



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:40 PM UTC

PDB ID : 6KDF / pdb\_00006kdf  
Title : Crystal structure of the alpha beta heterodimer of human IDH3 in APO form.  
Authors : Sun, P.; Ding, J.  
Deposited on : 2019-07-02  
Resolution : 3.05 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

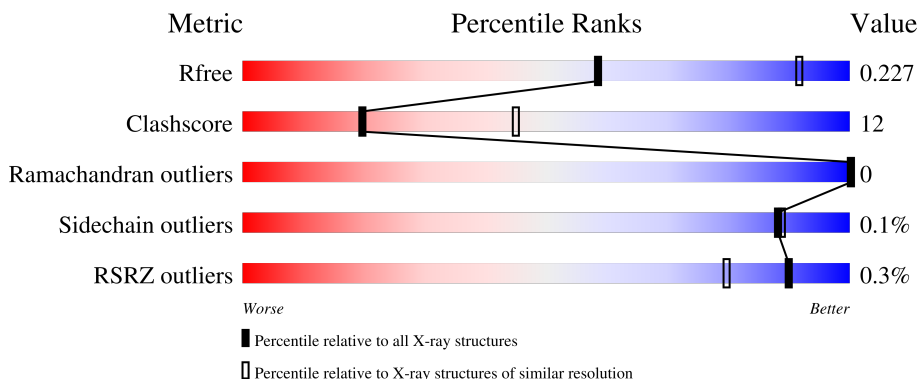
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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  $\geq 3$ , 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	341	 79% 19%
1	B	341	 76% 22%
1	E	341	 75% 24%
1	G	341	 70% 28%
1	I	341	 72% 26%

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Mol	Chain	Length	Quality of chain
1	K	341	 72% 26%
1	M	341	 68% 30%
1	O	341	 73% 26%
2	C	356	 69% 21% 10%
2	D	356	 69% 20% 10%
2	F	356	 69% 19% 12%
2	H	356	 68% 22% 10%
2	J	356	 69% 20% 11%
2	L	356	 63% 25% 11%
2	N	356	 68% 21% 11%
2	P	356	 69% 21% 10%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 39059 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 Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	333	Total 2474	C 1552	N 421	O 479	S 22	0	0	0
1	A	335	Total 2503	C 1572	N 429	O 481	S 21	0	0	0
1	E	338	Total 2518	C 1580	N 431	O 485	S 22	0	0	0
1	G	335	Total 2491	C 1565	N 427	O 477	S 22	0	0	0
1	I	333	Total 2468	C 1548	N 421	O 477	S 22	0	0	0
1	K	333	Total 2476	C 1555	N 422	O 477	S 22	0	0	0
1	M	335	Total 2490	C 1564	N 425	O 479	S 22	0	0	0
1	O	335	Total 2495	C 1566	N 427	O 481	S 21	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P50213
B	0	SER	-	expression tag	UNP P50213
A	-1	GLY	-	expression tag	UNP P50213
A	0	SER	-	expression tag	UNP P50213
E	-1	GLY	-	expression tag	UNP P50213
E	0	SER	-	expression tag	UNP P50213
G	-1	GLY	-	expression tag	UNP P50213
G	0	SER	-	expression tag	UNP P50213
I	-1	GLY	-	expression tag	UNP P50213
I	0	SER	-	expression tag	UNP P50213
K	-1	GLY	-	expression tag	UNP P50213
K	0	SER	-	expression tag	UNP P50213
M	-1	GLY	-	expression tag	UNP P50213

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Chain	Residue	Modelled	Actual	Comment	Reference
M	0	SER	-	expression tag	UNP P50213
O	-1	GLY	-	expression tag	UNP P50213
O	0	SER	-	expression tag	UNP P50213

- Molecule 2 is a protein called Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	319	Total 2413	C 1530	N 418	O 445	S 20	0	0	0
2	D	319	Total 2391	C 1509	N 414	O 448	S 20	0	0	0
2	F	315	Total 2383	C 1511	N 414	O 438	S 20	0	0	0
2	H	319	Total 2395	C 1512	N 416	O 447	S 20	0	0	0
2	J	316	Total 2393	C 1517	N 418	O 438	S 20	0	0	0
2	L	317	Total 2380	C 1505	N 415	O 440	S 20	0	0	0
2	N	316	Total 2388	C 1512	N 414	O 442	S 20	0	0	0
2	P	320	Total 2401	C 1516	N 416	O 449	S 20	0	0	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	341	GLU	-	expression tag	UNP O43837
C	342	ILE	-	expression tag	UNP O43837
C	343	CYS	-	expression tag	UNP O43837
C	344	ARG	-	expression tag	UNP O43837
C	345	ARG	-	expression tag	UNP O43837
C	346	VAL	-	expression tag	UNP O43837
C	347	LYS	-	expression tag	UNP O43837
C	348	ASP	-	expression tag	UNP O43837
C	349	LEU	-	expression tag	UNP O43837
C	350	ASP	-	expression tag	UNP O43837
C	351	GLU	-	expression tag	UNP O43837
C	352	ASN	-	expression tag	UNP O43837
C	353	LEU	-	expression tag	UNP O43837
C	354	TYR	-	expression tag	UNP O43837
C	355	PHE	-	expression tag	UNP O43837

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Chain	Residue	Modelled	Actual	Comment	Reference
C	356	GLN	-	expression tag	UNP O43837
D	341	GLU	-	expression tag	UNP O43837
D	342	ILE	-	expression tag	UNP O43837
D	343	CYS	-	expression tag	UNP O43837
D	344	ARG	-	expression tag	UNP O43837
D	345	ARG	-	expression tag	UNP O43837
D	346	VAL	-	expression tag	UNP O43837
D	347	LYS	-	expression tag	UNP O43837
D	348	ASP	-	expression tag	UNP O43837
D	349	LEU	-	expression tag	UNP O43837
D	350	ASP	-	expression tag	UNP O43837
D	351	GLU	-	expression tag	UNP O43837
D	352	ASN	-	expression tag	UNP O43837
D	353	LEU	-	expression tag	UNP O43837
D	354	TYR	-	expression tag	UNP O43837
D	355	PHE	-	expression tag	UNP O43837
D	356	GLN	-	expression tag	UNP O43837
F	341	GLU	-	expression tag	UNP O43837
F	342	ILE	-	expression tag	UNP O43837
F	343	CYS	-	expression tag	UNP O43837
F	344	ARG	-	expression tag	UNP O43837
F	345	ARG	-	expression tag	UNP O43837
F	346	VAL	-	expression tag	UNP O43837
F	347	LYS	-	expression tag	UNP O43837
F	348	ASP	-	expression tag	UNP O43837
F	349	LEU	-	expression tag	UNP O43837
F	350	ASP	-	expression tag	UNP O43837
F	351	GLU	-	expression tag	UNP O43837
F	352	ASN	-	expression tag	UNP O43837
F	353	LEU	-	expression tag	UNP O43837
F	354	TYR	-	expression tag	UNP O43837
F	355	PHE	-	expression tag	UNP O43837
F	356	GLN	-	expression tag	UNP O43837
H	341	GLU	-	expression tag	UNP O43837
H	342	ILE	-	expression tag	UNP O43837
H	343	CYS	-	expression tag	UNP O43837
H	344	ARG	-	expression tag	UNP O43837
H	345	ARG	-	expression tag	UNP O43837
H	346	VAL	-	expression tag	UNP O43837
H	347	LYS	-	expression tag	UNP O43837
H	348	ASP	-	expression tag	UNP O43837
H	349	LEU	-	expression tag	UNP O43837

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Chain	Residue	Modelled	Actual	Comment	Reference
H	350	ASP	-	expression tag	UNP O43837
H	351	GLU	-	expression tag	UNP O43837
H	352	ASN	-	expression tag	UNP O43837
H	353	LEU	-	expression tag	UNP O43837
H	354	TYR	-	expression tag	UNP O43837
H	355	PHE	-	expression tag	UNP O43837
H	356	GLN	-	expression tag	UNP O43837
J	341	GLU	-	expression tag	UNP O43837
J	342	ILE	-	expression tag	UNP O43837
J	343	CYS	-	expression tag	UNP O43837
J	344	ARG	-	expression tag	UNP O43837
J	345	ARG	-	expression tag	UNP O43837
J	346	VAL	-	expression tag	UNP O43837
J	347	LYS	-	expression tag	UNP O43837
J	348	ASP	-	expression tag	UNP O43837
J	349	LEU	-	expression tag	UNP O43837
J	350	ASP	-	expression tag	UNP O43837
J	351	GLU	-	expression tag	UNP O43837
J	352	ASN	-	expression tag	UNP O43837
J	353	LEU	-	expression tag	UNP O43837
J	354	TYR	-	expression tag	UNP O43837
J	355	PHE	-	expression tag	UNP O43837
J	356	GLN	-	expression tag	UNP O43837
L	341	GLU	-	expression tag	UNP O43837
L	342	ILE	-	expression tag	UNP O43837
L	343	CYS	-	expression tag	UNP O43837
L	344	ARG	-	expression tag	UNP O43837
L	345	ARG	-	expression tag	UNP O43837
L	346	VAL	-	expression tag	UNP O43837
L	347	LYS	-	expression tag	UNP O43837
L	348	ASP	-	expression tag	UNP O43837
L	349	LEU	-	expression tag	UNP O43837
L	350	ASP	-	expression tag	UNP O43837
L	351	GLU	-	expression tag	UNP O43837
L	352	ASN	-	expression tag	UNP O43837
L	353	LEU	-	expression tag	UNP O43837
L	354	TYR	-	expression tag	UNP O43837
L	355	PHE	-	expression tag	UNP O43837
L	356	GLN	-	expression tag	UNP O43837
N	341	GLU	-	expression tag	UNP O43837
N	342	ILE	-	expression tag	UNP O43837
N	343	CYS	-	expression tag	UNP O43837

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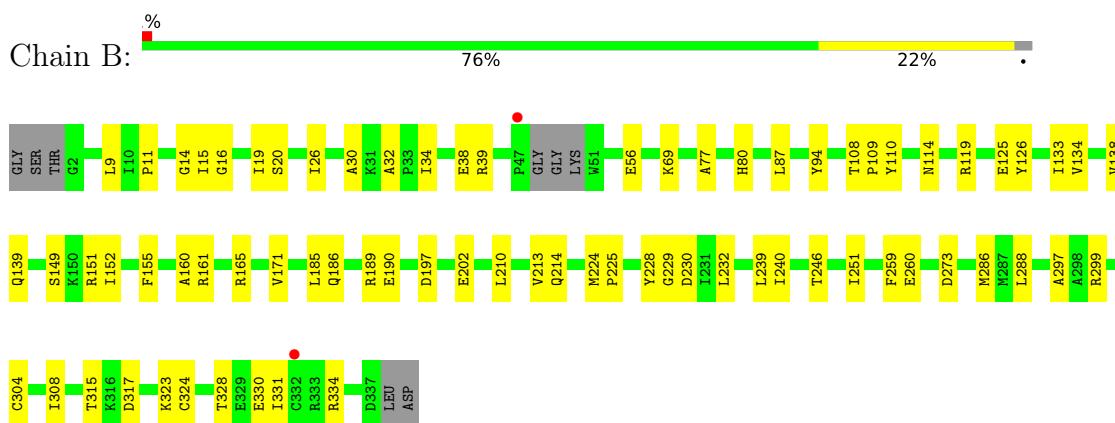
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Chain	Residue	Modelled	Actual	Comment	Reference
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N	345	ARG	-	expression tag	UNP O43837
N	346	VAL	-	expression tag	UNP O43837
N	347	LYS	-	expression tag	UNP O43837
N	348	ASP	-	expression tag	UNP O43837
N	349	LEU	-	expression tag	UNP O43837
N	350	ASP	-	expression tag	UNP O43837
N	351	GLU	-	expression tag	UNP O43837
N	352	ASN	-	expression tag	UNP O43837
N	353	LEU	-	expression tag	UNP O43837
N	354	TYR	-	expression tag	UNP O43837
N	355	PHE	-	expression tag	UNP O43837
N	356	GLN	-	expression tag	UNP O43837
P	341	GLU	-	expression tag	UNP O43837
P	342	ILE	-	expression tag	UNP O43837
P	343	CYS	-	expression tag	UNP O43837
P	344	ARG	-	expression tag	UNP O43837
P	345	ARG	-	expression tag	UNP O43837
P	346	VAL	-	expression tag	UNP O43837
P	347	LYS	-	expression tag	UNP O43837
P	348	ASP	-	expression tag	UNP O43837
P	349	LEU	-	expression tag	UNP O43837
P	350	ASP	-	expression tag	UNP O43837
P	351	GLU	-	expression tag	UNP O43837
P	352	ASN	-	expression tag	UNP O43837
P	353	LEU	-	expression tag	UNP O43837
P	354	TYR	-	expression tag	UNP O43837
P	355	PHE	-	expression tag	UNP O43837
P	356	GLN	-	expression tag	UNP O43837

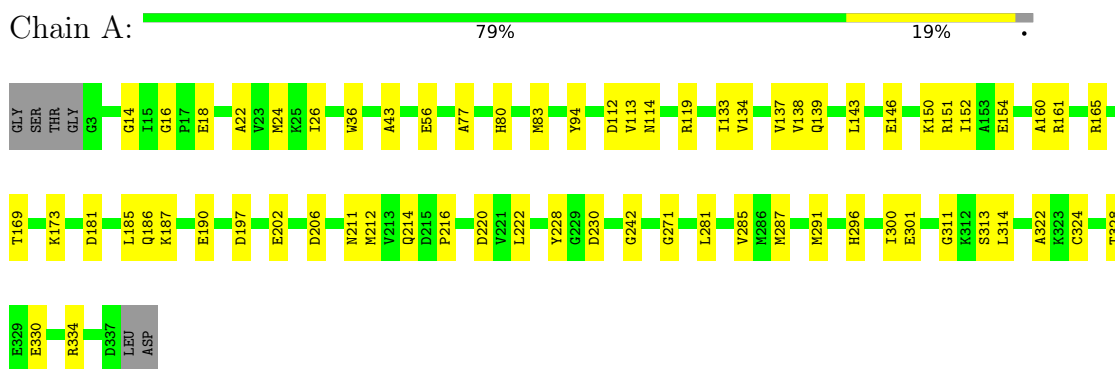
### 3 Residue-property plots [i](#)

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.

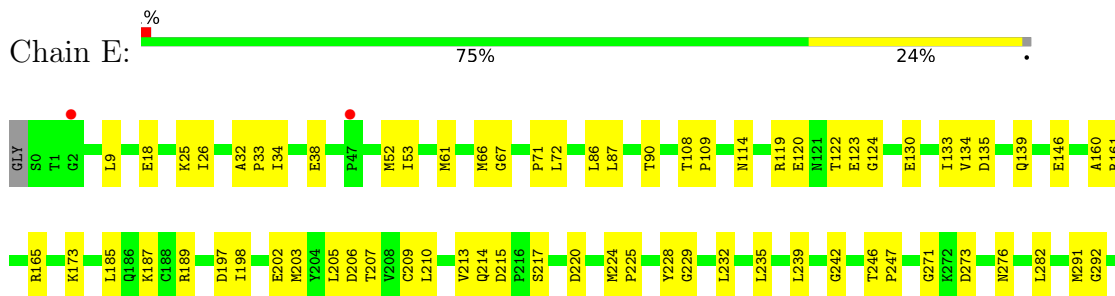
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

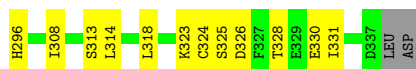


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial



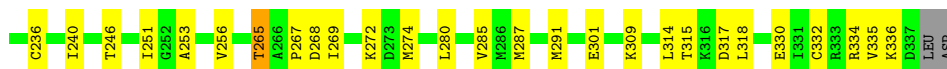
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial





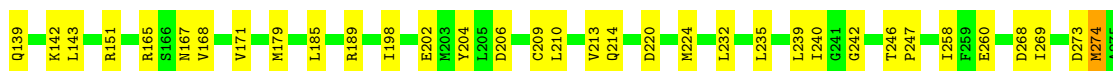
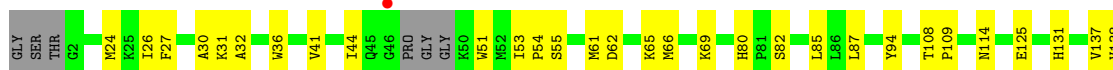
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

Chain G: 70% 28%



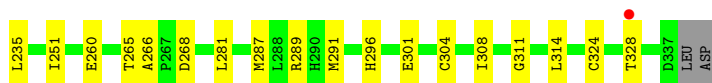
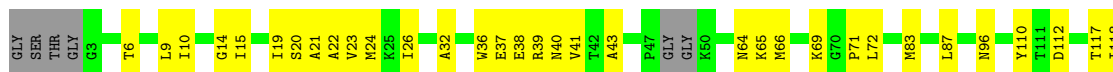
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

Chain I: 72% 26%



- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

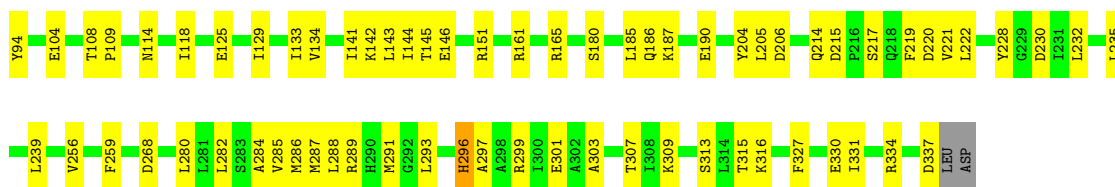
Chain K: 72% 26%



- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

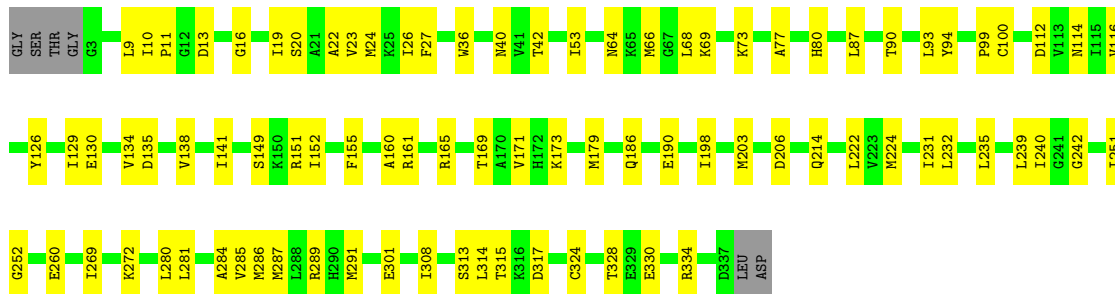
Chain M: 68% 30%





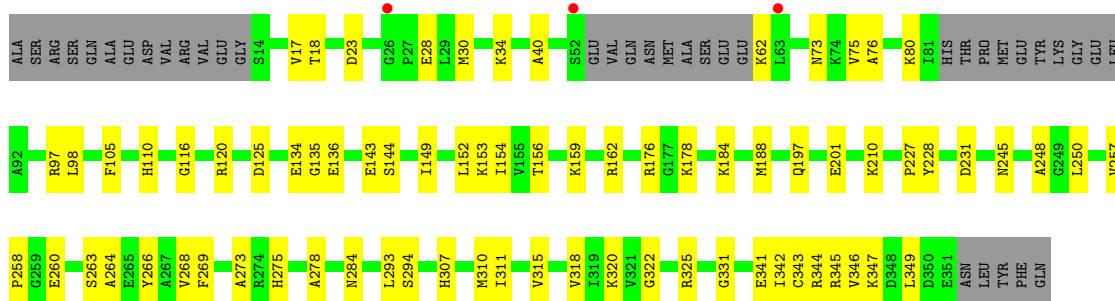
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

Chain O: 73% 26%



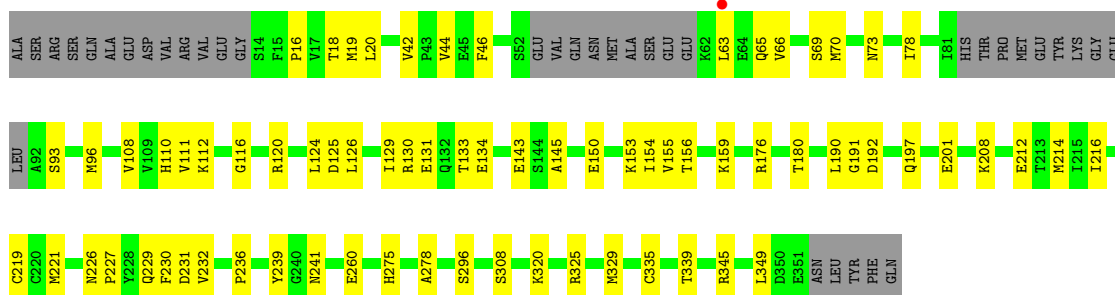
- Molecule 2: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain C: 69% 21% 10%



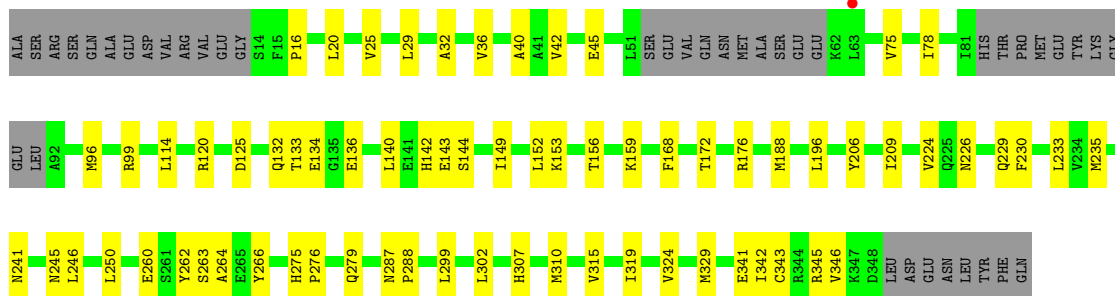
- Molecule 2: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain D: 69% 20% 10%

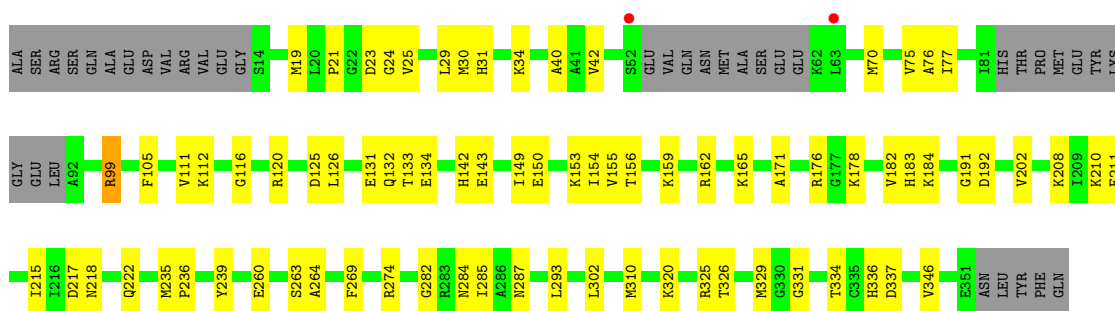


- Molecule 2: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

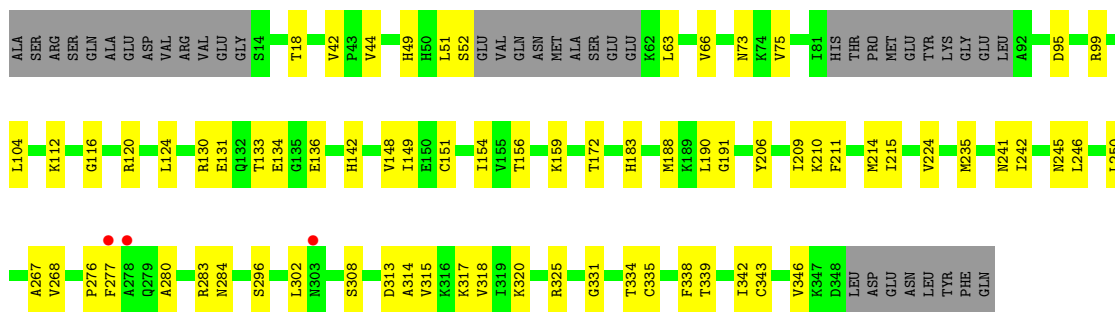
Chain F: 69% 19% 12%



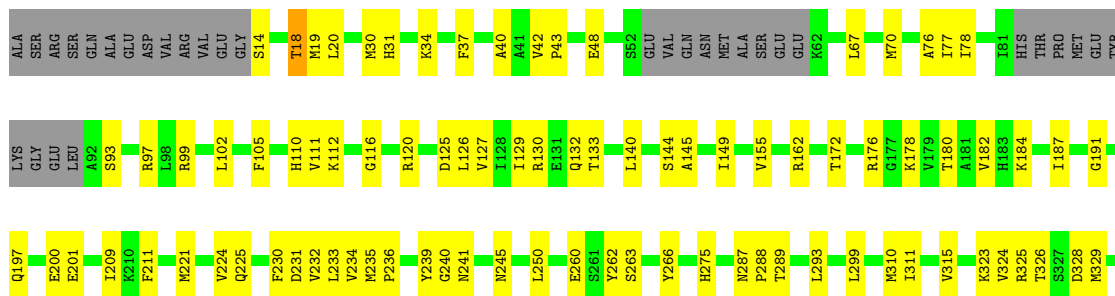
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

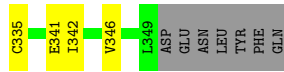


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

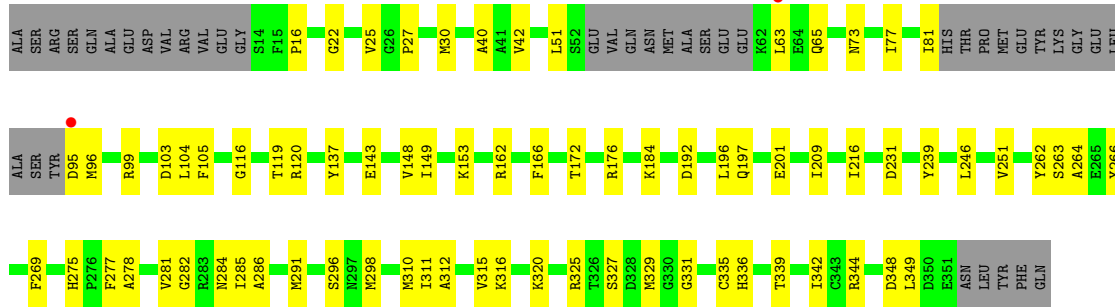


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

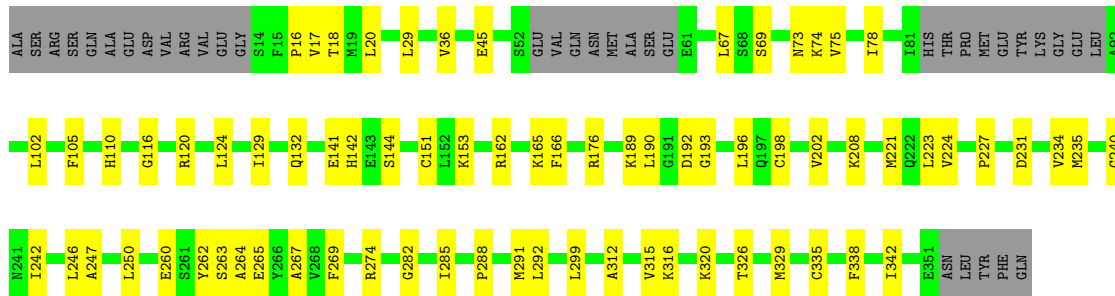




• Molecule 2: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	208.91Å 170.43Å 208.09Å 90.00° 103.43° 90.00°	Depositor
Resolution (Å)	49.75 – 3.05 49.75 – 3.05	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.75-3.05) 97.5 (49.75-3.05)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 3.07Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.177 , 0.227 0.179 , 0.227	Depositor DCC
$R_{free}$ test set	6602 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtrriage
Anisotropy	0.013	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	39059	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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	0.47	0/2546	0.66	0/3450
1	B	0.48	0/2514	0.67	0/3409
1	E	0.52	0/2561	0.68	0/3471
1	G	0.43	0/2534	0.63	2/3436 (0.1%)
1	I	0.54	0/2508	0.71	0/3401
1	K	0.52	0/2516	0.77	0/3411
1	M	0.52	0/2532	0.75	0/3433
1	O	0.48	0/2538	0.70	0/3442
2	C	0.46	0/2454	0.65	0/3315
2	D	0.47	0/2430	0.69	0/3286
2	F	0.43	0/2424	0.65	0/3275
2	H	0.45	0/2435	0.68	1/3292 (0.0%)
2	J	0.42	0/2434	0.67	0/3288
2	L	0.52	0/2420	0.74	0/3271
2	N	0.48	0/2428	0.71	0/3282
2	P	0.48	0/2442	0.68	0/3303
All	All	0.48	0/39716	0.69	3/53765 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	99	ARG	CG-CD-NE	-6.37	97.99	112.00
1	G	265	THR	CA-C-N	5.09	128.33	122.83
1	G	265	THR	C-N-CA	5.09	128.33	122.83

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	2503	0	2475	45	1
1	B	2474	0	2421	55	0
1	E	2518	0	2486	63	0
1	G	2491	0	2454	67	0
1	I	2468	0	2410	77	1
1	K	2476	0	2429	72	0
1	M	2490	0	2453	85	0
1	O	2495	0	2453	62	0
2	C	2413	0	2389	53	0
2	D	2391	0	2337	51	0
2	F	2383	0	2361	55	0
2	H	2395	0	2345	53	0
2	J	2393	0	2380	62	0
2	L	2380	0	2341	72	0
2	N	2388	0	2362	53	0
2	P	2401	0	2336	51	0
All	All	39059	0	38432	894	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 12.

The worst 5 of 894 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:I:273:ASP:O	1:I:324:CYS:N	1.71	1.21
1:I:51:TRP:HH2	1:I:80:HIS:NE2	1.52	1.08
1:M:289:ARG:NH2	1:M:301:GLU:OE2	1.86	1.08
1:M:32:ALA:HA	1:M:296:HIS:CE1	1.92	1.04
1:I:51:TRP:CH2	1:I:80:HIS:CD2	2.46	1.04

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:A:56:GLU:OE1	1:I:55:SER:OG[2_556]	2.09	0.11

### 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	333/341 (98%)	310 (93%)	23 (7%)	0	100	100
1	B	329/341 (96%)	309 (94%)	20 (6%)	0	100	100
1	E	336/341 (98%)	315 (94%)	21 (6%)	0	100	100
1	G	333/341 (98%)	311 (93%)	22 (7%)	0	100	100
1	I	329/341 (96%)	303 (92%)	26 (8%)	0	100	100
1	K	329/341 (96%)	305 (93%)	24 (7%)	0	100	100
1	M	333/341 (98%)	312 (94%)	21 (6%)	0	100	100
1	O	333/341 (98%)	308 (92%)	25 (8%)	0	100	100
2	C	313/356 (88%)	296 (95%)	17 (5%)	0	100	100
2	D	313/356 (88%)	293 (94%)	20 (6%)	0	100	100
2	F	309/356 (87%)	286 (93%)	23 (7%)	0	100	100
2	H	313/356 (88%)	295 (94%)	18 (6%)	0	100	100
2	J	310/356 (87%)	286 (92%)	24 (8%)	0	100	100
2	L	311/356 (87%)	294 (94%)	17 (6%)	0	100	100
2	N	310/356 (87%)	284 (92%)	26 (8%)	0	100	100
2	P	314/356 (88%)	292 (93%)	22 (7%)	0	100	100
All	All	5148/5576 (92%)	4799 (93%)	349 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 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	266/278 (96%)	266 (100%)	0	100	100
1	B	261/278 (94%)	261 (100%)	0	100	100
1	E	267/278 (96%)	267 (100%)	0	100	100
1	G	263/278 (95%)	263 (100%)	0	100	100
1	I	259/278 (93%)	258 (100%)	1 (0%)	84	84
1	K	261/278 (94%)	261 (100%)	0	100	100
1	M	263/278 (95%)	261 (99%)	2 (1%)	73	79
1	O	264/278 (95%)	264 (100%)	0	100	100
2	C	252/300 (84%)	252 (100%)	0	100	100
2	D	248/300 (83%)	248 (100%)	0	100	100
2	F	249/300 (83%)	249 (100%)	0	100	100
2	H	249/300 (83%)	249 (100%)	0	100	100
2	J	251/300 (84%)	251 (100%)	0	100	100
2	L	247/300 (82%)	246 (100%)	1 (0%)	84	84
2	N	251/300 (84%)	251 (100%)	0	100	100
2	P	248/300 (83%)	248 (100%)	0	100	100
All	All	4099/4624 (89%)	4095 (100%)	4 (0%)	88	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	274	MET
2	L	18	THR
1	M	293	LEU
1	M	296	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	336	HIS
2	L	226	ASN
1	K	163	ASN
2	L	47	GLN
2	L	287	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 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 [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	335/341 (98%)	-0.57	0 <b>100</b> <b>100</b>	25, 47, 85, 101	0
1	B	333/341 (97%)	-0.43	2 (0%) 85 69	32, 51, 79, 125	0
1	E	338/341 (99%)	-0.54	2 (0%) 85 69	27, 44, 71, 105	0
1	G	335/341 (98%)	-0.40	0 <b>100</b> <b>100</b>	33, 58, 92, 107	0
1	I	333/341 (97%)	-0.48	1 (0%) 90 80	34, 49, 79, 111	0
1	K	333/341 (97%)	-0.47	1 (0%) 90 80	27, 49, 83, 105	0
1	M	335/341 (98%)	-0.36	0 <b>100</b> <b>100</b>	26, 51, 87, 100	0
1	O	335/341 (98%)	-0.47	0 <b>100</b> <b>100</b>	30, 50, 87, 104	0
2	C	319/356 (89%)	-0.45	3 (0%) 81 61	32, 51, 92, 111	0
2	D	319/356 (89%)	-0.54	1 (0%) 90 80	33, 48, 85, 103	0
2	F	315/356 (88%)	-0.36	1 (0%) 90 80	38, 57, 93, 111	0
2	H	319/356 (89%)	-0.48	2 (0%) 85 69	38, 52, 91, 111	0
2	J	316/356 (88%)	-0.37	3 (0%) 81 61	40, 58, 88, 111	0
2	L	317/356 (89%)	-0.27	0 <b>100</b> <b>100</b>	34, 62, 98, 133	0
2	N	316/356 (88%)	-0.48	2 (0%) 85 69	31, 50, 87, 108	0
2	P	320/356 (89%)	-0.51	0 <b>100</b> <b>100</b>	32, 51, 86, 112	0
All	All	5218/5576 (93%)	-0.45	18 (0%) <b>90</b> <b>80</b>	25, 52, 87, 133	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	46	GLY	4.2
1	B	47	PRO	3.8
2	F	63	LEU	3.1
2	J	303	ASN	2.9
2	C	63	LEU	2.9

## 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.