



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 28, 2017 – 12:53 PM EST

PDB ID : 5XTB
EMDB ID: : EMD-6771
Title : Cryo-EM structure of human respiratory complex I matrix arm
Authors : Gu, J.; Wu, M.; Yang, M.
Deposited on : unknown
Resolution : 3.40 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

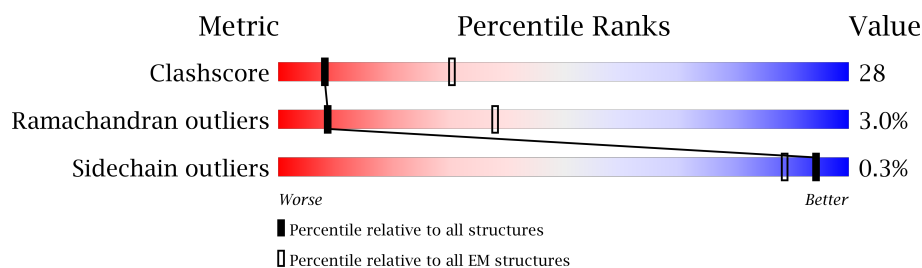
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



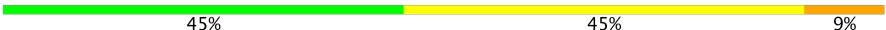



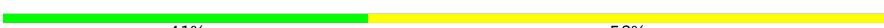




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	431	48% 50% .
2	B	176	51% 48% .
3	C	156	56% 43% .
4	E	113	49% 49% .
5	F	83	49% 51%
6	G	85	46% 52% .
7	H	112	54% 45% .
8	I	110	46% 36% . 14%
9	J	337	48% 50% .

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Mol	Chain	Length	Quality of chain
10	K	33	 45% 45% 9%
11	L	118	 43% 56% .
12	M	687	 47% 52% .
13	N	143	 59% 38% .
14	O	212	 41% 58% .
15	P	208	 49% 47% .
16	Q	385	 46% 53% .
17	T	95	 58% 39% .
18	W	22	 64% 32% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	SF4	A	501	-	-	X	-
19	SF4	B	302	-	-	X	-
19	SF4	M	801	-	-	X	-
20	FMN	A	502	-	-	X	-
22	NDP	J	401	-	-	X	-
23	FES	O	301	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 27962 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3322	2096	594	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	85	Total	C	N	O	S	0	0
			672	434	99	134	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	337	Total	C	N	O	S	0	0
			2712	1759	482	463	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	33	Total	C	N	O	S	0	0
			274	173	47	53	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	118	Total	C	N	O	S	0	0
			964	608	173	179	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	687	Total	C	N	O	S	0	0
			5274	3310	917	1009	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1195	770	210	212	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1643	1047	276	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1730	1117	297	313	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	385	Total	C	N	O	S	0	0
			3087	1971	536	558	22		

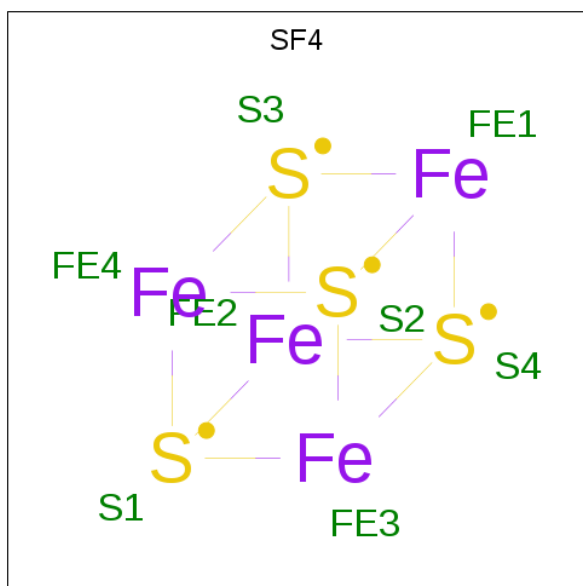
- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

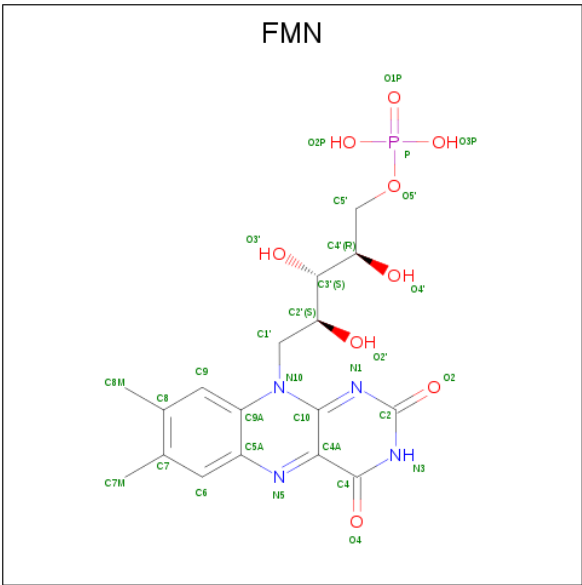
Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	22	Total	C	N	O	S	0	0
			179	113	35	30	1		

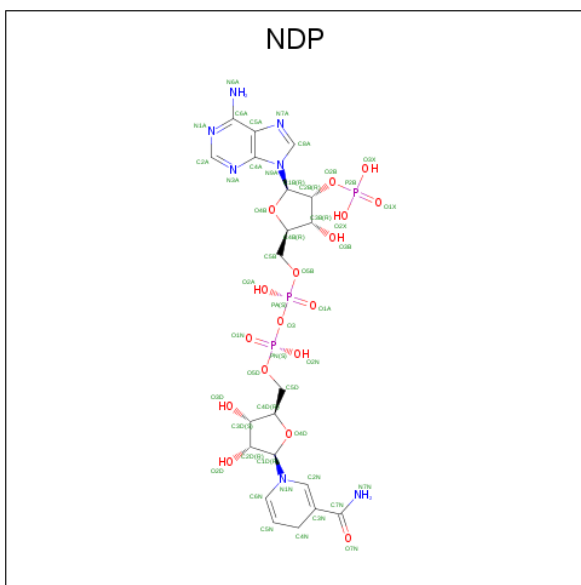
- Molecule 19 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	Fe	S	0
			8	4	4	
19	B	1	Total	Fe	S	0
			16	8	8	
19	B	1	Total	Fe	S	0
			16	8	8	
19	C	1	Total	Fe	S	0
			8	4	4	
19	M	1	Total	Fe	S	0
			16	8	8	
19	M	1	Total	Fe	S	0
			16	8	8	

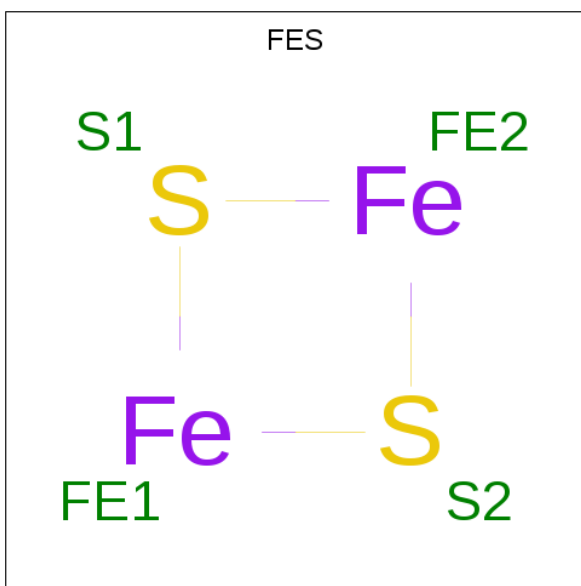
- Molecule 20 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).





Mol	Chain	Residues	Atoms					AltConf
22	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

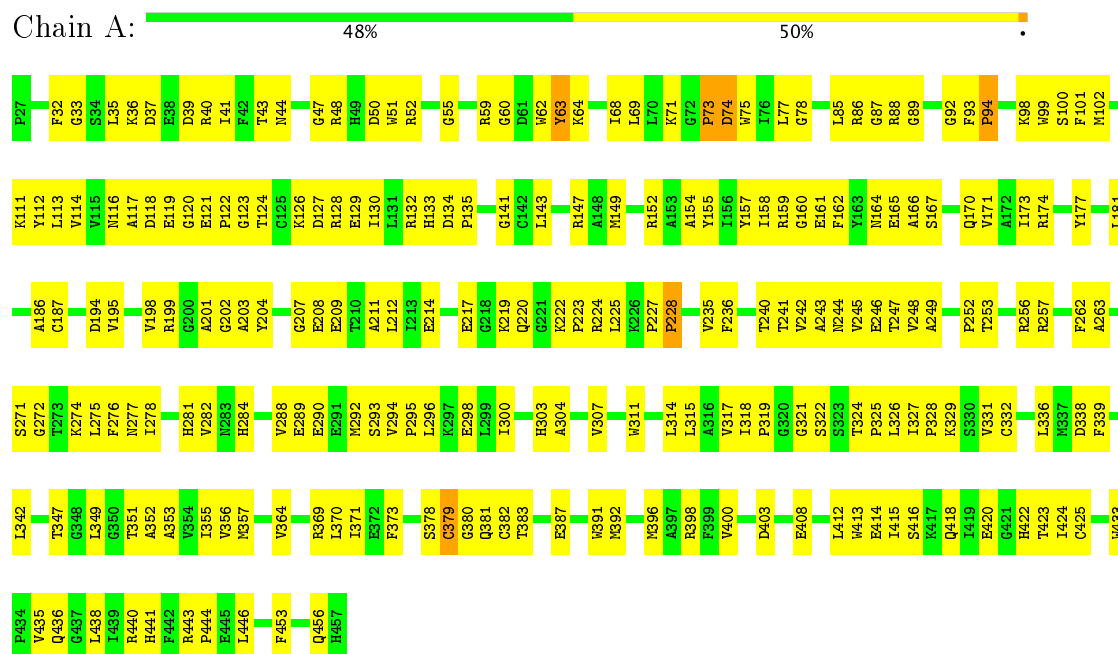


Mol	Chain	Residues	Atoms			AltConf
23	M	1	Total 4	Fe 2	S 2	0
23	O	1	Total 4	Fe 2	S 2	0

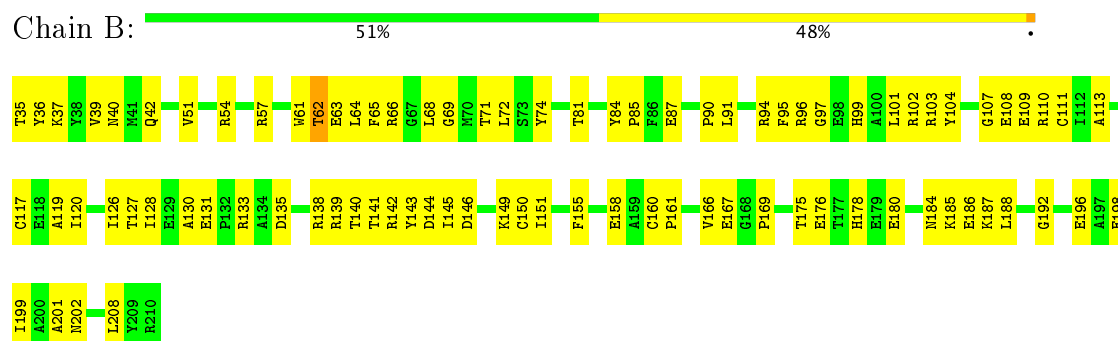
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

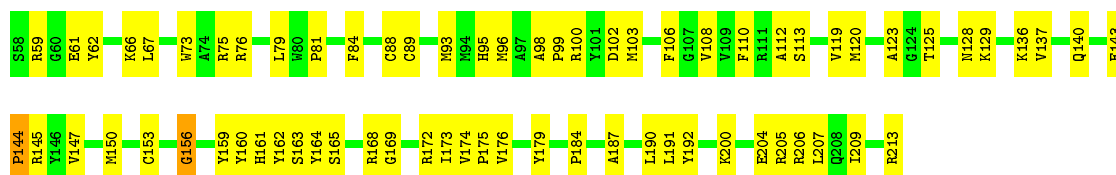


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

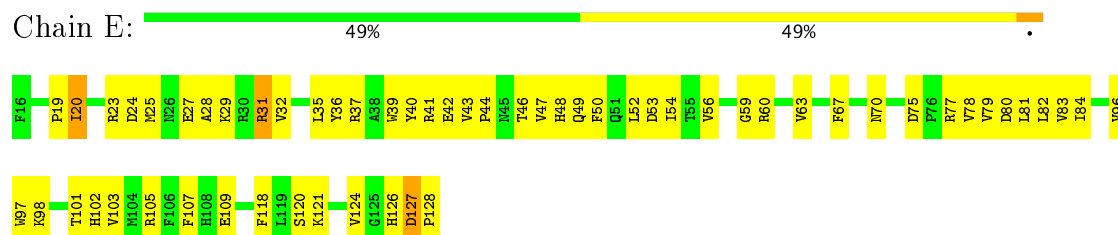


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

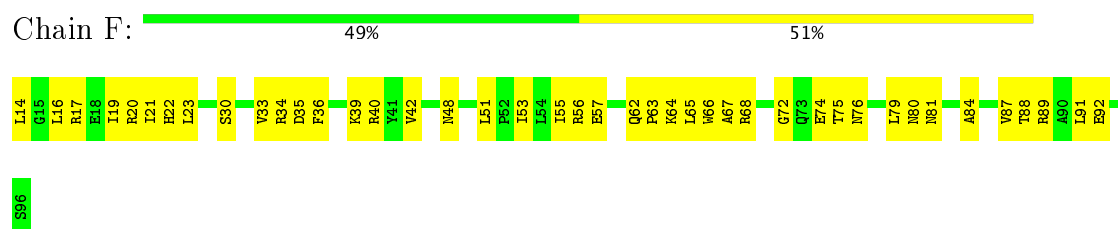




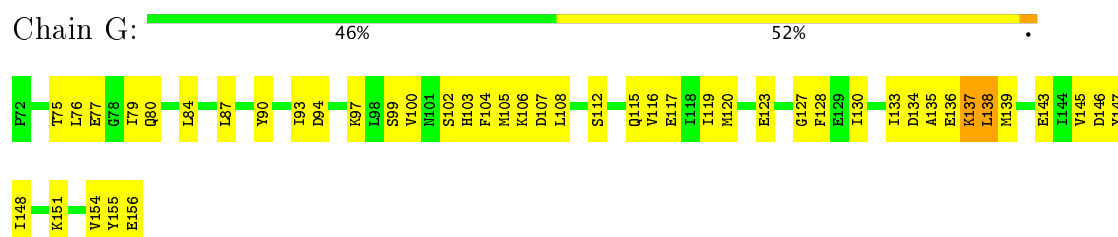
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



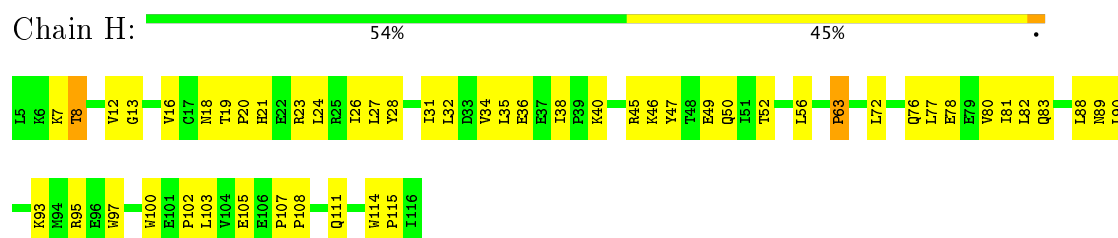
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 6: Acyl carrier protein, mitochondrial



- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

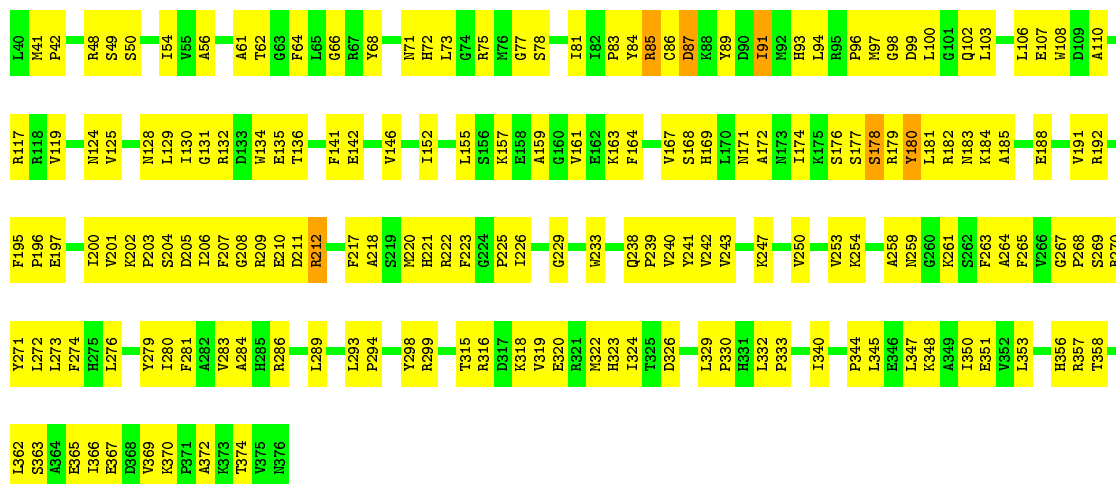


- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain J: 48% 50%



- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain K:  45% 45% 9%



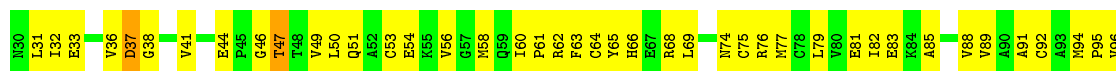
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

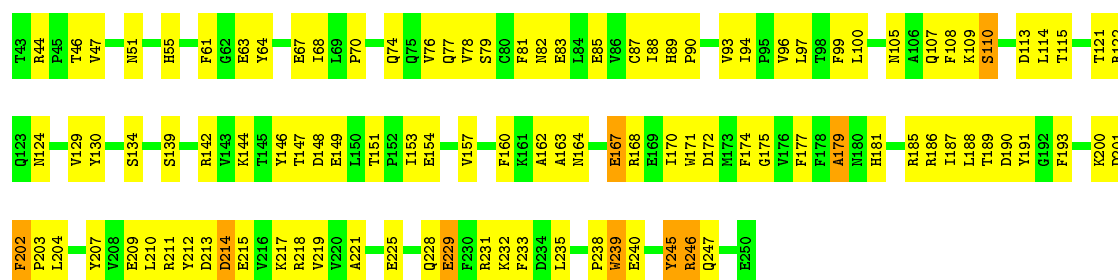
Chain L:  43% 56%



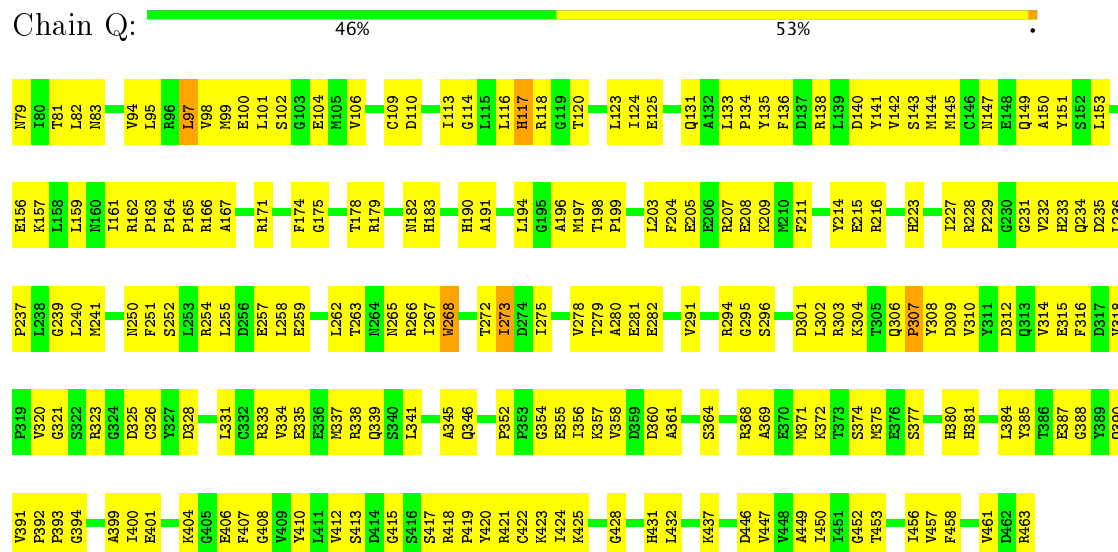
- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:  47% 52%

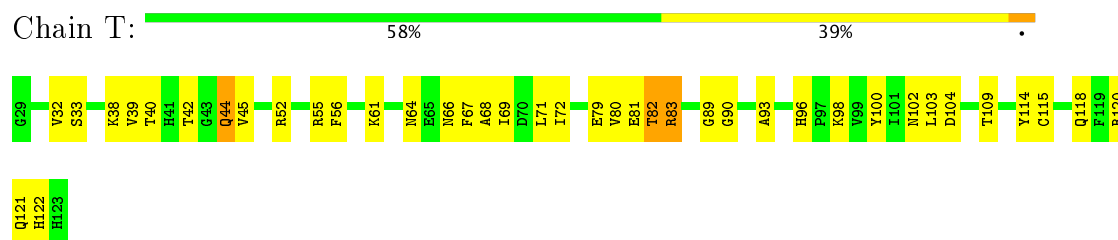




- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, 8Q1, SF4, FES, NDP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.30	0/3398	0.49	0/4590
10	K	0.27	0/282	0.47	0/381
11	L	0.33	0/987	0.53	0/1331
12	M	0.32	0/5362	0.53	0/7266
13	N	0.37	0/1236	0.55	0/1681
14	O	0.29	0/1682	0.51	0/2289
15	P	0.38	0/1780	0.59	0/2424
16	Q	0.44	0/3161	0.60	1/4275 (0.0%)
17	T	0.31	0/755	0.47	0/1017
18	W	0.34	0/185	0.65	0/249
2	B	0.50	0/1452	0.57	0/1964
3	C	0.58	0/1280	0.57	0/1732
4	E	0.34	0/993	0.53	0/1335
5	F	0.28	0/682	0.52	0/922
6	G	0.33	0/684	0.53	0/926
7	H	0.33	0/941	0.59	0/1275
8	I	0.29	0/788	0.54	0/1066
9	J	0.34	0/2785	0.52	0/3771
All	All	0.36	0/28433	0.54	1/38494 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	97	LEU	CA-CB-CG	5.67	128.34	115.30

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	3322	0	3289	209	0
2	B	1420	0	1371	99	0
3	C	1249	0	1253	65	0
4	E	968	0	982	62	0
5	F	670	0	679	37	0
6	G	672	0	650	32	0
7	H	922	0	950	58	0
8	I	769	0	788	45	0
9	J	2712	0	2757	227	0
10	K	274	0	257	24	0
11	L	964	0	962	65	0
12	M	5274	0	5312	329	0
13	N	1195	0	1155	47	0
14	O	1643	0	1646	111	0
15	P	1730	0	1685	114	0
16	Q	3087	0	3069	223	0
17	T	742	0	723	37	0
18	W	179	0	179	11	0
19	A	8	0	0	6	0
19	B	16	0	0	3	0
19	C	8	0	0	1	0
19	M	16	0	0	4	0
20	A	31	0	19	17	0
21	E	35	0	0	4	0
22	J	48	0	26	26	0
23	M	4	0	0	1	0
23	O	4	0	0	2	0
All	All	27962	0	27752	1536	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 28.

The worst 5 of 1536 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)
9:J:130:ILE:HG23	22:J:401:NDP:C8A	1.45	1.46
12:M:134:GLY:HA2	19:M:801:SF4:S3	1.57	1.42
16:Q:262:LEU:HD22	16:Q:268:TRP:CD1	1.64	1.32
9:J:206:ILE:HA	9:J:240:VAL:O	1.35	1.26
9:J:171:ASN:O	9:J:181:LEU:HD21	1.23	1.24

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	429/431 (100%)	396 (92%)	24 (6%)	9 (2%)	8	43
2	B	174/176 (99%)	163 (94%)	10 (6%)	1 (1%)	28	68
3	C	154/156 (99%)	137 (89%)	12 (8%)	5 (3%)	5	34
4	E	111/113 (98%)	101 (91%)	8 (7%)	2 (2%)	10	46
5	F	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
6	G	83/85 (98%)	78 (94%)	3 (4%)	2 (2%)	7	40
7	H	110/112 (98%)	100 (91%)	5 (4%)	5 (4%)	3	24
8	I	91/110 (83%)	79 (87%)	6 (7%)	6 (7%)	1	15
9	J	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	8	43
10	K	31/33 (94%)	27 (87%)	1 (3%)	3 (10%)	1	7
11	L	116/118 (98%)	104 (90%)	8 (7%)	4 (3%)	4	32
12	M	685/687 (100%)	608 (89%)	54 (8%)	23 (3%)	4	32
13	N	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	2	22
14	O	210/212 (99%)	188 (90%)	15 (7%)	7 (3%)	4	33
15	P	206/208 (99%)	173 (84%)	22 (11%)	11 (5%)	2	20
16	Q	383/385 (100%)	355 (93%)	23 (6%)	5 (1%)	14	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	T	93/95 (98%)	87 (94%)	2 (2%)	4 (4%)	3	26
18	W	20/22 (91%)	16 (80%)	1 (5%)	3 (15%)	0	2
All	All	3453/3506 (98%)	3119 (90%)	230 (7%)	104 (3%)	9	35

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	TYR
1	A	73	PRO
1	A	379	CYS
2	B	62	THR
12	M	37	ASP

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 PDB entries followed by that with respect to all EM entries.

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	346/346 (100%)	346 (100%)	0	100	100
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/106 (100%)	105 (99%)	1 (1%)	82	92
5	F	74/74 (100%)	74 (100%)	0	100	100
6	G	74/79 (94%)	74 (100%)	0	100	100
7	H	100/100 (100%)	100 (100%)	0	100	100
8	I	87/96 (91%)	87 (100%)	0	100	100
9	J	292/292 (100%)	288 (99%)	4 (1%)	71	88
10	K	32/32 (100%)	32 (100%)	0	100	100
11	L	107/107 (100%)	107 (100%)	0	100	100
12	M	576/577 (100%)	574 (100%)	2 (0%)	94	98
13	N	129/129 (100%)	129 (100%)	0	100	100
14	O	181/181 (100%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	190/190 (100%)	190 (100%)	0	100	100
16	Q	331/331 (100%)	329 (99%)	2 (1%)	89	95
17	T	79/79 (100%)	79 (100%)	0	100	100
18	W	19/19 (100%)	19 (100%)	0	100	100
All	All	3006/3021 (100%)	2997 (100%)	9 (0%)	94	98

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

Mol	Chain	Res	Type
9	J	212	ARG
16	Q	273	ILE
12	M	174	THR
9	J	91	ILE
12	M	130	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
11	L	86	ASN
12	M	514	ASN
16	Q	431	HIS
12	M	384	ASN
12	M	460	HIS

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

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	SF4	A	501	1	0,12,12	0.00	-	0,24,24	0.00	-
20	FMN	A	502	-	31,33,33	1.47	5 (16%)	38,50,50	1.96	7 (18%)
19	SF4	B	301	2	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	C	301	3	0,12,12	0.00	-	0,24,24	0.00	-
21	8Q1	E	201	-	32,34,34	1.65	6 (18%)	39,43,43	1.53	8 (20%)
22	NDP	J	401	-	43,52,52	0.98	2 (4%)	49,80,80	1.41	3 (6%)
19	SF4	M	801	12	0,12,12	0.00	-	0,24,24	0.00	-
19	SF4	M	802	12	0,12,12	0.00	-	0,24,24	0.00	-
23	FES	M	803	-	0,4,4	0.00	-	0,4,4	0.00	-
23	FES	O	301	14	0,4,4	0.00	-	0,4,4	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	SF4	A	501	1	-	0/0/48/48	0/6/5/5
20	FMN	A	502	-	-	0/16/18/18	0/3/3/3
19	SF4	B	301	2	-	0/0/48/48	0/6/5/5
19	SF4	B	302	2	-	0/0/48/48	0/6/5/5
19	SF4	C	301	3	-	0/0/48/48	0/6/5/5
21	8Q1	E	201	-	-	2/41/41/41	0/0/0/0
22	NDP	J	401	-	-	0/30/77/77	0/5/5/5
19	SF4	M	801	12	-	0/0/48/48	0/6/5/5
19	SF4	M	802	12	-	0/0/48/48	0/6/5/5
23	FES	M	803	-	-	0/0/4/4	0/1/1/1
23	FES	O	301	14	-	0/0/4/4	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	E	201	8Q1	O35-C34	-2.50	1.18	1.23
21	E	201	8Q1	O40-C39	-2.27	1.18	1.23
20	A	502	FMN	C6-C5A	-2.04	1.38	1.41
21	E	201	8Q1	C6-C1	2.11	1.53	1.50
22	J	401	NDP	C5A-C4A	2.59	1.46	1.40

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	401	NDP	N3A-C2A-N1A	-7.00	122.77	128.86
20	A	502	FMN	C4-C4A-C10	-3.98	116.74	119.96
20	A	502	FMN	C4A-C4-N3	-3.38	118.67	123.48
21	E	201	8Q1	O4-C1-C6	-3.38	120.99	123.95
22	J	401	NDP	C4A-C5A-N7A	-2.66	106.84	109.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	E	201	8Q1	C29-C32-C34-N36
21	E	201	8Q1	O35-C34-C32-C29

There are no ring outliers.

10 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	501	SF4	6	0
20	A	502	FMN	17	0
19	B	301	SF4	1	0
19	B	302	SF4	2	0
19	C	301	SF4	1	0
21	E	201	8Q1	4	0
22	J	401	NDP	26	0
19	M	801	SF4	4	0
23	M	803	FES	1	0
23	O	301	FES	2	0

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.