



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 12:42 pm BST

PDB ID : 6DV2
Title : Crystal Structure of Human Mitochondrial Trifunctional Protein
Authors : Fu, Z.; Xia, C.; Battaile, K.P.; Kim, J.P.
Deposited on : 2018-06-22
Resolution : 3.60 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 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	:	2.11
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)	:	2.11

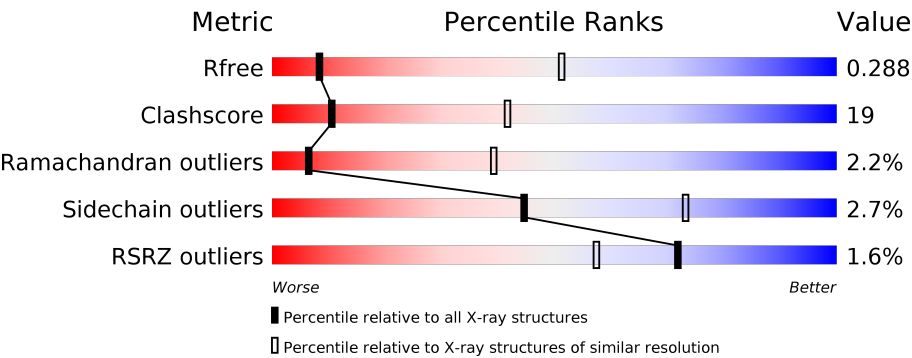
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 on 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	457	<div><div>5%</div><div><div></div><div>56%</div><div>34%</div><div>5%</div><div>5%</div></div></div>
1	B	457	<div><div>2%</div><div><div></div><div>55%</div><div>31%</div><div>5%</div><div>8%</div></div></div>
1	C	457	<div><div>2%</div><div><div></div><div>60%</div><div>29%</div><div>•</div><div>8%</div></div></div>
1	D	457	<div><div>4%</div><div><div></div><div>58%</div><div>32%</div><div>•</div><div>7%</div></div></div>
1	E	457	<div><div>2%</div><div><div></div><div>60%</div><div>29%</div><div>•</div><div>7%</div></div></div>
1	F	457	<div><div>2%</div><div><div></div><div>61%</div><div>29%</div><div>•</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	727	<div><div></div><div>64%34%</div><div></div></div>
2	H	727	<div><div>%</div><div></div><div>65%33%</div><div></div></div>
2	I	727	<div><div>2%</div><div></div><div>65%32%</div><div></div></div>
2	J	727	<div><div>%</div><div></div><div>68%29%</div><div></div></div>
2	K	727	<div><div>%</div><div></div><div>67%31%</div><div></div></div>
2	L	727	<div><div>%</div><div></div><div>65%32%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 51375 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 Trifunctional enzyme subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3267	2071	566	608	22			
1	B	419	Total	C	N	O	S	0	0	0
			3170	2012	548	589	21			
1	C	421	Total	C	N	O	S	0	0	0
			3073	1938	530	586	19			
1	D	424	Total	C	N	O	S	0	0	0
			3087	1946	533	589	19			
1	E	423	Total	C	N	O	S	0	0	0
			3082	1943	532	588	19			
1	F	425	Total	C	N	O	S	0	0	0
			3092	1949	534	590	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	HIS	-	expression tag	UNP P55084
A	19	HIS	-	expression tag	UNP P55084
A	20	HIS	-	expression tag	UNP P55084
A	21	HIS	-	expression tag	UNP P55084
A	22	HIS	-	expression tag	UNP P55084
A	23	HIS	-	expression tag	UNP P55084
A	24	SER	-	expression tag	UNP P55084
A	25	SER	-	expression tag	UNP P55084
A	26	GLY	-	expression tag	UNP P55084
A	27	LEU	-	expression tag	UNP P55084
A	28	VAL	-	expression tag	UNP P55084
A	29	PRO	-	expression tag	UNP P55084
A	30	ARG	-	expression tag	UNP P55084
A	31	GLY	-	expression tag	UNP P55084
A	32	SER	-	expression tag	UNP P55084
A	33	HIS	-	expression tag	UNP P55084
B	18	HIS	-	expression tag	UNP P55084

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Chain	Residue	Modelled	Actual	Comment	Reference
B	19	HIS	-	expression tag	UNP P55084
B	20	HIS	-	expression tag	UNP P55084
B	21	HIS	-	expression tag	UNP P55084
B	22	HIS	-	expression tag	UNP P55084
B	23	HIS	-	expression tag	UNP P55084
B	24	SER	-	expression tag	UNP P55084
B	25	SER	-	expression tag	UNP P55084
B	26	GLY	-	expression tag	UNP P55084
B	27	LEU	-	expression tag	UNP P55084
B	28	VAL	-	expression tag	UNP P55084
B	29	PRO	-	expression tag	UNP P55084
B	30	ARG	-	expression tag	UNP P55084
B	31	GLY	-	expression tag	UNP P55084
B	32	SER	-	expression tag	UNP P55084
B	33	HIS	-	expression tag	UNP P55084
C	18	HIS	-	expression tag	UNP P55084
C	19	HIS	-	expression tag	UNP P55084
C	20	HIS	-	expression tag	UNP P55084
C	21	HIS	-	expression tag	UNP P55084
C	22	HIS	-	expression tag	UNP P55084
C	23	HIS	-	expression tag	UNP P55084
C	24	SER	-	expression tag	UNP P55084
C	25	SER	-	expression tag	UNP P55084
C	26	GLY	-	expression tag	UNP P55084
C	27	LEU	-	expression tag	UNP P55084
C	28	VAL	-	expression tag	UNP P55084
C	29	PRO	-	expression tag	UNP P55084
C	30	ARG	-	expression tag	UNP P55084
C	31	GLY	-	expression tag	UNP P55084
C	32	SER	-	expression tag	UNP P55084
C	33	HIS	-	expression tag	UNP P55084
D	18	HIS	-	expression tag	UNP P55084
D	19	HIS	-	expression tag	UNP P55084
D	20	HIS	-	expression tag	UNP P55084
D	21	HIS	-	expression tag	UNP P55084
D	22	HIS	-	expression tag	UNP P55084
D	23	HIS	-	expression tag	UNP P55084
D	24	SER	-	expression tag	UNP P55084
D	25	SER	-	expression tag	UNP P55084
D	26	GLY	-	expression tag	UNP P55084
D	27	LEU	-	expression tag	UNP P55084
D	28	VAL	-	expression tag	UNP P55084

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Chain	Residue	Modelled	Actual	Comment	Reference
D	29	PRO	-	expression tag	UNP P55084
D	30	ARG	-	expression tag	UNP P55084
D	31	GLY	-	expression tag	UNP P55084
D	32	SER	-	expression tag	UNP P55084
D	33	HIS	-	expression tag	UNP P55084
E	18	HIS	-	expression tag	UNP P55084
E	19	HIS	-	expression tag	UNP P55084
E	20	HIS	-	expression tag	UNP P55084
E	21	HIS	-	expression tag	UNP P55084
E	22	HIS	-	expression tag	UNP P55084
E	23	HIS	-	expression tag	UNP P55084
E	24	SER	-	expression tag	UNP P55084
E	25	SER	-	expression tag	UNP P55084
E	26	GLY	-	expression tag	UNP P55084
E	27	LEU	-	expression tag	UNP P55084
E	28	VAL	-	expression tag	UNP P55084
E	29	PRO	-	expression tag	UNP P55084
E	30	ARG	-	expression tag	UNP P55084
E	31	GLY	-	expression tag	UNP P55084
E	32	SER	-	expression tag	UNP P55084
E	33	HIS	-	expression tag	UNP P55084
F	18	HIS	-	expression tag	UNP P55084
F	19	HIS	-	expression tag	UNP P55084
F	20	HIS	-	expression tag	UNP P55084
F	21	HIS	-	expression tag	UNP P55084
F	22	HIS	-	expression tag	UNP P55084
F	23	HIS	-	expression tag	UNP P55084
F	24	SER	-	expression tag	UNP P55084
F	25	SER	-	expression tag	UNP P55084
F	26	GLY	-	expression tag	UNP P55084
F	27	LEU	-	expression tag	UNP P55084
F	28	VAL	-	expression tag	UNP P55084
F	29	PRO	-	expression tag	UNP P55084
F	30	ARG	-	expression tag	UNP P55084
F	31	GLY	-	expression tag	UNP P55084
F	32	SER	-	expression tag	UNP P55084
F	33	HIS	-	expression tag	UNP P55084

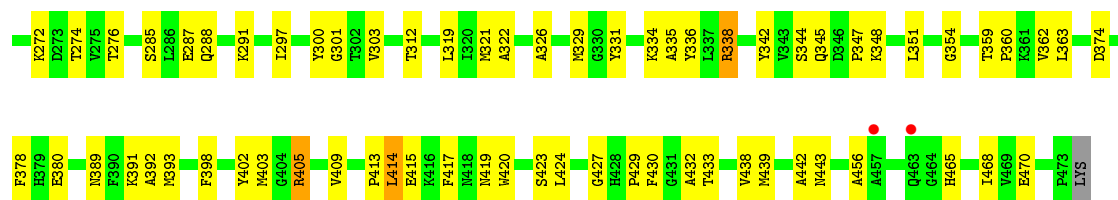
- Molecule 2 is a protein called Trifunctional enzyme subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	725	Total	C	N	O	S	0	0	0
			5440	3455	929	1027	29			

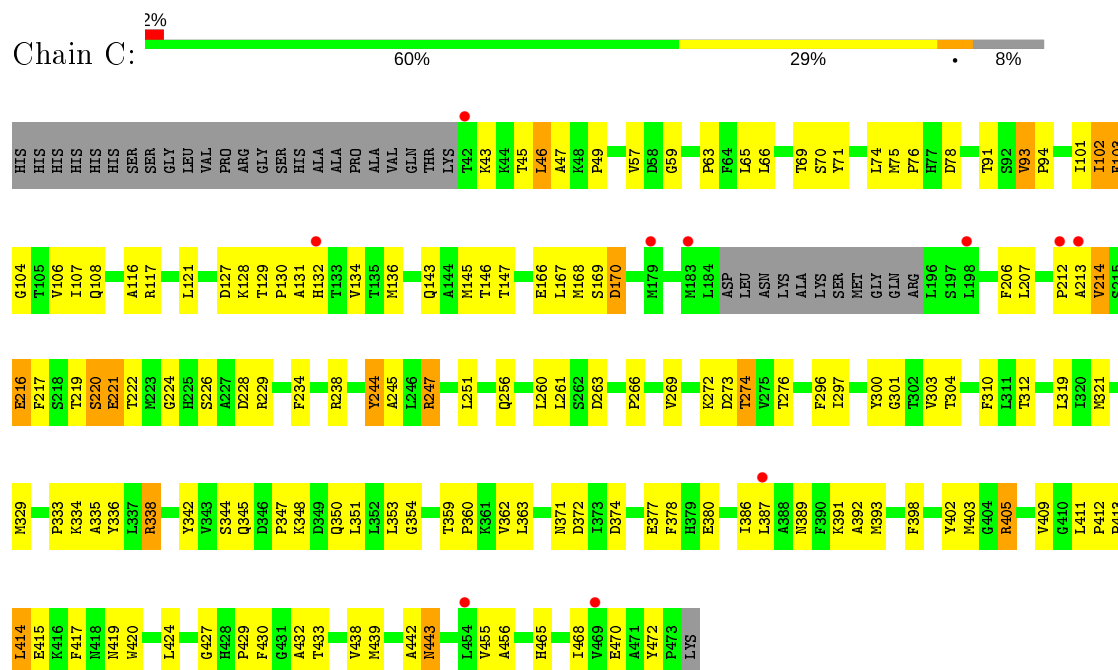
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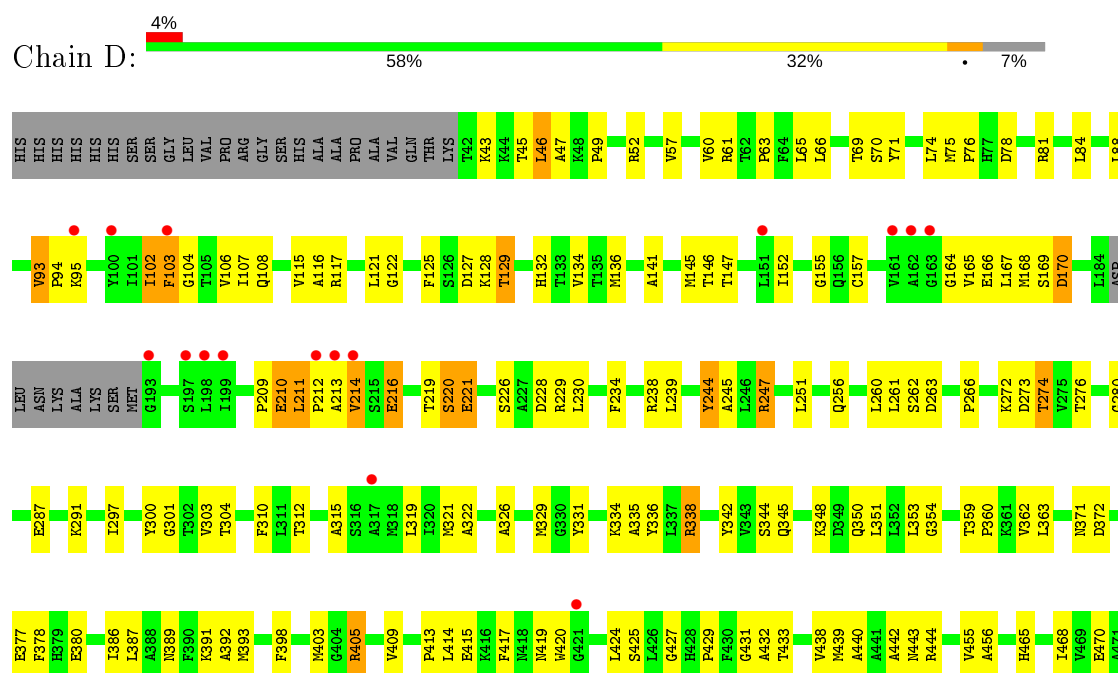
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	725	Total	C	N	O	S	0	0	0
			5440	3455	929	1027	29			
2	I	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	J	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	K	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			
2	L	714	Total	C	N	O	S	0	0	0
			5431	3454	928	1020	29			



- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial



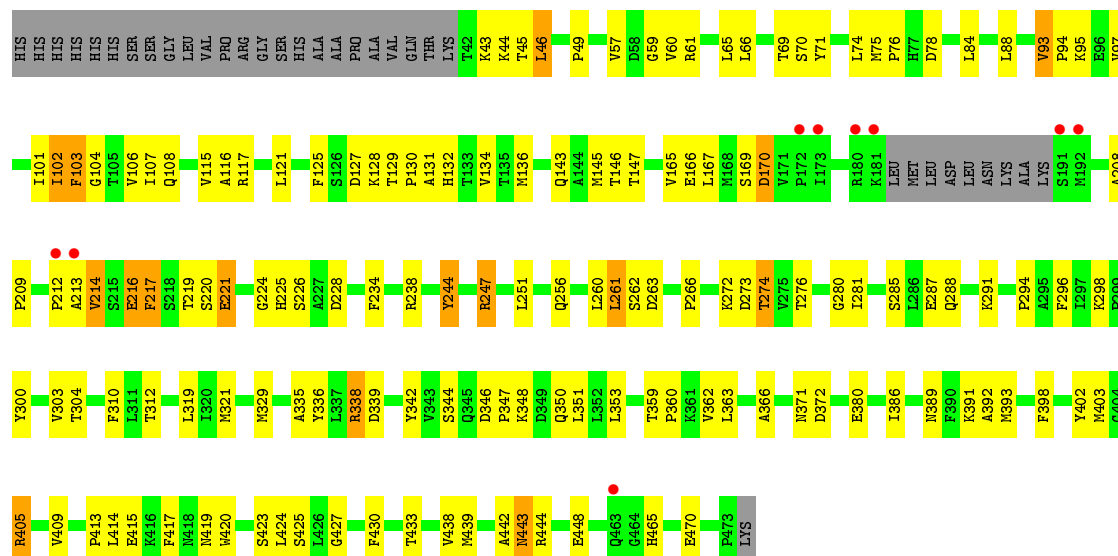
- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial



Y472
P473
LYS

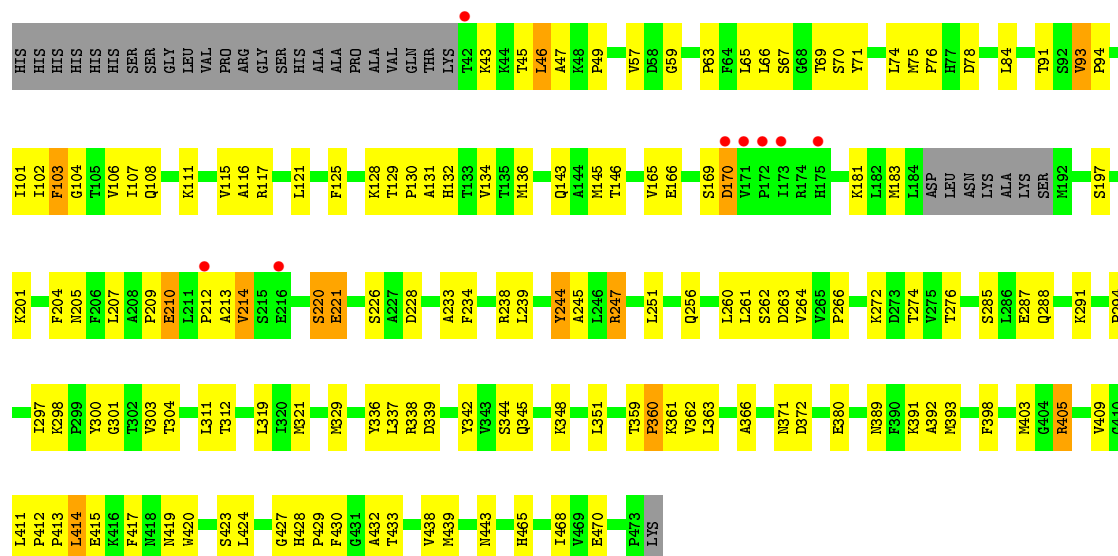
- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain E: 



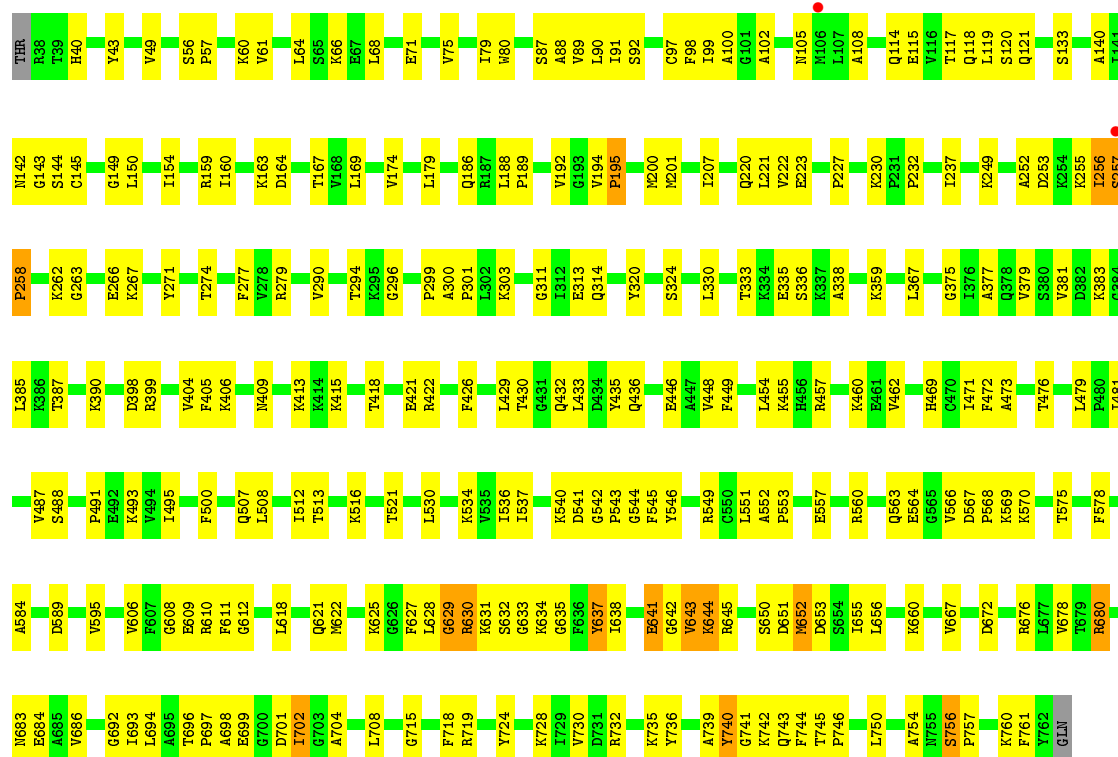
- Molecule 1: Trifunctional enzyme subunit beta, mitochondrial

Chain F: 

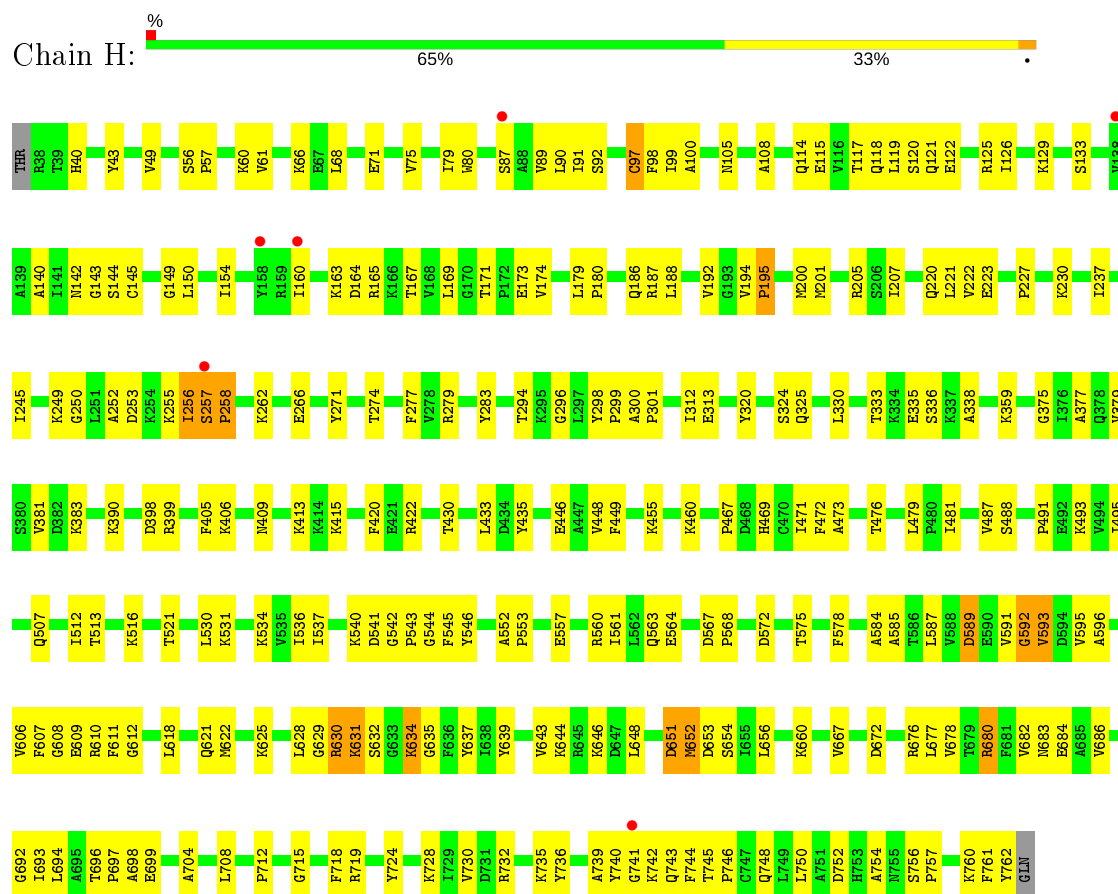


- Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial

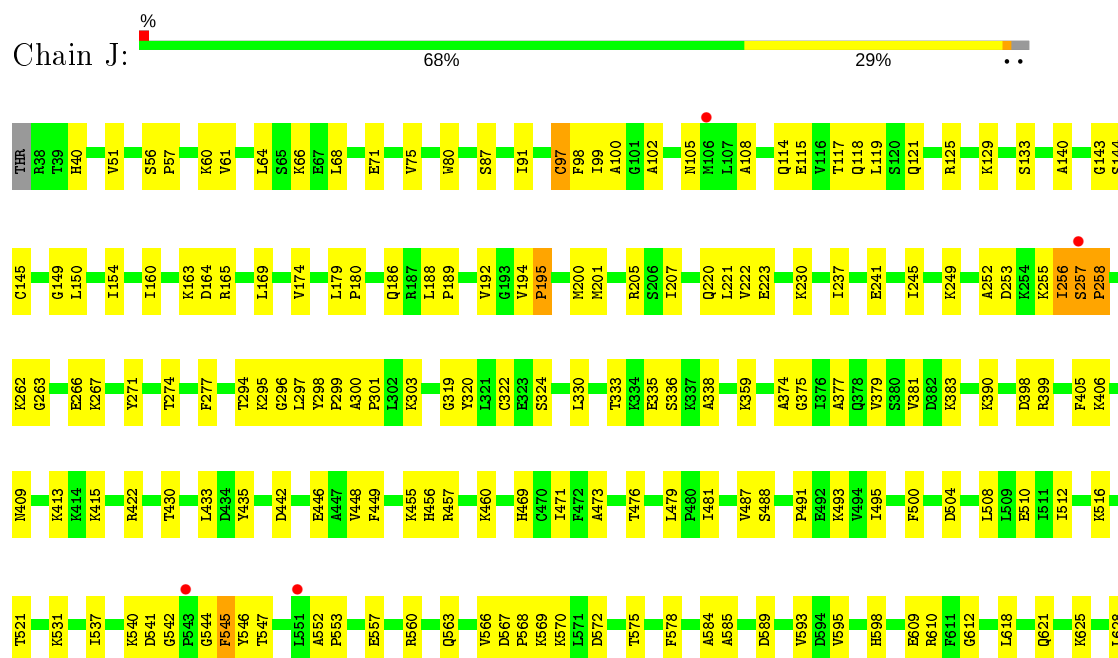
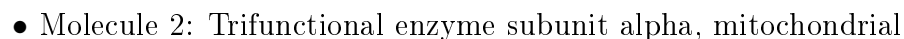
Chain G: 



• Molecule 2: Trifunctional enzyme subunit alpha, mitochondrial



- Chain I: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.54Å 237.94Å 141.32Å 90.00° 105.61° 90.00°	Depositor
Resolution (Å)	89.56 – 3.60 89.57 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (89.56-3.60) 98.7 (89.57-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.58Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.244 , 0.289 0.244 , 0.288	Depositor DCC
R_{free} test set	4957 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	110.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	51375	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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	0.29	0/3330	0.49	0/4498
1	B	0.29	0/3232	0.49	0/4368
1	C	0.24	0/3128	0.44	0/4238
1	D	0.24	0/3142	0.44	0/4257
1	E	0.25	0/3137	0.46	0/4250
1	F	0.26	0/3147	0.46	0/4264
2	G	0.25	0/5524	0.45	0/7453
2	H	0.24	0/5524	0.44	0/7453
2	I	0.23	0/5515	0.43	0/7431
2	J	0.23	0/5515	0.43	0/7431
2	K	0.23	0/5515	0.42	0/7431
2	L	0.23	0/5515	0.43	0/7431
All	All	0.25	0/52224	0.45	0/70505

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3267	0	3317	194	0
1	B	3170	0	3207	205	0
1	C	3073	0	2988	117	0
1	D	3087	0	2995	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3082	0	2993	117	0
1	F	3092	0	2997	115	0
2	G	5440	0	5569	213	0
2	H	5440	0	5569	198	0
2	I	5431	0	5632	175	0
2	J	5431	0	5632	178	0
2	K	5431	0	5632	172	0
2	L	5431	0	5632	180	0
All	All	51375	0	52163	1919	0

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 19.

The worst 5 of 1919 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:A:174:ARG:HB2	1:A:178:LYS:HG2	1.29	1.15
1:A:173:ILE:HG23	1:B:173:ILE:HG22	1.23	1.11
1:B:178:LYS:HD3	1:B:181:LYS:HD3	1.31	1.11
1:B:174:ARG:HB3	1:B:177:ARG:HB3	1.40	1.02
1:E:45:THR:O	1:E:46:LEU:HG	1.63	0.98

There are no symmetry-related clashes.

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	430/457 (94%)	353 (82%)	61 (14%)	16 (4%)	3	28
1	B	415/457 (91%)	347 (84%)	54 (13%)	14 (3%)	3	31
1	C	417/457 (91%)	355 (85%)	48 (12%)	14 (3%)	3	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	420/457 (92%)	347 (83%)	59 (14%)	14 (3%)	4	31
1	E	419/457 (92%)	357 (85%)	48 (12%)	14 (3%)	4	31
1	F	421/457 (92%)	357 (85%)	53 (13%)	11 (3%)	5	35
2	G	723/727 (99%)	613 (85%)	91 (13%)	19 (3%)	5	35
2	H	723/727 (99%)	619 (86%)	87 (12%)	17 (2%)	6	37
2	I	710/727 (98%)	621 (88%)	82 (12%)	7 (1%)	15	55
2	J	710/727 (98%)	608 (86%)	95 (13%)	7 (1%)	15	55
2	K	710/727 (98%)	614 (86%)	87 (12%)	9 (1%)	12	50
2	L	710/727 (98%)	617 (87%)	86 (12%)	7 (1%)	15	55
All	All	6808/7104 (96%)	5808 (85%)	851 (12%)	149 (2%)	6	39

5 of 149 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
1	A	208	ALA
1	A	216	GLU
1	A	221	GLU
1	B	49	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	345/365 (94%)	330 (96%)	15 (4%)	29	63
1	B	334/365 (92%)	316 (95%)	18 (5%)	22	57
1	C	305/365 (84%)	294 (96%)	11 (4%)	35	67
1	D	305/365 (84%)	295 (97%)	10 (3%)	38	69
1	E	305/365 (84%)	291 (95%)	14 (5%)	27	61
1	F	305/365 (84%)	292 (96%)	13 (4%)	29	63
2	G	580/603 (96%)	571 (98%)	9 (2%)	62	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	580/603 (96%)	566 (98%)	14 (2%)	49	75
2	I	591/603 (98%)	579 (98%)	12 (2%)	55	79
2	J	591/603 (98%)	580 (98%)	11 (2%)	57	80
2	K	591/603 (98%)	580 (98%)	11 (2%)	57	80
2	L	591/603 (98%)	582 (98%)	9 (2%)	65	84
All	All	5423/5808 (93%)	5276 (97%)	147 (3%)	44	73

5 of 147 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	433	THR
2	G	430	THR
2	K	719	ARG
1	F	93	VAL
1	F	247	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	108	GLN
1	F	108	GLN
2	K	621	GLN
1	E	345	GLN
1	F	288	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 carbohydrates 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	432/457 (94%)	0.34	24 (5%) 24 14	78, 115, 154, 202	0
1	B	419/457 (91%)	0.13	7 (1%) 70 55	77, 114, 150, 211	0
1	C	421/457 (92%)	0.14	10 (2%) 59 42	74, 116, 181, 239	0
1	D	424/457 (92%)	0.19	16 (3%) 40 26	78, 122, 186, 224	0
1	E	423/457 (92%)	0.04	9 (2%) 63 48	57, 91, 191, 228	0
1	F	425/457 (92%)	-0.05	8 (1%) 66 51	59, 93, 186, 231	0
2	G	725/727 (99%)	-0.14	2 (0%) 94 88	68, 123, 180, 234	0
2	H	725/727 (99%)	-0.15	6 (0%) 86 75	76, 130, 186, 241	0
2	I	714/727 (98%)	-0.04	11 (1%) 73 60	86, 128, 184, 234	0
2	J	714/727 (98%)	-0.14	8 (1%) 80 68	78, 123, 183, 237	0
2	K	714/727 (98%)	-0.18	5 (0%) 87 78	66, 121, 178, 226	0
2	L	714/727 (98%)	-0.22	6 (0%) 86 75	67, 119, 179, 214	0
All	All	6850/7104 (96%)	-0.04	112 (1%) 72 57	57, 119, 181, 241	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	212	PRO	6.9
1	E	213	ALA	4.4
1	A	453	GLY	4.2
2	J	257	SER	4.1
1	D	214	VAL	4.0

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 [i](#)

There are no carbohydrates 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.