



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:31 AM BST

PDB ID : 2ODX
Title : Solution structure of Zn(II)Cox4
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Deposited on : 2006-12-27

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
<http://wwpdb.org/validation/2016/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
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

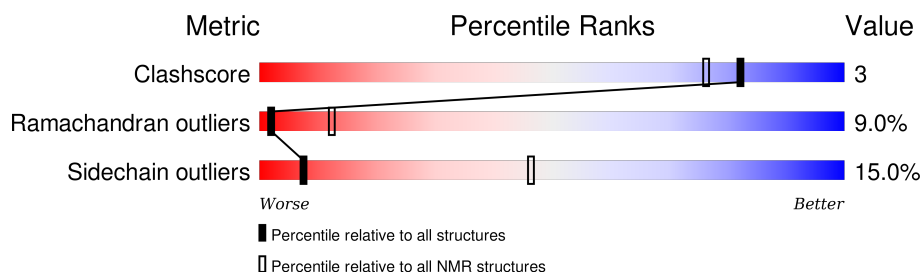
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	80	<div> <div>51%</div> <div>16%</div> <div>33%</div> </div>

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:94-A:147 (54)	0.40	1

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 5 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 3, 7, 11, 18
2	2, 4, 6, 14, 21
3	5, 9, 19
4	12, 13
5	15, 17
Single-model clusters	8; 10; 16; 20

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 828 atoms, of which 405 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytochrome c oxidase polypeptide IV.

Mol	Chain	Residues	Atoms						Trace
1	A	54	Total	C	H	N	O	S	0
			827	269	405	69	79	5	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	CLONING ARTIFACT	UNP P04037
A	77	MET	-	CLONING ARTIFACT	UNP P04037
A	78	ALA	-	CLONING ARTIFACT	UNP P04037

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

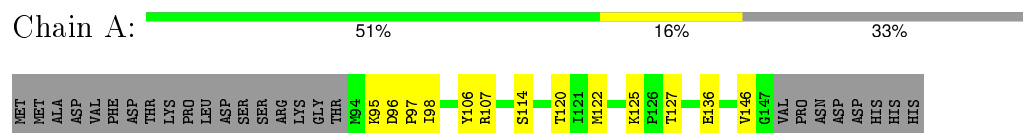
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: Cytochrome c oxidase polypeptide IV

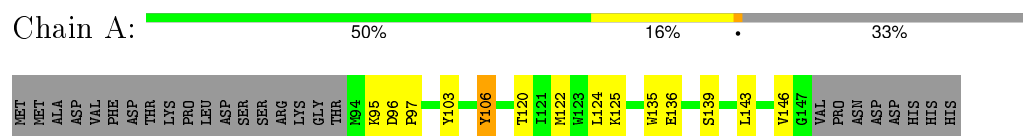


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

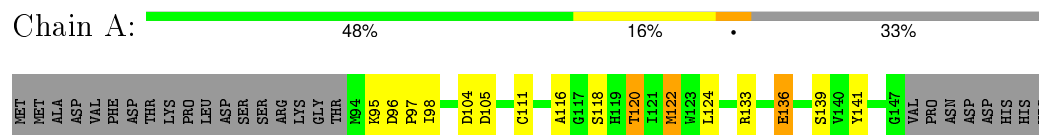
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Cytochrome c oxidase polypeptide IV



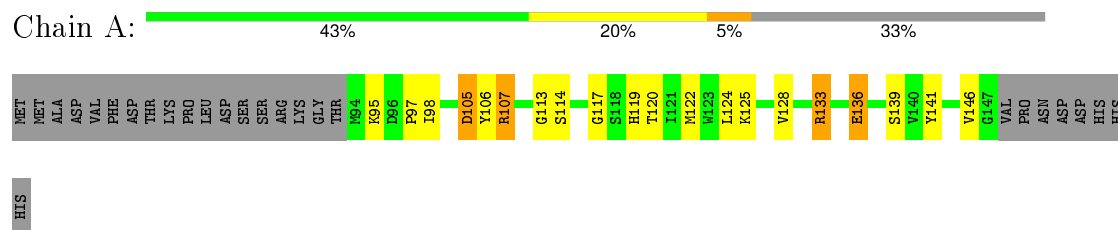
4.2.2 Score per residue for model 2

- Molecule 1: Cytochrome c oxidase polypeptide IV



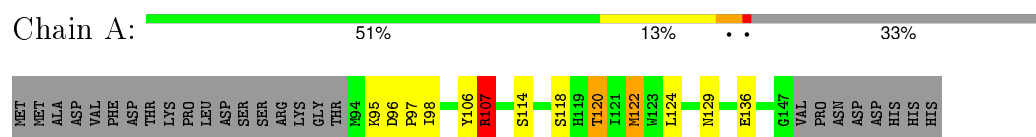
4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c oxidase polypeptide IV



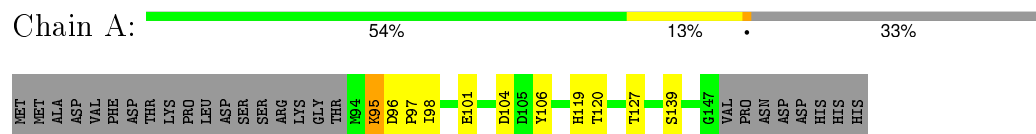
4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c oxidase polypeptide IV



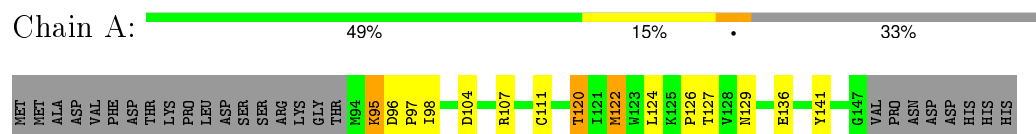
4.2.5 Score per residue for model 5

- Molecule 1: Cytochrome c oxidase polypeptide IV



4.2.6 Score per residue for model 6

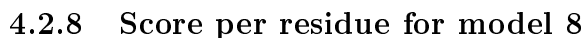
- Molecule 1: Cytochrome c oxidase polypeptide IV



4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c oxidase polypeptide IV





4.2.9 Score per residue for model 9



Met	Met	Ala	Asp	Val	Phe	Asp	Thr	Lys	Pro	Leu	Asp	Ser	Ser	Arg	Lys	Gly	Thr	K94	K95	D96	P97	I98	Y106	F107	Y108	G111	S114	M122	F123	I124	K125	S139	V140	Pro	Asn	Asp	Asp	His	His	Trp
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4.2.10 Score per residue for model 10



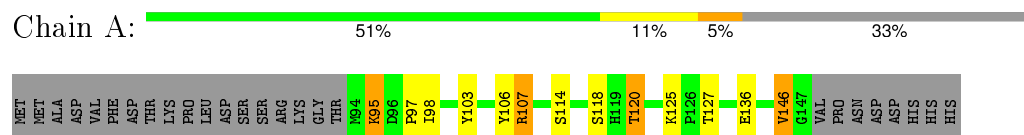
MET	ALA	ASP	VAL	PHE	ASP	THR	LYS	PRO	LEU	ASP	SER	ARG	SER	GLY	THR	P94	K95	D96	P97	I98	Y103	Y106	R107	G113	S114	P115	A116	G117	T120	T127	E136	S139	I143	N144	G147	VAL	PRO	ASN	ASP	ASP	HIS	THR
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4.2.11 Score per residue for model 11



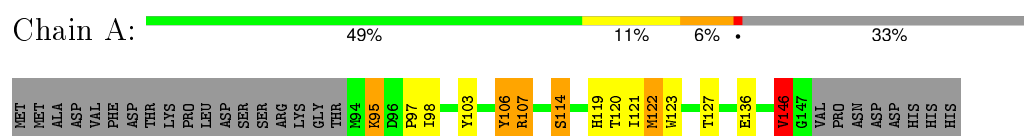
4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome c oxidase polypeptide IV



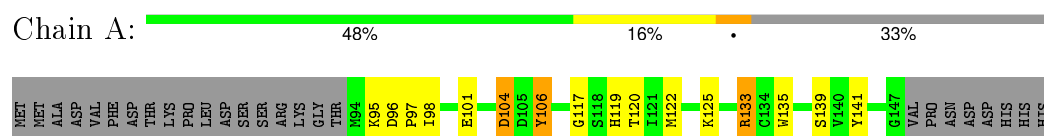
4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome c oxidase polypeptide IV



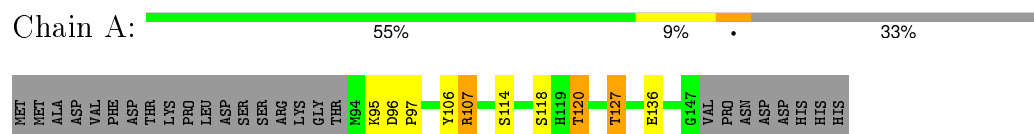
4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome c oxidase polypeptide IV



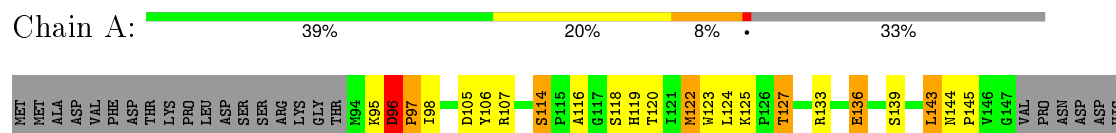
4.2.15 Score per residue for model 15

- Molecule 1: Cytochrome c oxidase polypeptide IV



4.2.16 Score per residue for model 16

- Molecule 1: Cytochrome c oxidase polypeptide IV



HIS
HIS

4.2.17 Score per residue for model 17

- Molecule 1: Cytochrome c oxidase polypeptide IV

Chain A: 

4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome c oxidase polypeptide IV

Chain A: 

4.2.19 Score per residue for model 19

- Molecule 1: Cytochrome c oxidase polypeptide IV

Chain A: 

4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome c oxidase polypeptide IV

Chain A: 

4.2.21 Score per residue for model 21

- Molecule 1: Cytochrome c oxidase polypeptide IV

Chain A: 

MET	MET	ALA	ASP	VAL	PHE	ASP	THR	LYS	PRO	LEU	ASP	SER	SER	ARG	LYS	GLY	THR	K94	K95	D96	P97	Y106	R107	C111	T112	G113	S114	T120	T121	M122	K125	E136	Y141	N144	G147	VAL	PRO	ASN	ASP	HIS	HIS
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 21 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
CYANA	structure solution	
AMBER	refinement	8.0

No chemical shift data was provided. 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](#)

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

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	0.72±0.01	0±0/434 (0.0±0.0%)	1.31±0.05	1±1/591 (0.2±0.2%)
All	All	0.72	0/9114 (0.0%)	1.31	30/12411 (0.2%)

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	1.9±1.4
All	All	0	39

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(°)	Ideal(°)	Models	
								Worst	Total
1	A	107	ARG	NE-CZ-NH1	10.24	125.42	120.30	4	9
1	A	107	ARG	NE-CZ-NH2	-7.42	116.59	120.30	20	4
1	A	146	VAL	CG1-CB-CG2	-7.39	99.07	110.90	18	2
1	A	133	ARG	NE-CZ-NH1	6.56	123.58	120.30	8	5
1	A	141	TYR	CB-CG-CD1	-6.07	117.36	121.00	14	2
1	A	146	VAL	CA-CB-CG2	5.79	119.58	110.90	18	1
1	A	96	ASP	N-CA-CB	-5.50	100.70	110.60	5	3
1	A	122	MET	CG-SD-CE	5.47	108.95	100.20	20	1
1	A	107	ARG	CD-NE-CZ	5.25	130.95	123.60	4	1
1	A	107	ARG	NH1-CZ-NH2	-5.13	113.75	119.40	4	1
1	A	130	GLU	C-N-CA	5.04	134.29	121.70	17	1

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	106	TYR	Sidechain	11
1	A	141	TYR	Sidechain	5
1	A	103	TYR	Peptide,Sidechain	3
1	A	117	GLY	Peptide	3
1	A	113	GLY	Peptide	3
1	A	146	VAL	Peptide	3
1	A	133	ARG	Sidechain	3
1	A	119	HIS	Peptide,Sidechain	2
1	A	107	ARG	Peptide,Sidechain	2
1	A	129	ASN	Peptide	2
1	A	116	ALA	Peptide	1
1	A	108	TYR	Sidechain	1

6.2 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 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	422	405	404	3±2
All	All	8883	8505	8484	53

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:120:THR:HG22	1:A:136:GLU:OE1	0.66	1.91	11	5
1:A:120:THR:HG22	1:A:136:GLU:OE2	0.62	1.93	7	11
1:A:105:ASP:OD1	1:A:128:VAL:HG12	0.57	1.98	20	3
1:A:143:LEU:HD23	1:A:144:ASN:N	0.56	2.15	10	1
1:A:103:TYR:CD1	1:A:146:VAL:HG23	0.53	2.39	18	1
1:A:143:LEU:HD23	1:A:144:ASN:H	0.53	1.63	10	2
1:A:122:MET:CE	1:A:124:LEU:HD21	0.52	2.34	3	3
1:A:122:MET:SD	1:A:124:LEU:HD21	0.51	2.46	17	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:HIS:CE1	1:A:122:MET:SD	0.47	3.07	13	2
1:A:103:TYR:H	1:A:146:VAL:CG2	0.47	2.23	12	3
1:A:102:SER:HB2	1:A:143:LEU:HD21	0.45	1.88	7	1
1:A:111:CYS:H	1:A:122:MET:CE	0.45	2.25	19	1
1:A:105:ASP:CG	1:A:128:VAL:HG12	0.43	2.34	20	1
1:A:119:HIS:CD2	1:A:136:GLU:HB3	0.42	2.49	18	2
1:A:113:GLY:CA	1:A:119:HIS:CD2	0.42	3.03	3	1
1:A:111:CYS:H	1:A:122:MET:HE2	0.42	1.74	19	1
1:A:122:MET:SD	1:A:135:TRP:NE1	0.42	2.92	7	2
1:A:103:TYR:CE1	1:A:146:VAL:HG22	0.42	2.50	1	1
1:A:122:MET:CE	1:A:135:TRP:CD1	0.41	3.03	1	1
1:A:107:ARG:CG	1:A:107:ARG:HH11	0.41	2.28	4	1
1:A:96:ASP:N	1:A:97:PRO:HD3	0.41	2.31	16	1
1:A:121:ILE:C	1:A:122:MET:SD	0.41	2.99	13	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	52/80 (65%)	39±2 (74±4%)	9±2 (17±4%)	5±1 (9±2%)	2	12
All	All	1092/1680 (65%)	810 (74%)	184 (17%)	98 (9%)	2	12

All 15 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	97	PRO	21
1	A	120	THR	15
1	A	114	SER	13
1	A	96	ASP	10
1	A	146	VAL	8
1	A	127	THR	8
1	A	95	LYS	8
1	A	105	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	116	ALA	4
1	A	118	SER	2
1	A	126	PRO	1
1	A	104	ASP	1
1	A	135	TRP	1
1	A	130	GLU	1
1	A	107	ARG	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	47/71 (66%)	40±3 (85±6%)	7±3 (15±6%)	7	46
All	All	987/1491 (66%)	839 (85%)	148 (15%)	7	46

All 25 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	95	LYS	20
1	A	98	ILE	17
1	A	125	LYS	13
1	A	106	TYR	12
1	A	139	SER	10
1	A	122	MET	9
1	A	114	SER	9
1	A	136	GLU	7
1	A	111	CYS	7
1	A	104	ASP	6
1	A	107	ARG	6
1	A	143	LEU	6
1	A	127	THR	4
1	A	118	SER	3
1	A	123	TRP	3
1	A	124	LEU	2
1	A	105	ASP	2
1	A	133	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	108	TYR	2
1	A	96	ASP	2
1	A	101	GLU	2
1	A	145	PRO	1
1	A	134	CYS	1
1	A	144	ASN	1
1	A	146	VAL	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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

No chemical shift data were provided