wwPDB X-ray Structure Validation Summary Report (i)

Sep 2, 2023 – 08:29 PM EDT

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*
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 (i)) were used in the production of this report:

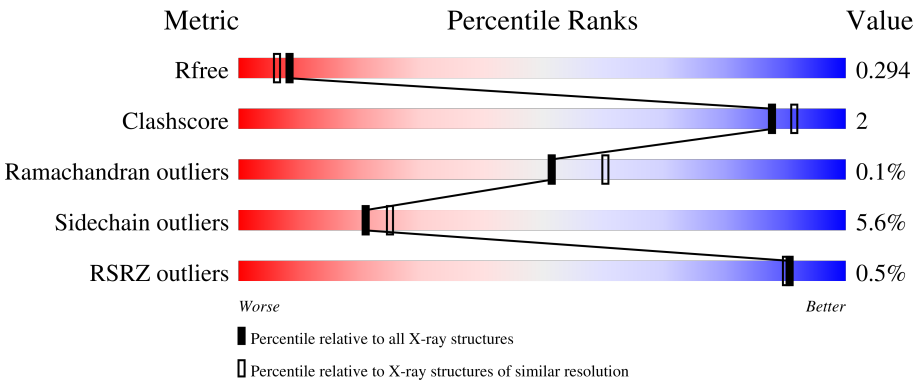
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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 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	538	.% 86% 9% • 5%
1	B	538	85% 10% •
1	C	538	.% 85% 10% • 5%
1	D	538	87% 8% 5%
1	E	538	87% 8% 5%

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Mol	Chain	Length	Quality of chain
1	F	538	% 86% 9% • 5%
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 (i)

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

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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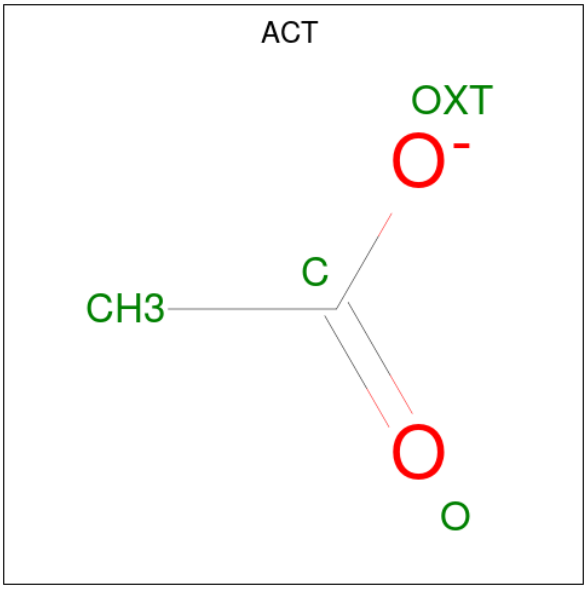
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	9	Total Cd 9 9	0	0
2	B	4	Total Cd 4 4	0	0
2	C	11	Total Cd 11 11	0	0
2	D	5	Total Cd 5 5	0	0
2	E	5	Total Cd 5 5	0	0
2	F	4	Total Cd 4 4	0	0
2	G	6	Total Cd 6 6	0	0
2	H	3	Total Cd 3 3	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
			Total	C	O		
3	D	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	E	1	4	2	2	0	0
3	F	1	4	2	2	0	0
3	F	1	4	2	2	0	0
3	H	1	4	2	2	0	0

- Molecule 4 is water.

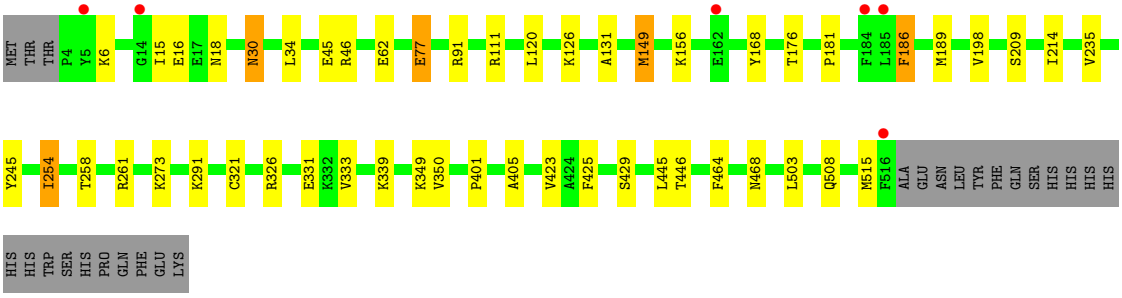
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	89	89	89	0	0
4	B	102	102	102	0	0
4	C	104	104	104	0	0
4	D	83	83	83	0	0
4	E	76	76	76	0	0
4	F	67	67	67	0	0
4	G	79	79	79	0	0
4	H	73	73	73	0	0

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: 1-pyrroline-5-carboxylate dehydrogenase

Chain A:

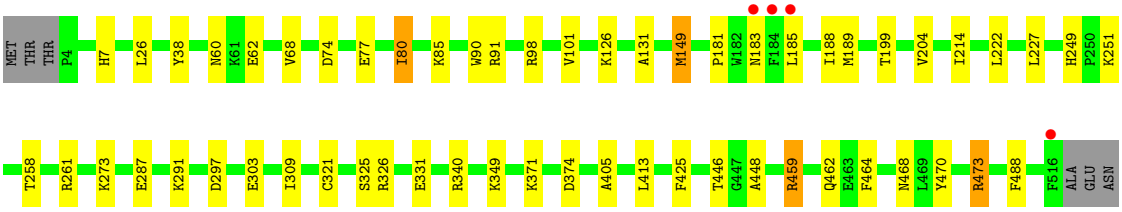


• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain B:

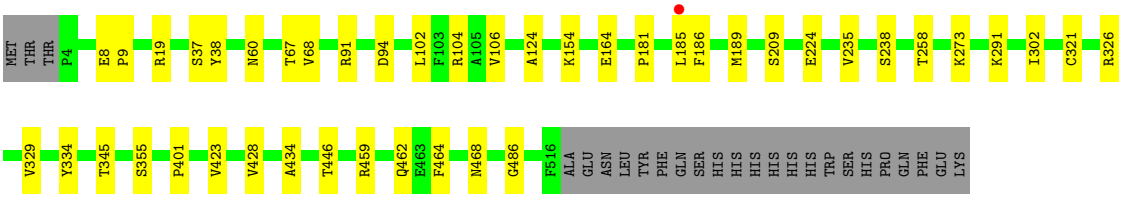
• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain C:



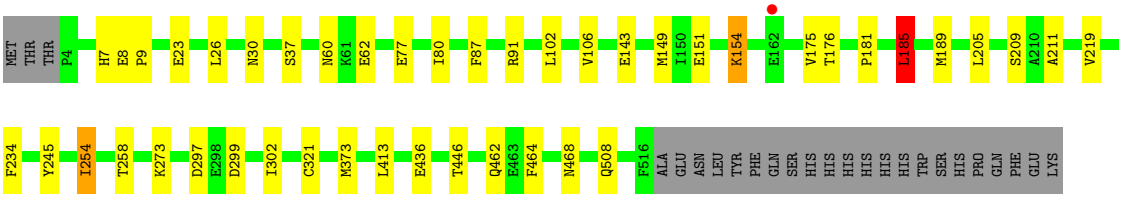
• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain D:



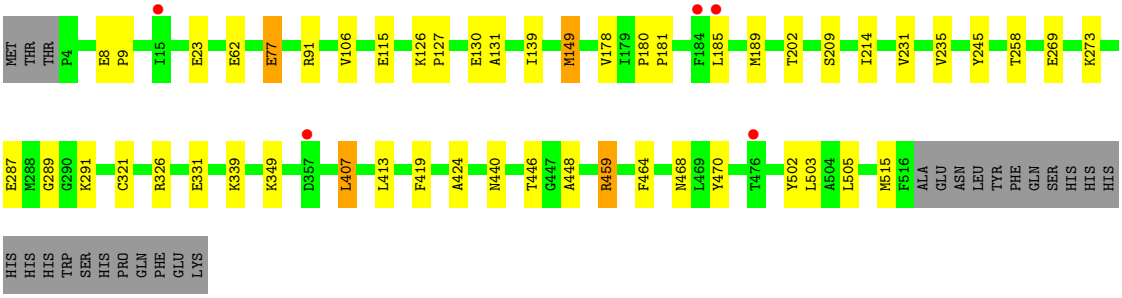
• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain E:



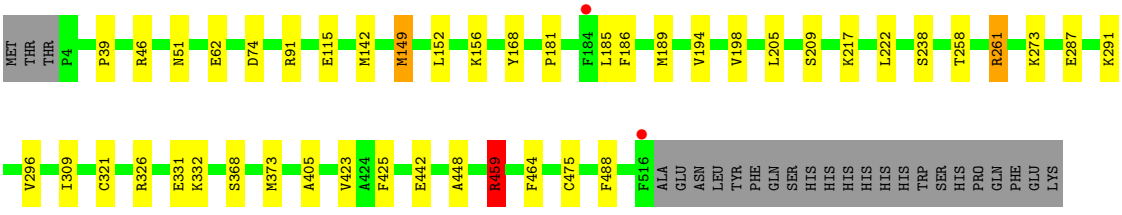
• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain F:



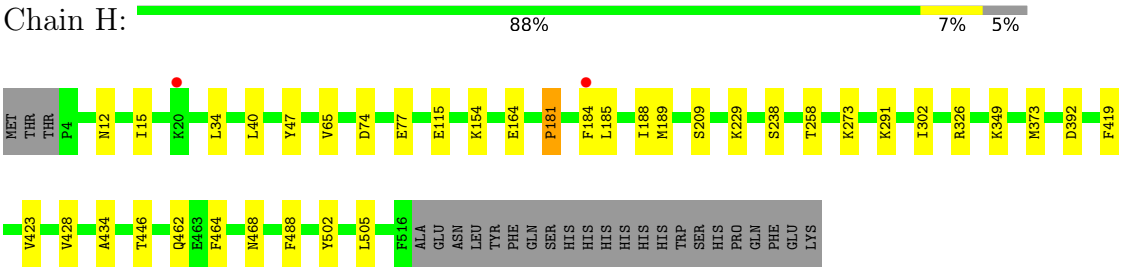
• Molecule 1: 1-pyrroline-5-carboxylate dehydrogenase

Chain G:



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

Chain H:


88%
7%
5%
MET THR THR P4 N12 I15 K20 L34 L40 Y47 V65 D74 E77 E115 K154 E164 P181 F184 L185 I188 M189 S209 K229 S238 T258 K273 K291 I302 R326 K349 M373 D392 F419
V423 V428 A434 T446 Q462 E463 F464 N468 F488 Y502 L505 F516 ALA GLU ASN LEU TYR PHE GLN SER HIS HIS HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	33.8	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 19.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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^2)	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.*

[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: ACT, CD

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(^{o})	Ideal(^{o})
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 (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	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:HG2	1:G:459:ARG:HH11	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 (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	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	E	189	MET
1	F	413	LEU
1	E	297	ASP
1	F	62	GLU
1	G	62	GLU

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

Mol	Chain	Res	Type
1	H	36	GLN
1	H	462	GLN
1	D	462	GLN

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Mol	Chain	Res	Type
1	D	468	ASN
1	E	30	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	D	544	2	3,3,3	0.77	0	3,3,3	1.34	0
3	ACT	F	543	2	3,3,3	0.77	0	3,3,3	1.35	0
3	ACT	E	544	2	3,3,3	0.80	0	3,3,3	1.64	1 (33%)
3	ACT	F	544	2	3,3,3	0.77	0	3,3,3	1.33	0
3	ACT	B	543	2	3,3,3	0.74	0	3,3,3	1.33	0
3	ACT	E	545	2	3,3,3	0.76	0	3,3,3	1.34	0
3	ACT	A	548	2	3,3,3	0.76	0	3,3,3	1.35	0
3	ACT	H	542	2	3,3,3	0.76	0	3,3,3	1.34	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	544	ACT	OXT-C-O	-2.13	114.21	122.05

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	D	544	ACT	1	0
3	B	543	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 (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	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 (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(Å^2)	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
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
3	ACT	F	544	4/4	0.91	0.10	75,76,77,78	0
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
2	CD	C	546	1/1	0.95	0.11	69,69,69,69	1
2	CD	A	547	1/1	0.95	0.10	92,92,92,92	1
2	CD	C	540	1/1	0.95	0.08	84,84,84,84	1
3	ACT	B	543	4/4	0.95	0.23	56,57,59,63	0
2	CD	B	541	1/1	0.95	0.13	68,68,68,68	1
2	CD	F	541	1/1	0.95	0.06	87,87,87,87	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
3	ACT	D	544	4/4	0.96	0.16	58,66,66,68	0
3	ACT	E	545	4/4	0.96	0.14	54,61,61,61	0
2	CD	A	545	1/1	0.96	0.08	80,80,80,80	1
2	CD	C	544	1/1	0.96	0.07	74,74,74,74	1
2	CD	D	541	1/1	0.97	0.09	87,87,87,87	1
2	CD	A	541	1/1	0.97	0.05	86,86,86,86	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	G	543	1/1	0.97	0.14	76,76,76,76	1
2	CD	A	544	1/1	0.97	0.05	76,76,76,76	1
2	CD	G	544	1/1	0.98	0.09	78,78,78,78	1
2	CD	H	541	1/1	0.98	0.05	67,67,67,67	1
2	CD	F	540	1/1	0.98	0.16	66,66,66,66	1
2	CD	C	543	1/1	0.98	0.08	76,76,76,76	1
2	CD	F	542	1/1	0.98	0.05	68,68,68,68	1
2	CD	C	539	1/1	0.98	0.07	77,77,77,77	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CD	C	545	1/1	0.98	0.13	74,74,74,74	1
3	ACT	F	543	4/4	0.98	0.10	76,76,76,77	0
2	CD	A	546	1/1	0.98	0.14	78,78,78,78	1
2	CD	C	547	1/1	0.98	0.08	75,75,75,75	1
2	CD	H	540	1/1	0.99	0.17	56,56,56,56	1
2	CD	B	539	1/1	0.99	0.13	47,47,47,47	1
2	CD	C	548	1/1	0.99	0.14	49,49,49,49	1
2	CD	C	549	1/1	0.99	0.12	49,49,49,49	0
2	CD	E	541	1/1	0.99	0.14	37,37,37,37	0
2	CD	E	543	1/1	0.99	0.14	55,55,55,55	1
2	CD	G	542	1/1	0.99	0.12	75,75,75,75	1
2	CD	D	540	1/1	0.99	0.10	52,52,52,52	1
2	CD	A	543	1/1	0.99	0.10	72,72,72,72	1
2	CD	H	539	1/1	0.99	0.12	58,58,58,58	0
2	CD	D	539	1/1	1.00	0.10	57,57,57,57	0
2	CD	E	542	1/1	1.00	0.11	48,48,48,48	1
2	CD	E	539	1/1	1.00	0.09	55,55,55,55	0
2	CD	A	539	1/1	1.00	0.15	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.