

Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 02:05 pm BST

PDB ID : 5OM0

> Title : CH2 chimera of human 14-3-3 sigma with the Gli1 phosphopeptide around

: Sluchanko, N.N.; Tugaeva, K.V.; Greive, S.J.; Antson, A.A. Authors

2017-07-28 Deposited on

3.20 Å(reported) Resolution

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 A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4 Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

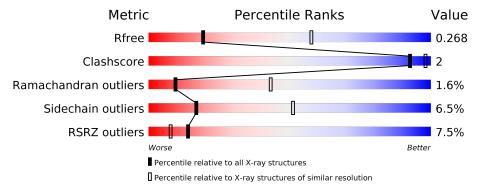
Validation Pipeline (wwPDB-VP) 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar resolution} \\ (\#{\rm Entries, resolution range(\AA)}) \end{array}$
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 >=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 <=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		
			3%		
1	A	248	84%	8%	8%
	_		10%		
	В	248	84%	7%	• 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TRS	В	303	-	-	-	X



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7214 atoms, of which 3559 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 14-3-3 protein sigma, Zinc finger protein GLI1.

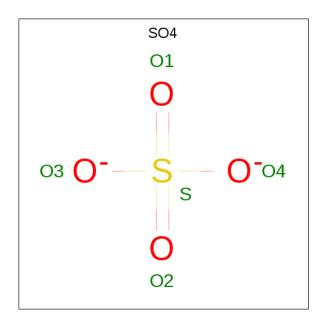
Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace		
1	A	228	Total 3566		H 1768	N 305	O 360	S 1	S 0	0	0	0
1	В	229	Total 3581		H 1767	N 312	O 364	P 1	S 9	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P31947
A	-1	PRO	-	expression tag	UNP P31947
A	0	HIS	_	expression tag	UNP P31947
A	77	ALA	LYS	engineered mutation	UNP P31947
A	232	GLY	_	linker	UNP P31947
A	233	SER	_	linker	UNP P31947
A	234	GLY	_	linker	UNP P31947
A	235	SER	_	linker	UNP P31947
A	236	LEU	_	linker	UNP P31947
В	-2	GLY	-	expression tag	UNP P31947
В	-1	PRO	_	expression tag	UNP P31947
В	0	HIS	_	expression tag	UNP P31947
В	77	ALA	LYS	engineered mutation	UNP P31947
В	232	GLY	_	linker	UNP P31947
В	233	SER	-	linker	UNP P31947
В	234	GLY		linker	UNP P31947
В	235	SER	-	linker	UNP P31947
В	236	LEU	-	linker	UNP P31947

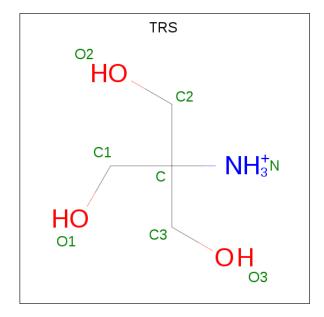
• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0
2	В	1	Total O S 5 4 1	0	0

• Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).





N	Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf			
	9	Λ	1	Total	С	Η	Ν	О	0	0	
	3 A	1	20	4	12	1	3	0			
	9	D	1	Total	С	Н	N	О	0	0	
	3	Ъ	1	20	4	12	1	3	0		

• Molecule 4 is water.

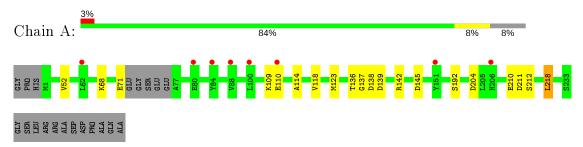
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
4	A	2	$\begin{array}{cc} \text{Total} & \text{O} \\ 2 & 2 \end{array}$	0	0
4	В	5	Total O 5 5	0	0



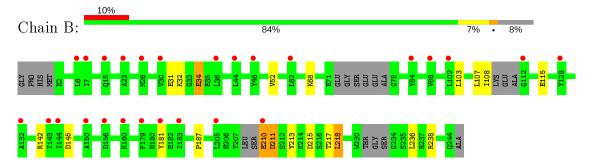
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 14-3-3 protein sigma, Zinc finger protein GLI1



• Molecule 1: 14-3-3 protein sigma, Zinc finger protein GLI1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants	110.43Å 110.43Å 174.11Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.00 - 3.20	Depositor
resolution (A)	47.82 - 3.14	EDS
% Data completeness	99.8 (47.00-3.20)	Depositor
(in resolution range)	99.5 (47.82-3.14)	EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.03 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.215 , 0.267	Depositor
It, It free	0.231 , 0.268	DCC
R_{free} test set	1035 reflections (9.04%)	wwPDB-VP
Wilson B-factor (\mathring{A}^2)	109.3	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41 , 121.7	EDS
L-test for twinning ²	$ < L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7214	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: TRS, SO4, SEP

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.53	0/1823	0.64	0/2452	
1	В	0.51	0/1826	0.63	0/2451	
All	All	0.52	0/3649	0.63	0/4903	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1798	1768	1779	2	0
1	В	1814	1767	1776	9	0
2	A	10	0	0	0	0
2	В	10	0	0	0	0
3	A	8	12	12	0	0
3	В	8	12	12	0	0
4	A	2	0	0	0	0
4	В	5	0	0	0	0
All	All	3655	3559	3579	11	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 2.



All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	Clash overlap (Å)
1:B:107:LEU:HD23	1:B:108:ILE:HG23	1.67	0.75
1:B:107:LEU:HD23	1:B:108:ILE:CG2	2.27	0.65
1:B:213:TYR:CZ	1:B:217:THR:HG21	2.38	0.57
1:B:107:LEU:HB3	1:B:108:ILE:HG23	1.91	0.53
1:B:103:LEU:O	1:B:107:LEU:HB2	2.14	0.47
1:A:114:ALA:O	1:A:118:VAL:HG23	2.14	0.47
1:B:32:LYS:HD3	1:B:32:LYS:N	2.32	0.45
1:B:181:TYR:CE2	1:B:187:PRO:HB3	2.52	0.44
1:A:218:LEU:O	1:A:218:LEU:HD12	2.19	0.42
1:B:210:GLU:HB3	1:B:211:ASP:H	1.69	0.42
1:B:218:LEU:O	1:B:218:LEU:HD12	2.19	0.41

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	Percentile	S
1	A	224/248 (90%)	215 (96%)	6 (3%)	3 (1%)	12 47	
1	В	218/248 (88%)	204 (94%)	10 (5%)	4 (2%)	8 41	
All	All	442/496 (89%)	419 (95%)	16 (4%)	7 (2%)	9 43	

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	GLY
1	В	34	GLU
1	В	31	GLU
1	В	211	ASP
1	A	211	ASP

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Mol	Chain	Res	Type
1	В	236	LEU
1	A	138	ASP

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	Percer	ntiles
1	A	192/205 (94%)	177 (92%)	15 (8%)	12	43
1	В	191/205 (93%)	181 (95%)	10 (5%)	23	59
All	All	383/410 (93%)	358 (94%)	25 (6%)	17	51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	68	LYS
1	A	71	GLU
1	A	109	LYS
1	A	110	GLU
1	A	123	MET
1	A	136	THR
1	A	139	ASP
1	A	142	ARG
1	A	145	ASP
1	A	192	SER
1	A	204	ASP
1	A	210	GLU
1	A	212	SER
1	A	218	LEU
1	В	34	GLU
1	В	52	VAL
1	В	68	LYS
1	В	115	GLU
1	В	142	ARG
1	В	145	ASP

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Mol	Chain	Res	Type
1	В	210	GLU
1	В	215	ASP
1	В	218	LEU
1	В	238	ARG

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Ros	Link	В	Bond lengths			Bond angles		
WIGI	Type	Chain	ites	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
1	SEP	В	240	1	8,9,10	1.56	2 (25%)	8,12,14	2.90	5 (62%)	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	${f Torsions}$	Rings
1	SEP	В	240	1	-	3/5/8/10	_

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	В	240	SEP	P-O1P	2.64	1.59	1.50
1	В	240	SEP	P-O2P	2.42	1.64	1.54



	All ((5)	bond	angle	outliers	are	listed	below
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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
1	В	240	SEP	O2P-P-OG	4.75	119.37	106.73
1	В	240	SEP	OG-CB-CA	4.56	112.58	108.14
1	В	240	SEP	OG-P-O1P	-2.99	98.09	106.47
1	В	240	SEP	O2P-P-O1P	2.83	121.78	110.68
1	В	240	SEP	P-OG-CB	-2.23	112.17	118.30

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	В	240	SEP	CB-OG-P-O2P
1	В	240	SEP	CB-OG-P-O3P
1	В	240	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Ty	Trees	Chain	Res	Link	Bond lengths			Bond angles		
	Type				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	В	302	-	4,4,4	0.47	0	6,6,6	0.38	0
2	SO4	В	301	_	4,4,4	0.50	0	6,6,6	0.51	0
3	TRS	A	303	-	7,7,7	0.31	0	9,9,9	0.32	0
3	TRS	В	303	_	7,7,7	0.26	0	9,9,9	0.24	0
2	SO4	A	302	-	4,4,4	0.18	0	6,6,6	0.34	0



Mol	Type	Chain	n Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	SO4	A	301	-	4,4,4	0.37	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

\mathbf{M}	ol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3	TRS	A	303	_	-	0/9/9/9	-
3	}	TRS	В	303	-	-	0/9/9/9	-

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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q<0.9
1	A	228/248 (91%)	0.53	8 (3%) 44 28	97, 124, 169, 223	0
1	В	228/248 (91%)	0.81	26 (11%) 5 3	107, 149, 197, 221	0
All	All	456/496 (91%)	0.67	34 (7%) 14 8	97, 136, 189, 223	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	112	GLY	5.1
1	В	88	VAL	4.7
1	В	7	ILE	3.4
1	В	183	ILE	3.4
1	В	128	TYR	3.2
1	A	110	GLU	3.1
1	A	88	VAL	3.1
1	В	48	TYR	2.7
1	В	6	LEU	2.7
1	В	23	ALA	2.7
1	В	30	VAL	2.7
1	В	210	GLU	2.6
1	В	102	LEU	2.6
1	В	156	ASP	2.5
1	A	206	HIS	2.5
1	В	181	TYR	2.5
1	В	144	ILE	2.4
1	В	132	ALA	2.4
1	A	84	TYR	2.4
1	В	205	LEU	2.3
1	В	84	TYR	2.3
1	A	62	LEU	2.3
1	В	143	ILE	2.3
1	В	36	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	В	26	MET	2.2
1	В	62	LEU	2.2
1	В	44	LEU	2.2
1	A	80	GLU	2.1
1	В	179	PHE	2.1
1	В	15	GLN	2.1
1	A	100	LEU	2.1
1	В	160	LYS	2.0
1	A	151	TYR	2.0
1	В	150	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	SEP	В	240	10/11	0.94	0.25	111,117,119,119	0

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
3	TRS	В	303	8/8	0.47	0.72	161,167,176,177	0
3	TRS	A	303	8/8	0.69	0.35	167,170,172,172	0
2	SO4	В	302	5/5	0.83	0.17	162,163,164,165	0
2	SO4	A	302	5/5	0.84	0.16	197,199,201,201	0
2	SO4	В	301	5/5	0.89	0.20	136,140,143,145	0
2	SO4	A	301	5/5	0.89	0.17	167,168,169,171	0



6.5 Other polymers (i)

There are no such residues in this entry.

