q462 E463 F464 N468 Q508 F516 ALA GLU ASN LEU TYR PHE GLN SER HIS HIS HIS HIS TRP SER PRO GLN GLU LYS

- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase


Chain F:  86% 9% 5%

MET THR THR P4 E8 P9 I115 E23 E62 E77 R91 V106 E115 K126 P127 E130 A131 I139 M149 V178 I179 P180 P181 F184 L185 M189 T202 S209 I214 V231 V235 Y245 T258 E269 K273

E287 F288 G289 K291 C321 R326 E331 K339 R349 R357 L407 L413 F419 A424 M440 T446 G447 A448 R459 F464 N468 F469 Y470 T476 Y502 L503 A504 L505 M515 F516 ALA GLU ASN LEU TYR PHE GLN SER HIS HIS

HIS  
HIS  
HIS  
TRP  
SER  
HIS  
PRO  
GLN  
PHE  
GLU  
LYS

- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain G:  87% 8% 5%

MET THR THR P4 P39 R46 N51 E62 D74 R91 E115 H142 M149 L152 K156 Y168 P181 F184 L185 F186 M189 V194 V198 L205 S209 K217 L222 S238 T258 R261 K273 E287 K291

V296 I309 C321 R326 E331 K332 S368 M373 A405 V423 A424 F425 E442 A448 R459 F464 C475 F488 F516 ALA GLU ASN LEU TYR PHE GLN SER HIS HIS HIS HIS TRP SER HIS HIS PRO GLN PHE GLU LYS

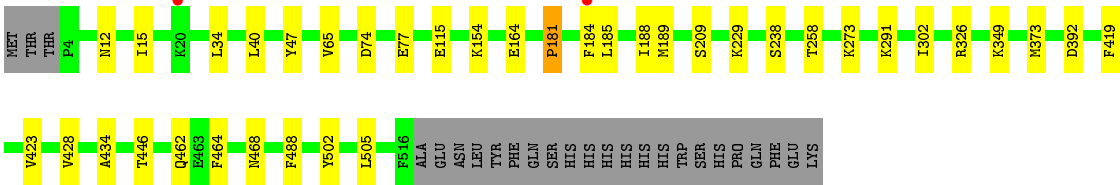
- Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain H: 

88%

7%

5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.27Å 116.11Å 181.77Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 39.35 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.9 (20.00-2.20) 86.8 (39.35-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.222 , 0.292 0.224 , 0.294	Depositor DCC
$R_{free}$ test set	5710 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.8	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 19.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32569	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.6344e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

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

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	0.42	0/4075	0.59	0/5516
1	B	0.45	0/4074	0.60	0/5516
1	C	0.44	0/4074	0.61	1/5513 (0.0%)
1	D	0.43	0/4081	0.58	1/5524 (0.0%)
1	E	0.44	0/4063	0.59	1/5500 (0.0%)
1	F	0.43	0/4063	0.59	0/5500
1	G	0.45	0/4050	0.61	2/5483 (0.0%)
1	H	0.42	0/4053	0.58	0/5488
All	All	0.44	0/32533	0.59	5/44040 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	374	ASP	CB-CG-OD2	6.04	123.74	118.30
1	G	459	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	94	ASP	CB-CG-OD1	5.50	123.25	118.30
1	E	185	LEU	CA-CB-CG	5.45	127.84	115.30
1	G	152	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	3984	0	3926	17	0
1	B	3983	0	3924	14	0
1	C	3983	0	3928	20	0
1	D	3987	0	3930	16	0
1	E	3975	0	3918	13	0
1	F	3975	0	3918	19	0
1	G	3965	0	3898	16	1
1	H	3965	0	3903	10	0
2	A	9	0	0	0	0
2	B	4	0	0	0	0
2	C	11	0	0	0	1
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	4	0	0	0	0
2	G	6	0	0	0	1
2	H	3	0	0	0	0
3	A	4	0	3	3	0
3	B	4	0	3	1	0
3	D	4	0	3	1	0
3	E	8	0	6	0	0
3	F	8	0	6	0	0
3	H	4	0	3	0	0
4	A	89	0	0	0	0
4	B	102	0	0	0	0
4	C	104	0	0	0	0
4	D	83	0	0	2	0
4	E	76	0	0	1	1
4	F	67	0	0	0	0
4	G	79	0	0	0	0
4	H	73	0	0	0	0
All	All	32569	0	31369	125	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 2.

The worst 5 of 125 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:D:321:CYS:SG	4:D:550:HOH:O	2.36	0.83
1:C:459:ARG:HG2	1:C:459:ARG:HH11	1.53	0.73
1:G:459:ARG:HH11	1:G:459:ARG:HG2	1.55	0.71
1:F:185:LEU:HG	1:F:214:ILE:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:HD3	1:A:258:THR:HB	1.79	0.65

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)
2:G:540:CD:CD	4:E:550:HOH:O[1_565]	2.02	0.18
1:G:74:ASP:OD2	2:C:543:CD:CD[1_455]	2.13	0.07

## 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	514/538 (96%)	497 (97%)	17 (3%)	0	100	100
1	B	514/538 (96%)	495 (96%)	18 (4%)	1 (0%)	47	55
1	C	513/538 (95%)	500 (98%)	12 (2%)	1 (0%)	47	55
1	D	514/538 (96%)	499 (97%)	15 (3%)	0	100	100
1	E	512/538 (95%)	489 (96%)	22 (4%)	1 (0%)	47	55
1	F	512/538 (95%)	492 (96%)	20 (4%)	0	100	100
1	G	511/538 (95%)	498 (98%)	13 (2%)	0	100	100
1	H	512/538 (95%)	496 (97%)	14 (3%)	2 (0%)	34	37
All	All	4102/4304 (95%)	3966 (97%)	131 (3%)	5 (0%)	51	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	496	LYS
1	C	183	ASN
1	E	185	LEU

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Mol	Chain	Res	Type
1	H	185	LEU
1	H	181	PRO

### 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	420/442 (95%)	390 (93%)	30 (7%)	14	16
1	B	420/442 (95%)	389 (93%)	31 (7%)	13	14
1	C	420/442 (95%)	392 (93%)	28 (7%)	16	18
1	D	421/442 (95%)	405 (96%)	16 (4%)	33	42
1	E	419/442 (95%)	395 (94%)	24 (6%)	20	24
1	F	419/442 (95%)	399 (95%)	20 (5%)	25	32
1	G	417/442 (94%)	394 (94%)	23 (6%)	21	26
1	H	417/442 (94%)	399 (96%)	18 (4%)	29	36
All	All	3353/3536 (95%)	3163 (94%)	190 (6%)	21	24

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	462	GLN
1	E	23	GLU
1	H	154	LYS
1	C	488	PHE
1	D	189	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	462	GLN
1	D	468	ASN
1	H	12	ASN

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Mol	Chain	Res	Type
1	D	73	GLN
1	H	36	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 55 ligands modelled in this entry, 47 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z  > 2$
3	ACT	E	544	2	1,3,3	1.37	0	0,3,3	0.00	-
3	ACT	F	544	2	1,3,3	1.39	0	0,3,3	0.00	-
3	ACT	B	543	2	1,3,3	1.01	0	0,3,3	0.00	-
3	ACT	F	543	2	1,3,3	1.34	0	0,3,3	0.00	-
3	ACT	D	544	2	1,3,3	1.35	0	0,3,3	0.00	-
3	ACT	E	545	2	1,3,3	1.39	0	0,3,3	0.00	-
3	ACT	A	548	2	1,3,3	1.34	0	0,3,3	0.00	-
3	ACT	H	542	2	1,3,3	1.32	0	0,3,3	0.00	-

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	543	ACT	1	0
3	D	544	ACT	1	0
3	A	548	ACT	3	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<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	513/538 (95%)	-0.29	6 (1%) 79 77	23, 45, 72, 97	0
1	B	514/538 (95%)	-0.38	1 (0%) 95 94	21, 42, 64, 78	0
1	C	513/538 (95%)	-0.35	4 (0%) 86 85	22, 43, 65, 81	0
1	D	513/538 (95%)	-0.37	1 (0%) 95 94	21, 45, 67, 80	0
1	E	513/538 (95%)	-0.39	1 (0%) 95 94	23, 41, 64, 78	0
1	F	513/538 (95%)	-0.31	5 (0%) 82 81	24, 44, 71, 95	0
1	G	513/538 (95%)	-0.34	2 (0%) 92 91	21, 44, 64, 78	0
1	H	513/538 (95%)	-0.37	2 (0%) 92 91	23, 46, 67, 80	0
All	All	4105/4304 (95%)	-0.35	22 (0%) 91 90	21, 44, 67, 97	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	516	PHE	4.8
1	A	185	LEU	3.4
1	C	184	PHE	3.4
1	F	185	LEU	3.4
1	D	185	LEU	3.2

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CD	A	542	1/1	0.86	0.07	88,88,88,88	1
2	CD	E	540	1/1	0.86	0.06	97,97,97,97	1
2	CD	G	539	1/1	0.88	0.08	80,80,80,80	1
2	CD	G	540	1/1	0.88	0.08	93,93,93,93	1
3	ACT	A	548	4/4	0.89	0.17	62,67,69,71	0
2	CD	A	540	1/1	0.90	0.06	88,88,88,88	1
3	ACT	F	544	4/4	0.91	0.10	75,76,77,78	0
2	CD	C	542	1/1	0.91	0.14	72,72,72,72	1
2	CD	D	543	1/1	0.91	0.09	82,82,82,82	1
2	CD	B	540	1/1	0.91	0.09	97,97,97,97	1
2	CD	F	539	1/1	0.92	0.07	71,71,71,71	1
3	ACT	H	542	4/4	0.93	0.24	61,65,67,72	0
2	CD	B	542	1/1	0.94	0.06	100,100,100,100	1
3	ACT	B	543	4/4	0.95	0.23	56,57,59,63	0
2	CD	C	540	1/1	0.95	0.08	84,84,84,84	1
2	CD	A	547	1/1	0.95	0.10	92,92,92,92	1
2	CD	F	541	1/1	0.95	0.06	87,87,87,87	1
2	CD	B	541	1/1	0.95	0.13	68,68,68,68	1
2	CD	C	546	1/1	0.95	0.11	69,69,69,69	1
2	CD	C	541	1/1	0.96	0.04	85,85,85,85	1
2	CD	D	542	1/1	0.96	0.05	76,76,76,76	1
2	CD	A	545	1/1	0.96	0.08	80,80,80,80	1
3	ACT	E	545	4/4	0.96	0.14	54,61,61,61	0
2	CD	C	544	1/1	0.96	0.07	74,74,74,74	1
3	ACT	D	544	4/4	0.96	0.16	58,66,66,68	0
2	CD	A	544	1/1	0.97	0.05	76,76,76,76	1
3	ACT	E	544	4/4	0.97	0.12	59,59,60,61	0
2	CD	G	541	1/1	0.97	0.10	81,81,81,81	1
2	CD	A	541	1/1	0.97	0.05	86,86,86,86	1
2	CD	D	541	1/1	0.97	0.09	87,87,87,87	1
2	CD	G	543	1/1	0.97	0.14	76,76,76,76	1
2	CD	A	546	1/1	0.98	0.14	78,78,78,78	1
2	CD	C	543	1/1	0.98	0.08	76,76,76,76	1
2	CD	G	544	1/1	0.98	0.09	78,78,78,78	1
3	ACT	F	543	4/4	0.98	0.10	76,76,76,77	0
2	CD	F	540	1/1	0.98	0.16	66,66,66,66	1
2	CD	F	542	1/1	0.98	0.05	68,68,68,68	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CD	C	547	1/1	0.98	0.08	75,75,75,75	1
2	CD	H	541	1/1	0.98	0.05	67,67,67,67	1
2	CD	C	545	1/1	0.98	0.13	74,74,74,74	1
2	CD	C	539	1/1	0.98	0.07	77,77,77,77	1
2	CD	B	539	1/1	0.99	0.13	47,47,47,47	1
2	CD	A	543	1/1	0.99	0.10	72,72,72,72	1
2	CD	C	548	1/1	0.99	0.14	49,49,49,49	1
2	CD	E	541	1/1	0.99	0.14	37,37,37,37	0
2	CD	C	549	1/1	0.99	0.12	49,49,49,49	0
2	CD	H	540	1/1	0.99	0.17	56,56,56,56	1
2	CD	H	539	1/1	0.99	0.12	58,58,58,58	0
2	CD	D	540	1/1	0.99	0.10	52,52,52,52	1
2	CD	G	542	1/1	0.99	0.12	75,75,75,75	1
2	CD	E	543	1/1	0.99	0.14	55,55,55,55	1
2	CD	A	539	1/1	1.00	0.15	43,43,43,43	0
2	CD	E	542	1/1	1.00	0.11	48,48,48,48	1
2	CD	D	539	1/1	1.00	0.10	57,57,57,57	0
2	CD	E	539	1/1	1.00	0.09	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.