Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1LM0
Title	:	Solution structure and characterization of the heme chaperone CcmE
Authors	:	Arnesano, F.; Banci, L.; Barker, P.D.; Bertini, I.; Rosato, A.; Su, X.C.; Viezzoli, M.S.
Deposited on	:	2002-04-30

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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

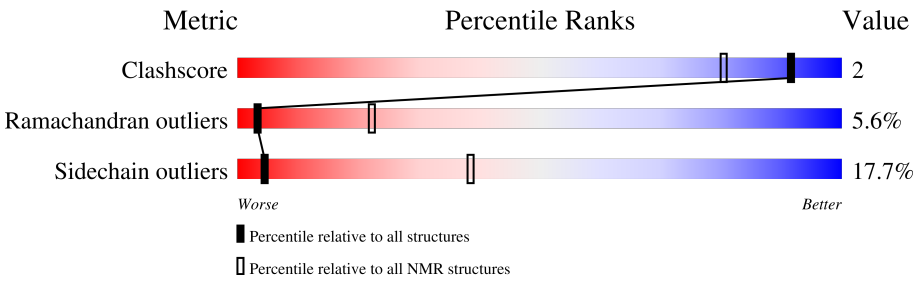
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 was not calculated.

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)	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	136	56% 12% 6% 26%

2 Ensemble composition and analysis (i)

This entry contains 35 models. Model 8 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:36-A:86, A:90-A:131 (93)	0.45	8

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 3 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 6, 7, 8, 9, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 23, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35
2	5, 22
3	4, 10
Single-model clusters	24

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1504 atoms, of which 749 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called cytochrome c maturation protein E.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1504	472	749	131	150	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	PHE	-	cloning artifact	UNP O52690
A	27	ALA	-	cloning artifact	UNP O52690
A	28	ALA	-	cloning artifact	UNP O52690
A	29	ASP	-	cloning artifact	UNP O52690

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: cytochrome c maturation protein E

Chain A: 56% 12% 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 I43 K47 T50 K53 T67 R73 L78 S87 L88 G89 I92 Y96 P101 D102 L103 F104 R105 Q113 K121 L128 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET

GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

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: cytochrome c maturation protein E

Chain A: 55% 12% • 6% 26%

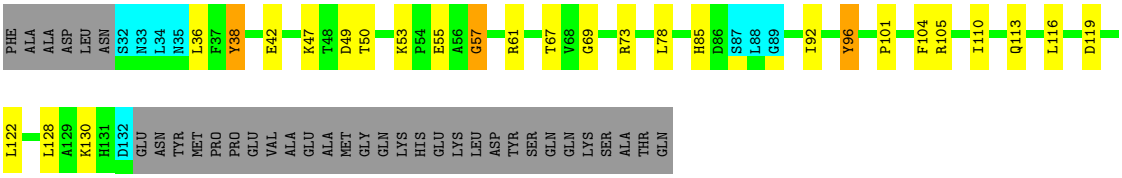
PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 L36 F37 Y38 I43 D49 T50 K53 Q58 T67 R73 L78 H79 V80 S87 L88 G89 I92 F104 L116 D119 G120 K121 L122 K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA

MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.2 Score per residue for model 2

• Molecule 1: cytochrome c maturation protein E

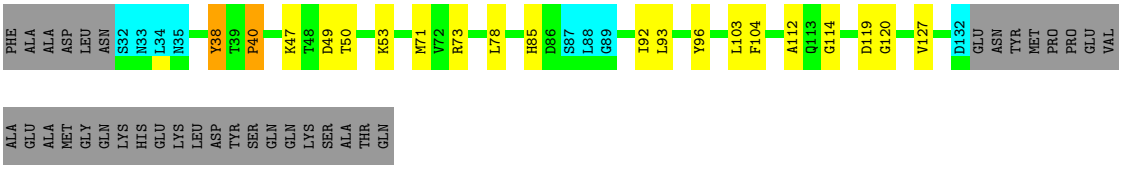
Chain A: 49% 18% • 6% 26%



4.2.3 Score per residue for model 3

- Molecule 1: cytochrome c maturation protein E

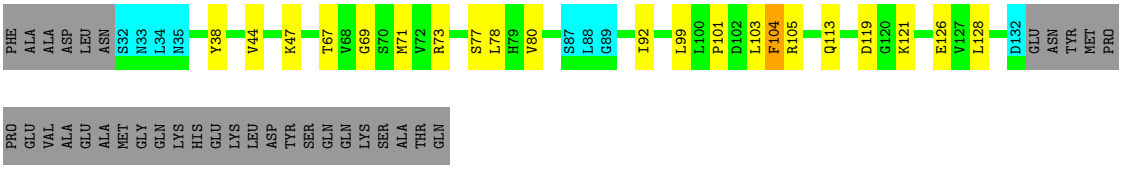
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: cytochrome c maturation protein E

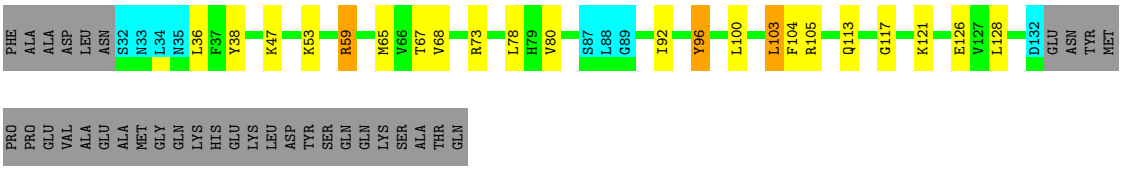
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: cytochrome c maturation protein E

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: cytochrome c maturation protein E

Chain A: 58% 10% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 T39 I43 T50 M65 L78 H79 V80 S87 L88 G89 I92 Y96 D97 D98 L99 L100 P101 R105 K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS

LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.7 Score per residue for model 7

• Molecule 1: cytochrome c maturation protein E

Chain A: 54% 12% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 E42 I43 V44 T50 K53 M65 V66 T67 V68 D74 L78 H79 V80 H85 D86 S87 L88 G89 I92 L103 F104 R105 K121 L128 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA

MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.8 Score per residue for model 8 (medoid)

• Molecule 1: cytochrome c maturation protein E

Chain A: 53% 13% •• 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 L36 F37 Y38 E42 I43 D49 K53 R59 M65 V66 R73 L78 H85 D86 S87 L88 G89 I92 Y96 F104 Q113 L116 G117 L122 T125 L128 D132 GLU ASN TYR MET PRO PRO

GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.9 Score per residue for model 9

• Molecule 1: cytochrome c maturation protein E

Chain A: 47% 21% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 L36 F37 Y38 K47 T48 D49 T50 K53 R59 I60 R61 V66 T67 M71 D74 L78 A83 V84 H85 D86 S87 L88 G89 I92 D97 P101 D102 L103 F104 R105 A112 Q113 D119 V127 L128 A129

K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.10 Score per residue for model 10

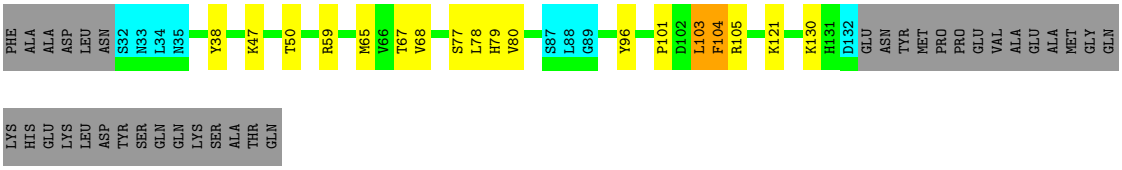
- Molecule 1: cytochrome c maturation protein E

Chain A: 59% 9% • 6% 26%

4.2.11 Score per residue for model 11

- Molecule 1: cytochrome c maturation protein E

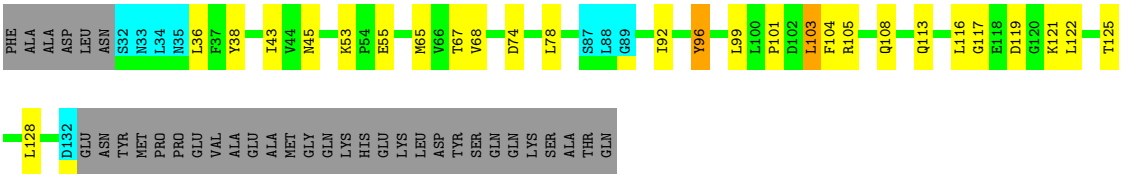
Chain A: 55% 12% • 6% 26%



4.2.12 Score per residue for model 12

- Molecule 1: cytochrome c maturation protein E

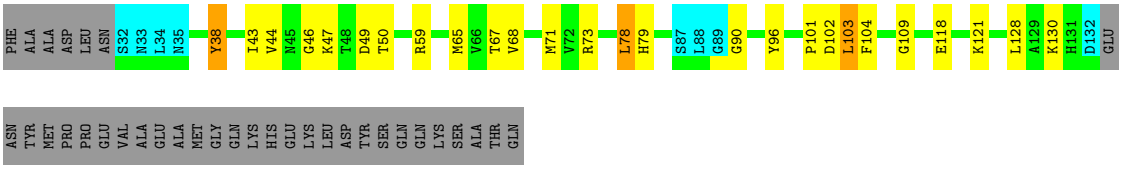
Chain A: 49% 18% • 6% 26%



4.2.13 Score per residue for model 13

- Molecule 1: cytochrome c maturation protein E

Chain A: 49% 17% • 6% 26%



4.2.14 Score per residue for model 14

- Molecule 1: cytochrome c maturation protein E

Chain A: 58% 10% 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 K47 M65 M71 V72 R73 V80 S87 L88 G89 I92 Y96 L103 F104 D119 G120 K121 L128 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS

LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.15 Score per residue for model 15

- Molecule 1: cytochrome c maturation protein E

Chain A: 46% 19% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 L36 F37 Y38 I43 K47 V52 E55 A56 T67 V68 G69 S70 M71 D74 L78 H79 V80 H85 D86 S87 L88 G89 I92 Y96 D97 P101 D102 L103 F104 R105 E106 G109 L116 G117 K121 L122

T125 L128 A129 K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.16 Score per residue for model 16

- Molecule 1: cytochrome c maturation protein E

Chain A: 55% 12% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 K47 T48 D49 T50 K53 R59 M71 D74 V80 S87 L88 G89 I92 P101 D102 L103 F104 R105 Q113 E118 D119 G120 K121 K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU

ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.17 Score per residue for model 17

- Molecule 1: cytochrome c maturation protein E

Chain A: 55% 12% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 E42 I43 T50 K53 M71 L78 F82 S87 L88 G89 L93 V94 T95 Y96 P101 D102 L103 F104 R105 Q108 Q113 K121 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET

GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.18 Score per residue for model 18

- Molecule 1: cytochrome c maturation protein E

Chain A: 55% 12% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 I43 V44 K47 T50 M65 V66 T67 D74 L78 S87 L88 G89 I92 D97 P101 D102 L103 F104 A112 K121 V127 L128 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY

GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.19 Score per residue for model 19

- Molecule 1: cytochrome c maturation protein E

Chain A: 54% 12% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 E42 I43 K47 T50 R59 T67 M71 V72 R73 L78 S87 L88 G89 Y96 L99 L103 F104 R105 Q113 D119 G120 K121 L128 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU

ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.20 Score per residue for model 20

- Molecule 1: cytochrome c maturation protein E

Chain A: 54% 12% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 V44 R59 M65 M71 V72 R73 L78 Q81 S87 L88 G89 P101 D102 L103 F104 G109 Q113 L116 G117 K121 L122 K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA

MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.21 Score per residue for model 21

- Molecule 1: cytochrome c maturation protein E

Chain A: 50% 18% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 T39 E42 I43 T48 D49 T50 M65 V66 T67 V68 L78 H79 V80 H85 D86 S87 L88 G89 L99 L100 P101 D102 L103 F104 Q108 L116 D119 G120 K121 L128 H131 D132 GLU ASN TYR MET PRO

PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.22 Score per residue for model 22

- Molecule 1: cytochrome c maturation protein E

Chain A: 53% 13% •• 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 S41 K47 K53 R59 M65 V66 T67 V68 M71 V80 H85 D86 S87 L88 G89 G90 E91 Y96 D97 D98 L103 F104 R105 Q108 G109 L128 A129 K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL

ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.23 Score per residue for model 23

- Molecule 1: cytochrome c maturation protein E

Chain A: 52% 12% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 V44 T48 E55 R59 I60 T67 V68 G69 D74 F82 S87 L88 G89 I92 Y96 L100 P101 F104 Q113 L116 G117 E118 D119 G120 K121 L122 V127 D132 GLU ASN TYR MET

PRO PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.24 Score per residue for model 24

- Molecule 1: cytochrome c maturation protein E

Chain A: 54% 13% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 T50 K53 V62 V68 G69 S70 M71 L78 H85 D86 S87 L88 G89 I92 Y96 P101 D102 L103 F104 I110 Q113 D119 L122 L128 A129 K130 H131 D132 GLU ASN TYR MET PRO PRO

GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.25 Score per residue for model 25

- Molecule 1: cytochrome c maturation protein E

Chain A: 52% 15% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 L36 F37 Y38 K47 T50 K53 R59 M71 V72 R73 L78 H79 V80 H85 D86 S87 L88 G89 I92 L99 D102 L103 F104 Q113 G117 K121 L128 A129 K130 H131 D132 GLU ASN TYR MET PRO

PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.26 Score per residue for model 26

- Molecule 1: cytochrome c maturation protein E

Chain A: 49% 18% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 L36 F37 Y38 S41 K47 T50 K53 R59 I60 M65 R73 L78 H85 D86 S87 L88 G89 G90 E91 I92 Y96 D102 L103 F104 R105 A112 D119 G120 K121 V127 L128 H131 D132 GLU ASN

TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.27 Score per residue for model 27

- Molecule 1: cytochrome c maturation protein E

Chain A: 56% 8% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 I43 V44 N45 T50 M71 V72 R73 L78 H79 V80 H85 D86 S87 L88 G89 D102 L103 F104 R105 E106 G120 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU

LYS LEU ASP TYR SER GLN GLN GLN LYS SER ALA THR GLN

4.2.28 Score per residue for model 28

- Molecule 1: cytochrome c maturation protein E

Chain A: 54% 12% • 6% 26%

PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 Y38 T39 E42 K47 T50 L78 F82 H85 D86 S87 L88 G89 I92 P101 D102 L103 F104 R105 Q113 D119 L128 A129 K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY

GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.29 Score per residue for model 29

- Molecule 1: cytochrome c maturation protein E

Chain A: 48% 17% • 6% 26%

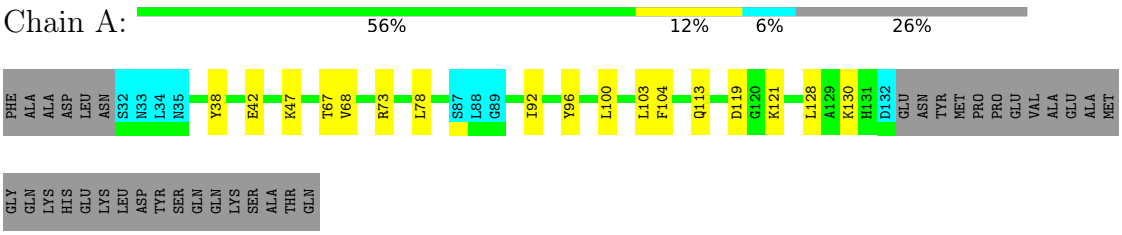
PHE ALA ALA ASP LEU ASN S32 N33 L34 N35 T50 K53 M65 V66 T67 V68 G69 S70 M71 V72 R73 S77 L78 H79 V80 Q81 F82 S87 L88 G89 V94 T95 Y96 L99 L100 P101 D102 L103 F104 R105 Q113 L116 G117 K121 L122 E126 V127 L128 A129

K130 H131 D132 GLU ASN TYR MET PRO PRO GLU VAL ALA GLU ALA MET GLY GLN LYS HIS GLU LYS LEU ASP TYR SER GLN GLN LYS SER ALA THR GLN

4.2.30 Score per residue for model 30

- Molecule 1: cytochrome c maturation protein E

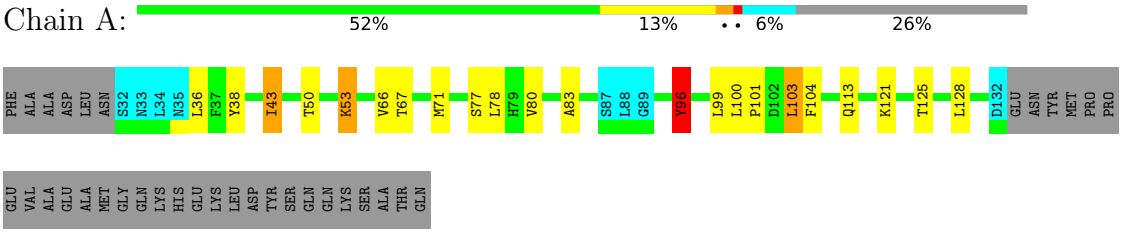
Chain A:



4.2.31 Score per residue for model 31

- Molecule 1: cytochrome c maturation protein E

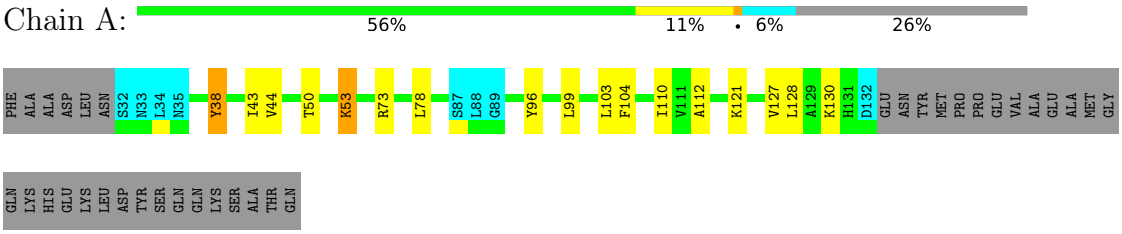
Chain A:



4.2.32 Score per residue for model 32

- Molecule 1: cytochrome c maturation protein E

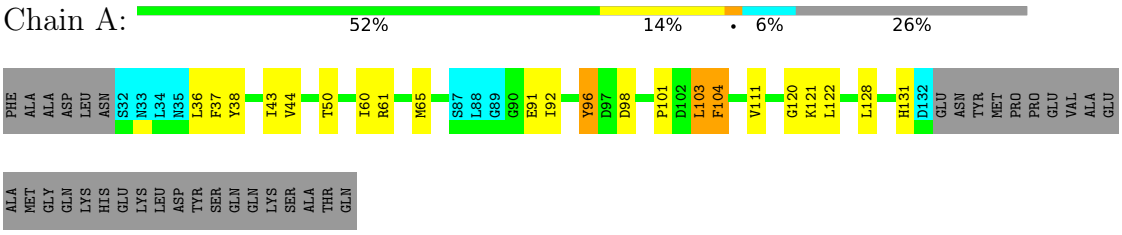
Chain A:



4.2.33 Score per residue for model 33

- Molecule 1: cytochrome c maturation protein E

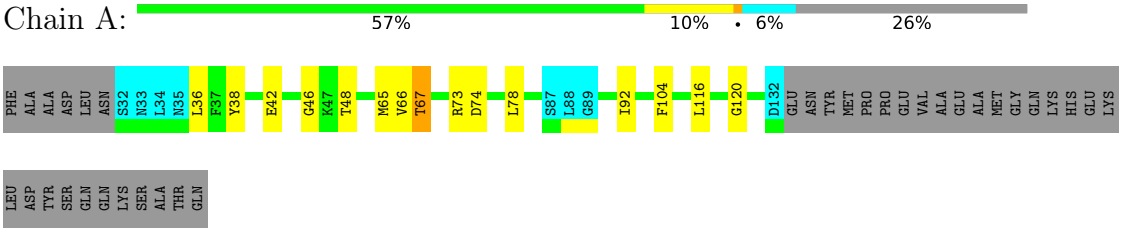
Chain A:



4.2.34 Score per residue for model 34

- Molecule 1: cytochrome c maturation protein E

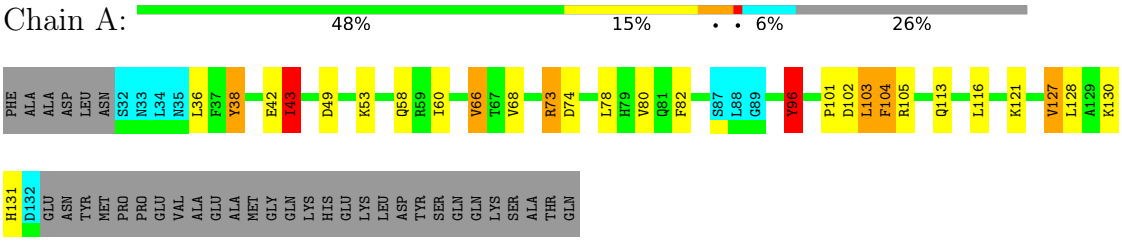
Chain A:



4.2.35 Score per residue for model 35

- Molecule 1: cytochrome c maturation protein E

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, torsion angle dyanamics, restrained energy minimization.*

Of the 400 calculated structures, 35 were deposited, based on the following criterion: *the submitted conformer models are the 35 structures with the lowest target function.*

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

Software name	Classification	Version
DYANA	structure solution	1.5
Amber	refinement	5.0

No chemical shift data was provided.

6 Model quality (i)

6.1 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 (average) 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	0.52±0.01	0±0/711 (0.0± 0.0%)	0.94±0.04	0±1/965 (0.0± 0.1%)
All	All	0.52	0/24885 (0.0%)	0.94	13/33775 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.2	1.8±1.1
All	All	1	64

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	96	TYR	CB-CG-CD2	-6.60	117.04	121.00	2	4
1	A	86	ASP	CB-CG-OD2	-5.77	113.11	118.30	15	1
1	A	105	ARG	NE-CZ-NH2	-5.62	117.49	120.30	29	2
1	A	73	ARG	NE-CZ-NH2	-5.61	117.50	120.30	27	1
1	A	93	LEU	CB-CA-C	-5.41	99.92	110.20	3	1
1	A	93	LEU	N-CA-CB	-5.24	99.92	110.40	3	1
1	A	106	GLU	CB-CA-C	5.22	120.84	110.40	15	1
1	A	61	ARG	NE-CZ-NH2	-5.14	117.73	120.30	2	1
1	A	57	GLY	N-CA-C	-5.10	100.35	113.10	2	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	40	PRO	CA	1

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	96	TYR	Sidechain	16
1	A	104	PHE	Sidechain,Peptide	13
1	A	105	ARG	Peptide,Sidechain	11
1	A	38	TYR	Sidechain	9
1	A	59	ARG	Sidechain	4
1	A	82	PHE	Sidechain	3
1	A	103	LEU	Peptide	2
1	A	73	ARG	Sidechain	1
1	A	57	GLY	Peptide	1
1	A	61	ARG	Sidechain	1

6.2 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 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	699	698	698	2±2
All	All	24465	24430	24430	75

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
1:A:116:LEU:HD22	1:A:122:LEU:HD22	0.81	1.48	23	2
1:A:43:ILE:HD13	1:A:43:ILE:H	0.63	1.52	35	1
1:A:96:TYR:OH	1:A:127:VAL:HG13	0.61	1.94	23	2
1:A:48:THR:HG23	1:A:116:LEU:HD11	0.61	1.72	21	1
1:A:38:TYR:OH	1:A:43:ILE:HD12	0.60	1.96	35	1
1:A:38:TYR:CZ	1:A:43:ILE:HD12	0.59	2.31	35	1
1:A:48:THR:HG21	1:A:116:LEU:HD11	0.59	1.72	34	1
1:A:80:VAL:HG21	1:A:100:LEU:CD2	0.59	2.28	31	1
1:A:48:THR:CG2	1:A:122:LEU:HD21	0.58	2.29	23	1
1:A:105:ARG:CD	1:A:105:ARG:H	0.57	2.11	10	1
1:A:66:VAL:HG13	1:A:104:PHE:CE2	0.56	2.36	35	1
1:A:48:THR:HG21	1:A:122:LEU:HD21	0.55	1.78	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ILE:CD1	1:A:116:LEU:HD21	0.53	2.33	23	1
1:A:116:LEU:HG	1:A:122:LEU:HD22	0.52	1.81	20	2
1:A:121:LYS:C	1:A:122:LEU:HD23	0.51	2.25	1	2
1:A:82:PHE:CE1	1:A:104:PHE:CE1	0.51	2.99	29	2
1:A:103:LEU:HD13	1:A:106:GLU:OE1	0.50	2.07	27	1
1:A:38:TYR:CZ	1:A:60:ILE:HD12	0.50	2.42	35	1
1:A:48:THR:CG2	1:A:116:LEU:HD11	0.50	2.37	21	1
1:A:37:PHE:CE1	1:A:61:ARG:HB3	0.49	2.42	33	1
1:A:66:VAL:HG22	1:A:104:PHE:CZ	0.49	2.42	29	1
1:A:112:ALA:HB2	1:A:127:VAL:HG12	0.49	1.85	32	3
1:A:102:ASP:O	1:A:103:LEU:HD12	0.48	2.08	27	1
1:A:44:VAL:HG21	1:A:90:GLY:HA3	0.48	1.84	13	1
1:A:66:VAL:HG21	1:A:104:PHE:CE1	0.48	2.44	34	1
1:A:80:VAL:HG21	1:A:100:LEU:HD21	0.47	1.86	31	1
1:A:66:VAL:HG23	1:A:83:ALA:O	0.47	2.09	31	2
1:A:116:LEU:HG	1:A:122:LEU:HD12	0.47	1.85	29	2
1:A:82:PHE:CD1	1:A:104:PHE:CZ	0.47	3.02	29	2
1:A:112:ALA:CB	1:A:127:VAL:HG12	0.47	2.40	18	2
1:A:60:ILE:HD12	1:A:116:LEU:HD21	0.47	1.86	23	1
1:A:60:ILE:HD11	1:A:122:LEU:HD11	0.46	1.87	33	1
1:A:116:LEU:HD23	1:A:116:LEU:N	0.46	2.26	23	1
1:A:66:VAL:HG21	1:A:104:PHE:CZ	0.46	2.46	34	1
1:A:96:TYR:CD2	1:A:100:LEU:HD21	0.45	2.46	5	1
1:A:56:ALA:HB1	1:A:117:GLY:HA2	0.44	1.89	15	1
1:A:80:VAL:HG21	1:A:100:LEU:HG	0.44	1.89	6	1
1:A:44:VAL:HG23	1:A:45:ASN:H	0.44	1.72	27	1
1:A:82:PHE:CE1	1:A:94:VAL:CG2	0.44	3.00	29	2
1:A:67:THR:HG22	1:A:68:VAL:HG12	0.44	1.89	22	1
1:A:116:LEU:HD11	1:A:122:LEU:HD23	0.44	1.89	8	1
1:A:44:VAL:HG21	1:A:90:GLY:CA	0.43	2.43	13	1
1:A:80:VAL:HG23	1:A:96:TYR:HB3	0.43	1.89	6	1
1:A:66:VAL:HG13	1:A:104:PHE:CZ	0.43	2.48	35	1
1:A:113:GLN:HB2	1:A:126:GLU:HB2	0.43	1.89	4	1
1:A:37:PHE:CE1	1:A:111:VAL:HB	0.43	2.49	33	1
1:A:43:ILE:H	1:A:43:ILE:CD1	0.43	2.26	35	1
1:A:100:LEU:HD13	1:A:104:PHE:CB	0.42	2.44	23	1
1:A:58:GLN:O	1:A:116:LEU:HD12	0.42	2.14	35	1
1:A:42:GLU:OE2	1:A:47:LYS:NZ	0.42	2.51	2	2
1:A:122:LEU:HD23	1:A:122:LEU:N	0.42	2.30	1	1
1:A:66:VAL:HG11	1:A:104:PHE:CE2	0.41	2.50	18	1
1:A:36:LEU:HD11	1:A:38:TYR:CD2	0.41	2.50	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ARG:NH1	1:A:126:GLU:OE2	0.41	2.54	5	1
1:A:66:VAL:HG11	1:A:104:PHE:CE1	0.41	2.51	8	1
1:A:77:SER:O	1:A:99:LEU:HD13	0.41	2.16	4	1
1:A:96:TYR:CE2	1:A:125:THR:HA	0.41	2.50	8	1
1:A:104:PHE:CZ	1:A:110:ILE:HD12	0.41	2.51	24	1
1:A:118:GLU:OE1	1:A:121:LYS:NZ	0.40	2.49	16	1
1:A:116:LEU:CD1	1:A:116:LEU:N	0.40	2.85	8	1
1:A:73:ARG:CB	1:A:80:VAL:HG12	0.40	2.46	35	1
1:A:78:LEU:HD12	1:A:79:HIS:N	0.40	2.32	13	1

6.3 Torsion angles (i)

6.3.1 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 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	93/136 (68%)	74±3 (79±3%)	14±3 (15±3%)	5±2 (6±2%)	3 22
All	All	3255/4760 (68%)	2585 (79%)	489 (15%)	181 (6%)	3 22

All 27 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	104	PHE	22
1	A	101	PRO	20
1	A	53	LYS	19
1	A	103	LEU	16
1	A	119	ASP	15
1	A	43	ILE	14
1	A	68	VAL	12
1	A	67	THR	10
1	A	47	LYS	9
1	A	117	GLY	9
1	A	69	GLY	5
1	A	120	GLY	4
1	A	109	GLY	4

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Mol	Chain	Res	Type	Models (Total)
1	A	102	ASP	4
1	A	77	SER	3
1	A	46	GLY	2
1	A	99	LEU	2
1	A	90	GLY	2
1	A	40	PRO	1
1	A	114	GLY	1
1	A	98	ASP	1
1	A	49	ASP	1
1	A	45	ASN	1
1	A	118	GLU	1
1	A	52	VAL	1
1	A	97	ASP	1
1	A	86	ASP	1

6.3.2 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	75/111 (68%)	62±3 (82±4%)	13±3 (18±4%)	4 38
All	All	2625/3885 (68%)	2161 (82%)	464 (18%)	4 38

All 56 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	38	TYR	30
1	A	78	LEU	29
1	A	103	LEU	27
1	A	121	LYS	25
1	A	128	LEU	24
1	A	50	THR	23
1	A	92	ILE	23
1	A	130	LYS	17
1	A	113	GLN	17
1	A	73	ARG	16
1	A	71	MET	16

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Mol	Chain	Res	Type	Models (Total)
1	A	65	MET	16
1	A	80	VAL	14
1	A	36	LEU	13
1	A	85	HIS	13
1	A	67	THR	10
1	A	47	LYS	10
1	A	131	HIS	10
1	A	49	ASP	9
1	A	96	TYR	9
1	A	59	ARG	9
1	A	74	ASP	9
1	A	44	VAL	8
1	A	42	GLU	8
1	A	105	ARG	6
1	A	99	LEU	6
1	A	122	LEU	5
1	A	55	GLU	4
1	A	108	GLN	4
1	A	102	ASP	4
1	A	43	ILE	4
1	A	110	ILE	3
1	A	39	THR	3
1	A	53	LYS	3
1	A	60	ILE	3
1	A	104	PHE	3
1	A	125	THR	3
1	A	116	LEU	2
1	A	97	ASP	2
1	A	119	ASP	2
1	A	66	VAL	2
1	A	86	ASP	2
1	A	41	SER	2
1	A	91	GLU	2
1	A	98	ASP	2
1	A	127	VAL	2
1	A	58	GLN	1
1	A	40	PRO	1
1	A	79	HIS	1
1	A	52	VAL	1
1	A	93	LEU	1
1	A	81	GLN	1
1	A	62	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	70	SER	1
1	A	126	GLU	1
1	A	100	LEU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided