WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:49 pm BST

PDB ID	:	2L0Y
Title	:	Complex hMia40-hCox17
Authors	:	Bertini, I.; Ciofi-Baffoni, S.; Gallo, A.
Deposited on	:	2010-07-20

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp
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:

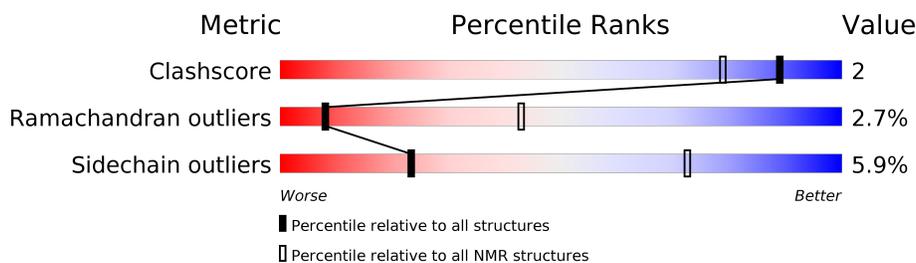|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	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:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 68%.

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
Clashscore		2
Ramachandran outliers		2.7%
Sidechain outliers		5.9%

Worse   *Better*

■ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	146	29% • 8% 59%
2	B	67	18% 13% 69%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:7, A:11-A:53, B:66-B:77 (60)	0.39	14

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 7, 9, 13, 17, 18, 20
2	4, 5, 6, 10, 14
3	3, 12, 16
4	2, 19
Single-model clusters	8; 11; 15

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1214 atoms, of which 580 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Mitochondrial intermembrane space import and assembly protein 40.

Mol	Chain	Residues	Atoms						Trace
1	A	60	Total 881	C 289	H 415	N 77	O 92	S 8	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-48	GLY	-	expression tag	UNP Q8N4Q1
A	-47	SER	-	expression tag	UNP Q8N4Q1
A	-46	PHE	-	expression tag	UNP Q8N4Q1
A	-45	THR	-	expression tag	UNP Q8N4Q1
A	8	SER	CYS	engineered mutation	UNP Q8N4Q1

- Molecule 2 is a protein called COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17).

Mol	Chain	Residues	Atoms						Trace
2	B	21	Total 333	C 105	H 165	N 32	O 29	S 2	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	GLY	-	expression tag	UNP Q5W0Q5
B	16	SER	-	expression tag	UNP Q5W0Q5
B	17	PHE	-	expression tag	UNP Q5W0Q5
B	18	THR	-	expression tag	UNP Q5W0Q5
B	73	SER	CYS	engineered mutation	UNP Q5W0Q5

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B: 16% · 13% 69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65 L66 I67** **G78 F79 K80 I81**

4.2.2 Score per residue for model 2

- Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A: 32% · 8% 59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER SER ALA GLU VAL ALA ASP ASP ASN ASP PRO TYR GLU HIS GLY ILE LEU ILE LEU PRO **N1 G2** **S8 P9 C10** **K38** **Q54 K55**

Y56 P57 D58 L59 Y60 PRO GLN GLU ASP GLU ASP GLU GLU GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR ALA THR LYS GLU GLU GLU GLY SER SER

- Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B: 15% ·· 13% 69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65 L66** **M74** **G78 F79 K80 I81**
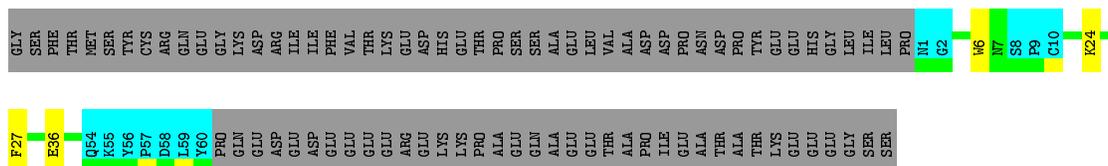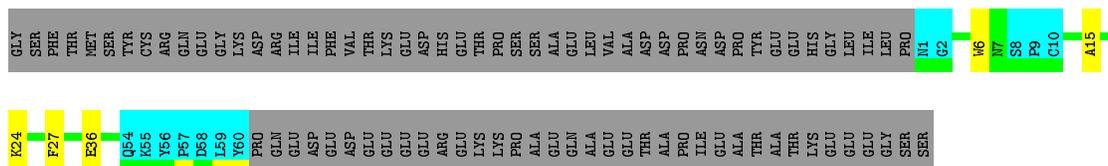
4.2.3 Score per residue for model 3

- Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A: 29% · 8% 59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER SER ALA GLU VAL ALA ASP ASP ASN ASP PRO TYR GLU HIS GLY ILE LEU ILE LEU PRO **N1 G2 N3 I4 N5 W6 N7 S8 P9 C10**

K24 **F27** **E36** **Q54 K55 Y56 P57 D58 L59 Y60** PRO GLN GLU ASP GLU ASP GLU GLU GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR ALA THR LYS GLU GLU GLU GLY SER SER

- Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B: 18% 13% 69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65** **G78 F79 K80 I81**

4.2.4 Score per residue for model 4

- Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A: 29% • 8% 59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER SER ALA GLU LEU VAL ALA ASP PRO ASN ASP TYR GLU HIS LEU ILE LEU PRO **N1** **G2** **N3** **W6** **N7** **S8** **P9** **C10** **K24**

F27 **Y32** **E36** **Q54** **K55** **Y56** **P57** **D58** **L59** **Y60** PRO GLN GLU ASP GLU GLU GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR ALA THR LYS GLU GLU GLY GLY SER SER

● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B: 16% • 13% 69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN PRO ALA LEU PRO GLU SER GLU GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU **E61** **H62** **C63** **G64** **H65** **L66** **I67** **G78** **F79** **K80** **I81**

4.2.5 Score per residue for model 5

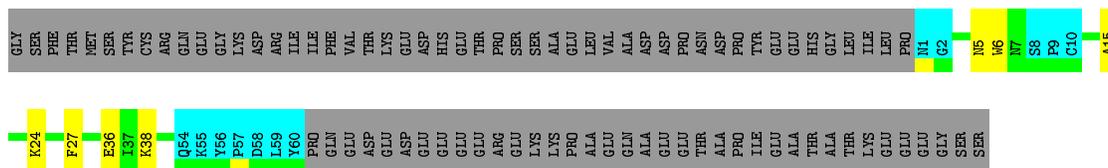● Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A: 30% • 8% 59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER SER ALA GLU LEU VAL ALA ASP PRO ASN ASP TYR GLU HIS LEU ILE LEU PRO **N1** **G2** **W6** **N7** **S8** **P9** **C10** **K24**

F27 **E36** **Q54** **K55** **Y56** **P57** **D58** **L59** **Y60** PRO GLN GLU ASP GLU GLU GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR ALA THR LYS GLU GLU GLY GLY SER SER

● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B: 16% • 13% 69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN PRO ALA LEU PRO GLU SER GLU GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU **E61** **H62** **C63** **G64** **H65** **R75** **G78** **F79** **K80** **I81**
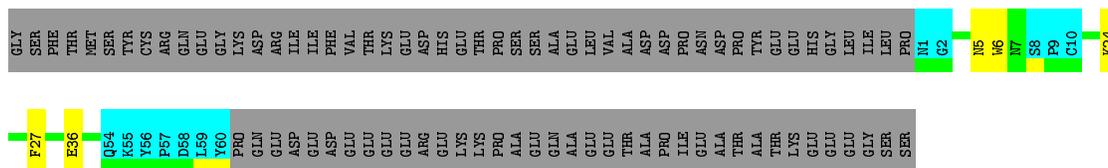
4.2.6 Score per residue for model 6

● Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A: 29% • 8% 59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER SER ALA GLU LEU VAL ALA ASP PRO ASN ASP TYR GLU HIS LEU ILE LEU PRO **N1** **G2** **W6** **N7** **S8** **P9** **C10** **A15**

K24 **F27** **E36** **Q54** **K55** **Y56** **P57** **D58** **L59** **Y60** PRO GLN GLU ASP GLU ASP GLU GLU GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR ALA THR LYS GLU GLU GLY GLY SER SER

● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:

16%   •   13%   69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS GLU THR LYS LYS ALA ASP ALA ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65 L66 I67** **G78 F79 K80 I81**

4.2.7 Score per residue for model 7

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:

29%   •   8%   59%
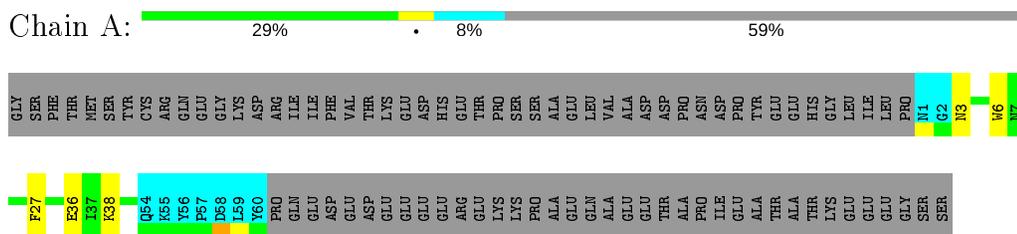
GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS ASP HIS GLU THR PRO SER SER ALA GLU LEU VAL ALA ASP ASP ASN ASP PRO TYR GLU HIS GLY LEU ILE LEU PRO **N1 G2** **W6 N7 S8 P9 C10** **K24**

F27 Y32 K38 E51 **Q54 K55 Y56 P57 D58 L59 Y60** PRO GLN GLU ASP GLU GLU GLU GLU ARG GLU LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR ALA THR LYS GLU GLU GLU GLY SER SER

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:

16%   •   13%   69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS GLU THR LYS LYS ALA ASP ALA ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65 L66 I67** **G78 F79 K80 I81**

4.2.8 Score per residue for model 8

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:

30%   •   8%   59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS ASP HIS GLU THR PRO SER SER ALA GLU LEU VAL ALA ASP ASP ASN ASP PRO TYR GLU HIS GLY LEU ILE LEU PRO **N1 G2** **W6 N7 S8 P9 C10** **K24**

E36 I37 K38 **Q54 K55 Y56 P57 D58 L59 Y60** PRO GLN GLU ASP GLU GLU GLU GLU ARG GLU LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR ALA THR LYS GLU GLU GLU GLY SER SER

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:

18%   13%   69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS GLU THR LYS LYS ALA ASP ALA ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65** **G78 F79 K80 I81**

4.2.9 Score per residue for model 9

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:
28%   5% 8%   59%

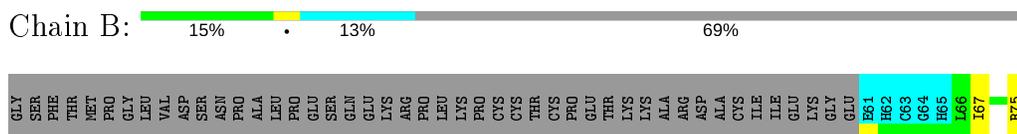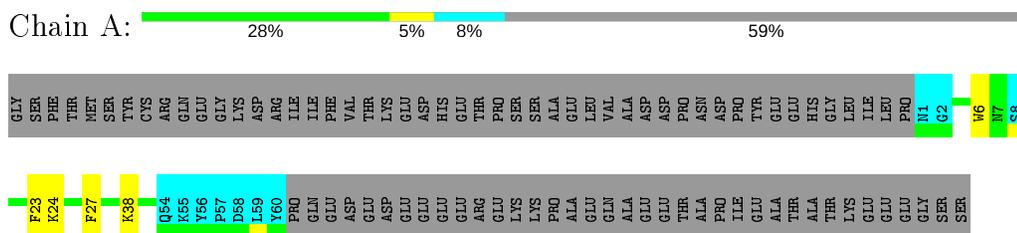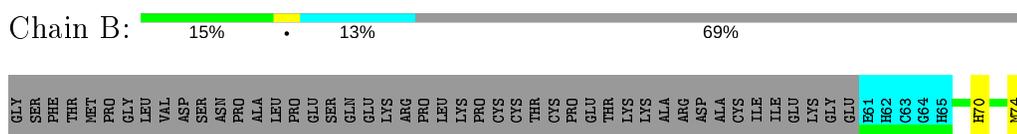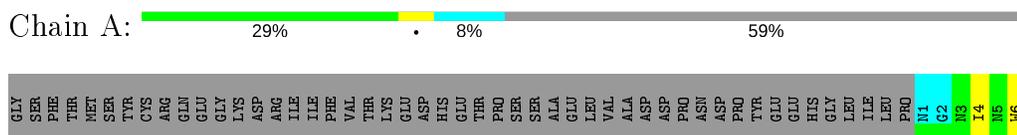● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:
16%   · 13%   69%

4.2.10 Score per residue for model 10

● Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:
29%   · 8%   59%

● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:
15%   · 13%   69%

4.2.11 Score per residue for model 11

● Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:
29%   ·· 8%   59%

● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:

18%   13%   69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN PRO ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS ALA ASP ALA CYS ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65** G78 F79 K80 I81

4.2.12 Score per residue for model 12

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:

29%   •   8%   59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER SER ALA GLU LEU VAL ALA ASP ASP PRO ASN ASP PRO TYR GLU HIS GLU LEU LEU ILE LEU PRO **N1 G2 N3 I4 N5 W6 N7 S8 P9 C10**

K24 E36 I37 K38 Q54 K55 Y56 P57 D58 L59 Y60 PRO GLN GLU ASP GLU GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR LYS GLU GLU GLY SER SER

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:

13%   •   13%   69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN PRO ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65 L66 I67** M74 L77 G78 F79 K80

I81

4.2.13 Score per residue for model 13

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:

27%   5%   8%   59%

GLY SER PHE THR MET SER TYR CYS ARG GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER SER ALA GLU LEU VAL ALA ASP ASP PRO ASN ASP PRO TYR GLU HIS GLU GLY LEU ILE LEU PRO **N1 G2 N5 W6 N7 S8 P9 C10 M14**

K24 F27 F30 E35 E36 Q54 K55 Y56 P57 D58 L59 Y60 PRO GLN GLU ASP GLU GLU GLU GLU GLU LYS ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU GLU THR ALA PRO ILE GLU ALA THR LYS GLU GLU GLY SER SER

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:

18%   13%   69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN PRO ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU **E61 H62 C63 G64 H65** G78 F79 K80 I81

4.2.14 Score per residue for model 14 (medoid)

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:

4.2.15 Score per residue for model 15

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B:

4.2.16 Score per residue for model 16

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A:

K24 F27 E36 I37 K38 Q54 K55 Y56 P57 D58 L59 Y60 PRO GLN GLU ASP GLU ASP GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU THR ALA PRO ILE GLU ALA THR ALA LYS GLU GLU GLU GLY SER SER

● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B: 16% · 13% 69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN PRO ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU E61 H62 C63 G64 H65 L66 I67 G78 F79 K80 I81

4.2.17 Score per residue for model 17

● Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A: 28% · · 8% 59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER ALA GLU LEU VAL ALA ASP ASP PRO ASN ASP PRO TYR GLU HIS GLY LEU ILE LEU PRO N1 G2 W6 N7 S8 P9 C10 K24

F27 F30 H31 E35 K38 Q54 K55 Y56 P57 D58 L59 Y60 PRO GLN ASP GLU ASP GLU GLU GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU THR ALA PRO ILE GLU ALA THR ALA LYS GLU GLU GLU GLY SER SER

● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B: 18% 13% 69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN PRO ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU E61 H62 C63 G64 H65 G78 F79 K80 I81

4.2.18 Score per residue for model 18

● Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

Chain A: 27% 5% 8% 59%

GLY SER PHE THR MET SER TYR CYS ARG GLN GLU GLY LYS ASP ARG ILE ILE PHE VAL THR LYS GLU ASP HIS GLU THR PRO SER ALA GLU LEU VAL ALA ASP ASP PRO ASN ASP PRO TYR GLU HIS GLY LEU ILE LEU PRO N1 G2 W6 N7 S8 P9 C10 K24

F27 H31 E36 I37 K38 G39 S40 E51 Q54 K55 Y56 P57 D58 L59 Y60 PRO GLN GLU ASP GLU ASP GLU GLU GLU GLU ARG GLU LYS LYS PRO ALA GLU GLN ALA GLU THR ALA PRO ILE GLU ALA THR ALA LYS GLU GLU GLU GLY SER SER

● Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

Chain B: 15% · 13% 69%

GLY SER PHE THR MET PRO GLY LEU VAL ASP SER ASN PRO ALA LEU PRO GLU SER GLN GLU LYS ARG PRO LEU LYS PRO CYS CYS THR CYS PRO GLU THR LYS LYS ALA ARG ASP ALA CYS ILE ILE GLU LYS GLY GLU E61 H62 C63 G64 H65 L66 I67 L77 G78 F79 K80 I81

4.2.19 Score per residue for model 19

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

4.2.20 Score per residue for model 20

• Molecule 1: Mitochondrial intermembrane space import and assembly protein 40

• Molecule 2: COX17 cytochrome c oxidase assembly homolog (S. cerevisiae) pseudogene (COX17)

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing, molecular dynamics*.

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Amber	refinement	10.0
CYANA	structure solution	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1135
Number of shifts mapped to atoms	1115
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	370	329	329	2±1
2	B	96	102	102	0±0
All	All	9320	8620	8620	33

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 2.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
2:B:66:LEU:H	2:B:66:LEU:HD23	0.55	1.60	2	1
1:A:11:LEU:HD23	1:A:23:PHE:CE2	0.53	2.39	19	2
1:A:6:TRP:CH2	1:A:24:LYS:HA	0.52	2.40	3	13
1:A:4:ILE:HG21	1:A:11:LEU:HD22	0.49	1.85	19	1
1:A:15:ALA:HB1	1:A:24:LYS:CE	0.48	2.38	6	2
1:A:6:TRP:CE2	1:A:24:LYS:HD2	0.48	2.44	8	11
1:A:4:ILE:HG21	1:A:6:TRP:CE3	0.47	2.44	12	2
2:B:66:LEU:H	2:B:66:LEU:CD2	0.42	2.27	2	1

5.2 Torsion angles (i)

5.2.1 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 NMR 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	48/146 (33%)	42±1 (87±3%)	5±1 (10±3%)	2±1 (3±1%)	6	37
2	B	12/67 (18%)	12±0 (99±2%)	0±0 (1±3%)	0±0 (0±0%)	100	100
All	All	1200/4260 (28%)	1070 (89%)	98 (8%)	32 (3%)	8	43

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	36	GLU	15
1	A	38	LYS	12
1	A	5	ASN	3
1	A	3	ASN	1
1	A	35	GLU	1

5.2.2 Protein sidechains (i)

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 NMR 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	40/126 (32%)	38±1 (96±3%)	2±1 (4±3%)	31	80
2	B	10/57 (18%)	9±1 (88±9%)	1±1 (11±9%)	9	52
All	All	1000/3660 (27%)	941 (94%)	59 (6%)	23	72

All 18 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	27	PHE	17
2	B	67	ILE	8
2	B	74	MET	6
1	A	38	LYS	5
1	A	51	GLU	3
2	B	66	LEU	3
1	A	35	GLU	2
2	B	75	ARG	2
1	A	14	MET	2
1	A	31	HIS	2
2	B	77	LEU	2
2	B	72	GLU	1
1	A	4	ILE	1
2	B	70	HIS	1
1	A	40	SER	1
1	A	3	ASN	1
1	A	5	ASN	1
1	A	30	PHE	1

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.4 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.5 Ligand geometry (i)

There are no ligands in this entry.

5.6 Other polymers (i)

There are no such molecules in this entry.

5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 68% for the well-defined parts and 64% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

6.1.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1135
Number of shifts mapped to atoms	1115
Number of unparsed shifts	0
Number of shifts with mapping errors	20
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 20 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	22	LYS	C	171.6	0.3	1
B	30	SER	CB	60.6	0.3	1
B	30	SER	N	116.7	0.3	1
B	22	LYS	CB	29.7	0.3	1
B	40	SER	CB	60.9	0.3	1
B	29	ALA	N	126.6	0.3	1
B	22	LYS	N	124.0	0.3	1
B	29	ALA	CB	16.6	0.3	1
B	40	SER	C	171.8	0.3	1
B	29	ALA	C	174.5	0.3	1
B	30	SER	C	170.2	0.3	1
B	30	SER	CA	53.5	0.3	1
B	29	ALA	CA	49.6	0.3	1
B	30	SER	H	8.26	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	40	SER	H	8.27	0.02	1
B	29	ALA	H	8.35	0.02	1
B	22	LYS	H	8.22	0.02	1
B	22	LYS	CA	51.3	0.3	1
B	40	SER	CA	56.2	0.3	1
B	40	SER	N	114.6	0.3	1

6.1.2   Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	155	2.36 ± 0.30	Should be applied
$^{13}C_\beta$	144	3.24 ± 0.08	Should be applied
$^{13}C'$	148	2.33 ± 0.30	Should be applied
^{15}N	148	0.33 ± 0.26	None needed (< 0.5 ppm)

6.1.3   Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 68%, i.e. 487 atoms were assigned a chemical shift out of a possible 713. 2 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	285/298 (96%)	107/119 (90%)	119/120 (99%)	59/59 (100%)
Sidechain	189/345 (55%)	101/206 (49%)	88/124 (71%)	0/15 (0%)
Aromatic	13/70 (19%)	13/38 (34%)	0/29 (0%)	0/3 (0%)
Overall	487/713 (68%)	221/363 (61%)	207/273 (76%)	59/77 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 615 atoms were assigned a chemical shift out of a possible 967. 3 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	360/399 (90%)	133/159 (84%)	152/162 (94%)	75/78 (96%)
Sidechain	242/459 (53%)	130/276 (47%)	112/164 (68%)	0/19 (0%)
Aromatic	13/109 (12%)	13/59 (22%)	0/45 (0%)	0/5 (0%)
Overall	615/967 (64%)	276/494 (56%)	264/371 (71%)	75/102 (74%)

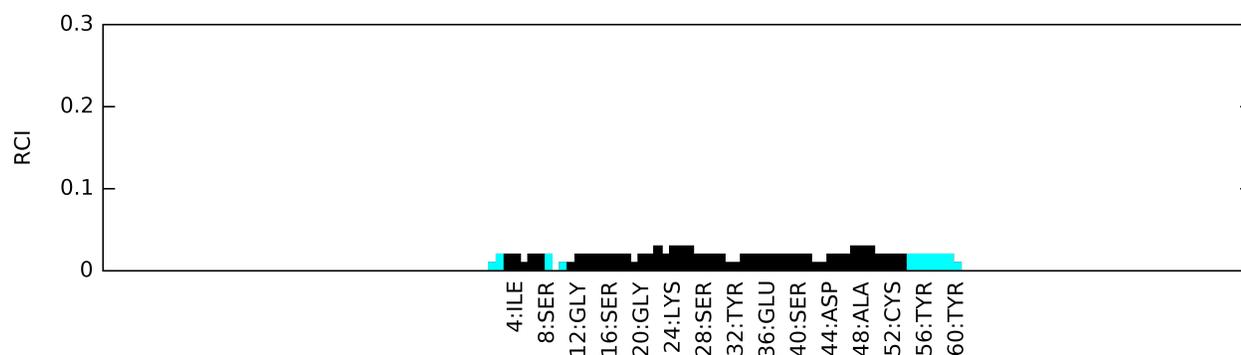### 6.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	53	MET	CE	47.90	26.97 − 7.37	15.7
1	A	49	MET	CE	39.30	26.97 − 7.37	11.3
1	A	11	LEU	CD2	6.80	32.60 − 15.60	-10.2
1	A	85	ILE	CG1	14.70	36.54 − 18.94	-7.4
1	A	91	LYS	HE2	1.55	3.87 − 1.97	-7.2
1	A	82	THR	HB	1.88	5.82 − 2.52	-6.9
1	A	11	LEU	CD1	13.90	32.77 − 16.57	-6.6
1	A	85	ILE	CD1	24.50	21.91 − 5.01	6.5
1	A	59	LEU	CD2	14.10	32.60 − 15.60	-5.9
1	A	8	SER	HB3	2.27	5.25 − 2.45	-5.6
1	A	91	LYS	HD3	2.87	2.75 − 0.45	5.5
1	A	36	GLU	CG	29.40	42.24 − 29.94	-5.4
1	A	85	ILE	CG2	10.10	24.63 − 10.43	-5.2

6.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

Random coil index (RCI) for chain B: