



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2022 – 12:18 PM JST

PDB ID : 8GS5
Title : Crystal structure of a constitutively active mutant of human IDH3 holoenzyme in apo form
Authors : Sun, P.; Chen, X.; Ding, J.
Deposited on : 2022-09-04
Resolution : 4.49 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

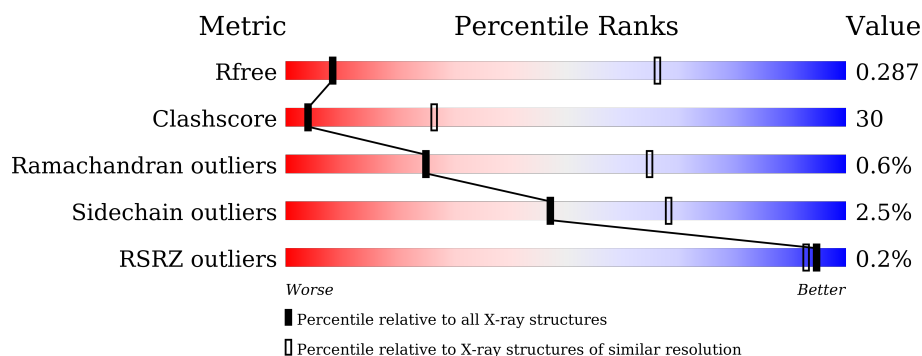
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.49 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	1051 (5.12-3.80)
Clashscore	141614	1119 (5.12-3.80)
Ramachandran outliers	138981	1065 (5.12-3.80)
Sidechain outliers	138945	1047 (5.12-3.80)
RSRZ outliers	127900	1099 (5.20-3.70)

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	A	339	
1	C	339	
1	E	339	
1	G	339	
1	I	339	
1	K	339	

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Mol	Chain	Length	Quality of chain
1	M	339	<div><div>%</div><div><div></div><div>66%</div><div>33%</div><div></div></div><div></div></div>
1	O	339	<div><div></div><div>53%</div><div>42%</div><div></div></div> <div><div></div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39351 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
1	C	328	Total	C	N	O	S	0	0	0
			2389	1503	406	459	21			
1	A	336	Total	C	N	O	S	0	0	0
			2412	1510	412	470	20			
1	G	324	Total	C	N	O	S	0	0	0
			2444	1537	417	470	20			
1	E	336	Total	C	N	O	S	0	0	0
			2400	1502	411	465	22			
1	K	327	Total	C	N	O	S	0	0	0
			2480	1561	424	473	22			
1	I	336	Total	C	N	O	S	0	0	0
			2439	1530	414	473	22			
1	O	329	Total	C	N	O	S	0	0	0
			2454	1546	419	467	22			
1	M	336	Total	C	N	O	S	0	0	0
			2436	1524	416	474	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	ALA	GLN	engineered mutation	UNP P50213
A	139	ALA	GLN	engineered mutation	UNP P50213
G	139	ALA	GLN	engineered mutation	UNP P50213
E	139	ALA	GLN	engineered mutation	UNP P50213
K	139	ALA	GLN	engineered mutation	UNP P50213
I	139	ALA	GLN	engineered mutation	UNP P50213
O	139	ALA	GLN	engineered mutation	UNP P50213
M	139	ALA	GLN	engineered mutation	UNP P50213

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	339	Total	C	N	O	S	0	0	0
			2496	1556	456	466	18			
2	H	347	Total	C	N	O	S	0	0	0
			2555	1594	467	476	18			
2	L	347	Total	C	N	O	S	0	0	0
			2569	1606	469	477	17			
2	P	346	Total	C	N	O	S	0	0	0
			2539	1590	462	469	18			

- Molecule 3 is a protein called Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	335	Total	C	N	O	S	0	0	0
			2466	1557	425	465	19			
3	F	335	Total	C	N	O	S	0	0	0
			2400	1516	420	446	18			
3	J	335	Total	C	N	O	S	0	0	0
			2465	1557	429	459	20			
3	N	334	Total	C	N	O	S	0	0	0
			2407	1515	417	456	19			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	341	GLU	-	expression tag	UNP O43837-2
B	342	ILE	-	expression tag	UNP O43837-2
B	343	CYS	-	expression tag	UNP O43837-2
B	344	ARG	-	expression tag	UNP O43837-2
B	345	ARG	-	expression tag	UNP O43837-2
B	346	VAL	-	expression tag	UNP O43837-2
B	347	LYS	-	expression tag	UNP O43837-2
B	348	ASP	-	expression tag	UNP O43837-2
B	349	LEU	-	expression tag	UNP O43837-2
B	350	ASP	-	expression tag	UNP O43837-2
B	351	GLU	-	expression tag	UNP O43837-2
B	352	ASN	-	expression tag	UNP O43837-2
F	341	GLU	-	expression tag	UNP O43837-2
F	342	ILE	-	expression tag	UNP O43837-2
F	343	CYS	-	expression tag	UNP O43837-2
F	344	ARG	-	expression tag	UNP O43837-2
F	345	ARG	-	expression tag	UNP O43837-2
F	346	VAL	-	expression tag	UNP O43837-2

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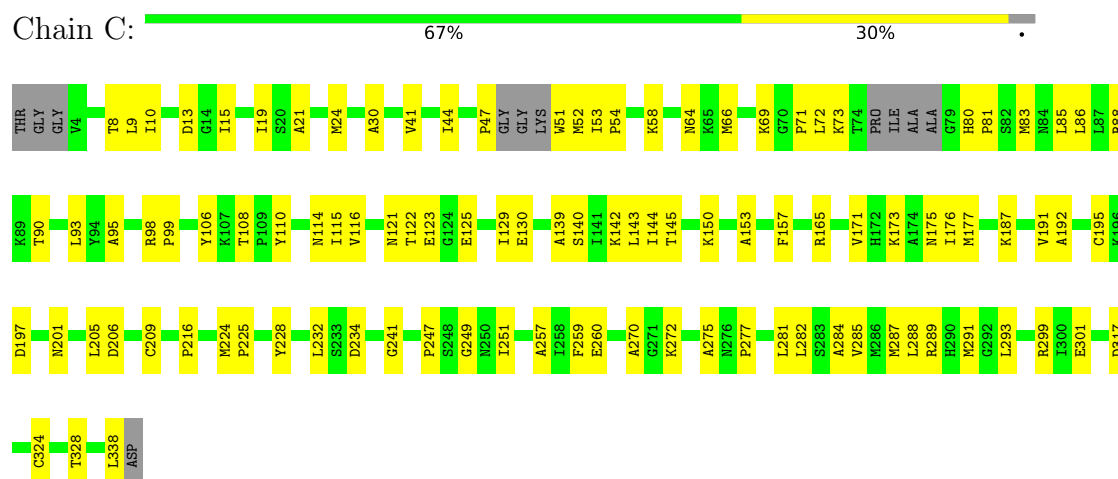
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Chain	Residue	Modelled	Actual	Comment	Reference
F	347	LYS	-	expression tag	UNP O43837-2
F	348	ASP	-	expression tag	UNP O43837-2
F	349	LEU	-	expression tag	UNP O43837-2
F	350	ASP	-	expression tag	UNP O43837-2
F	351	GLU	-	expression tag	UNP O43837-2
F	352	ASN	-	expression tag	UNP O43837-2
J	341	GLU	-	expression tag	UNP O43837-2
J	342	ILE	-	expression tag	UNP O43837-2
J	343	CYS	-	expression tag	UNP O43837-2
J	344	ARG	-	expression tag	UNP O43837-2
J	345	ARG	-	expression tag	UNP O43837-2
J	346	VAL	-	expression tag	UNP O43837-2
J	347	LYS	-	expression tag	UNP O43837-2
J	348	ASP	-	expression tag	UNP O43837-2
J	349	LEU	-	expression tag	UNP O43837-2
J	350	ASP	-	expression tag	UNP O43837-2
J	351	GLU	-	expression tag	UNP O43837-2
J	352	ASN	-	expression tag	UNP O43837-2
N	341	GLU	-	expression tag	UNP O43837-2
N	342	ILE	-	expression tag	UNP O43837-2
N	343	CYS	-	expression tag	UNP O43837-2
N	344	ARG	-	expression tag	UNP O43837-2
N	345	ARG	-	expression tag	UNP O43837-2
N	346	VAL	-	expression tag	UNP O43837-2
N	347	LYS	-	expression tag	UNP O43837-2
N	348	ASP	-	expression tag	UNP O43837-2
N	349	LEU	-	expression tag	UNP O43837-2
N	350	ASP	-	expression tag	UNP O43837-2
N	351	GLU	-	expression tag	UNP O43837-2
N	352	ASN	-	expression tag	UNP O43837-2

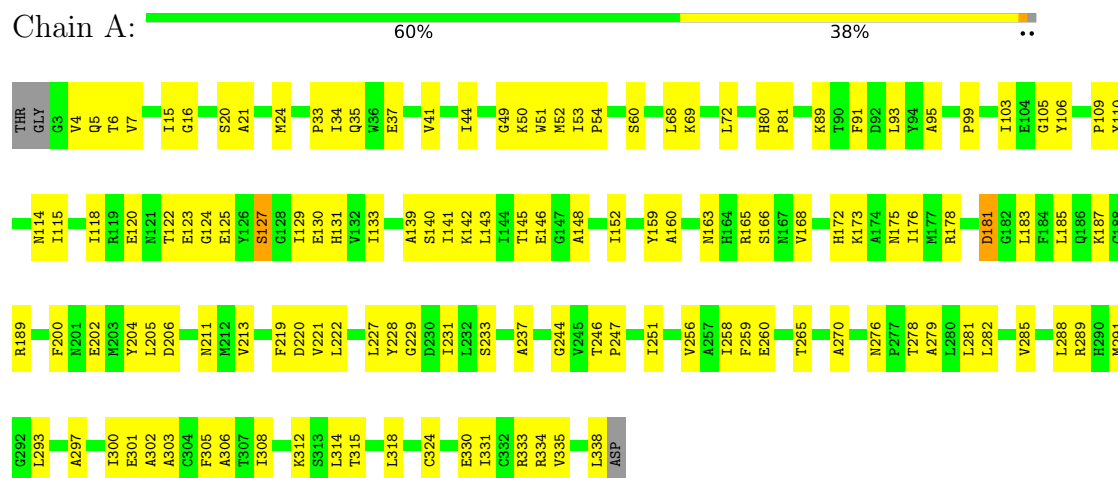
3 Residue-property plots

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: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

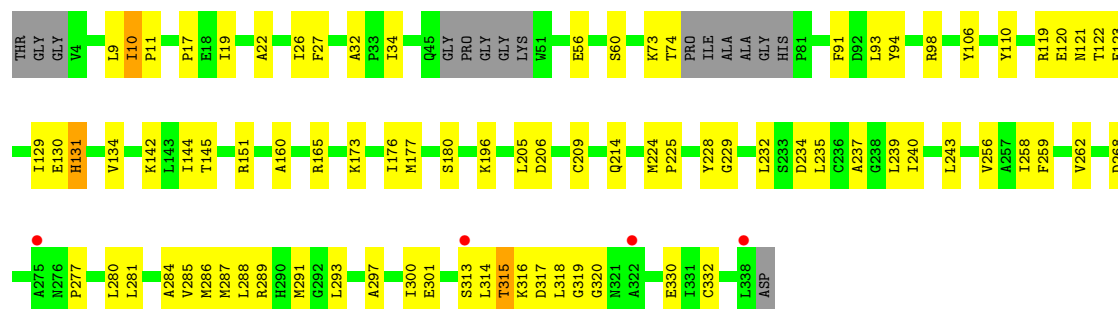


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial



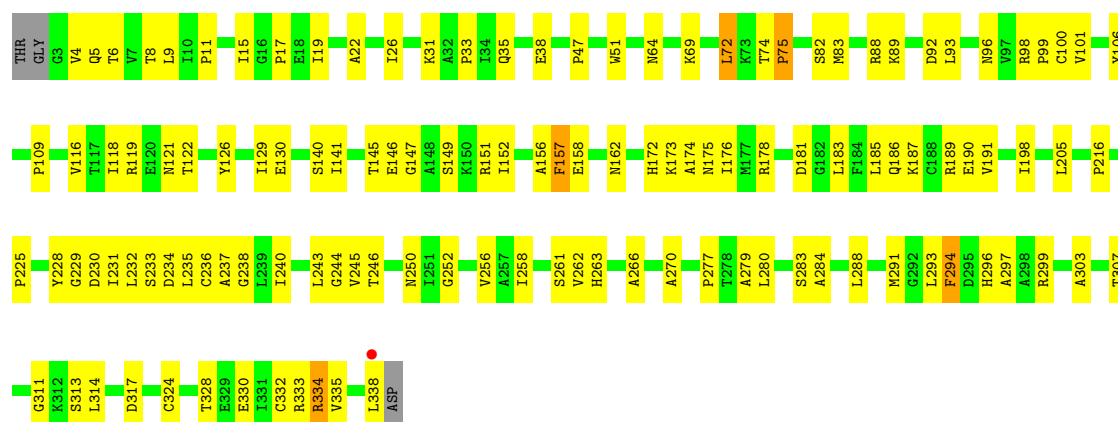
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial





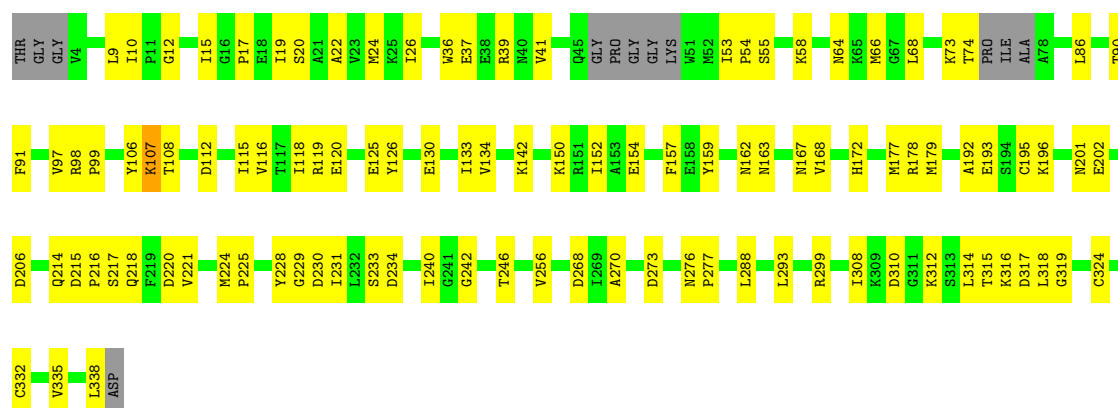
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

Chain E: 63% 35% ..



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

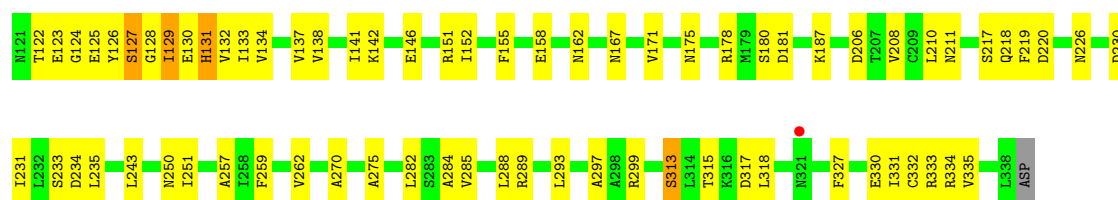
Chain K: 66% 30% .

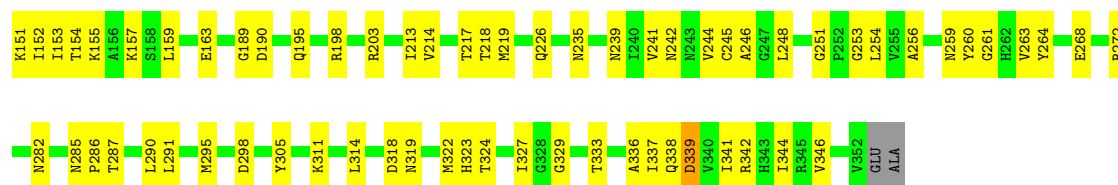


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

Chain I: 68% 29% ..

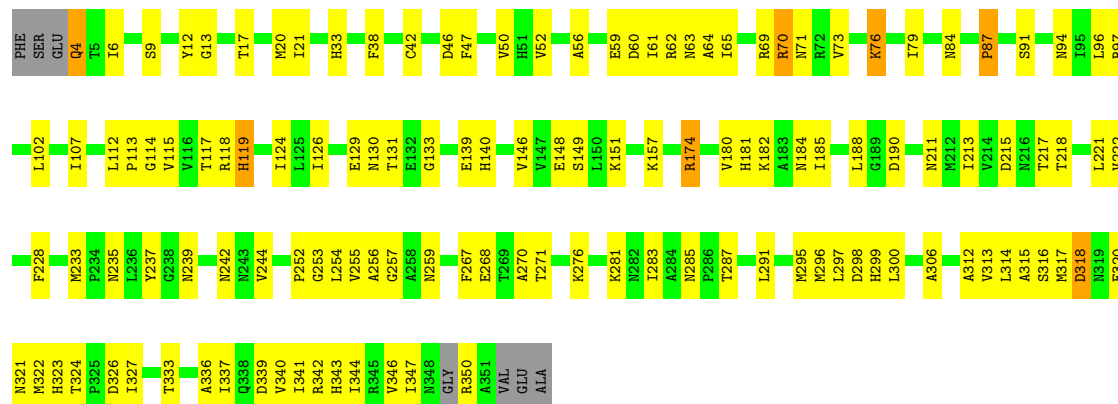






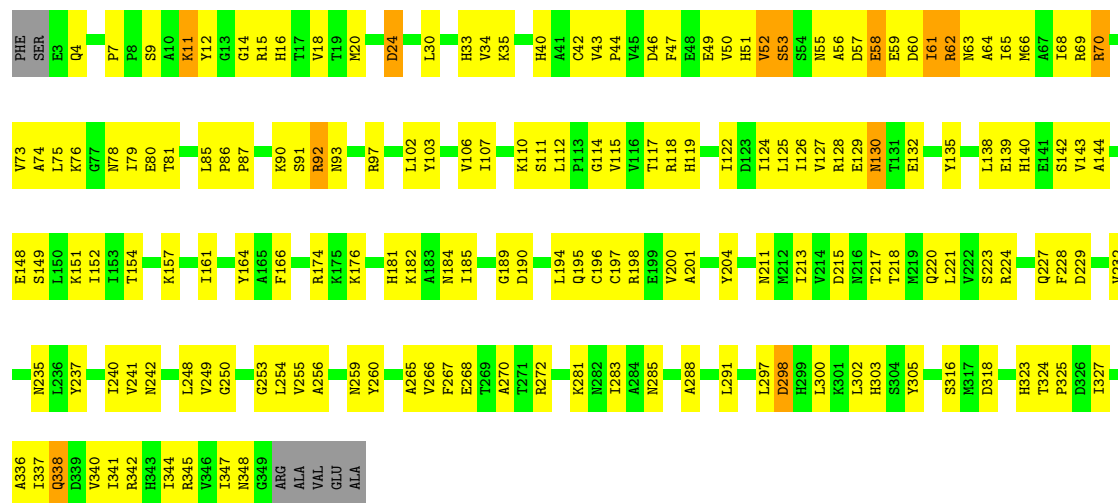
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial

Chain H: 62% 34% ..



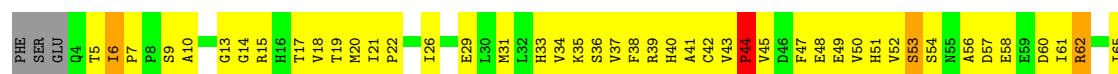
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial

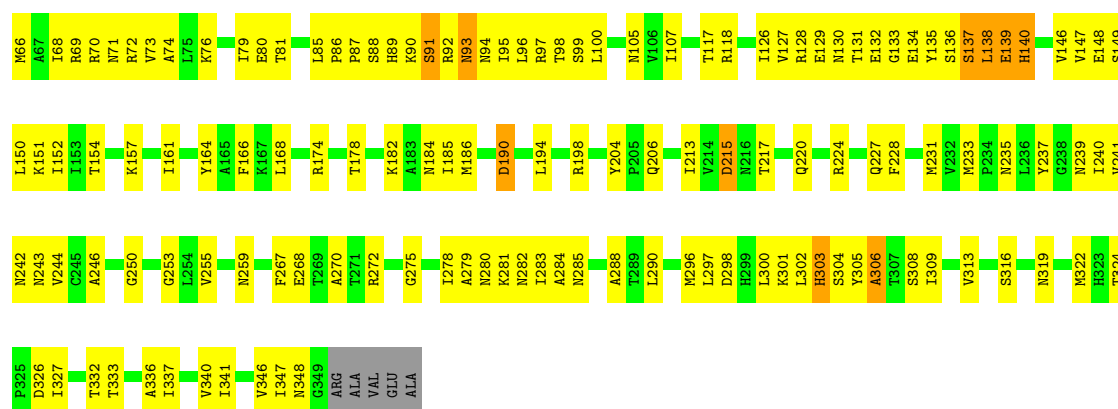
Chain L: 50% 45% ..



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

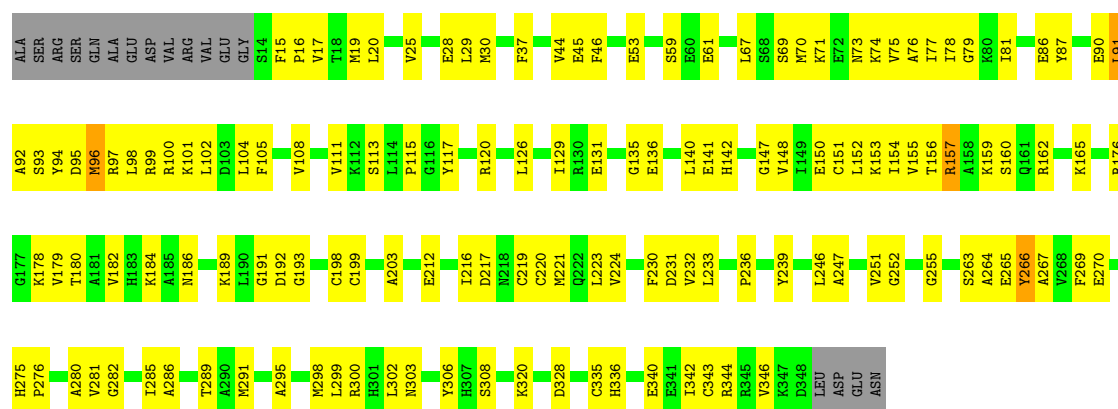
Chain P: 47% 47% ..





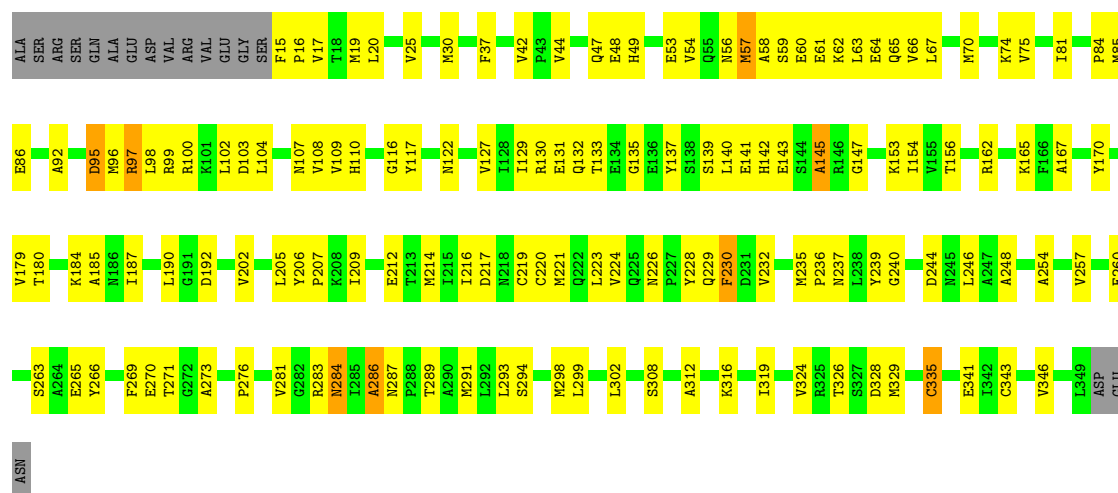
- Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain B: 56% 38% 5%



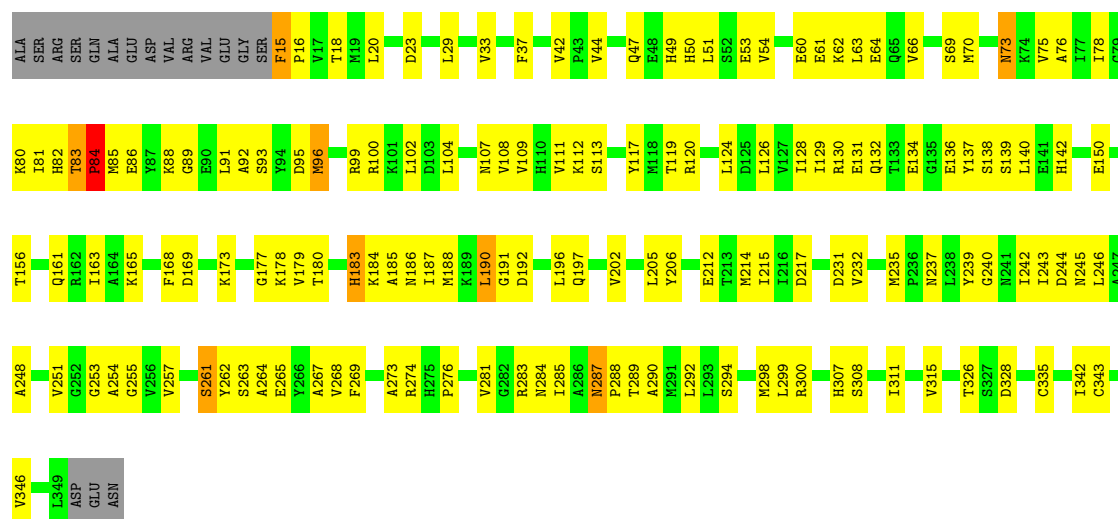
- Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain F: 55% 38% 5%



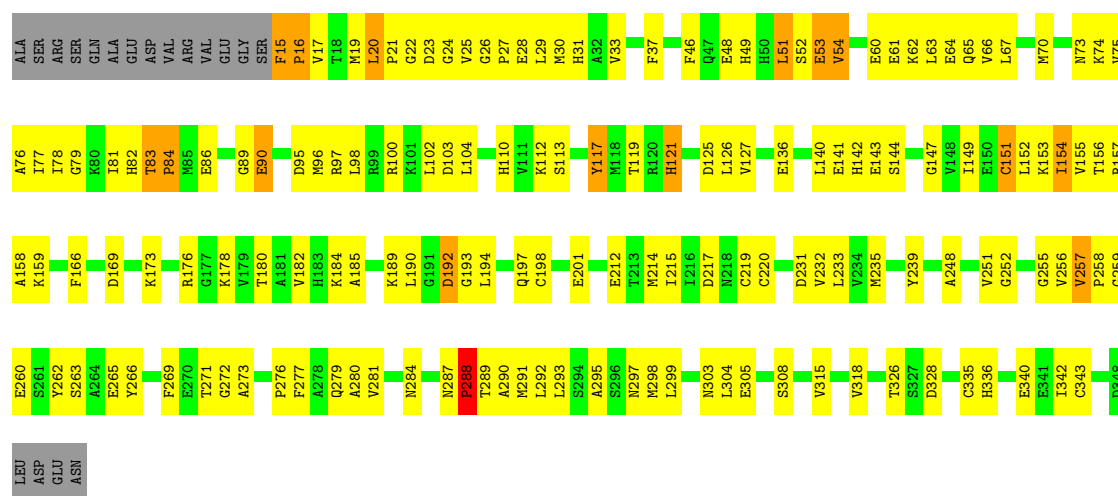
- Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain J:  53% 40% 5%



• Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain N:  50% 40% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	159.26Å 490.33Å 330.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.54 – 4.49 30.54 – 4.49	Depositor EDS
% Data completeness (in resolution range)	84.4 (30.54-4.49) 84.4 (30.54-4.49)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 4.42Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.268 , 0.286 0.268 , 0.287	Depositor DCC
R_{free} test set	3246 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	39351	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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 [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	0.34	0/2452	0.56	3/3339 (0.1%)
1	C	0.26	0/2427	0.46	0/3295
1	E	0.44	2/2439 (0.1%)	0.54	1/3321 (0.0%)
1	G	0.25	0/2482	0.48	2/3355 (0.1%)
1	I	0.48	1/2482 (0.0%)	0.62	2/3379 (0.1%)
1	K	0.27	0/2518	0.52	1/3400 (0.0%)
1	M	0.36	0/2476	0.50	0/3366
1	O	0.34	0/2493	0.59	1/3372 (0.0%)
2	D	0.35	0/2534	0.61	1/3438 (0.0%)
2	H	0.36	0/2592	0.62	3/3516 (0.1%)
2	L	0.43	0/2609	0.75	6/3541 (0.2%)
2	P	0.48	1/2578 (0.0%)	0.78	6/3501 (0.2%)
3	B	0.46	1/2508 (0.0%)	0.77	5/3402 (0.1%)
3	F	0.38	0/2442	0.76	8/3322 (0.2%)
3	J	0.47	2/2507 (0.1%)	0.73	5/3400 (0.1%)
3	N	0.44	1/2447 (0.0%)	0.72	5/3324 (0.2%)
All	All	0.39	8/39986 (0.0%)	0.64	49/54271 (0.1%)

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	E	0	1
2	H	0	1
3	B	0	1
3	F	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	81	PRO	N-CD	-14.24	1.27	1.47
1	E	75	PRO	N-CD	-13.11	1.29	1.47
2	P	44	PRO	N-CD	6.10	1.56	1.47
1	E	109	PRO	N-CD	6.06	1.56	1.47
3	J	261	SER	CA-CB	-5.88	1.44	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	230	PHE	CB-CA-C	-21.91	66.59	110.40
3	B	252	GLY	N-CA-C	-13.39	79.63	113.10
3	B	92	ALA	N-CA-C	-10.75	81.97	111.00
2	P	302	LEU	CB-CA-C	-10.58	90.10	110.20
2	P	44	PRO	CA-N-CD	-9.81	97.76	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	59	SER	Mainchain
1	E	72	LEU	Mainchain
3	F	230	PHE	Peptide
2	H	4	GLN	Peptide

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	2412	0	2284	108	0
1	C	2389	0	2310	76	0
1	E	2400	0	2277	124	0
1	G	2444	0	2435	62	0
1	I	2439	0	2329	130	0
1	K	2480	0	2498	94	0
1	M	2436	0	2329	126	0
1	O	2454	0	2436	199	0
2	D	2496	0	2451	171	0
2	H	2555	0	2508	169	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2569	0	2526	236	0
2	P	2539	0	2498	328	0
3	B	2466	0	2365	181	1
3	F	2400	0	2236	174	0
3	J	2465	0	2376	195	1
3	N	2407	0	2245	242	0
All	All	39351	0	38103	2346	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 30.

The worst 5 of 2346 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)
3:N:29:LEU:CD1	3:N:288:PRO:HB3	1.24	1.65
3:J:20:LEU:CB	3:J:78:ILE:HG21	1.20	1.61
3:J:20:LEU:HB2	3:J:78:ILE:CG2	1.26	1.61
2:P:138:LEU:HD23	1:M:131:HIS:CD2	1.15	1.61
2:D:50:VAL:CG2	2:D:64:ALA:HB1	1.20	1.60

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)
3:B:282:GLY:O	3:J:85:MET:CB[8_545]	1.48	0.72

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	334/339 (98%)	292 (87%)	42 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	322/339 (95%)	276 (86%)	46 (14%)	0	100	100
1	E	334/339 (98%)	310 (93%)	24 (7%)	0	100	100
1	G	318/339 (94%)	282 (89%)	36 (11%)	0	100	100
1	I	334/339 (98%)	291 (87%)	42 (13%)	1 (0%)	41	76
1	K	321/339 (95%)	292 (91%)	29 (9%)	0	100	100
1	M	334/339 (98%)	292 (87%)	42 (13%)	0	100	100
1	O	323/339 (95%)	287 (89%)	33 (10%)	3 (1%)	17	56
2	D	335/354 (95%)	301 (90%)	33 (10%)	1 (0%)	41	76
2	H	343/354 (97%)	300 (88%)	42 (12%)	1 (0%)	41	76
2	L	345/354 (98%)	307 (89%)	34 (10%)	4 (1%)	13	50
2	P	344/354 (97%)	296 (86%)	42 (12%)	6 (2%)	9	43
3	B	333/352 (95%)	295 (89%)	38 (11%)	0	100	100
3	F	333/352 (95%)	294 (88%)	37 (11%)	2 (1%)	25	65
3	J	333/352 (95%)	285 (86%)	45 (14%)	3 (1%)	17	56
3	N	332/352 (94%)	283 (85%)	39 (12%)	10 (3%)	4	31
All	All	5318/5536 (96%)	4683 (88%)	604 (11%)	31 (1%)	25	65

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	87	PRO
3	F	57	MET
2	L	85	LEU
2	L	87	PRO
3	J	84	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	241/276 (87%)	235 (98%)	6 (2%)	47	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	245/276 (89%)	244 (100%)	1 (0%)	91	94
1	E	239/276 (87%)	232 (97%)	7 (3%)	42	64
1	G	263/276 (95%)	260 (99%)	3 (1%)	73	85
1	I	249/276 (90%)	240 (96%)	9 (4%)	35	60
1	K	269/276 (98%)	266 (99%)	3 (1%)	73	85
1	M	248/276 (90%)	244 (98%)	4 (2%)	62	79
1	O	260/276 (94%)	251 (96%)	9 (4%)	36	60
2	D	259/299 (87%)	254 (98%)	5 (2%)	57	75
2	H	263/299 (88%)	257 (98%)	6 (2%)	50	70
2	L	265/299 (89%)	257 (97%)	8 (3%)	41	63
2	P	261/299 (87%)	252 (97%)	9 (3%)	37	61
3	B	247/296 (83%)	242 (98%)	5 (2%)	55	73
3	F	226/296 (76%)	220 (97%)	6 (3%)	44	66
3	J	246/296 (83%)	236 (96%)	10 (4%)	30	56
3	N	231/296 (78%)	222 (96%)	9 (4%)	32	57
All	All	4012/4588 (87%)	3912 (98%)	100 (2%)	47	68

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	313	SER
1	O	91	PHE
3	N	197	GLN
3	J	15	PHE
3	J	183	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	172	HIS
2	P	348	ASN
1	I	131	HIS
2	P	280	ASN
1	I	121	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](#)

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	A	336/339 (99%)	-0.40	0	100	100	44, 95, 154, 197	0
1	C	328/339 (96%)	-0.11	0	100	100	77, 153, 193, 206	0
1	E	336/339 (99%)	-0.09	1 (0%)	94	90	125, 184, 217, 231	0
1	G	324/339 (95%)	-0.08	4 (1%)	79	70	108, 167, 200, 216	0
1	I	336/339 (99%)	-0.47	1 (0%)	94	90	36, 85, 145, 184	0
1	K	327/339 (96%)	-0.36	0	100	100	35, 91, 134, 152	0
1	M	336/339 (99%)	-0.21	3 (0%)	84	77	54, 144, 180, 197	0
1	O	329/339 (97%)	-0.41	0	100	100	46, 87, 142, 156	0
2	D	339/354 (95%)	-0.32	0	100	100	76, 138, 164, 200	0
2	H	347/354 (98%)	-0.45	0	100	100	64, 104, 138, 166	0
2	L	347/354 (98%)	-0.59	0	100	100	30, 59, 99, 129	0
2	P	346/354 (97%)	-0.54	0	100	100	45, 65, 102, 145	0
3	B	335/352 (95%)	-0.64	0	100	100	40, 62, 78, 102	0
3	F	335/352 (95%)	-0.36	0	100	100	125, 149, 169, 185	0
3	J	335/352 (95%)	-0.66	0	100	100	33, 49, 75, 92	0
3	N	334/352 (94%)	-0.46	0	100	100	54, 87, 142, 226	0
All	All	5370/5536 (97%)	-0.39	9 (0%)	95	93	30, 106, 188, 231	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	78	ALA	3.5
1	I	321	ASN	3.1
1	G	338	LEU	2.5
1	G	275	ALA	2.4
1	G	313	SER	2.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.