



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 03:43 AM UTC

PDB ID : 9AXW / pdb_00009axw
Title : Nanobody NbJRI bound to yeast Pdc1
Authors : Carrasco-Lopez, C.; Avalos, J.L.
Deposited on : 2024-03-06
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

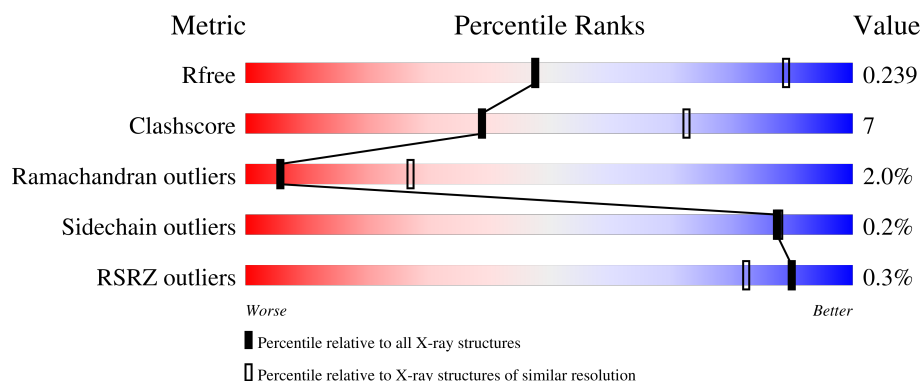
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA1	573	
1	BA1	573	
1	CA1	573	
1	DA1	573	
1	EA1	573	

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Mol	Chain	Length	Quality of chain
1	FA1	573	 79%12%9%
1	GA1	573	 82%10%8%
1	HA1	573	 82%10%8%
2	I	152	 %55%22%5%18%
2	J	152	 61%20%•18%
2	K	152	 59%19%•18%
2	L	152	 %59%20%•18%
2	M	152	 %63%16%•18%
2	N	152	 61%16%5%18%
2	O	152	 55%25%•18%
2	P	152	 57%20%•20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39941 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 branched-chain-2-oxoacid decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA1	519	Total	C	N	O	S	0	0	0
			3989	2549	667	757	16			
1	BA1	527	Total	C	N	O	S	0	0	0
			4052	2588	677	771	16			
1	CA1	532	Total	C	N	O	S	0	0	0
			4092	2615	686	775	16			
1	DA1	523	Total	C	N	O	S	0	0	0
			4008	2559	672	761	16			
1	EA1	534	Total	C	N	O	S	0	0	0
			4110	2625	686	783	16			
1	FA1	520	Total	C	N	O	S	0	0	0
			3990	2549	667	758	16			
1	GA1	525	Total	C	N	O	S	0	0	0
			4025	2570	670	769	16			
1	HA1	529	Total	C	N	O	S	0	0	0
			4063	2595	677	775	16			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA1	-1	MET	-	initiating methionine	UNP A0A7I9FNH9
AA1	0	ALA	-	expression tag	UNP A0A7I9FNH9
AA1	1	SER	-	expression tag	UNP A0A7I9FNH9
AA1	564	LEU	-	expression tag	UNP A0A7I9FNH9
AA1	565	GLU	-	expression tag	UNP A0A7I9FNH9
AA1	566	HIS	-	expression tag	UNP A0A7I9FNH9
AA1	567	HIS	-	expression tag	UNP A0A7I9FNH9
AA1	568	HIS	-	expression tag	UNP A0A7I9FNH9
AA1	569	HIS	-	expression tag	UNP A0A7I9FNH9
AA1	570	HIS	-	expression tag	UNP A0A7I9FNH9
AA1	571	HIS	-	expression tag	UNP A0A7I9FNH9
BA1	-1	MET	-	initiating methionine	UNP A0A7I9FNH9
BA1	0	ALA	-	expression tag	UNP A0A7I9FNH9

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Chain	Residue	Modelled	Actual	Comment	Reference
BA1	1	SER	-	expression tag	UNP A0A7I9FNH9
BA1	564	LEU	-	expression tag	UNP A0A7I9FNH9
BA1	565	GLU	-	expression tag	UNP A0A7I9FNH9
BA1	566	HIS	-	expression tag	UNP A0A7I9FNH9
BA1	567	HIS	-	expression tag	UNP A0A7I9FNH9
BA1	568	HIS	-	expression tag	UNP A0A7I9FNH9
BA1	569	HIS	-	expression tag	UNP A0A7I9FNH9
BA1	570	HIS	-	expression tag	UNP A0A7I9FNH9
BA1	571	HIS	-	expression tag	UNP A0A7I9FNH9
CA1	-1	MET	-	initiating methionine	UNP A0A7I9FNH9
CA1	0	ALA	-	expression tag	UNP A0A7I9FNH9
CA1	1	SER	-	expression tag	UNP A0A7I9FNH9
CA1	564	LEU	-	expression tag	UNP A0A7I9FNH9
CA1	565	GLU	-	expression tag	UNP A0A7I9FNH9
CA1	566	HIS	-	expression tag	UNP A0A7I9FNH9
CA1	567	HIS	-	expression tag	UNP A0A7I9FNH9
CA1	568	HIS	-	expression tag	UNP A0A7I9FNH9
CA1	569	HIS	-	expression tag	UNP A0A7I9FNH9
CA1	570	HIS	-	expression tag	UNP A0A7I9FNH9
CA1	571	HIS	-	expression tag	UNP A0A7I9FNH9
DA1	-1	MET	-	initiating methionine	UNP A0A7I9FNH9
DA1	0	ALA	-	expression tag	UNP A0A7I9FNH9
DA1	1	SER	-	expression tag	UNP A0A7I9FNH9
DA1	564	LEU	-	expression tag	UNP A0A7I9FNH9
DA1	565	GLU	-	expression tag	UNP A0A7I9FNH9
DA1	566	HIS	-	expression tag	UNP A0A7I9FNH9
DA1	567	HIS	-	expression tag	UNP A0A7I9FNH9
DA1	568	HIS	-	expression tag	UNP A0A7I9FNH9
DA1	569	HIS	-	expression tag	UNP A0A7I9FNH9
DA1	570	HIS	-	expression tag	UNP A0A7I9FNH9
DA1	571	HIS	-	expression tag	UNP A0A7I9FNH9
EA1	-1	MET	-	initiating methionine	UNP A0A7I9FNH9
EA1	0	ALA	-	expression tag	UNP A0A7I9FNH9
EA1	1	SER	-	expression tag	UNP A0A7I9FNH9
EA1	564	LEU	-	expression tag	UNP A0A7I9FNH9
EA1	565	GLU	-	expression tag	UNP A0A7I9FNH9
EA1	566	HIS	-	expression tag	UNP A0A7I9FNH9
EA1	567	HIS	-	expression tag	UNP A0A7I9FNH9
EA1	568	HIS	-	expression tag	UNP A0A7I9FNH9
EA1	569	HIS	-	expression tag	UNP A0A7I9FNH9
EA1	570	HIS	-	expression tag	UNP A0A7I9FNH9
EA1	571	HIS	-	expression tag	UNP A0A7I9FNH9

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Chain	Residue	Modelled	Actual	Comment	Reference
FA1	-1	MET	-	initiating methionine	UNP A0A7I9FNH9
FA1	0	ALA	-	expression tag	UNP A0A7I9FNH9
FA1	1	SER	-	expression tag	UNP A0A7I9FNH9
FA1	564	LEU	-	expression tag	UNP A0A7I9FNH9
FA1	565	GLU	-	expression tag	UNP A0A7I9FNH9
FA1	566	HIS	-	expression tag	UNP A0A7I9FNH9
FA1	567	HIS	-	expression tag	UNP A0A7I9FNH9
FA1	568	HIS	-	expression tag	UNP A0A7I9FNH9
FA1	569	HIS	-	expression tag	UNP A0A7I9FNH9
FA1	570	HIS	-	expression tag	UNP A0A7I9FNH9
FA1	571	HIS	-	expression tag	UNP A0A7I9FNH9
GA1	-1	MET	-	initiating methionine	UNP A0A7I9FNH9
GA1	0	ALA	-	expression tag	UNP A0A7I9FNH9
GA1	1	SER	-	expression tag	UNP A0A7I9FNH9
GA1	564	LEU	-	expression tag	UNP A0A7I9FNH9
GA1	565	GLU	-	expression tag	UNP A0A7I9FNH9
GA1	566	HIS	-	expression tag	UNP A0A7I9FNH9
GA1	567	HIS	-	expression tag	UNP A0A7I9FNH9
GA1	568	HIS	-	expression tag	UNP A0A7I9FNH9
GA1	569	HIS	-	expression tag	UNP A0A7I9FNH9
GA1	570	HIS	-	expression tag	UNP A0A7I9FNH9
GA1	571	HIS	-	expression tag	UNP A0A7I9FNH9
HA1	-1	MET	-	initiating methionine	UNP A0A7I9FNH9
HA1	0	ALA	-	expression tag	UNP A0A7I9FNH9
HA1	1	SER	-	expression tag	UNP A0A7I9FNH9
HA1	564	LEU	-	expression tag	UNP A0A7I9FNH9
HA1	565	GLU	-	expression tag	UNP A0A7I9FNH9
HA1	566	HIS	-	expression tag	UNP A0A7I9FNH9
HA1	567	HIS	-	expression tag	UNP A0A7I9FNH9
HA1	568	HIS	-	expression tag	UNP A0A7I9FNH9
HA1	569	HIS	-	expression tag	UNP A0A7I9FNH9
HA1	570	HIS	-	expression tag	UNP A0A7I9FNH9
HA1	571	HIS	-	expression tag	UNP A0A7I9FNH9

- Molecule 2 is a protein called NbJRI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	124	Total	C	N	O	S	0	0	0
			953	596	167	187	3			
2	J	124	Total	C	N	O	S	0	0	0
			953	596	167	187	3			
2	K	124	Total	C	N	O	S	0	0	0
			953	596	167	187	3			

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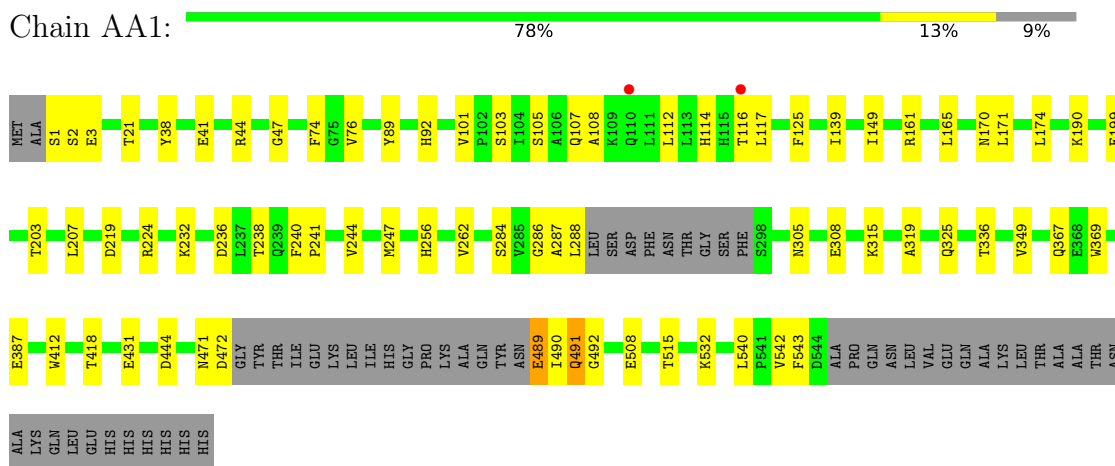
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	124	Total 953	C 596	N 167	O 187	S 3	0	0	0
2	N	124	Total 953	C 596	N 167	O 187	S 3	0	0	0
2	O	124	Total 953	C 596	N 167	O 187	S 3	0	0	0
2	P	122	Total 941	C 590	N 165	O 183	S 3	0	0	0
2	M	124	Total 953	C 596	N 167	O 187	S 3	0	0	0

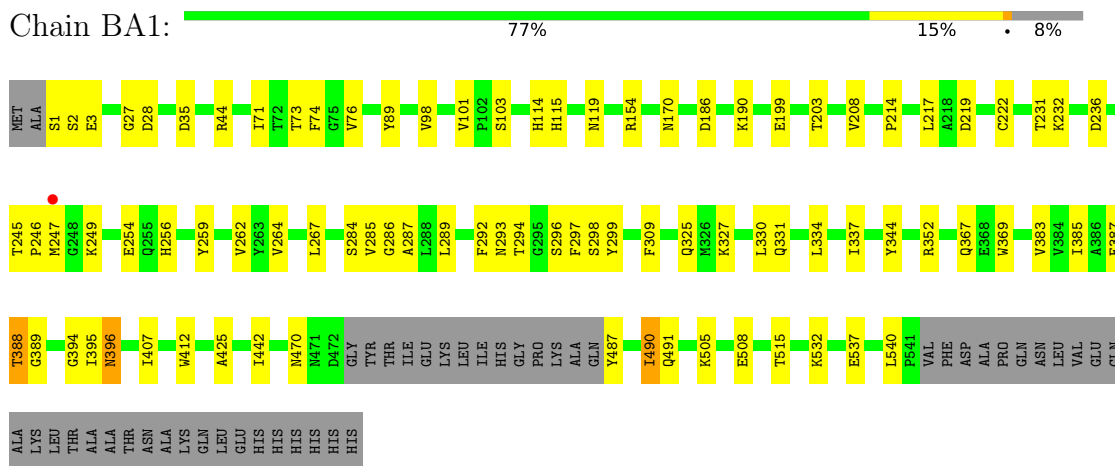
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

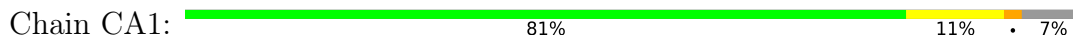
- Molecule 1: branched-chain-2-oxoacid decarboxylase

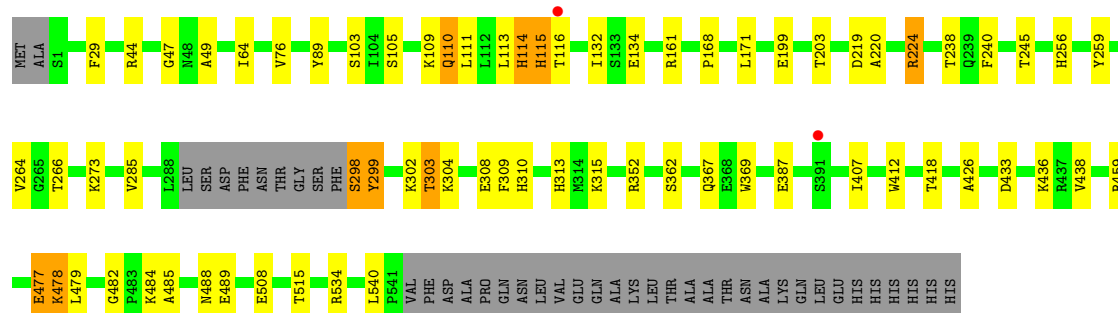


- Molecule 1: branched-chain-2-oxoacid decarboxylase



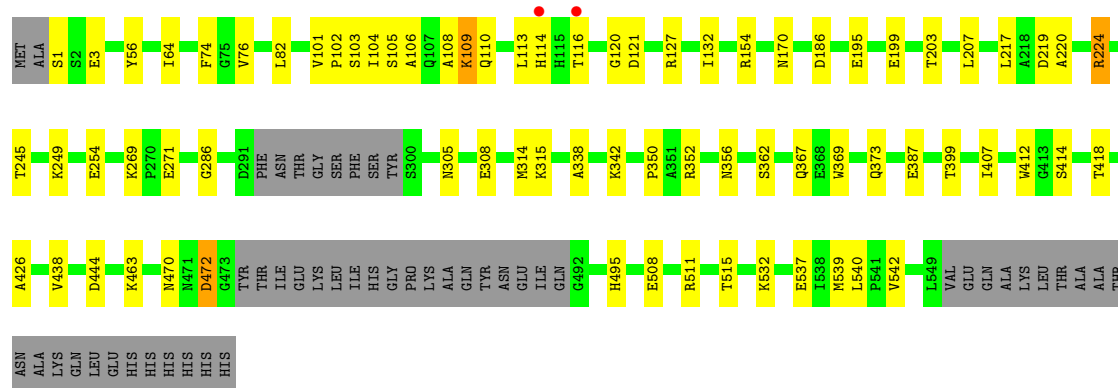
- Molecule 1: branched-chain-2-oxoacid decarboxylase





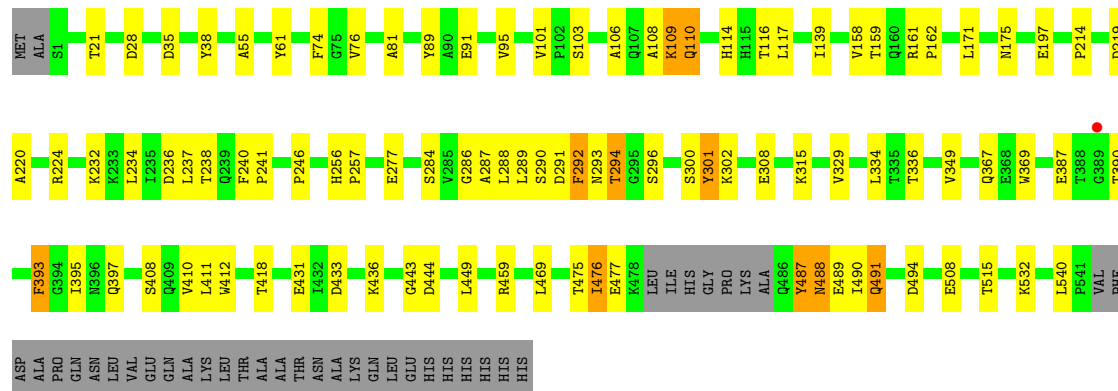
- Molecule 1: branched-chain-2-oxoacid decarboxylase

Chain DA1: 78% 12% 9%



- Molecule 1: branched-chain-2-oxoacid decarboxylase

Chain EA1: 76% 15% 7%



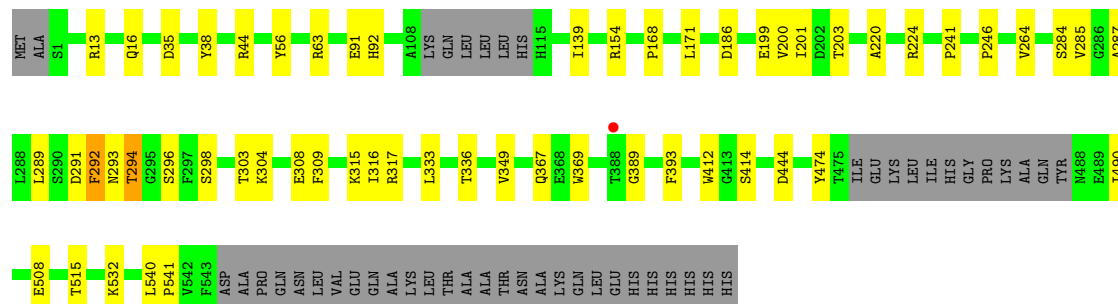
- Molecule 1: branched-chain-2-oxoacid decarboxylase

Chain FA1: 79% 12% 9%



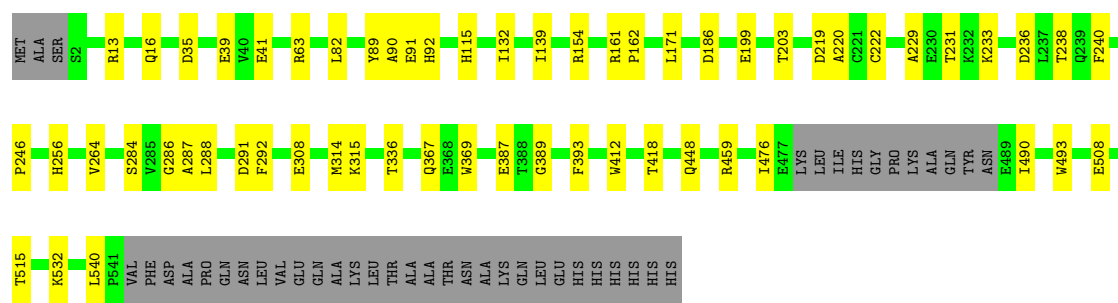
- Molecule 1: branched-chain-2-oxoacid decarboxylase

Chain GA1: 82% 10% 8%



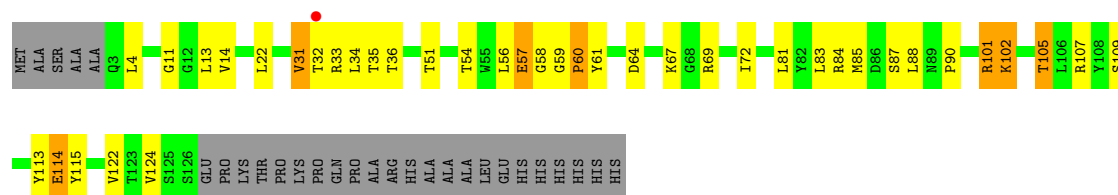
- Molecule 1: branched-chain-2-oxoacid decarboxylase

Chain HA1:  82% 10% 8%



- Molecule 2: NbJRi

Chain I: 



- Molecule 2: NbJRi

Chain J: 61% 20% 1% 18%



GLN
PRO
ALA
SER
ALA
ARG
HIS
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS

• Molecule 2: NbJRi

Chain K:  59% 19% 18%

MET ALA SER ALA ALA LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
Q3 E8 G12 C24 T30 V31 T32 R33 L34 T35 T36 V50 T54 W55 L56 P60 Y61 V66 L81 P90 R101 K102 A103 G104 T105 L106 R107 Y108 S109 A110 S111 E112 Y113 E114 Y115 W116 G117 Q121 V124 S125 GLU

PRO LYS THR PRO LYS LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
HIS

• Molecule 2: NbJRi

Chain L:  % 59% 20% 18%

MET ALA SER ALA ALA LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
Q3 T9 G11 V14 L20 S23 C24 G29 T30 V31 T32 T35 K45 E46 W55 L56 E57 G58 G59 P60 Y61 R69 N79 T90 L81 D86 P90 R101 K102 A103 G104 T105 L106 R107 E112 Y113 E114 Y115 V124

S125 S126 GLU PRO LYS LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
HIS

• Molecule 2: NbJRi

Chain N:  61% 16% 5% 18%

MET ALA SER ALA ALA LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
Q3 V14 V31 T35 R47 V50 T54 W55 L56 E57 G58 V66 R69 R74 D75 N76 L81 D86 S87 L88 Y97 R101 K102 A103 G104 T105 L106 R107 Y108 S109 A110 S111 E112 Y113 E114 G119 S126 GLU PRO LYS

THR PRO LYS LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
HIS

• Molecule 2: NbJRi

Chain O:  55% 25% 18%

MET ALA SER ALA ALA LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
Q3 L4 E8 T16 G28 G29 T30 V31 T32 R33 L34 T35 W55 L56 E57 G58 G59 P60 Y61 R69 F70 T71 R74 D75 N76 L81 M85 D86 V95 R101 K102 A103 G104 T105 L106 R107 Y108 S109 A110 S111 E112 Y113 E114 Y115 W116

G117 Q121 V122 S125 S126 GLU PRO LYS LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
HIS

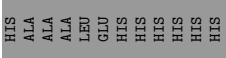
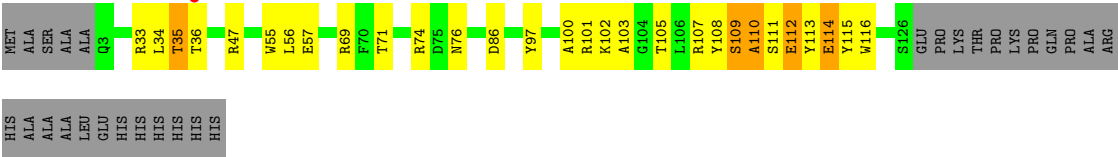
• Molecule 2: NbJRi

Chain P:  57% 20% 20%

MET ALA SER ALA ALA LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
Q3 E8 C24 R33 L34 T35 T36 R40 R47 E48 T54 W55 L56 E57 G58 G59 P60 Y61 R69 N76 L81 D86 Y97 A100 R101 K102 A103 G104 T105 L106 R107 Y108 S109 A110 S111 E112 Y113 E114 Y115 W116 G117 V124

SER SER GLU PRO LYS LYS PRO GLN PRO ALA ARG HIS HIS HIS HIS
HIS

● Molecule 2: NbJRi



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.45Å 113.05Å 155.50Å 79.42° 78.06° 67.02°	Depositor
Resolution (Å)	29.59 – 3.30 29.59 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (29.59-3.30) 92.1 (29.59-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.31Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.196 , 0.239 0.196 , 0.239	Depositor DCC
R_{free} test set	6496 reflections (6.95%)	wwPDB-VP
Wilson B-factor (Å ²)	96.5	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 90.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39941	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	AA1	0.10	0/4071	0.26	0/5533
1	BA1	0.09	0/4137	0.28	0/5624
1	CA1	0.12	0/4178	0.33	1/5679 (0.0%)
1	DA1	0.09	0/4090	0.27	0/5560
1	EA1	0.10	0/4196	0.32	0/5703
1	FA1	0.09	0/4072	0.26	0/5535
1	GA1	0.09	0/4109	0.27	0/5587
1	HA1	0.08	0/4148	0.26	0/5640
2	I	0.13	0/972	0.41	0/1318
2	J	0.09	0/972	0.33	0/1318
2	K	0.11	0/972	0.36	0/1318
2	L	0.10	0/972	0.36	0/1318
2	M	0.11	0/972	0.37	0/1318
2	N	0.11	0/972	0.33	0/1318
2	O	0.09	0/972	0.33	0/1318
2	P	0.11	0/960	0.42	0/1302
All	All	0.10	0/40765	0.30	1/55389 (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	AA1	0	1
1	CA1	0	1
1	FA1	0	1
2	I	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA1	115	HIS	N-CA-C	-5.67	106.74	113.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA1	489	GLU	Peptide
1	CA1	298	SER	Peptide
1	FA1	117	LEU	Peptide
2	I	101	ARG	Peptide

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	AA1	3989	0	3995	59	0
1	BA1	4052	0	4048	54	0
1	CA1	4092	0	4103	55	1
1	DA1	4008	0	4016	47	1
1	EA1	4110	0	4105	66	0
1	FA1	3990	0	3995	45	0
1	GA1	4025	0	4003	38	0
1	HA1	4063	0	4053	38	0
2	I	953	0	922	37	0
2	J	953	0	922	28	0
2	K	953	0	922	25	0
2	L	953	0	922	23	0
2	M	953	0	922	20	0
2	N	953	0	922	24	0
2	O	953	0	922	26	0
2	P	941	0	912	27	0
All	All	39941	0	39684	544	1

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 7.

The worst 5 of 544 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:FA1:111:LEU:HD11	1:FA1:120:GLY:HA2	1.53	0.91
1:FA1:117:LEU:HB2	1:FA1:119:ASN:HB3	1.56	0.85
2:O:55:TRP:NE1	2:O:102:LYS:O	2.10	0.82
2:L:101:ARG:HH12	2:L:107:ARG:HD2	1.50	0.77
2:I:101:ARG:NH2	2:I:105:THR:O	2.16	0.76

All (1) 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)
1:CA1:362:SER:OG	1:DA1:362:SER:O[1_645]	2.10	0.10

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	AA1	513/573 (90%)	486 (95%)	24 (5%)	3 (1%)	21	52
1	BA1	523/573 (91%)	494 (94%)	24 (5%)	5 (1%)	12	40
1	CA1	528/573 (92%)	485 (92%)	36 (7%)	7 (1%)	9	35
1	DA1	517/573 (90%)	491 (95%)	22 (4%)	4 (1%)	16	45
1	EA1	530/573 (92%)	490 (92%)	28 (5%)	12 (2%)	5	25
1	FA1	514/573 (90%)	486 (95%)	26 (5%)	2 (0%)	30	60
1	GA1	519/573 (91%)	496 (96%)	18 (4%)	5 (1%)	12	40
1	HA1	525/573 (92%)	504 (96%)	19 (4%)	2 (0%)	30	60
2	I	122/152 (80%)	104 (85%)	11 (9%)	7 (6%)	1	9
2	J	122/152 (80%)	104 (85%)	12 (10%)	6 (5%)	1	12
2	K	122/152 (80%)	108 (88%)	8 (7%)	6 (5%)	1	12
2	L	122/152 (80%)	101 (83%)	12 (10%)	9 (7%)	1	6
2	M	122/152 (80%)	103 (84%)	11 (9%)	8 (7%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	122/152 (80%)	104 (85%)	8 (7%)	10 (8%)	0	5
2	O	122/152 (80%)	102 (84%)	12 (10%)	8 (7%)	1	7
2	P	120/152 (79%)	103 (86%)	9 (8%)	8 (7%)	1	7
All	All	5143/5800 (89%)	4761 (93%)	280 (5%)	102 (2%)	6	27

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA1	491	GLN
1	BA1	490	ILE
1	CA1	110	GLN
1	CA1	114	HIS
1	DA1	105	SER

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	AA1	430/476 (90%)	429 (100%)	1 (0%)	87	88
1	BA1	437/476 (92%)	435 (100%)	2 (0%)	81	83
1	CA1	440/476 (92%)	439 (100%)	1 (0%)	87	88
1	DA1	432/476 (91%)	431 (100%)	1 (0%)	87	88
1	EA1	443/476 (93%)	442 (100%)	1 (0%)	87	88
1	FA1	430/476 (90%)	429 (100%)	1 (0%)	87	88
1	GA1	433/476 (91%)	432 (100%)	1 (0%)	87	88
1	HA1	438/476 (92%)	437 (100%)	1 (0%)	87	88
2	I	98/119 (82%)	98 (100%)	0	100	100
2	J	98/119 (82%)	98 (100%)	0	100	100
2	K	98/119 (82%)	98 (100%)	0	100	100
2	L	98/119 (82%)	98 (100%)	0	100	100
2	M	98/119 (82%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	98/119 (82%)	98 (100%)	0	100	100
2	O	98/119 (82%)	98 (100%)	0	100	100
2	P	96/119 (81%)	96 (100%)	0	100	100
All	All	4265/4760 (90%)	4256 (100%)	9 (0%)	87	88

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	GA1	336	THR
1	HA1	336	THR
1	CA1	224	ARG
1	DA1	224	ARG
1	EA1	336	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	P	5	GLN
2	M	5	GLN
2	K	5	GLN
2	L	3	GLN
2	N	5	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 oligosaccharides 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

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, 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	AA1	519/573 (90%)	-0.54	2 (0%) 88 79	64, 100, 142, 237	0
1	BA1	527/573 (91%)	-0.51	1 (0%) 91 86	67, 100, 160, 258	0
1	CA1	532/573 (92%)	-0.53	2 (0%) 88 79	70, 107, 165, 272	0
1	DA1	523/573 (91%)	-0.52	2 (0%) 88 79	74, 111, 161, 265	0
1	EA1	534/573 (93%)	-0.42	1 (0%) 91 86	74, 132, 192, 327	0
1	FA1	520/573 (90%)	-0.54	1 (0%) 91 86	71, 113, 167, 249	0
1	GA1	525/573 (91%)	-0.46	1 (0%) 91 86	89, 138, 195, 272	0
1	HA1	529/573 (92%)	-0.40	0 100 100	100, 166, 226, 309	0
2	I	124/152 (81%)	-0.38	1 (0%) 82 68	79, 105, 143, 200	0
2	J	124/152 (81%)	-0.43	0 100 100	99, 144, 190, 226	0
2	K	124/152 (81%)	-0.38	0 100 100	74, 103, 146, 169	0
2	L	124/152 (81%)	-0.39	1 (0%) 82 68	84, 113, 157, 216	0
2	M	124/152 (81%)	-0.27	1 (0%) 82 68	167, 214, 252, 282	0
2	N	124/152 (81%)	-0.41	0 100 100	111, 153, 204, 240	0
2	O	124/152 (81%)	-0.15	0 100 100	120, 158, 205, 255	0
2	P	122/152 (80%)	-0.42	0 100 100	144, 177, 220, 266	0
All	All	5199/5800 (89%)	-0.46	13 (0%) 90 82	64, 121, 207, 327	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA1	116	THR	3.3
1	BA1	247	MET	2.8
1	EA1	389	GLY	2.6
1	DA1	116	THR	2.6
2	L	59	GLY	2.5

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 oligosaccharides 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.