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Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 04:43 PM BST

PDB ID : 1P6T

Title : Structure characterization of the water soluble region of P-type ATPase CopA from Bacillus subtilis

Authors : Banci, L.; Bertini, I.; Ciofi-Baffoni, S.; Gonnelli, L.; Su, X.C.; Structural Proteomics in Europe (SPINE)

Deposited on : 2003-04-30

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

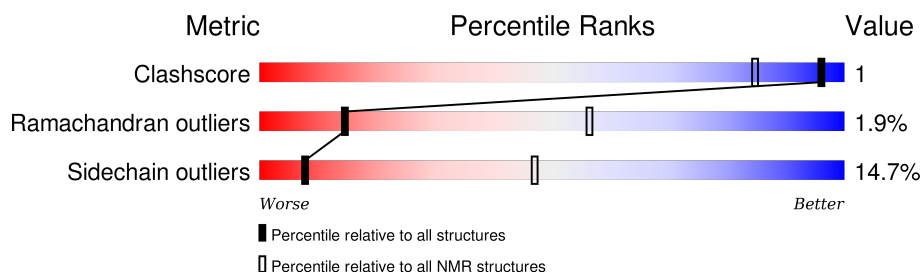|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 84%.

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		1
Ramachandran outliers		1.9%
Sidechain outliers		14.7%

■ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	151	80% 9% 11%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:5-A:83, A:87-A:142 (135)	0.37	13

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 6 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2303 atoms, of which 1161 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Potential copper-transporting ATPase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	151	2303	708	1161	194	231	9	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	VAL	SER	ENGINEERED	UNP O32220
A	148	ILE	-	CLONING ARTIFACT	UNP O32220
A	149	GLU	-	CLONING ARTIFACT	UNP O32220
A	150	GLY	-	CLONING ARTIFACT	UNP O32220
A	151	ARG	-	CLONING ARTIFACT	UNP O32220

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.

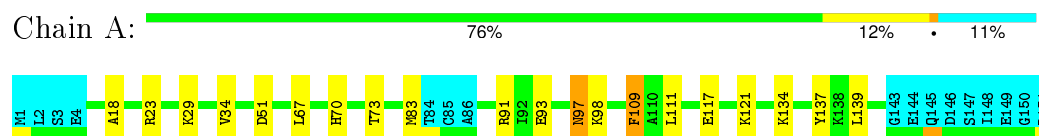• Molecule 1: Potential copper-transporting ATPase
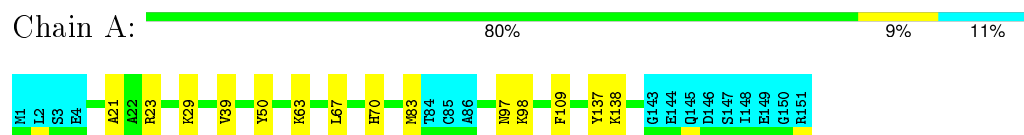
4.2 Scores per residue for each member of the ensemble
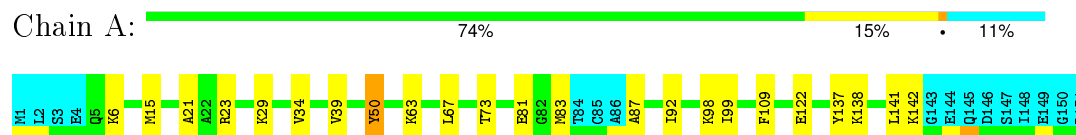
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1
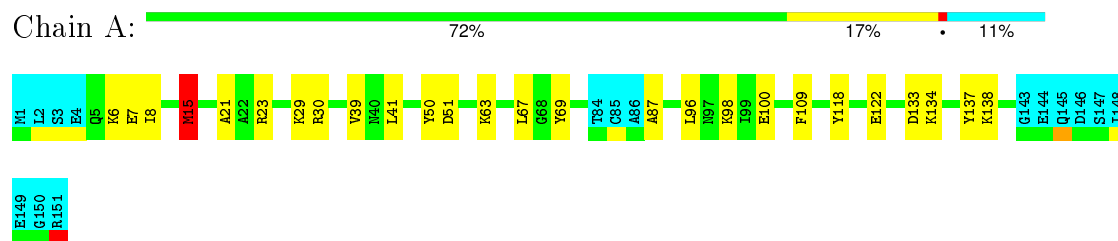
• Molecule 1: Potential copper-transporting ATPase

4.2.2 Score per residue for model 2

• Molecule 1: Potential copper-transporting ATPase

4.2.3 Score per residue for model 3

• Molecule 1: Potential copper-transporting ATPase

4.2.4 Score per residue for model 4

• Molecule 1: Potential copper-transporting ATPase

4.2.5 Score per residue for model 5

• Molecule 1: Potential copper-transporting ATPase

4.2.6 Score per residue for model 6

• Molecule 1: Potential copper-transporting ATPase

4.2.7   Score per residue for model 7

• Molecule 1: Potential copper-transporting ATPase

4.2.8   Score per residue for model 8

• Molecule 1: Potential copper-transporting ATPase

4.2.9   Score per residue for model 9

• Molecule 1: Potential copper-transporting ATPase

4.2.10   Score per residue for model 10

• Molecule 1: Potential copper-transporting ATPase

4.2.11 Score per residue for model 11

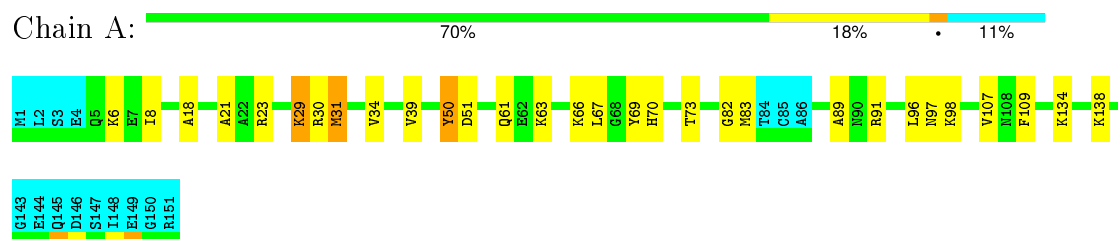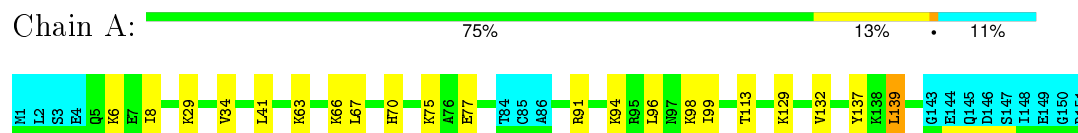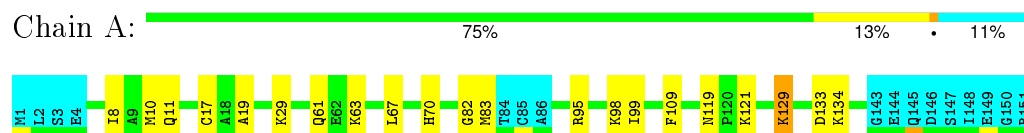• Molecule 1: Potential copper-transporting ATPase

Chain A:

4.2.12 Score per residue for model 12

• Molecule 1: Potential copper-transporting ATPase

Chain A:

4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: Potential copper-transporting ATPase

Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: Potential copper-transporting ATPase

Chain A:

4.2.15 Score per residue for model 15

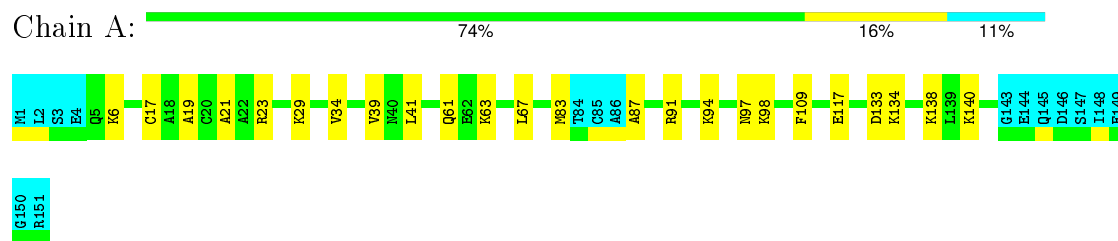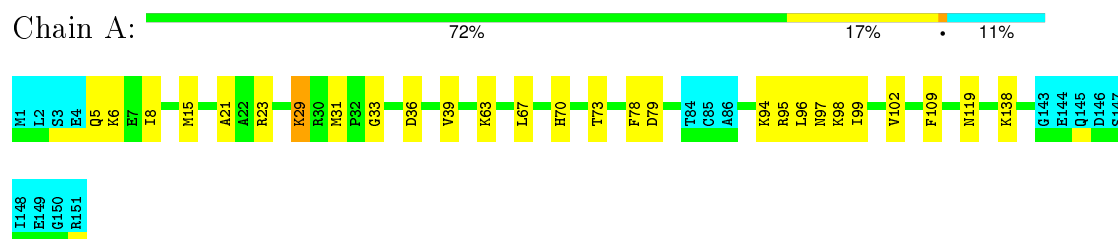• Molecule 1: Potential copper-transporting ATPase

Chain A:

81% | 9% | 11%

M1 L2 S3 E4 Q5 K6 Q11 A18 K29 V34 Y50 L67 E81 G82 M83 T84 C85 A86 L96 N97 K98 K138 G143 E144 Q145 D146 S147 I148 E149 G150 R151

4.2.16 Score per residue for model 16

• Molecule 1: Potential copper-transporting ATPase

Chain A:

74% | 15% | • | 11%

M1 L2 S3 E4 Q5 K6 A21 A22 R23 K29 V39 N40 L41 K63 L67 H70 K75 G82 M83 T84 C85 A86 A89 I92 K98 I99 E100 V107 N108 F109 Y118 K121 K134 Y137 K138 L139 G143 E144 Q145 D146 S147 I148 E149

G150 R151

4.2.17 Score per residue for model 17

• Molecule 1: Potential copper-transporting ATPase

Chain A:

70% | 19% | • | 11%

M1 L2 S3 E4 E7 I8 M15 A21 A22 R23 I24 K29 R30 V39 N40 L41 K63 L67 H70 M83 T84 C85 A86 I92 L96 N97 K98 I99 E100 G101 V102 F109 K121 E122 D133 K134 Y137 K138 L139 K140 G143 E144 Q145 D146

S147 I148 E149 G150 R151

4.2.18 Score per residue for model 18

• Molecule 1: Potential copper-transporting ATPase

Chain A:

77% | 11% | • | 11%

M1 L2 S3 E4 R23 I24 Y50 D51 K63 K66 L67 G68 Y69 H70 T73 E77 G82 M83 T84 C85 A86 N90 R91 I92 E93 K94 N97 K98 K142 G143 E144 Q145 D146 S147 I148 E149 G150 R151

4.2.19 Score per residue for model 19

• Molecule 1: Potential copper-transporting ATPase

Chain A:

4.2.20 Score per residue for model 20
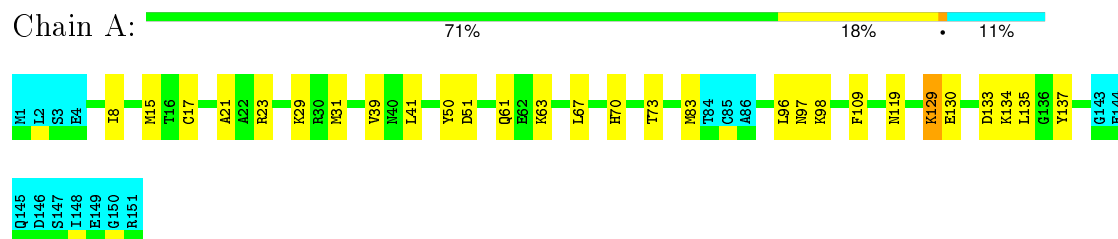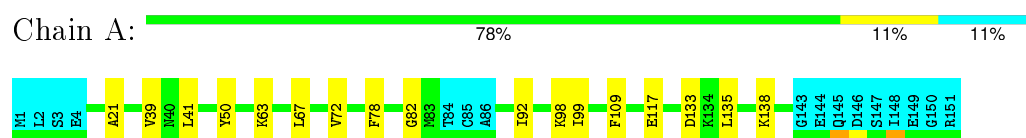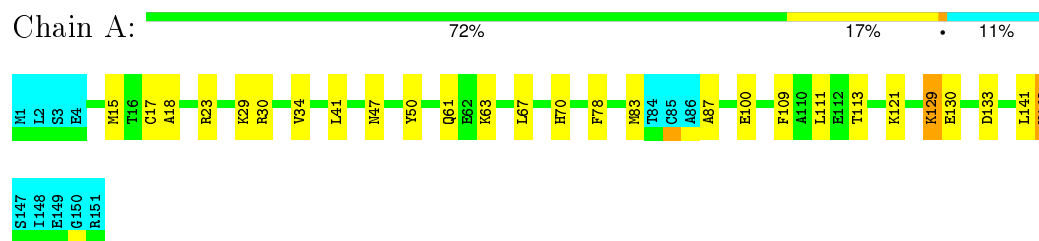
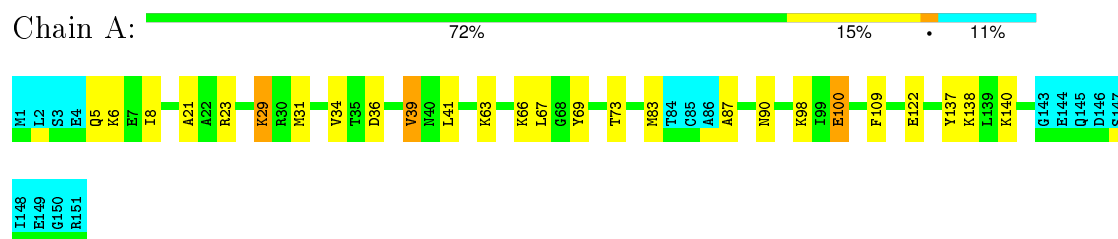• Molecule 1: Potential copper-transporting ATPase

Chain A:

4.2.21 Score per residue for model 21

• Molecule 1: Potential copper-transporting ATPase

Chain A:

4.2.22 Score per residue for model 22

• Molecule 1: Potential copper-transporting ATPase

Chain A:

4.2.23 Score per residue for model 23

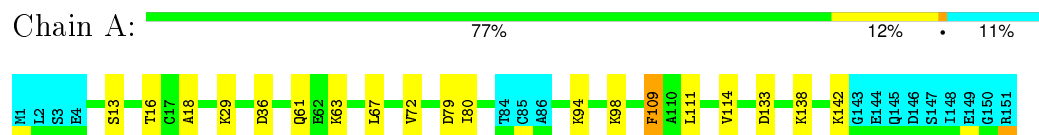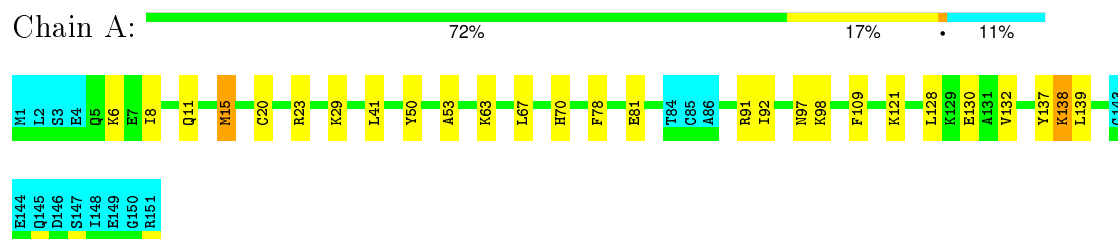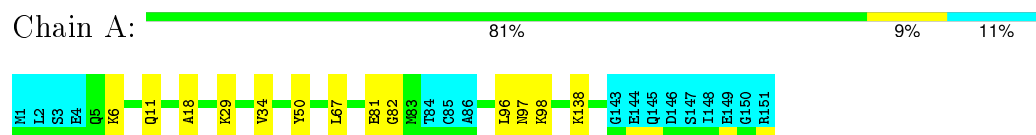• Molecule 1: Potential copper-transporting ATPase

Chain A:

M1 L2 S3 E4 Q5 K6 E7 C17 A18 A19 C20 A21 K29 V39 Y50 D51 E62 K66 L67 T73 E81 G82 M83 T84 C85 A86 N90 K98 F109 N119 P120 K121 E122 G143 E144 Q145 D146 S147 I148 E149 G150 R151

4.2.24 Score per residue for model 24

- Molecule 1: Potential copper-transporting ATPase

Chain A: 79%   10% • 11%

M1 L2 S3 E4 M15 A21 V34 V39 Y50 Q61 E62 K63 L67 G68 Y69 G82 M83 T84 C85 A86 F109 E122 E130 A131 V132 L139 G143 E144 Q145 D146 S147 I148 E149 G150 R151

4.2.25 Score per residue for model 25

- Molecule 1: Potential copper-transporting ATPase

Chain A: 75%   15%   11%

M1 L2 S3 E4 Q5 S13 A18 R23 Q61 E62 K63 L67 G68 Y69 H70 V71 V72 T73 F78 G82 M83 T84 C85 A86 K94 R95 L96 N97 K98 F109 E130 K134 K138 G143 E144 Q145 D146 S147 I148 E149 G150 R151
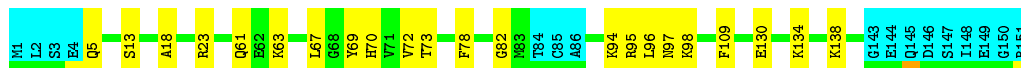
4.2.26 Score per residue for model 26

- Molecule 1: Potential copper-transporting ATPase

Chain A: 72%   18%   11%

M1 L2 S3 E4 Q11 V12 S13 A18 A21 A22 R23 I24 K29 V34 V39 K63 L67 G68 Y69 T73 G82 M83 T84 C85 A86 A89 E93 K94 R95 L96 N97 E100 V107 N108 F109 N119 P120 K121 E122 G143 E144 Q145 D146 S147

I148 E149 G150 R151
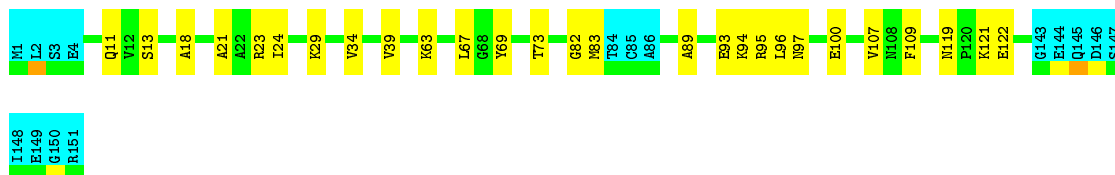
4.2.27 Score per residue for model 27

- Molecule 1: Potential copper-transporting ATPase

Chain A: 73%   15% • 11%

M1 L2 S3 E4 Q11 M15 A21 A22 R23 L28 K29 R30 M31 V39 Y50 T57 I60 K63 L67 H70 E77 G82 M83 T84 C85 A86 A89 I92 N97 K98 F109 A110 L111 E112 T113 K138 G143 E144 Q145 D146 S147

I148 E149 G150 R151
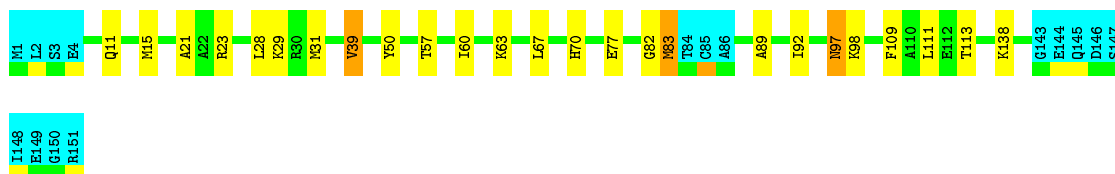
4.2.28 Score per residue for model 28

• Molecule 1: Potential copper-transporting ATPase

Chain A:
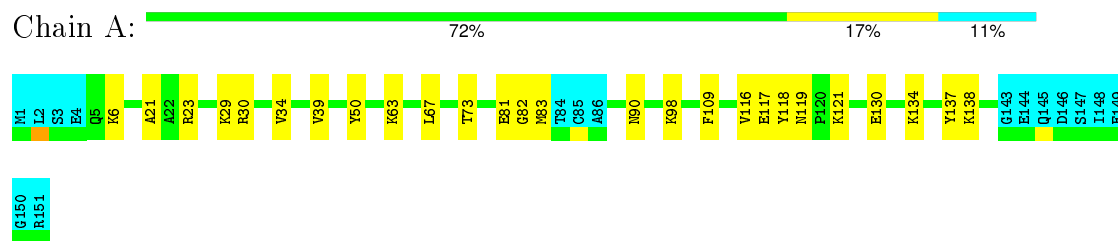
4.2.29 Score per residue for model 29

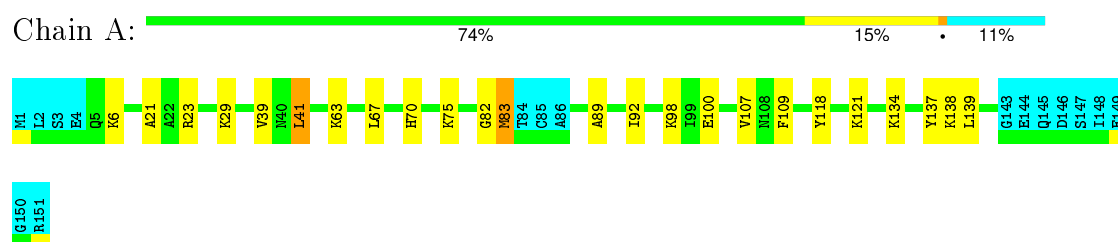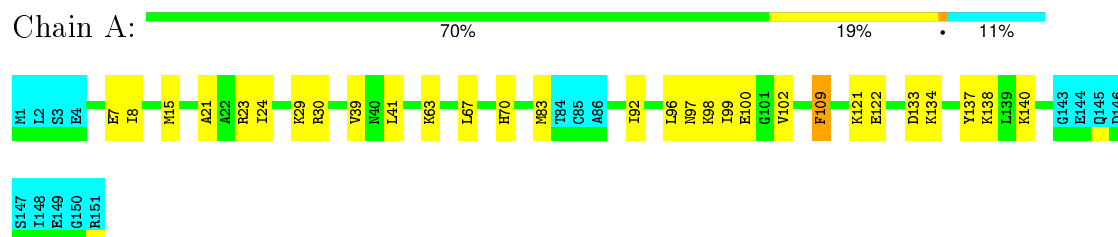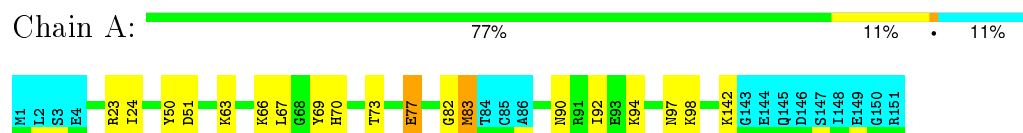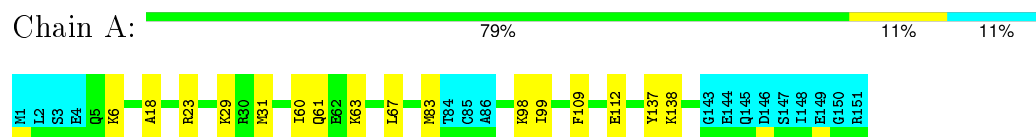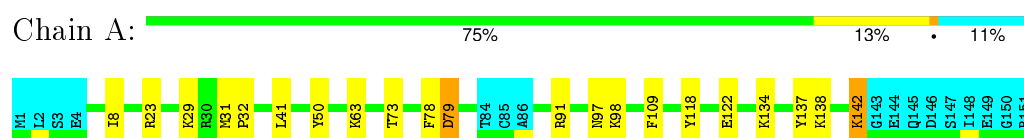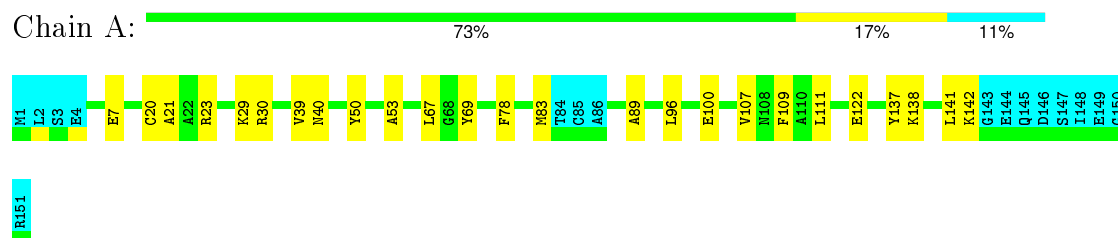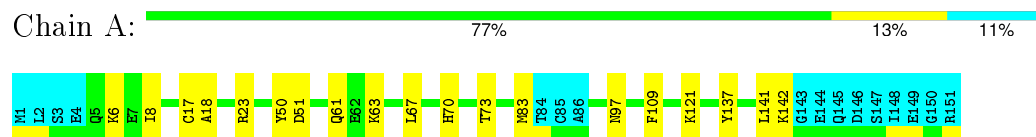• Molecule 1: Potential copper-transporting ATPase

Chain A:
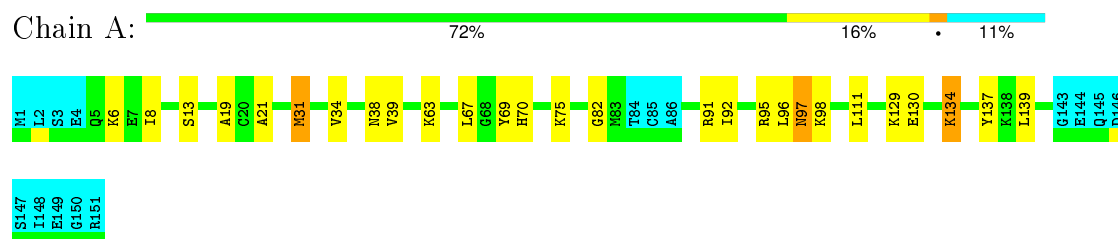
4.2.30 Score per residue for model 30

• Molecule 1: Potential copper-transporting ATPase

Chain A:
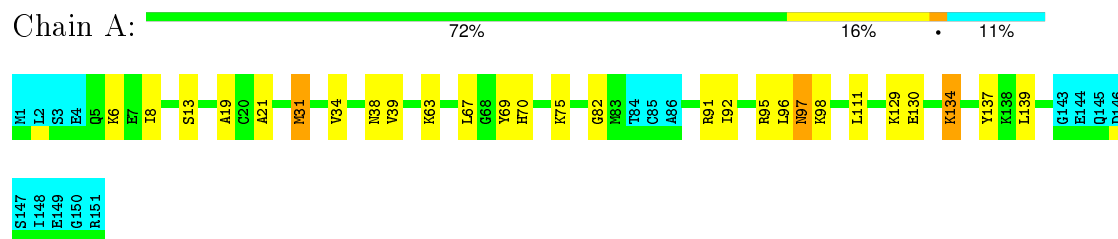
5 Refinement protocol and experimental data overview ⓘ

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

Of the 300 calculated structures, 30 were deposited, based on the following criterion: *The submitted conformer models are the 30 structures with the lowest violations.*.

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

Software name	Classification	Version
DYANA	structure solution	1.5
Xeasy	structure solution	1.3
AMBER	refinement	5.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 5813
Number of chemical shift lists	1
Total number of shifts	1655
Number of shifts mapped to atoms	1655
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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

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	0.49±0.00	0±0/1035 (0.0±0.0%)	0.87±0.01	0±0/1397 (0.0±0.0%)
All	All	0.49	0/31050 (0.0%)	0.87	2/41910 (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±0.0	1.7±0.9
All	All	0	51

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	50	TYR	CB-CG-CD2	-5.21	117.87	121.00	4	2

There are no chirality outliers.

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	137	TYR	Sidechain	16
1	A	50	TYR	Sidechain	16
1	A	69	TYR	Sidechain	8
1	A	78	PHE	Sidechain	6
1	A	109	PHE	Sidechain	3
1	A	118	TYR	Sidechain	2

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	1024	1052	1052	2±2
All	All	30720	31560	31560	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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:21:ALA:HB1	1:A:39:VAL:HG11	0.87	1.45	3	13
1:A:132:VAL:HG11	1:A:139:LEU:CB	0.72	2.15	24	2
1:A:132:VAL:HG11	1:A:139:LEU:HB3	0.66	1.68	24	1
1:A:89:ALA:HB1	1:A:107:VAL:HG11	0.63	1.69	26	3
1:A:83:MET:HB2	1:A:89:ALA:HB2	0.61	1.70	16	1
1:A:83:MET:SD	1:A:89:ALA:HB2	0.61	2.34	27	3
1:A:132:VAL:HG11	1:A:139:LEU:HB2	0.60	1.73	14	2
1:A:21:ALA:HB1	1:A:39:VAL:CG1	0.57	2.30	17	3
1:A:89:ALA:HB1	1:A:107:VAL:HG21	0.55	1.78	21	1
1:A:89:ALA:HB3	1:A:109:PHE:CZ	0.50	2.41	26	2
1:A:15:MET:SD	1:A:21:ALA:HB2	0.50	2.47	3	1
1:A:78:PHE:CZ	1:A:128:LEU:HD12	0.49	2.42	14	1
1:A:111:LEU:O	1:A:113:THR:HG23	0.49	2.08	11	1
1:A:21:ALA:HB1	1:A:39:VAL:HG13	0.48	1.86	17	5
1:A:89:ALA:HB3	1:A:109:PHE:CE1	0.47	2.44	26	1
1:A:29:LYS:HA	1:A:34:VAL:HG11	0.47	1.86	4	2
1:A:21:ALA:CB	1:A:41:LEU:HD22	0.46	2.41	16	1
1:A:28:LEU:HD21	1:A:60:ILE:HG23	0.46	1.87	27	1
1:A:24:ILE:HD11	1:A:69:TYR:CD2	0.45	2.46	18	1
1:A:62:GLU:OE2	1:A:66:LYS:NZ	0.44	2.51	23	1
1:A:41:LEU:HD23	1:A:41:LEU:H	0.43	1.74	16	1
1:A:81:GLU:HB2	1:A:138:LYS:HE2	0.43	1.89	2	1
1:A:80:ILE:HD11	1:A:114:VAL:HB	0.43	1.91	13	1
1:A:29:LYS:NZ	1:A:36:ASP:OD1	0.42	2.51	8	3
1:A:31:MET:O	1:A:34:VAL:HG12	0.42	2.14	30	4
1:A:99:ILE:O	1:A:102:VAL:HG23	0.42	2.13	17	1
1:A:129:LYS:NZ	1:A:133:ASP:OD1	0.42	2.52	11	2

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:81:GLU:CB	1:A:138:LYS:HE2	0.42	2.45	2	1
1:A:113:THR:HG21	1:A:142:LYS:HD2	0.42	1.92	11	1
1:A:77:GLU:OE2	1:A:142:LYS:NZ	0.41	2.53	18	1
1:A:15:MET:HE2	1:A:24:ILE:HD12	0.41	1.91	17	1
1:A:130:GLU:OE2	1:A:134:LYS:NZ	0.41	2.54	9	2
1:A:130:GLU:OE1	1:A:134:LYS:NZ	0.41	2.51	30	2
1:A:79:ASP:OD2	1:A:142:LYS:NZ	0.41	2.54	20	1
1:A:92:ILE:HG22	1:A:135:LEU:HG	0.41	1.91	10	1
1:A:129:LYS:NZ	1:A:133:ASP:OD2	0.41	2.54	6	1
1:A:24:ILE:HD11	1:A:69:TYR:CE2	0.40	2.50	26	1
1:A:132:VAL:HG21	1:A:139:LEU:HG	0.40	1.93	5	1
1:A:89:ALA:HB1	1:A:107:VAL:CG1	0.40	2.47	4	1
1:A:96:LEU:O	1:A:102:VAL:HG11	0.40	2.17	8	1
1:A:81:GLU:HB3	1:A:138:LYS:CG	0.40	2.46	14	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	135/151 (89%)	114±3 (85±2%)	18±2 (13±2%)	3±1 (2±1%)	14	56
All	All	4050/4530 (89%)	3426 (85%)	546 (13%)	78 (2%)	14	56

All 16 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	82	GLY	14
1	A	97	ASN	11
1	A	18	ALA	9
1	A	34	VAL	8
1	A	99	ILE	6
1	A	87	ALA	5
1	A	19	ALA	5
1	A	83	MET	4

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Mol	Chain	Res	Type	Models (Total)
1	A	15	MET	3
1	A	17	CYS	3
1	A	72	VAL	3
1	A	53	ALA	2
1	A	100	GLU	2
1	A	5	GLN	1
1	A	32	PRO	1
1	A	33	GLY	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	109/122 (89%)	93±4 (85±3%)	16±4 (15±3%)	8	47
All	All	3270/3660 (89%)	2790 (85%)	480 (15%)	8	47

All 65 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	67	LEU	29
1	A	63	LYS	26
1	A	98	LYS	25
1	A	109	PHE	23
1	A	29	LYS	22
1	A	23	ARG	21
1	A	138	LYS	17
1	A	70	HIS	16
1	A	6	LYS	15
1	A	83	MET	14
1	A	73	THR	13
1	A	8	ILE	13
1	A	96	LEU	11
1	A	134	LYS	11
1	A	41	LEU	11
1	A	61	GLN	10
1	A	121	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	122	GLU	9
1	A	97	ASN	9
1	A	91	ARG	8
1	A	15	MET	8
1	A	31	MET	8
1	A	92	ILE	8
1	A	51	ASP	7
1	A	94	LYS	7
1	A	95	ARG	6
1	A	30	ARG	6
1	A	119	ASN	6
1	A	100	GLU	6
1	A	129	LYS	6
1	A	111	LEU	6
1	A	142	LYS	5
1	A	133	ASP	5
1	A	139	LEU	5
1	A	13	SER	5
1	A	11	GLN	5
1	A	141	LEU	4
1	A	75	LYS	4
1	A	7	GLU	4
1	A	66	LYS	4
1	A	90	ASN	4
1	A	117	GLU	4
1	A	130	GLU	4
1	A	81	GLU	3
1	A	5	GLN	3
1	A	140	LYS	3
1	A	79	ASP	3
1	A	17	CYS	3
1	A	77	GLU	3
1	A	118	TYR	2
1	A	113	THR	2
1	A	20	CYS	2
1	A	38	ASN	2
1	A	93	GLU	2
1	A	39	VAL	2
1	A	116	VAL	1
1	A	34	VAL	1
1	A	47	ASN	1
1	A	60	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	112	GLU	1
1	A	10	MET	1
1	A	57	THR	1
1	A	135	LEU	1
1	A	40	ASN	1
1	A	16	THR	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 carbohydrates 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 ⓘ

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5813

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

7.1.1 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	1655
Number of shifts mapped to atoms	1655
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	127	2.54 ± 0.11	Should be applied
$^{13}C_\beta$	131	2.61 ± 0.14	Should be applied
$^{13}C'$	142	2.69 ± 0.12	Should be applied
^{15}N	144	0.83 ± 0.21	Should be applied

7.1.3 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 84%, i.e. 1341 atoms were assigned a chemical shift out of a possible 1599. 20 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	640/667 (96%)	263/266 (99%)	247/270 (91%)	130/131 (99%)
Sidechain	690/875 (79%)	417/506 (82%)	262/332 (79%)	11/37 (30%)

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	Total	**^{1}H**	**^{13}C**	**^{15}N**
Aromatic	11/57 (19%)	11/30 (37%)	0/26 (0%)	0/1 (0%)
Overall	1341/1599 (84%)	691/802 (86%)	509/628 (81%)	141/169 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1448 atoms were assigned a chemical shift out of a possible 1773. 20 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	**^{1}H**	**^{13}C**	**^{15}N**
Backbone	702/747 (94%)	289/298 (97%)	269/302 (89%)	144/147 (98%)
Sidechain	735/969 (76%)	449/561 (80%)	274/367 (75%)	12/41 (29%)
Aromatic	11/57 (19%)	11/30 (37%)	0/26 (0%)	0/1 (0%)
Overall	1448/1773 (82%)	749/889 (84%)	543/695 (78%)	156/189 (83%)

7.1.4　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	95	ARG	HD2	1.47	4.27 − 1.97	-7.2
1	A	151	ARG	HD3	1.64	4.36 − 1.86	-5.9

7.1.5　Random Coil Index (RCI) plots ⓘ

The image below reports *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: