



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:58 AM UTC

PDB ID : 4BK4 / pdb_00004bk4
Title : crystal structure of the human EphA4 ectodomain
Authors : Seiradake, E.; Schaupp, A.; del Toro Ruiz, D.; Kaufmann, R.; Mitakidis, N.; Harlos, K.; Aricescu, A.R.; Klein, R.; Jones, E.Y.
Deposited on : 2013-04-22
Resolution : 3.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

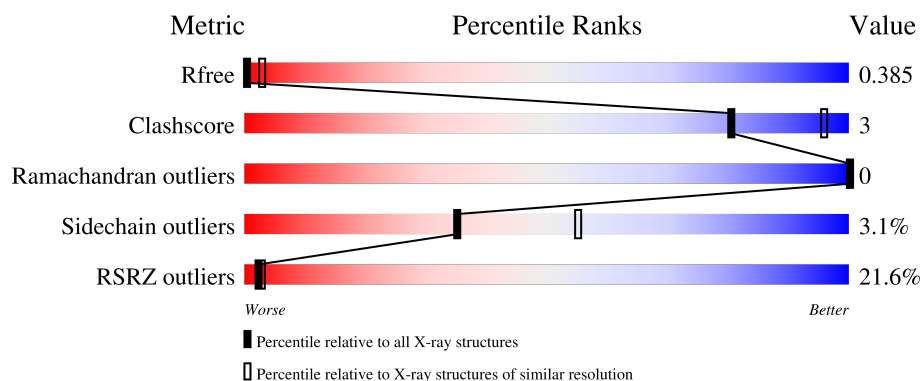
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	568	17% 83% 7% 10%
1	B	568	14% 46% 6% 47%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6344 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 EPHRIN TYPE-A RECEPTOR 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4002	2496	692	788	26			
1	B	300	Total	C	N	O	S	0	0	0
			2342	1460	398	462	22			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P54764
A	-10	GLY	-	expression tag	UNP P54764
A	-9	ILE	-	expression tag	UNP P54764
A	-8	LEU	-	expression tag	UNP P54764
A	-7	PRO	-	expression tag	UNP P54764
A	-6	SER	-	expression tag	UNP P54764
A	-5	PRO	-	expression tag	UNP P54764
A	-4	GLY	-	expression tag	UNP P54764
A	-3	MET	-	expression tag	UNP P54764
A	-2	PRO	-	expression tag	UNP P54764
A	-1	ALA	-	expression tag	UNP P54764
A	0	LEU	-	expression tag	UNP P54764
A	1	LEU	-	expression tag	UNP P54764
A	2	SER	-	expression tag	UNP P54764
A	3	LEU	-	expression tag	UNP P54764
A	4	VAL	-	expression tag	UNP P54764
A	5	SER	-	expression tag	UNP P54764
A	6	LEU	-	expression tag	UNP P54764
A	7	LEU	-	expression tag	UNP P54764
A	8	SER	-	expression tag	UNP P54764
A	9	VAL	-	expression tag	UNP P54764
A	10	LEU	-	expression tag	UNP P54764
A	11	LEU	-	expression tag	UNP P54764
A	12	MET	-	expression tag	UNP P54764
A	13	GLY	-	expression tag	UNP P54764

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	-	expression tag	UNP P54764
A	15	VAL	-	expression tag	UNP P54764
A	16	ALA	-	expression tag	UNP P54764
A	17	GLU	-	expression tag	UNP P54764
A	18	THR	-	expression tag	UNP P54764
A	19	GLY	-	expression tag	UNP P54764
A	548	GLY	-	expression tag	UNP P54764
A	549	THR	-	expression tag	UNP P54764
A	550	LYS	-	expression tag	UNP P54764
A	551	HIS	-	expression tag	UNP P54764
A	552	HIS	-	expression tag	UNP P54764
A	553	HIS	-	expression tag	UNP P54764
A	554	HIS	-	expression tag	UNP P54764
A	555	HIS	-	expression tag	UNP P54764
A	556	HIS	-	expression tag	UNP P54764
B	-11	MET	-	expression tag	UNP P54764
B	-10	GLY	-	expression tag	UNP P54764
B	-9	ILE	-	expression tag	UNP P54764
B	-8	LEU	-	expression tag	UNP P54764
B	-7	PRO	-	expression tag	UNP P54764
B	-6	SER	-	expression tag	UNP P54764
B	-5	PRO	-	expression tag	UNP P54764
B	-4	GLY	-	expression tag	UNP P54764
B	-3	MET	-	expression tag	UNP P54764
B	-2	PRO	-	expression tag	UNP P54764
B	-1	ALA	-	expression tag	UNP P54764
B	0	LEU	-	expression tag	UNP P54764
B	1	LEU	-	expression tag	UNP P54764
B	2	SER	-	expression tag	UNP P54764
B	3	LEU	-	expression tag	UNP P54764
B	4	VAL	-	expression tag	UNP P54764
B	5	SER	-	expression tag	UNP P54764
B	6	LEU	-	expression tag	UNP P54764
B	7	LEU	-	expression tag	UNP P54764
B	8	SER	-	expression tag	UNP P54764
B	9	VAL	-	expression tag	UNP P54764
B	10	LEU	-	expression tag	UNP P54764
B	11	LEU	-	expression tag	UNP P54764
B	12	MET	-	expression tag	UNP P54764
B	13	GLY	-	expression tag	UNP P54764
B	14	CYS	-	expression tag	UNP P54764
B	15	VAL	-	expression tag	UNP P54764

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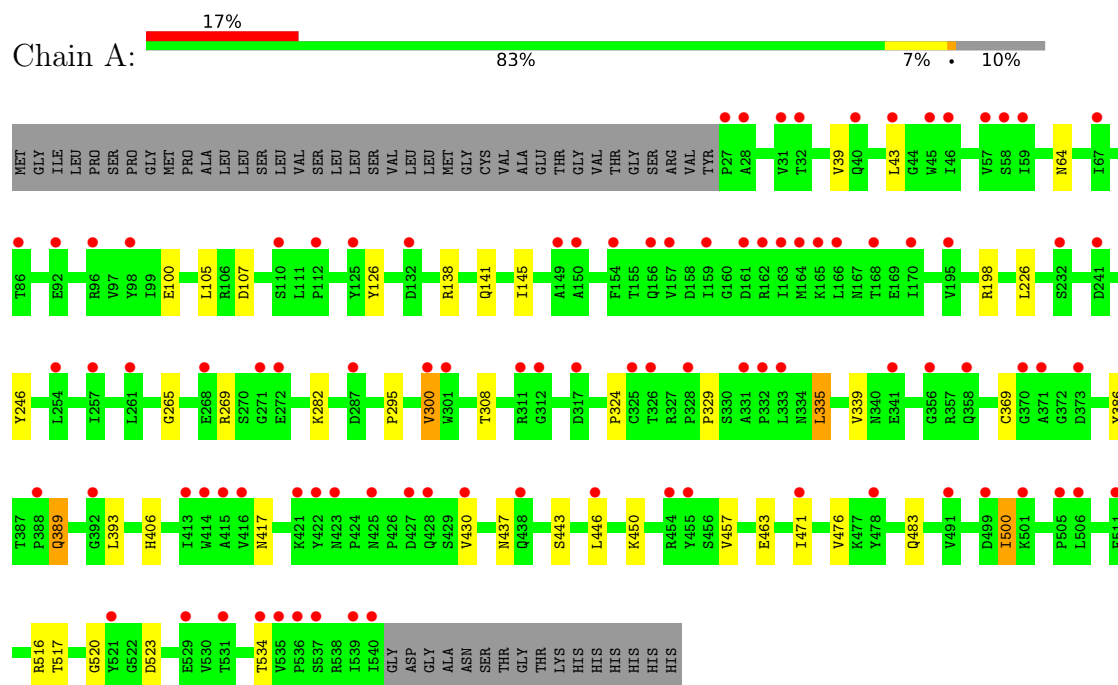
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Chain	Residue	Modelled	Actual	Comment	Reference
B	16	ALA	-	expression tag	UNP P54764
B	17	GLU	-	expression tag	UNP P54764
B	18	THR	-	expression tag	UNP P54764
B	19	GLY	-	expression tag	UNP P54764
B	548	GLY	-	expression tag	UNP P54764
B	549	THR	-	expression tag	UNP P54764
B	550	LYS	-	expression tag	UNP P54764
B	551	HIS	-	expression tag	UNP P54764
B	552	HIS	-	expression tag	UNP P54764
B	553	HIS	-	expression tag	UNP P54764
B	554	HIS	-	expression tag	UNP P54764
B	555	HIS	-	expression tag	UNP P54764
B	556	HIS	-	expression tag	UNP P54764

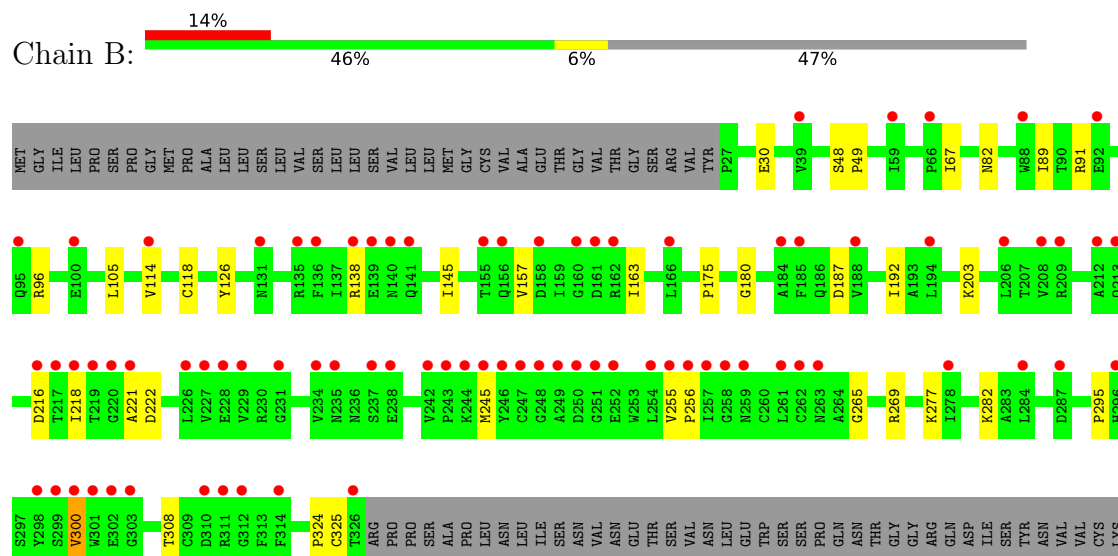
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: EPHRIN TYPE-A RECEPTOR 4



• Molecule 1: EPHRIN TYPE-A RECEPTOR 4



LYS	GLN	TYR	GLY
CYS	SER	ARG	THR
GLY	VAL	ILE	LYS
ALA	SER	VAL	HIS
GLY	VAL	ARG	HIS
ASP	THR	THR	HIS
PRO	VAL	ALA	HIS
SER	THR	ALA	HIS
LYS	THR	ARG	HIS
CYS	ASN	ARG	
ARG	GLN	THR	
PRO	ALA	ASP	
CYS	ALA	ILE	
GLY	PRO	LYS	
GLY	SER	GLY	
GLY	SER	LEU	
VAL	ILE	ASN	
HIS	ALA	PRO	
TYR	LEU	LEU	
THR	VAL	THR	
PRO	GLN	SER	
GLN	ALA	TYR	
LYS	LYS	VAL	
ASN	GLU	PHE	
GLY	VAL	HIS	
LEU	THR	VAL	
LYS	ARG	ARG	
THR	TYR	ALA	
THR	SER	ARG	
LYS	VAL	THR	
VAL	ALA	ALA	
SER	LEU	ALA	
ILE	ALA	GLY	
THR	TRP	TYR	
ASP	LEU	GLY	
LEU	GLU	ASP	
ALA	PRO	PHE	
HIS	ASP	SER	
THR	ALA	GLU	
THR	HIS	PRO	
ASN	ASN	LEU	
GLY	ASN	GLY	
THR	TYR	VAL	
PHE	ILE	THR	
GLU	THR	THR	
ILE	ILE	ASN	
TRP	TYR	THR	
ALA	GLU	VAL	
VAL	VAL	PRO	
ASN	LYS	SER	
GLY	TYR	ARG	
VAL	TYR	ILE	
LYS	GLU	ILE	
LYS	LYS	GLY	
TYR	ASP	ASP	
ASN	GLN	GLY	
PRO	ASN	ALA	
ASN	GLU	ASN	
PRO	ARG	SER	
ASP	SER	THR	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.89Å 166.89Å 192.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.18 – 3.65 48.18 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.18-3.65) 99.9 (48.18-3.65)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.67Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.349 , 0.386 0.382 , 0.385	Depositor DCC
R_{free} test set	1751 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	178.5	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6344	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.70	0/4088	1.10	3/5563 (0.1%)
1	B	0.70	0/2390	1.09	2/3240 (0.1%)
All	All	0.70	0/6478	1.09	5/8803 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	GLY	N-CA-C	5.90	119.11	110.80
1	B	138	ARG	CA-C-N	5.29	128.14	120.79
1	B	138	ARG	C-N-CA	5.29	128.14	120.79
1	A	269	ARG	CA-C-N	5.08	127.34	120.38
1	A	269	ARG	C-N-CA	5.08	127.34	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	4002	0	3865	15	0
1	B	2342	0	2236	17	0
All	All	6344	0	6101	32	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 3.

The worst 5 of 32 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:126:TYR:HB3	1:A:145:ILE:HD11	1.88	0.56
1:B:126:TYR:HB3	1:B:145:ILE:HD11	1.88	0.55
1:B:82:ASN:HB2	1:B:187:ASP:HB3	1.89	0.54
1:A:457:VAL:H	1:A:500:ILE:HG13	1.73	0.53
1:B:245:MET:HE2	1:B:256:PRO:HB3	1.91	0.53

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	512/568 (90%)	483 (94%)	29 (6%)	0	100	100
1	B	298/568 (52%)	280 (94%)	18 (6%)	0	100	100
All	All	810/1136 (71%)	763 (94%)	47 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 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 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	446/489 (91%)	429 (96%)	17 (4%)	29	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	259/489 (53%)	254 (98%)	5 (2%)	50 64
All	All	705/978 (72%)	683 (97%)	22 (3%)	35 55

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	500	ILE
1	B	67	ILE
1	A	534	THR
1	B	89	ILE
1	A	369	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	B	131	ASN
1	B	296	HIS
1	B	236	ASN
1	B	266	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th 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 ²)	Q<0.9
1	A	514/568 (90%)	1.14	95 (18%) 3 4	77, 116, 186, 300	0
1	B	300/568 (52%)	1.41	81 (27%) 1 2	65, 115, 228, 300	0
All	All	814/1136 (71%)	1.24	176 (21%) 2 3	65, 116, 212, 300	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	ASN	9.5
1	A	287	ASP	8.3
1	B	254	LEU	7.8
1	B	298	TYR	7.6
1	A	373	ASP	7.6

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.