W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 22, 2023 – 03:36 PM JST

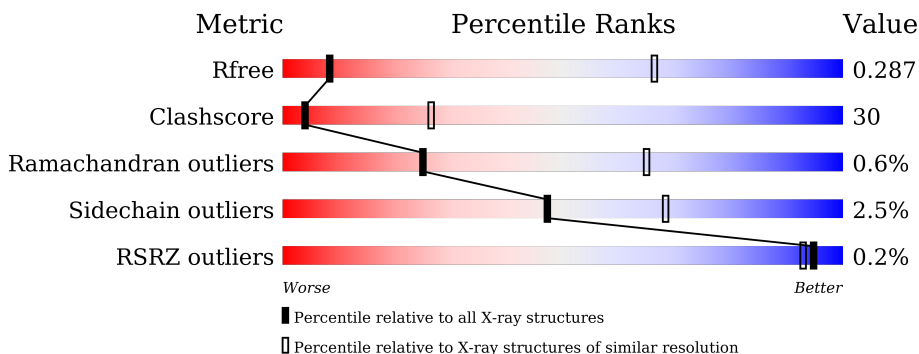|		
PDB ID	:	8GS5
Title	:	Crystal structure of a constitutively active mutant of human IDH3 holoenzyme in apo form
Authors	:	Sun, P.; Chen, X.; Ding, J.
Deposited on	:	2022-09-04
Resolution	:	4.49 Å(reported)

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 — Percentile Ranks — Value

- Rfree — 0.287
- Clashscore — 30
- Ramachandran outliers — 0.6%
- Sidechain outliers — 2.5%
- RSRZ outliers — 0.2%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 <=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	60% / 38% / ..
1	C	339	67% / 30% / .
1	E	339	63% / 35% / ..
1	G	339	.% / 71% / 24% / . .
1	I	339	68% / 29% / . .
1	K	339	66% / 30% / .

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Mol	Chain	Length	Quality of chain
1	M	339	66% 33%
1	O	339	53% 42%
2	D	354	57% 37%
2	H	354	62% 34%
2	L	354	50% 45%
2	P	354	47% 47%
3	B	352	56% 38% 5%
3	F	352	55% 38% 5%
3	J	352	53% 40% 5%
3	N	352	50% 40% 5%

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 2496	C 1556	N 456	O 466	S 18	0	0	0
2	H	347	Total 2555	C 1594	N 467	O 476	S 18	0	0	0
2	L	347	Total 2569	C 1606	N 469	O 477	S 17	0	0	0
2	P	346	Total 2539	C 1590	N 462	O 469	S 18	0	0	0

- 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 2466	C 1557	N 425	O 465	S 19	0	0	0
3	F	335	Total 2400	C 1516	N 420	O 446	S 18	0	0	0
3	J	335	Total 2465	C 1557	N 429	O 459	S 20	0	0	0
3	N	334	Total 2407	C 1515	N 417	O 456	S 19	0	0	0

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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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

Chain C:

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

Chain A:

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

Chain G:

THR GLY GLY V4 L9 I10 P11 P17 E18 I19 A22 I26 F27 A32 P33 I34 Q45 GLY PRO GLY LYS W51 E56 S60 K73 T74 PRO ILE ALA GLY HIS P81 F91 D92 L93 Y94 R98 Y106 Y110 R119 E120 N121 T122 E123

I129 E130 H131 V134 K142 L143 I144 T145 R151 A160 R165 K173 I176 M177 S180 K196 L205 D206 C209 Q214 M224 P225 Y228 G229 L232 S233 D234 L235 C236 A237 G238 L239 I240 L243 V256 A257 I258 F259 V262 D268

A275 N276 P277 L280 L281 A284 V285 M286 M287 L288 R289 H290 M291 G292 L293 A297 I300 E301 S313 L314 T315 K316 D317 L318 G319 G320 N321 A322 E330 I331 C332 L338 ASP

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

Chain E: 63% 35%

THR GLY G3 V4 Q5 T6 V7 T8 L9 I10 P11 I15 G16 P17 E18 I19 A22 I26 K31 A32 P33 I34 Q35 E38 P47 W51 N64 K69 L72 K73 T74 P75 S82 M83 R88 K89 D92 L93 N96 V97 R98 P99 C100 V101 Y106

P109 V116 T117 I118 R119 E120 N121 T122 Y126 I129 E130 S140 I141 T145 E146 G147 A148 S149 K150 R151 I152 A156 F157 E158 N162 H172 K173 A174 N175 I176 M177 R178 D181 G182 L183 F184 L185 Q186 K187 C188 R189 E190 V191 I198 L205 P216

P225 Y228 G229 D230 I231 L232 S233 D234 L235 C236 A237 G238 L239 I240 L243 G244 V245 T246 N250 I251 G252 V256 A257 I258 S261 V262 H263 A266 A270 P277 T278 A279 L280 S283 A284 L288 M291 G292 L293 F294 D295 H296 A297 A298 R299 A303 T307

G311 K312 S313 L314 D317 C324 T328 E329 E330 I331 C332 R333 R334 V335 L338 ASP

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

Chain K: 66% 30%

THR GLY GLY V4 L9 I10 P11 G12 I15 G16 P17 E18 I19 S20 A21 A22 V23 M24 K25 I26 W36 E37 E38 R39 N40 V41 Q45 GLY PRO GLY LYS W51 M52 I53 P54 S55 K58 N64 K65 M66 G67 L68 K73 T74 PRO ILE ALA A78 L86 T90

F91 V97 R98 P99 Y106 K107 T108 D112 I115 V116 T117 I118 R119 E120 E125 Y126 E130 I133 V134 K142 K150 R151 I152 A153 E154 F157 E158 Y159 N162 N163 N167 V168 H172 M177 R178 M179 A192 E193 S194 C195 K196 N201 E202

D206 Q214 D215 P216 S217 Q218 F219 D220 V221 M224 P225 Y228 G229 D230 I231 L232 S233 D234 I240 G241 G242 T246 V256 D268 I269 A270 D273 N276 P277 L288 L293 R299 I308 K309 D310 G311 K312 S313 L314 T315 K316 D317 L318 G319 C324

C332 V335 L338 ASP

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

Chain I: 68% 29%

THR GLY G3 V4 Q5 P11 I15 G16 P17 K25 I26 F27 D28 A29 A30 Q35 A43 K50 W51 M66 G67 L68 H80 P81 S82 M83 N84 L85 L86 L87 R88 F91 D92 L93 Y94 A95 R98 I103 E104 G105 Y106 Y110 I115 I118 R119 E120

N121 T122 E123 G124 E125 Y126 S127 G128 I129 E130 H131 V132 I133 V134 V137 V138 I141 K142 E146 R151 I152 F155 E158 N162 N167 V171 N175 R178 M179 S180 D181 K187 D206 T207 V208 C209 L210 N211 S217 Q218 F219 D220 N226 D230

I231 L232 S233 D234 L235 L243 N250 I251 A257 I258 F259 V262 A270 A275 L282 S283 A284 V285 L288 R289 L293 A297 A298 R299 S313 L314 T315 K316 D317 L318 N321 F327 E330 I331 C332 R333 R334 V335 L338 ASP

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

Chain O:

THR GLY GLY V4 V7 P11 I15 G16 P17 E18 I19 S20 A21 M24 K25 I34 Q35 W36 E37 E38 R39 N40 V41 I44 P47 GLY GLY LYS W51 P54 S55 K58 M66 K73 A77 ALA GLY HIS P81 S82 M83 L86 L87 R88 K89 T90 F91

D92 L93 Y94 A95 N96 V97 R98 P99 C100 Y106 D112 V113 N114 I115 V116 T117 I118 R119 E120 N121 T122 E125 N129 E130 H131 V132 I133 V134 D135 G136 V137 V138 S140 I141 K142 L143 I144 T145 A156 F157 E158 Y159 A160 R165 S166 N167 V168 V171 H172 K173 A174 N175

I176 M177 R178 M179 S180 D181 G182 L183 F184 L185 A192 C195 K199 F200 N201 Y204 L205 D206 T207 V208 C209 L210 N211 M212 V213 Q214 D215 P216 S217 Q218 F219 D220 M224 P225 G229 D230 I231 L232 S233 D234 I240 L243 N250 V256 V262 S261 V262 T265 A266

P267 D268 I269 A270 G271 K272 D273 M274 A275 N276 P277 T278 A279 L280 L281 L282 S283 A284 V285 L288 R289 L293 H296 A297 A298 R299 I300 E301 C304 F305 A306 K309 S313 L314 T315 K316 D317 L318 G319 G320 C324 F327 E330 I331 C332 R333 R334 L338 ASP

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

Chain M:

THR GLY G3 T8 P11 I15 G16 P17 E18 I19 V23 M24 W36 E37 N40 V41 T42 A43 I44 Q45 G46 G49 K50 W51 M52 I53 P54 K58 E59 S60 M61 D62 K63 N64 K65 M66 G67 L68 K69 L72 A77 A78 G79 H80 P81 S82 M83 L86 L87

R88 F91 D92 L93 Y94 A95 N96 V97 R98 P99 S102 Y106 V113 N114 I115 I118 R119 E120 N121 T122 E125 N129 E130 H131 V132 I133 V134 V137 S140 I141 K142 E146 G147 A148 I152 R161 N167 H172 N175 R178 M179 S180 L183

F184 L185 Q186 R189 E193 S194 C195 E202 M203 Y204 F219 D220 P225 M226 L227 Y228 G229 D230 I231 L232 S233 D234 L235 C236 L239 L243 P247 N250 I251 V256 A257 I258 F259 E260 H263 G264 T265 A266 P267 A270 P277 L280 L288 R289 H290

M291 E301 I308 S313 L314 F327 E330 R334 D337 L338 ASP

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

Chain D:

PHE SER GLU GLN THR ILE P7 P8 S9 A10 G13 G14 R15 H16 T17 V18 T19 M20 I21 P22 G23 I26 G27 P28 E29 L30 M31 L32 H33 V34 V43 D46 E49 V50 H51 V52 A56 D60 I61 R62 N63 A64 I65 M66 A67 I68 R69 R70 N71 R72 V73 A74

N78 I79 E80 THR ASN HIS ASN LEU PRO PRO S88 R92 N93 N94 I95 L96 R97 L102 Y103 A104 N105 V106 I107 S111 G114 V115 V116 T117 R118 H119 K120 D121 I122 I126 V127 R128 E129 N130 T131 E132 G133 E134 Y135 L138 E139 H140 E141 S142 V143 V146 V147 E148

K151 I152 I153 T154 K155 A156 K157 S158 L159 E163 G189 D190 Q195 R198 R203 I213 V214 T217 T218 M219 Q226 N235 N239 I240 V241 N242 N243 V244 C245 A246 G247 L248 G251 P252 G253 L254 V255 A256 N259 Y260 G261 H262 V263 Y264 E268 R272

N282 N285 P286 T287 L290 L291 M295 D298 Y305 K311 L314 D318 N319 M322 H323 T324 I327 G328 G329 T333 A336 I337 Q338 D339 V340 I341 R342 H343 I344 R345 V346 V352 GLU ALA

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

Chain H: ▬▬▬▬▬▬▬▬▬▬▬▬ 62% ▬▬▬▬▬▬▬▬ 34% ▬ • •

PHE SER GLU Q4 T5 I6 S9 Y12 G13 T17 M20 I21 H33 F38 C42 D46 F47 V50 H51 V52 A56 E59 D60 I61 R62 N63 A64 I65 R69 R70 N71 R72 V73 K76 I79 N84 P87 S91 N94 I95 L96 R97

L102 I107 L112 P113 G114 V115 V116 T117 R118 H119 I124 L125 I126 E129 N130 T131 E132 G133 E139 H140 V146 V147 E148 S149 L150 K151 K157 R174 V180 H181 K182 A183 N184 I185 L188 G189 D190 N211 M212 I213 V214 D215 N216 T217 T218 L221 V222

F228 M233 P234 N235 L236 Y237 G238 N239 N242 N243 V244 P252 G253 L254 V255 A256 G257 A258 N259 F267 E268 T269 A270 T271 K276 K281 N282 I283 A284 N285 P286 T287 L291 M295 M296 L297 D298 H299 L300 A306 A312 V313 L314 A315 S316 M317 D318 N319 E320

N321 M322 H323 T324 P325 D326 I327 T333 A336 I337 Q338 D339 V340 I341 R342 H343 I344 R345 V346 I347 N348 GLY R350 A351 VAL GLU ALA

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

Chain L: ▬▬▬▬▬▬▬▬▬▬ 50% ▬▬▬▬▬▬▬▬▬ 45% ▬ • •

PHE SER E3 Q4 P7 P8 S9 A10 K11 Y12 G13 G14 R15 H16 T17 V18 T19 M20 D24 L30 H33 V34 K35 H40 A41 C42 V43 P44 V45 D46 F47 E48 E49 V50 H51 V52 S53 S54 N55 A56 D57 E58 E59 D60 I61 R62 N63 A64 I65 M66 A67 I68 R69 R70

V73 A74 L75 K76 G77 N78 I79 E80 T81 L85 P86 P87 K90 S91 R92 N93 R97 L102 Y103 V106 I107 K110 S111 L112 P113 G114 V115 V116 T117 R118 H119 I122 D123 I124 L125 I126 V127 R128 E129 N130 T131 E132 Y135 L138 E139 H140 E141 S142 V143 A144

E148 S149 L150 K151 I152 I153 T154 K157 I161 Y164 A165 F166 R174 K175 K176 H181 K182 A183 N184 I185 G189 D190 L194 Q195 C196 C197 R198 E199 V200 A201 Y204 N211 M212 I213 V214 D215 N216 T217 T218 M219 Q220 L221 V222 S223 R224 Q227 F228 D229 V232

N235 L236 Y237 I240 V241 N242 L248 V249 C250 G253 L254 V255 A256 N259 Y260 A265 V266 F267 E268 T269 A270 T271 R272 K281 N282 I283 A284 N285 A288 L291 L297 D298 H299 L300 K301 L302 H303 S304 Y305 S316 M317 D318 H323 T324 P325 D326 I327

A336 I337 Q338 D339 V340 I341 R342 H343 I344 R345 V346 I347 N348 G349 ARG ALA VAL GLU ALA

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

Chain P: ▬▬▬▬▬▬▬▬▬▬ 47% ▬▬▬▬▬▬▬▬▬ 47% ▬ • •

PHE SER GLU Q4 T5 I6 P7 P8 S9 A10 G13 G14 R15 H16 T17 V18 T19 M20 I21 P22 I26 E29 L30 M31 L32 H33 V34 K35 S36 V37 F38 R39 H40 A41 C42 V43 P44 V45 D46 F47 E48 E49 V50 H51 V52 S53 S54 N55 A56 D57 E58 E59 D60 I61 R62 I65
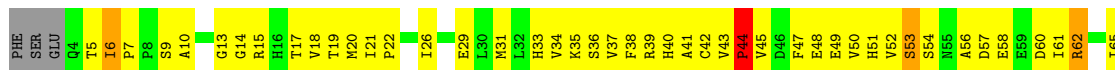
• Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial
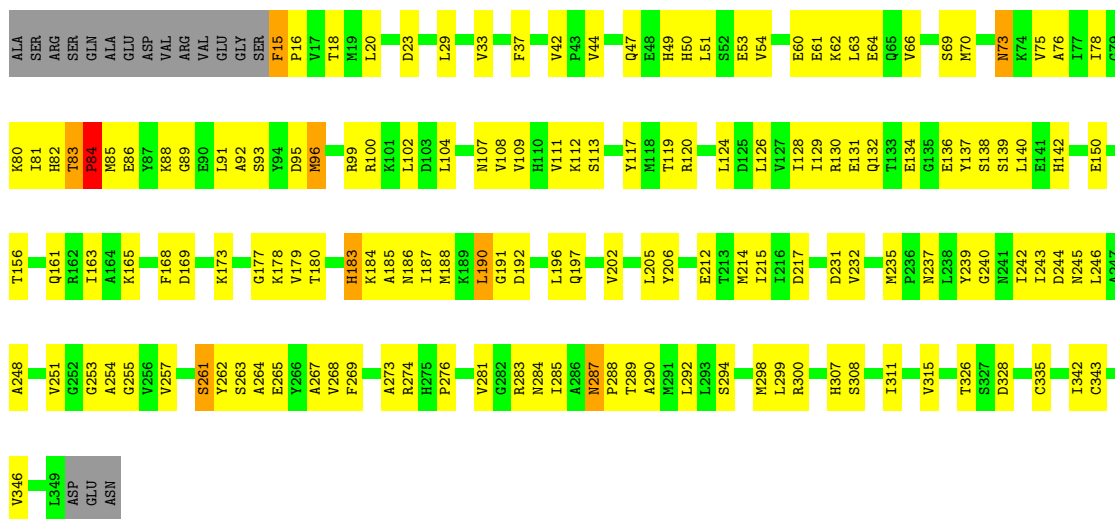

• Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

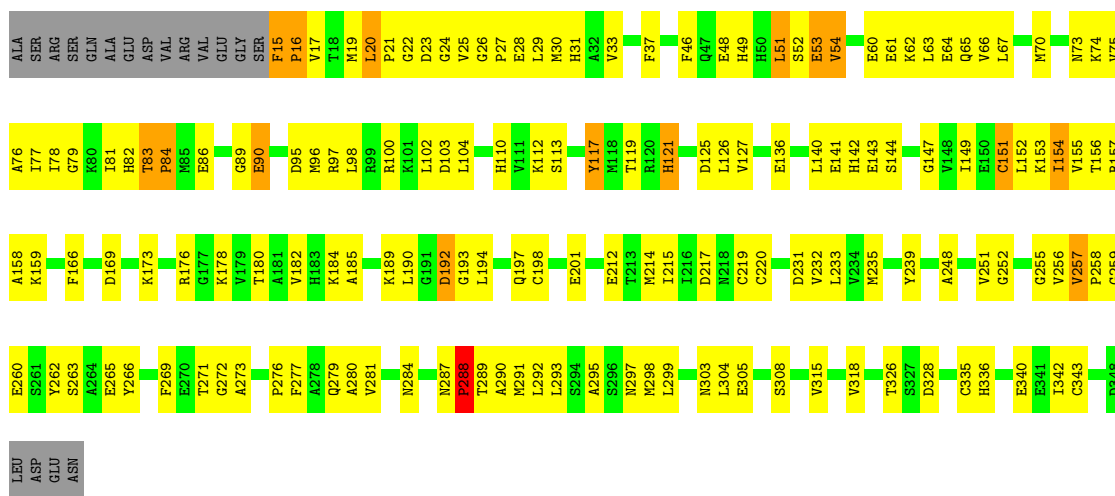• Molecule 3: Isoform A of Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial

Chain J:

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

Chain N:

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
$< I/\sigma(I) >$ [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 (Å²)	76.0	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.23 , 44.1	EDS
L-test for twinning [2]	$< |L| > = 0.45, < L^2 > = 0.28$	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 (Å²)	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.*

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[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 ⓘ

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	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(^{o})	Ideal(^{o})
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 ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 ⓘ

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

There are no ligands in this entry.

6.5   Other polymers ⓘ

There are no such residues in this entry.