



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2016 – 12:49 AM EDT

PDB ID : 5KL1  
Title : Crystal structure of the Pumilio-Nos-hunchback RNA complex  
Authors : Qiu, C.; Hall, T.M.T.  
Deposited on : 2016-06-23  
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

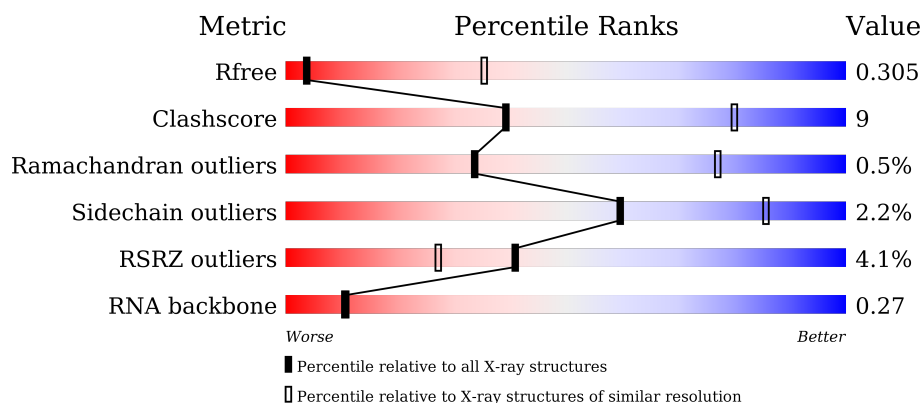
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	<div> <div>5%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
2	B	114	<div> <div>52%</div> <div>10%</div> <div>39%</div> </div>
3	C	16	<div> <div>19%</div> <div>44%</div> <div>13%</div> <div>25%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3446 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Maternal protein pumilio.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2648	1668	474	489	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1090	SER	-	expression tag	UNP P25822

- Molecule 2 is a protein called Protein nanos.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O	S	0	0	0
			544	336	99	102	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	288	SER	-	expression tag	UNP P25724

- Molecule 3 is a RNA chain called RNA (5'-R(\*AP\*AP\*AP\*UP\*UP\*GP\*UP\*AP\*CP\*AP\*UP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	12	Total	C	N	O	P	0	0	0
			252	115	46	80	11			

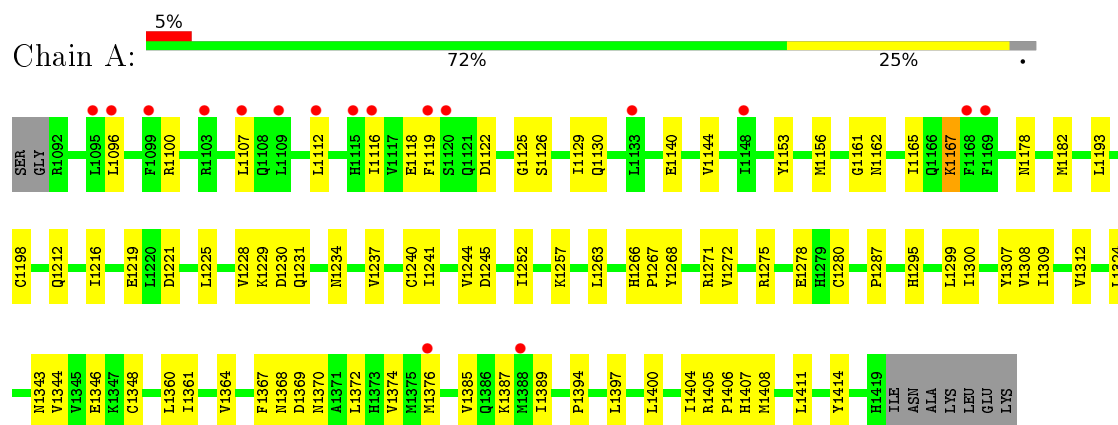
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		

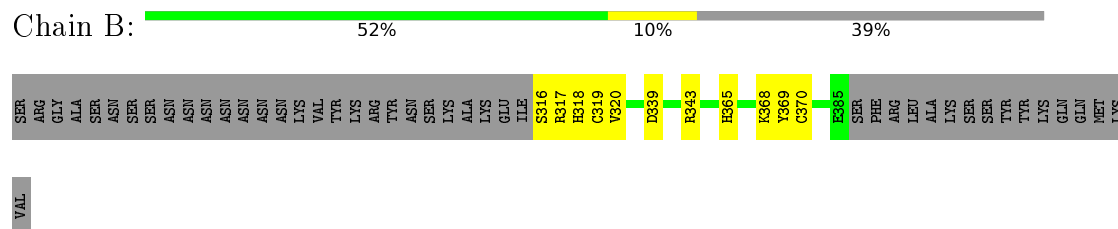
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

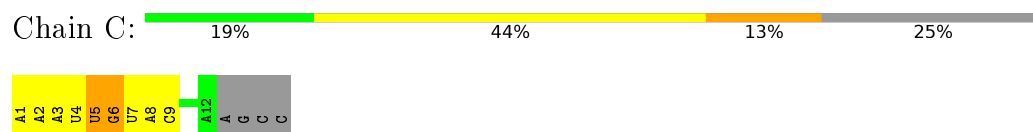
#### • Molecule 1: Maternal protein pumilio



#### • Molecule 2: Protein nanos



#### • Molecule 3: RNA (5'-R(\*AP\*AP\*AP\*UP\*UP\*GP\*UP\*AP\*CP\*AP\*UP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.01Å 137.01Å 221.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.33 – 3.70 46.24 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.33-3.70) 90.6 (46.24-3.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 3.66Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.264 , 0.300 0.265 , 0.305	Depositor DCC
$R_{free}$ test set	1293 reflections (10.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	137.3	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 113.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 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 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	0.26	0/2696	0.43	0/3636
2	B	0.26	0/555	0.42	0/751
3	C	0.30	0/282	0.83	0/437
All	All	0.26	0/3533	0.48	0/4824

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2648	0	2649	53	0
2	B	544	0	529	7	0
3	C	252	0	130	8	0
4	B	2	0	0	0	0
All	All	3446	0	3308	60	0

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 9.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:ASN:O	1:A:1370:ASN:N	2.21	0.73
1:A:1346:GLU:HB3	1:A:1387:LYS:HD2	1.73	0.70
1:A:1299:LEU:HD23	1:A:1309:ILE:HD11	1.85	0.58
1:A:1107:LEU:HD21	1:A:1112:LEU:HD21	1.86	0.57
1:A:1096:LEU:HD22	1:A:1118:GLU:HG2	1.86	0.57
3:C:1:A:O2'	3:C:2:A:H5'	2.05	0.57
1:A:1385:VAL:O	1:A:1389:ILE:HG13	2.08	0.54
1:A:1376:MET:HB3	1:A:1411:LEU:HD11	1.89	0.53
2:B:320:VAL:HG11	3:C:5:U:OP1	2.09	0.53
1:A:1178:ASN:O	1:A:1182:MET:HG3	2.10	0.51
1:A:1309:ILE:HG23	1:A:1324:LEU:HD13	1.92	0.51
2:B:320:VAL:HG11	3:C:5:U:P	2.50	0.51
2:B:369:TYR:OH	3:C:4:U:OP2	2.20	0.51
1:A:1394:PRO:HA	1:A:1397:LEU:HB3	1.93	0.51
1:A:1119:PHE:HD1	1:A:1125:GLY:HA3	1.76	0.50
1:A:1130:GLN:HE21	1:A:1167:LYS:HE3	1.77	0.49
1:A:1300:ILE:HG23	1:A:1344:VAL:HG21	1.94	0.49
2:B:316:SER:O	2:B:317:ARG:HG2	2.12	0.49
1:A:1237:VAL:O	1:A:1241:ILE:HG13	2.13	0.48
1:A:1228:VAL:HG13	1:A:1272:VAL:HG21	1.96	0.48
1:A:1275:ARG:HA	1:A:1278:GLU:HG2	1.94	0.48
1:A:1308:VAL:O	1:A:1312:VAL:HG23	2.13	0.47
1:A:1230:ASP:O	1:A:1234:ASN:ND2	2.34	0.47
1:A:1153:TYR:HA	1:A:1156:MET:HE2	1.96	0.47
1:A:1116:ILE:HD13	1:A:1144:VAL:HG13	1.96	0.46
1:A:1126:SER:O	1:A:1130:GLN:HB2	2.15	0.46
1:A:1361:ILE:HG23	1:A:1400:LEU:HD11	1.96	0.46
1:A:1229:LYS:HE2	1:A:1263:LEU:HD21	1.96	0.46
1:A:1372:LEU:O	1:A:1376:MET:HG2	2.16	0.46
1:A:1414:TYR:HE1	2:B:368:LYS:HE2	1.81	0.45
1:A:1271:ARG:O	1:A:1275:ARG:HG2	2.16	0.45
1:A:1212:GLN:O	1:A:1216:ILE:HG13	2.17	0.45
1:A:1116:ILE:HG23	1:A:1129:ILE:HD13	1.98	0.45
1:A:1271:ARG:NH1	3:C:9:C:O2'	2.50	0.45
2:B:365:HIS:CD2	2:B:370:CYS:HA	2.52	0.45
2:B:339:ASP:HB3	2:B:343:ARG:H	1.82	0.44
1:A:1216:ILE:O	1:A:1219:GLU:HB3	2.17	0.43
1:A:1370:ASN:O	1:A:1374:VAL:HG23	2.18	0.43
1:A:1411:LEU:HA	1:A:1411:LEU:HD23	1.86	0.43
1:A:1405:ARG:N	1:A:1406:PRO:HD2	2.34	0.43
1:A:1307:TYR:CZ	3:C:8:A:N7	2.87	0.42
1:A:1116:ILE:HA	1:A:1119:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1295:HIS:O	1:A:1299:LEU:HB2	2.19	0.42
1:A:1405:ARG:O	1:A:1408:MET:HB2	2.20	0.42
1:A:1360:LEU:O	1:A:1364:VAL:HG23	2.19	0.42
1:A:1343:ASN:OD1	3:C:6:G:N2	2.53	0.41
1:A:1240:CYS:O	1:A:1244:VAL:HG23	2.20	0.41
1:A:1346:GLU:OE2	3:C:6:G:N1	2.41	0.41
1:A:1100:ARG:NH1	1:A:1122:ASP:OD2	2.52	0.41
1:A:1193:LEU:HD23	1:A:1193:LEU:HA	1.91	0.41
1:A:1364:VAL:HG13	1:A:1367:PHE:CE2	2.56	0.41
1:A:1404:ILE:HG22	1:A:1407:HIS:HB2	2.03	0.41
1:A:1161:GLY:O	1:A:1165:ILE:HG12	2.20	0.41
1:A:1257:LYS:HE2	1:A:1287:PRO:HB2	2.03	0.41
1:A:1231:GLN:HG3	1:A:1268:TYR:OH	2.20	0.41
1:A:1252:ILE:HG13	1:A:1252:ILE:H	1.72	0.41
1:A:1266:HIS:CG	1:A:1267:PRO:HD2	2.56	0.41
1:A:1140:GLU:O	1:A:1144:VAL:HG23	2.21	0.40
1:A:1156:MET:HE2	1:A:1156:MET:HB2	1.94	0.40
1:A:1244:VAL:HG12	1:A:1245:ASP:H	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	326/337 (97%)	291 (89%)	33 (10%)	2 (1%)	30	75
2	B	68/114 (60%)	61 (90%)	7 (10%)	0	100	100
All	All	394/451 (87%)	352 (89%)	40 (10%)	2 (0%)	34	77

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	1369	ASP
1	A	1225	LEU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	294/301 (98%)	288 (98%)	6 (2%)	63	87
2	B	63/103 (61%)	61 (97%)	2 (3%)	46	80
All	All	357/404 (88%)	349 (98%)	8 (2%)	60	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1162	ASN
1	A	1167	LYS
1	A	1198	CYS
1	A	1221	ASP
1	A	1280	CYS
1	A	1348	CYS
2	B	318	HIS
2	B	319	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	11/16 (68%)	3 (27%)	1 (9%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	3	A

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Mol	Chain	Res	Type
3	C	5	U
3	C	7	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	6	G

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	328/337 (97%)	0.24	17 (5%) 31 21	120, 180, 246, 258	0
2	B	70/114 (61%)	-0.02	0 100 100	91, 120, 160, 164	0
3	C	12/16 (75%)	0.26	0 100 100	104, 126, 212, 228	0
All	All	410/467 (87%)	0.19	17 (4%) 41 27	91, 171, 243, 258	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1133	LEU	4.0
1	A	1107	LEU	3.5
1	A	1109	LEU	3.3
1	A	1103	ARG	3.1
1	A	1120	SER	3.1
1	A	1168	PHE	3.1
1	A	1116	ILE	2.9
1	A	1115	HIS	2.8
1	A	1096	LEU	2.7
1	A	1119	PHE	2.4
1	A	1112	LEU	2.3
1	A	1388	MET	2.3
1	A	1169	PHE	2.2
1	A	1099	PHE	2.1
1	A	1148	ILE	2.1
1	A	1095	LEU	2.1
1	A	1376	MET	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	B	602	1/1	0.99	0.27	-0.20	104,104,104,104	0
4	ZN	B	601	1/1	0.99	0.22	-	92,92,92,92	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.