Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2YT9
Title	:	Solution structure of C2H2 type Zinc finger domain 345 in Zinc finger protein 278
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Deposited on	:	2007-04-05

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:

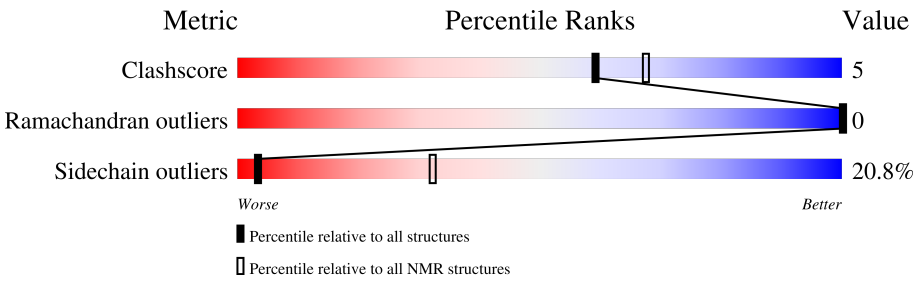
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	95	57% 18% • 24%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:362-A:382 (21)	0.13	15
2	A:388-A:412 (25)	0.08	18
3	A:418-A:443 (26)	0.10	3

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 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1428 atoms, of which 699 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called zinc finger-containing protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1425	445	699	144	130	7	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	GLY	-	expression tag	UNP Q9HBE1
A	356	SER	-	expression tag	UNP Q9HBE1
A	357	SER	-	expression tag	UNP Q9HBE1
A	358	GLY	-	expression tag	UNP Q9HBE1
A	359	SER	-	expression tag	UNP Q9HBE1
A	360	SER	-	expression tag	UNP Q9HBE1
A	361	GLY	-	expression tag	UNP Q9HBE1
A	444	SER	-	expression tag	UNP Q9HBE1
A	445	GLY	-	expression tag	UNP Q9HBE1
A	446	PRO	-	expression tag	UNP Q9HBE1
A	447	SER	-	expression tag	UNP Q9HBE1
A	448	SER	-	expression tag	UNP Q9HBE1
A	449	GLY	-	expression tag	UNP Q9HBE1

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	3	3	3

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: zinc finger-containing protein 1

Chain A: 57% 18% • 24%

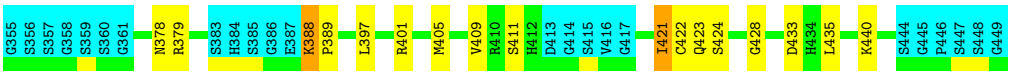
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: zinc finger-containing protein 1

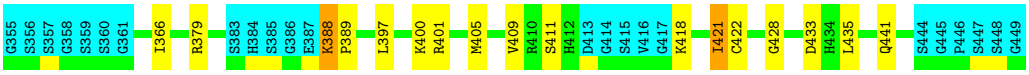
Chain A: 58% 16% • 24%



4.2.2 Score per residue for model 2

• Molecule 1: zinc finger-containing protein 1

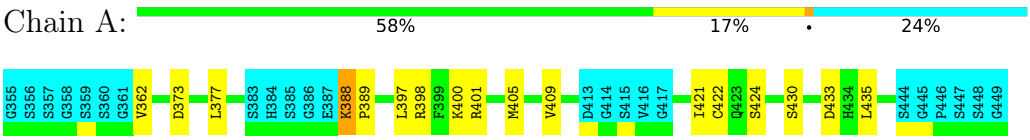
Chain A: 58% 16% • 24%



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: zinc finger-containing protein 1

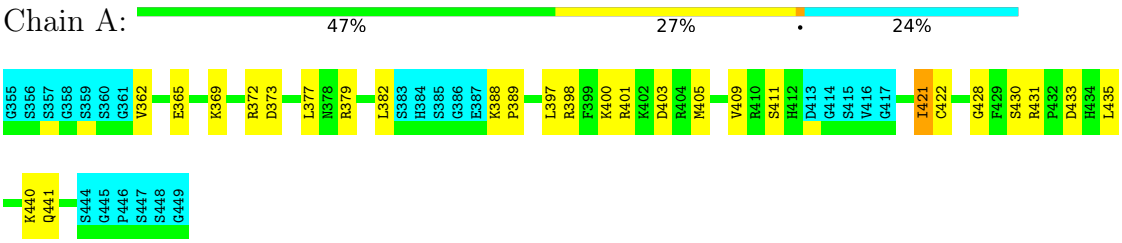
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: zinc finger-containing protein 1

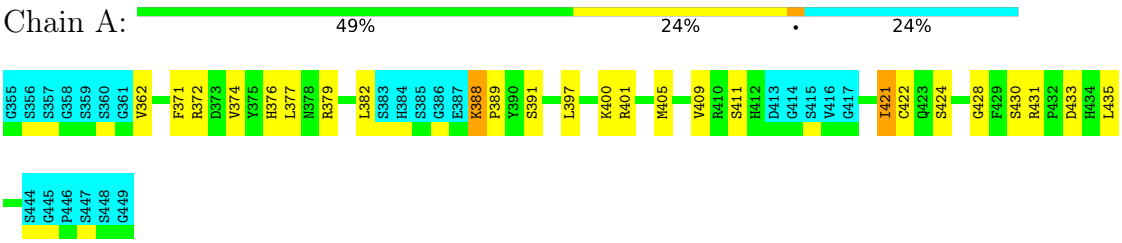
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: zinc finger-containing protein 1

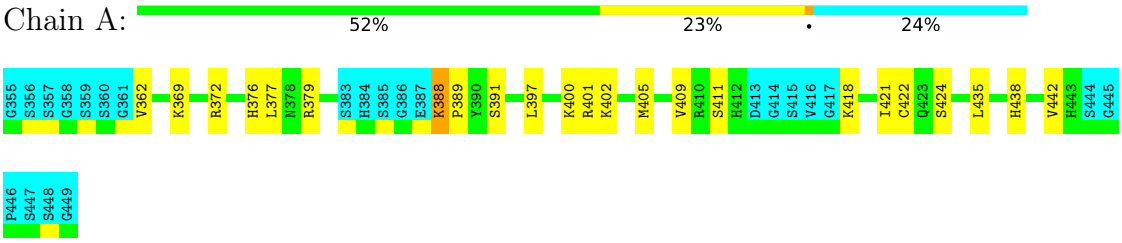
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: zinc finger-containing protein 1

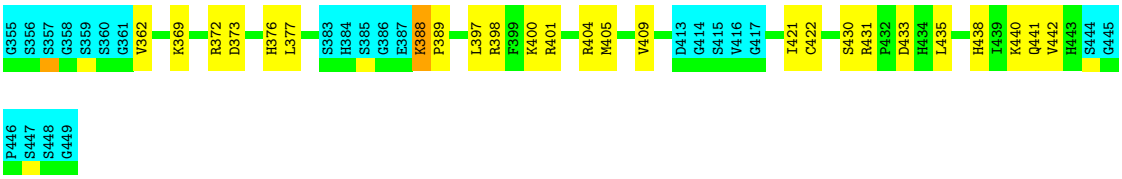
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: zinc finger-containing protein 1

Chain A: 49% 25% • 24%



4.2.8 Score per residue for model 8

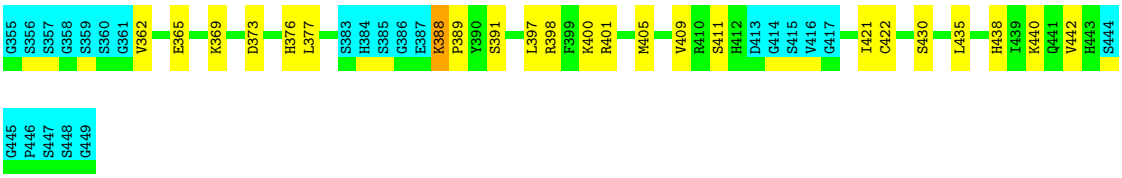
- Molecule 1: zinc finger-containing protein 1

Chain A: 54% 21% • 24%

4.2.9 Score per residue for model 9

- Molecule 1: zinc finger-containing protein 1

Chain A: 52% 23% • 24%



4.2.10 Score per residue for model 10

- Molecule 1: zinc finger-containing protein 1

Chain A: 58% 18% 24%

4.2.11 Score per residue for model 11

- Molecule 1: zinc finger-containing protein 1

Chain A: 48% 25% • 24%

G355 S356 S357 G358 S359 S360 G361 V362 D373 V374 Y375 H376 L377 H378 R379 S383 H384 S385 G386 E387 K388 P389 Y390 S391 L397 R398 R401 K402 D403 R404 M405 V409 R410 S411 H412 D413 G414 S415 V416 G417 K418 I421 C422 S430 D433 H434 L435 N436 I439 K440

S444 G445 P446 S447 S448 G449

4.2.12 Score per residue for model 12

- Molecule 1: zinc finger-containing protein 1

Chain A: 54% 19% • 24%

G355 S356 S357 G358 S359 S360 G361 E365 R379 L382 S383 H384 S385 G386 E387 K388 P389 Y390 S391 L397 R401 K402 M405 V409 D413 G414 S415 V416 G417 K418 I421 C422 Q423 G428 R431 L435 H438 I439 K440 Q441 V442 H443 S444 G445 P446 S447 S448

G449

4.2.13 Score per residue for model 13

- Molecule 1: zinc finger-containing protein 1

Chain A: 53% 22% • 24%

G355 S356 S357 G358 S359 S360 G361 F371 R372 D373 H376 L377 S383 H384 S385 G386 E387 K388 P389 Y390 S391 L397 K400 R401 M405 V409 R410 S411 H412 D413 G414 S415 V416 G417 K418 I421 C422 Q423 S424 R431 L435 H438 V442 H443 S444 G445 P446 S447

S448 G449

4.2.14 Score per residue for model 14

- Molecule 1: zinc finger-containing protein 1

Chain A: 49% 24% • 24%

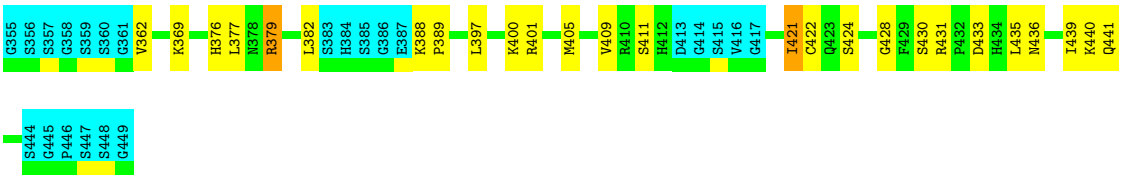
G355 S356 S357 G358 S359 S360 G361 V362 K369 R372 D373 L377 S383 H384 S385 G386 E387 K388 P389 Y390 S391 L397 R398 F399 K400 R401 K402 D403 R404 M405 V409 R410 S411 H412 D413 G414 S415 V416 G417 I421 C422 Q423 S430 R431 L435 N436 I439 K440 S444

G445 P446 S447 S448 G449

4.2.15 Score per residue for model 15

- Molecule 1: zinc finger-containing protein 1

Chain A: 48% 25% • 24%



4.2.16 Score per residue for model 16

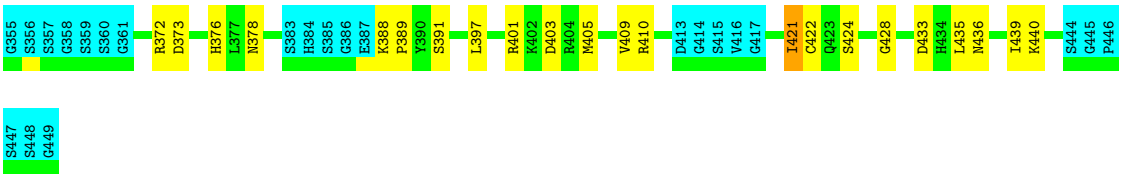
- Molecule 1: zinc finger-containing protein 1

Chain A: 54% 21% • 24%

4.2.17 Score per residue for model 17

- Molecule 1: zinc finger-containing protein 1

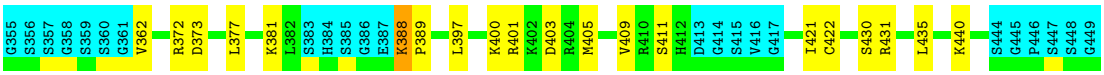
Chain A: 53% 22% • 24%



4.2.18 Score per residue for model 18

- Molecule 1: zinc finger-containing protein 1

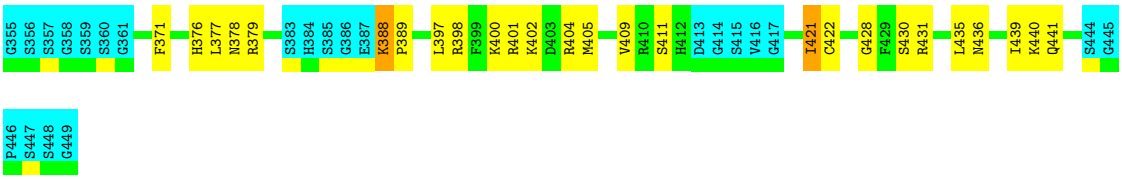
Chain A: 55% 20% • 24%



4.2.19 Score per residue for model 19

- Molecule 1: zinc finger-containing protein 1

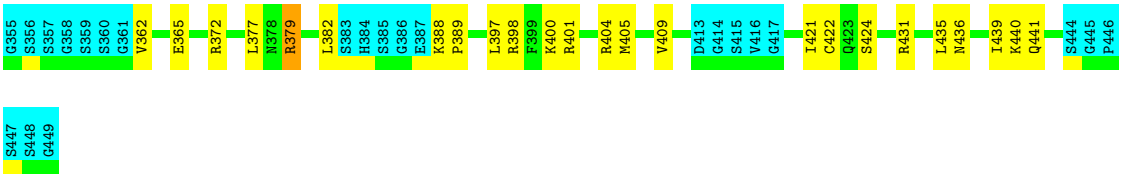
Chain A: 48% 25% • 24%



4.2.20 Score per residue for model 20

- Molecule 1: zinc finger-containing protein 1

Chain A: 51% 24% • 24%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy, target function.*

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	593	592	592	6±2
All	All	11920	11840	11840	115

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:362:VAL:HG11	1:A:374:VAL:HG22	0.77	1.55	5	1
1:A:362:VAL:HG21	1:A:377:LEU:HD22	0.59	1.74	15	6
1:A:362:VAL:HG11	1:A:377:LEU:HD22	0.59	1.75	11	3
1:A:379:ARG:HA	1:A:382:LEU:HD12	0.57	1.76	15	4
1:A:362:VAL:CG2	1:A:377:LEU:HD22	0.57	2.29	8	4
1:A:438:HIS:CE1	1:A:442:VAL:HG21	0.57	2.34	7	5
1:A:422:CYS:HA	1:A:435:LEU:HD11	0.57	1.77	11	18
1:A:422:CYS:CA	1:A:435:LEU:HD11	0.56	2.31	14	7
1:A:405:MET:O	1:A:409:VAL:HG23	0.52	2.04	3	20
1:A:371:PHE:CD1	1:A:377:LEU:HD13	0.50	2.42	5	4
1:A:362:VAL:HG21	1:A:374:VAL:HG22	0.50	1.84	11	1
1:A:362:VAL:CG1	1:A:377:LEU:HD22	0.49	2.37	11	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:436:ASN:HA	1:A:439:ILE:HD12	0.48	1.86	15	6
1:A:388:LYS:HA	1:A:389:PRO:C	0.45	2.32	12	20
1:A:421:ILE:HG22	1:A:428:GLY:CA	0.43	2.44	17	9
1:A:362:VAL:HG23	1:A:377:LEU:HD22	0.41	1.93	8	1
1:A:377:LEU:HD21	1:A:381:LYS:NZ	0.41	2.30	18	1
1:A:421:ILE:HG22	1:A:428:GLY:HA2	0.40	1.94	19	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	72/95 (76%)	60±1 (83±2%)	12±1 (17±2%)	0±0 (0±0%)	100	100
All	All	1440/1900 (76%)	1201 (83%)	239 (17%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	66/81 (81%)	52±2 (79±3%)	14±2 (21±3%)	3	32
All	All	1320/1620 (81%)	1045 (79%)	275 (21%)	3	32

All 29 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	397	LEU	20
1	A	401	ARG	20

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Mol	Chain	Res	Type	Models (Total)
1	A	421	ILE	20
1	A	400	LYS	16
1	A	411	SER	15
1	A	388	LYS	14
1	A	440	LYS	13
1	A	373	ASP	12
1	A	430	SER	12
1	A	379	ARG	11
1	A	431	ARG	11
1	A	424	SER	10
1	A	376	HIS	10
1	A	433	ASP	9
1	A	441	GLN	8
1	A	398	ARG	8
1	A	369	LYS	8
1	A	372	ARG	8
1	A	391	SER	8
1	A	418	LYS	7
1	A	402	LYS	6
1	A	423	GLN	5
1	A	365	GLU	5
1	A	403	ASP	5
1	A	404	ARG	5
1	A	378	ASN	3
1	A	382	LEU	2
1	A	436	ASN	2
1	A	410	ARG	2

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)

Of 3 ligands modelled in this entry, 3 are 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 (i)

No chemical shift data were provided