



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:30 am GMT

PDB ID : 1HR8
Title : Yeast Mitochondrial Processing Peptidase beta-E73Q Mutant Complexed with Cytochrome C Oxidase IV Signal Peptide
Authors : Taylor, A.B.; Smith, B.S.; Kitada, S.; Kojima, K.; Miyaura, H.; Otwinowski, Z.; Ito, A.; Deisenhofer, J.
Deposited on : 2000-12-21
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

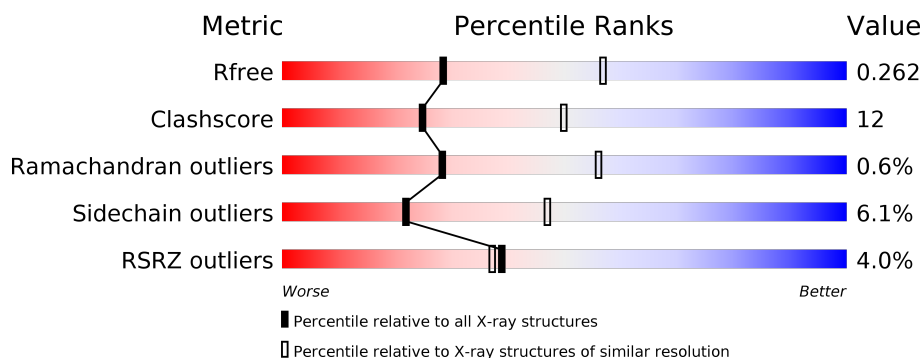
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 on the lower 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 $\leq 5\%$. 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	475	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	C	475	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>• 6%</div> </div> </div>
1	E	475	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	G	475	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 6%</div> </div> </div>
2	B	443	<div> <div></div> <div> <div></div> <div>71%</div> <div>24%</div> <div>• •</div> </div> </div>
2	D	443	<div> <div>•</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	443	
2	H	443	
3	O	24	
3	P	24	
3	Q	24	
3	R	24	

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
5	EPE	A	489	-	-	-	X
5	EPE	G	489	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27990 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 MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3499	2213	594	673	19			
1	C	448	Total	C	N	O	S	0	0	0
			3471	2198	587	667	19			
1	E	445	Total	C	N	O	S	0	0	0
			3459	2190	586	664	19			
1	G	448	Total	C	N	O	S	0	0	0
			3475	2198	589	669	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	GLU	SEE REMARK 999	UNP P11914
A	217	GLY	GLU	SEE REMARK 999	UNP P11914
A	483	HIS	-	EXPRESSION TAG	UNP P11914
A	484	HIS	-	EXPRESSION TAG	UNP P11914
A	485	HIS	-	EXPRESSION TAG	UNP P11914
A	486	HIS	-	EXPRESSION TAG	UNP P11914
A	487	HIS	-	EXPRESSION TAG	UNP P11914
A	488	HIS	-	EXPRESSION TAG	UNP P11914
C	177	GLY	GLU	SEE REMARK 999	UNP P11914
C	217	GLY	GLU	SEE REMARK 999	UNP P11914
C	483	HIS	-	EXPRESSION TAG	UNP P11914
C	484	HIS	-	EXPRESSION TAG	UNP P11914
C	485	HIS	-	EXPRESSION TAG	UNP P11914
C	486	HIS	-	EXPRESSION TAG	UNP P11914
C	487	HIS	-	EXPRESSION TAG	UNP P11914
C	488	HIS	-	EXPRESSION TAG	UNP P11914
E	177	GLY	GLU	SEE REMARK 999	UNP P11914
E	217	GLY	GLU	SEE REMARK 999	UNP P11914
E	483	HIS	-	EXPRESSION TAG	UNP P11914
E	484	HIS	-	EXPRESSION TAG	UNP P11914

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Chain	Residue	Modelled	Actual	Comment	Reference
E	485	HIS	-	EXPRESSION TAG	UNP P11914
E	486	HIS	-	EXPRESSION TAG	UNP P11914
E	487	HIS	-	EXPRESSION TAG	UNP P11914
E	488	HIS	-	EXPRESSION TAG	UNP P11914
G	177	GLY	GLU	SEE REMARK 999	UNP P11914
G	217	GLY	GLU	SEE REMARK 999	UNP P11914
G	483	HIS	-	EXPRESSION TAG	UNP P11914
G	484	HIS	-	EXPRESSION TAG	UNP P11914
G	485	HIS	-	EXPRESSION TAG	UNP P11914
G	486	HIS	-	EXPRESSION TAG	UNP P11914
G	487	HIS	-	EXPRESSION TAG	UNP P11914
G	488	HIS	-	EXPRESSION TAG	UNP P11914

- Molecule 2 is a protein called MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	439	Total	C	N	O	S	0	0	0
			3414	2148	591	668	7			
2	D	443	Total	C	N	O	S	0	0	0
			3442	2165	596	674	7			
2	F	443	Total	C	N	O	S	0	0	0
			3442	2165	596	674	7			
2	H	441	Total	C	N	O	S	0	0	0
			3431	2159	594	671	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	20	ALA	-	CLONING ARTIFACT	UNP P10507
B	73	GLN	GLU	ENGINEERED	UNP P10507
B	84	PRO	SER	SEE REMARK 999	UNP P10507
B	350	ARG	GLN	SEE REMARK 999	UNP P10507
D	20	ALA	-	CLONING ARTIFACT	UNP P10507
D	73	GLN	GLU	ENGINEERED	UNP P10507
D	84	PRO	SER	SEE REMARK 999	UNP P10507
D	350	ARG	GLN	SEE REMARK 999	UNP P10507
F	20	ALA	-	CLONING ARTIFACT	UNP P10507
F	73	GLN	GLU	ENGINEERED	UNP P10507
F	84	PRO	SER	SEE REMARK 999	UNP P10507
F	350	ARG	GLN	SEE REMARK 999	UNP P10507
H	20	ALA	-	CLONING ARTIFACT	UNP P10507

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Chain	Residue	Modelled	Actual	Comment	Reference
H	73	GLN	GLU	ENGINEERED	UNP P10507
H	84	PRO	SER	SEE REMARK 999	UNP P10507
H	350	ARG	GLN	SEE REMARK 999	UNP P10507

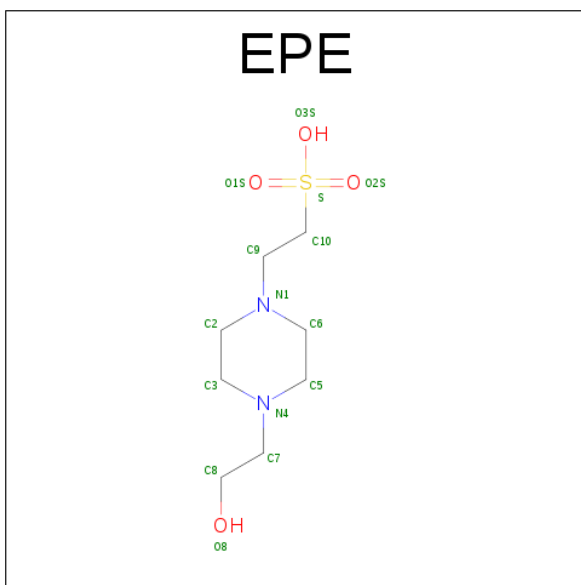
- Molecule 3 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	13	Total	C	N	O	S	0	0	0
			107	70	20	16	1			
3	P	9	Total	C	N	O		0	0	0
			76	52	13	11				
3	Q	10	Total	C	N	O	S	0	0	0
			82	55	14	12	1			
3	R	7	Total	C	N	O		0	0	0
			54	34	11	9				

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

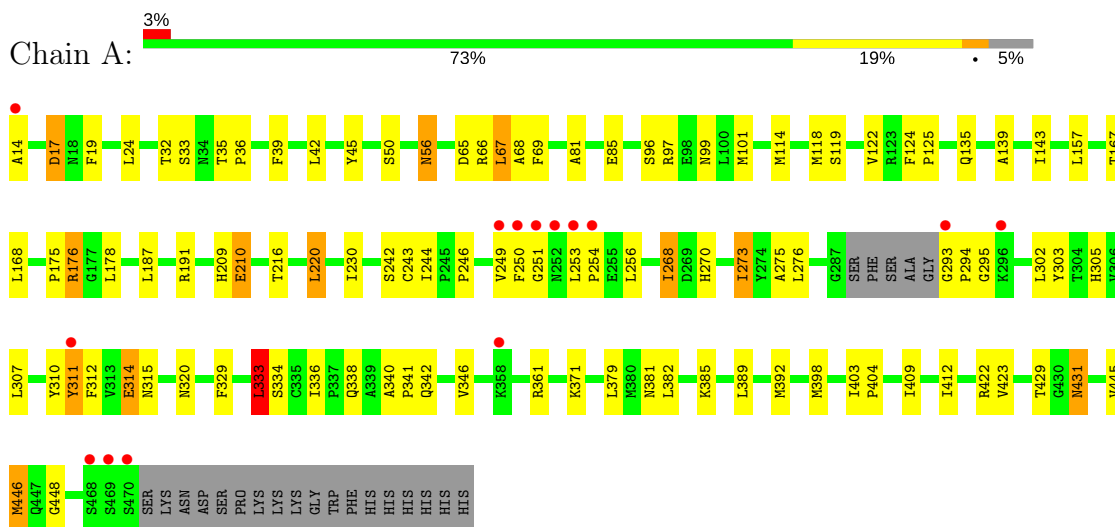
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	O	0	0
			1	1		
6	H	1	Total	O	0	0
			1	1		
6	O	1	Total	O	0	0
			1	1		
6	P	1	Total	O	0	0
			1	1		

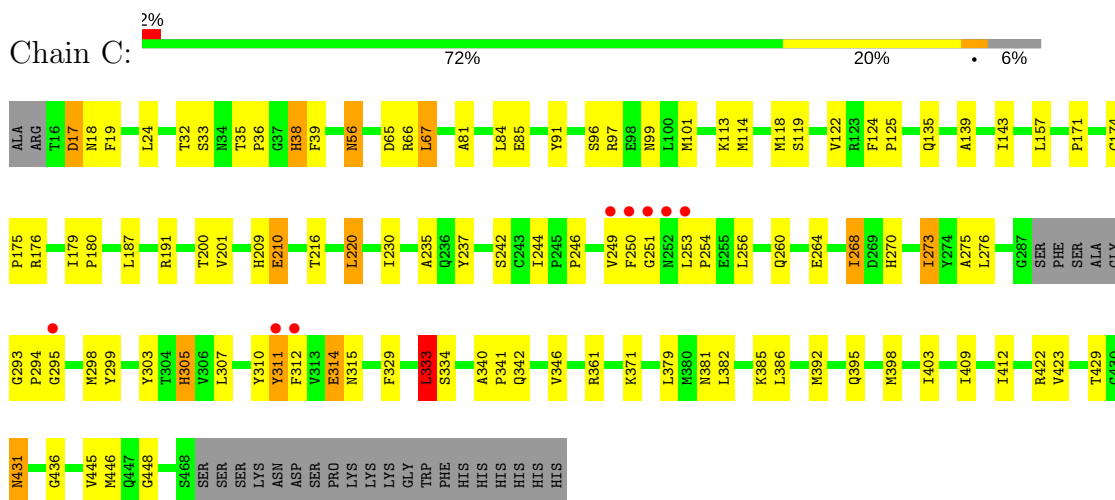
3 Residue-property plots [i](#)

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 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: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

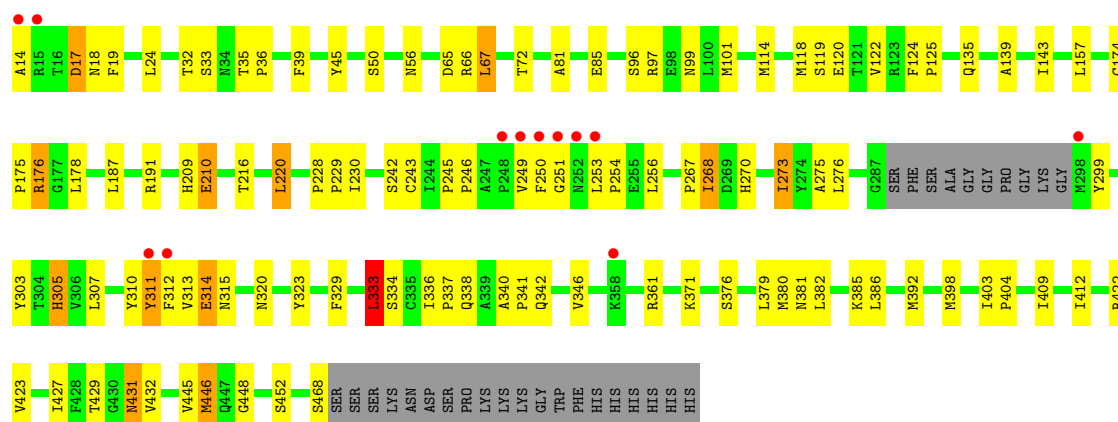


• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

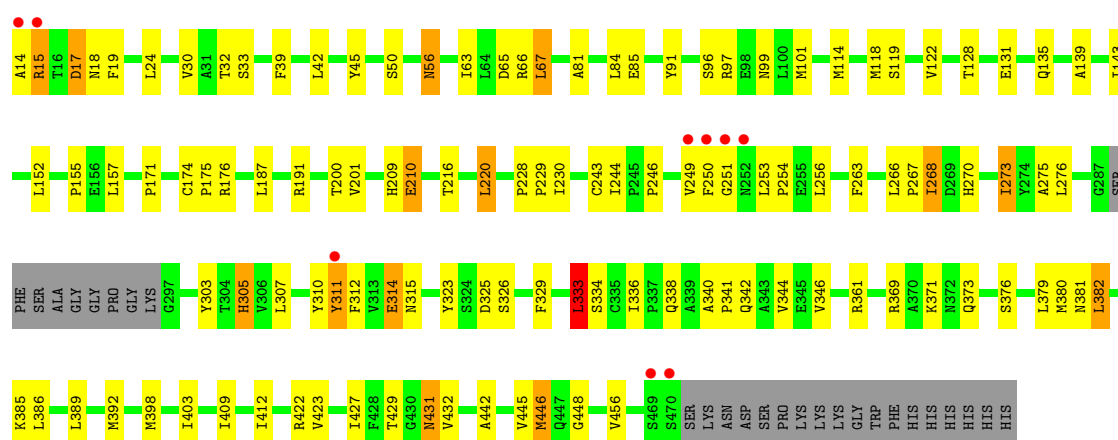


• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

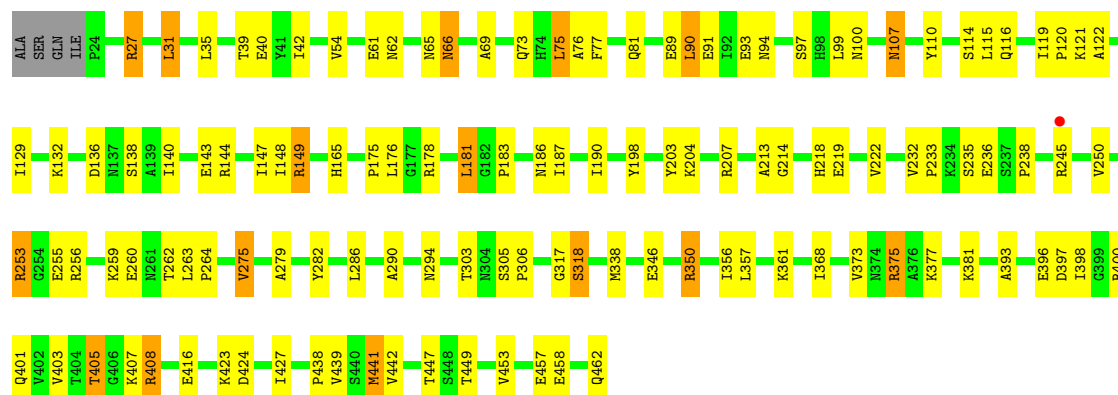




• Molecule 1: MITOCHONDRIAL PROCESSING PEPTIDASE ALPHA SUBUNIT

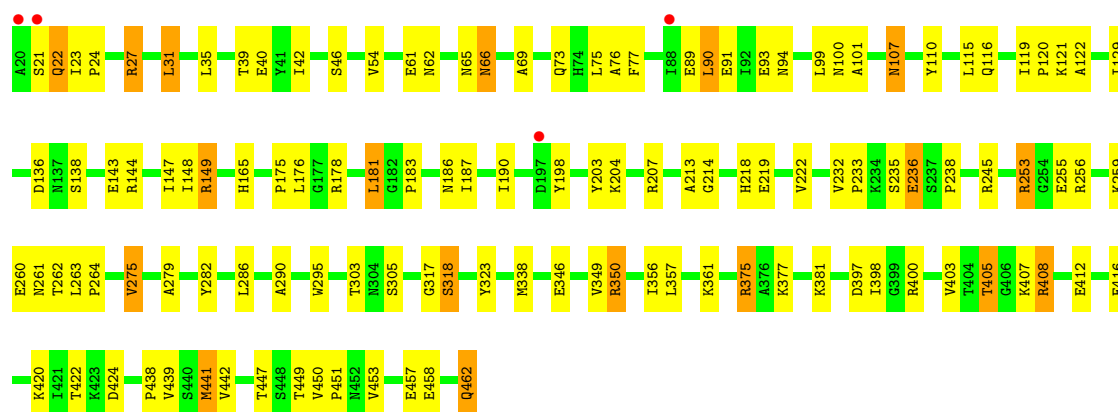


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

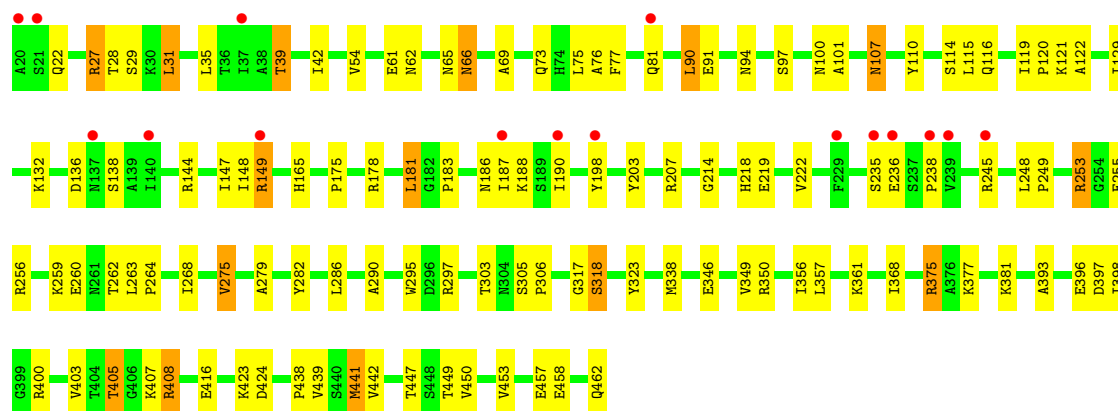


• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT

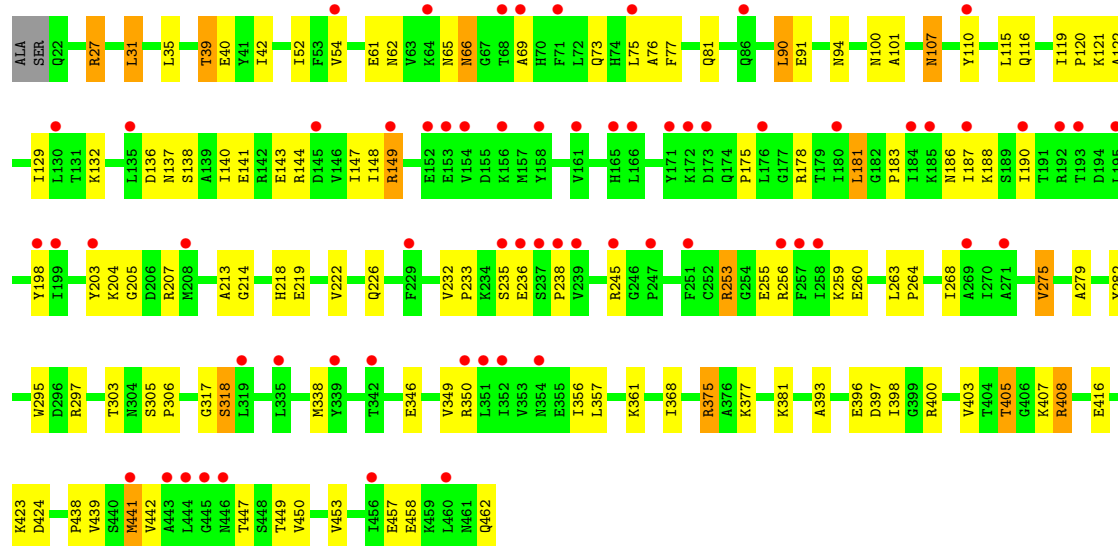




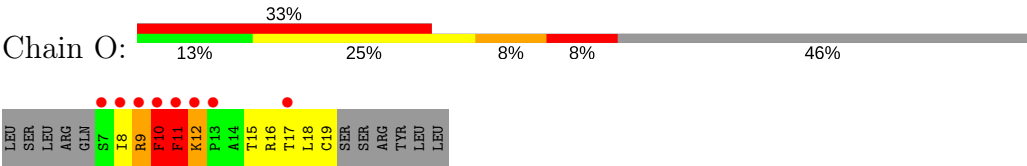
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



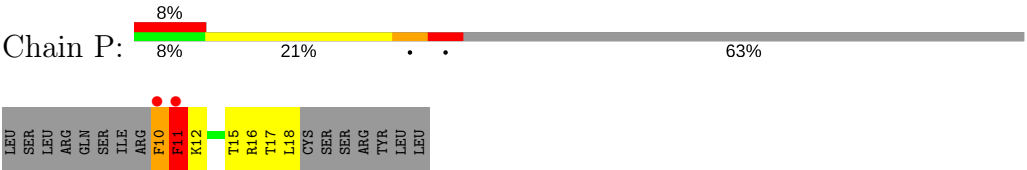
• Molecule 2: MITOCHONDRIAL PROCESSING PEPTIDASE BETA SUBUNIT



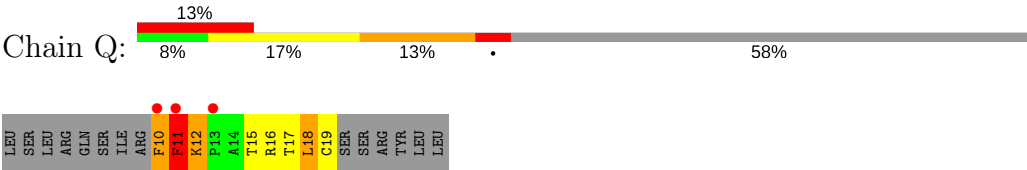
• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE IV



• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE IV



• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE IV



• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE IV



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.26Å 178.12Å 202.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.63 – 2.70 48.63 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.63-2.70) 99.5 (48.63-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.264 0.228 , 0.262	Depositor DCC
R_{free} test set	2016 reflections (1.51%)	DCC
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27990	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EPE

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	0.67	2/3570 (0.1%)	0.77	3/4830 (0.1%)
1	C	0.65	2/3542 (0.1%)	0.76	4/4793 (0.1%)
1	E	0.60	2/3529 (0.1%)	0.85	4/4776 (0.1%)
1	G	0.62	3/3545 (0.1%)	0.74	3/4797 (0.1%)
2	B	0.62	0/3478	0.82	7/4720 (0.1%)
2	D	0.66	4/3506 (0.1%)	0.91	8/4759 (0.2%)
2	F	0.51	0/3506	0.87	10/4759 (0.2%)
2	H	0.47	0/3495	0.97	10/4744 (0.2%)
3	O	0.99	0/109	1.37	3/145 (2.1%)
3	P	1.11	0/78	0.96	0/104
3	Q	1.02	0/84	1.08	1/112 (0.9%)
3	R	0.86	0/54	0.86	0/72
All	All	0.61	13/28496 (0.0%)	0.84	53/38611 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	462	GLN	CD-NE2	-10.01	1.07	1.32
2	D	261	ASN	CG-OD1	-9.49	1.03	1.24
2	D	462	GLN	CD-OE1	-9.15	1.03	1.24
2	D	261	ASN	CG-ND2	-9.05	1.10	1.32
1	A	431	ASN	CG-ND2	-6.59	1.16	1.32

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	149	ARG	NE-CZ-NH2	-21.41	109.60	120.30
2	D	253	ARG	NE-CZ-NH1	-21.33	109.63	120.30
2	D	253	ARG	NE-CZ-NH2	20.88	130.74	120.30
2	H	149	ARG	NE-CZ-NH1	20.82	130.71	120.30
1	E	422	ARG	NE-CZ-NH1	-20.01	110.30	120.30

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	3499	0	3460	77	0
1	C	3471	0	3432	77	0
1	E	3459	0	3421	76	0
1	G	3475	0	3434	86	0
2	B	3414	0	3414	97	0
2	D	3442	0	3442	101	0
2	F	3442	0	3442	92	0
2	H	3431	0	3432	87	0
3	O	107	0	114	14	0
3	P	76	0	80	10	0
3	Q	82	0	85	13	0
3	R	54	0	62	7	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	A	15	0	17	0	0
5	G	15	0	17	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
All	All	27990	0	27852	683	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 12.

The worst 5 of 683 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:G:33:SER:HB3	1:G:392:MET:HE3	1.18	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:ALA:N	1:G:19:PHE:HB3	1.64	1.11
1:C:33:SER:HB3	1:C:392:MET:HE1	1.28	1.10
1:A:33:SER:HB3	1:A:392:MET:HE1	1.27	1.10
1:E:33:SER:HB3	1:E:392:MET:HE1	1.42	1.02

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 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	448/475 (94%)	427 (95%)	19 (4%)	2 (0%)	38	66
1	C	444/475 (94%)	426 (96%)	15 (3%)	3 (1%)	25	53
1	E	441/475 (93%)	423 (96%)	15 (3%)	3 (1%)	25	53
1	G	444/475 (94%)	424 (96%)	16 (4%)	4 (1%)	20	46
2	B	437/443 (99%)	420 (96%)	16 (4%)	1 (0%)	51	79
2	D	441/443 (100%)	420 (95%)	19 (4%)	2 (0%)	32	60
2	F	441/443 (100%)	425 (96%)	15 (3%)	1 (0%)	51	79
2	H	439/443 (99%)	422 (96%)	16 (4%)	1 (0%)	51	79
3	O	11/24 (46%)	6 (54%)	4 (36%)	1 (9%)	1	1
3	P	7/24 (29%)	5 (71%)	1 (14%)	1 (14%)	0	0
3	Q	8/24 (33%)	3 (38%)	4 (50%)	1 (12%)	0	0
3	R	5/24 (21%)	4 (80%)	1 (20%)	0	100	100
All	All	3566/3768 (95%)	3405 (96%)	141 (4%)	20 (1%)	28	56

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	O	11	PHE

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Mol	Chain	Res	Type
3	P	11	PHE
3	Q	11	PHE
1	C	250	PHE
1	G	15	ARG

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	381/401 (95%)	360 (94%)	21 (6%)	25	52
1	C	378/401 (94%)	356 (94%)	22 (6%)	23	50
1	E	377/401 (94%)	353 (94%)	24 (6%)	20	45
1	G	379/401 (94%)	357 (94%)	22 (6%)	23	50
2	B	376/379 (99%)	352 (94%)	24 (6%)	20	45
2	D	379/379 (100%)	356 (94%)	23 (6%)	22	47
2	F	379/379 (100%)	358 (94%)	21 (6%)	25	52
2	H	378/379 (100%)	358 (95%)	20 (5%)	26	54
3	O	12/23 (52%)	9 (75%)	3 (25%)	1	2
3	P	8/23 (35%)	5 (62%)	3 (38%)	0	0
3	Q	9/23 (39%)	5 (56%)	4 (44%)	0	0
3	R	6/23 (26%)	5 (83%)	1 (17%)	2	6
All	All	3062/3212 (95%)	2874 (94%)	188 (6%)	22	47

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	403	VAL
1	E	320	ASN
2	H	405	THR
2	D	408	ARG
1	E	176	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	354	ASN
1	E	349	GLN
2	H	186	ASN
1	E	99	ASN
2	F	44	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
5	EPE	A	489	-	15,15,15	1.59	3 (20%)	18,20,20	0.95	1 (5%)
5	EPE	G	489	-	15,15,15	1.22	1 (6%)	18,20,20	1.14	2 (11%)

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
5	EPE	A	489	-	-	0/9/19/19	0/1/1/1
5	EPE	G	489	-	-	0/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	489	EPE	C10-S	2.01	1.80	1.77
5	A	489	EPE	C2-N1	2.05	1.52	1.47
5	A	489	EPE	C6-N1	2.51	1.53	1.47
5	A	489	EPE	C10-S	3.81	1.83	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	489	EPE	C7-N4-C5	-2.16	105.73	111.26
5	G	489	EPE	C7-N4-C5	-2.11	105.85	111.26
5	G	489	EPE	O1S-S-C10	-2.02	105.05	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	452/475 (95%)	-0.03	14 (3%)	49	49	22, 43, 88, 101	0
1	C	448/475 (94%)	-0.11	8 (1%)	69	70	25, 43, 80, 101	0
1	E	445/475 (93%)	0.06	12 (2%)	55	55	27, 51, 88, 101	0
1	G	448/475 (94%)	-0.04	9 (2%)	65	66	29, 49, 86, 101	0
2	B	439/443 (99%)	-0.14	1 (0%)	94	96	22, 43, 76, 101	0
2	D	443/443 (100%)	-0.07	4 (0%)	84	85	27, 52, 84, 101	0
2	F	443/443 (100%)	0.15	16 (3%)	43	42	33, 68, 98, 101	0
2	H	441/443 (99%)	0.77	65 (14%)	3	2	43, 91, 101, 101	0
3	O	13/24 (54%)	2.66	8 (61%)	0	0	52, 95, 101, 101	0
3	P	9/24 (37%)	1.37	2 (22%)	1	1	61, 77, 99, 101	0
3	Q	10/24 (41%)	1.97	3 (30%)	1	0	64, 101, 101, 101	0
3	R	7/24 (29%)	0.85	1 (14%)	3	2	89, 96, 101, 101	0
All	All	3598/3768 (95%)	0.09	143 (3%)	39	37	22, 53, 100, 101	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	250	PHE	7.2
3	Q	11	PHE	7.0
3	O	11	PHE	6.5
1	G	250	PHE	6.4
3	O	8	ILE	5.9

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	EPE	G	489	15/15	0.88	0.33	9.45	87,87,87,87	0
5	EPE	A	489	15/15	0.91	0.23	3.16	81,81,81,81	0
4	ZN	B	501	1/1	0.91	0.07	-2.18	72,72,72,72	0
4	ZN	D	502	1/1	0.95	0.07	-2.50	91,91,91,91	0
4	ZN	H	504	1/1	0.96	0.07	-2.78	101,101,101,101	0
4	ZN	F	503	1/1	0.93	0.08	-2.89	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.