



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2025 – 09:46 PM EST

PDB ID : 9MK7
Title : Crystal structure of the WDR domain of WDR91 in complex with DR3634
Authors : Zeng, H.; Ahmad, H.; Dong, A.; Seitova, A.; Owen, D.; Arrowsmith, C.H.;
Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)
Deposited on : 2024-12-16
Resolution : 2.31 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.3

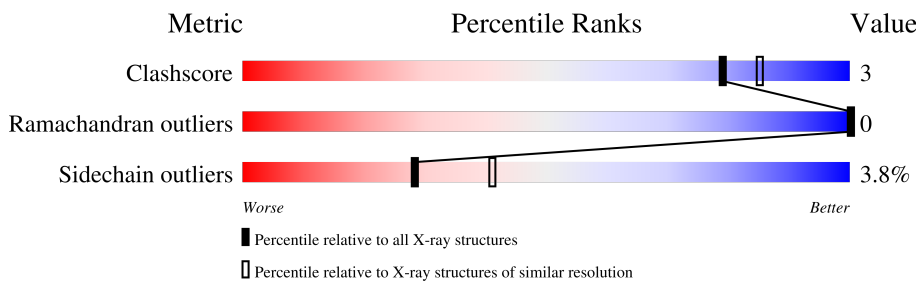
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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))
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	374	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2645 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.

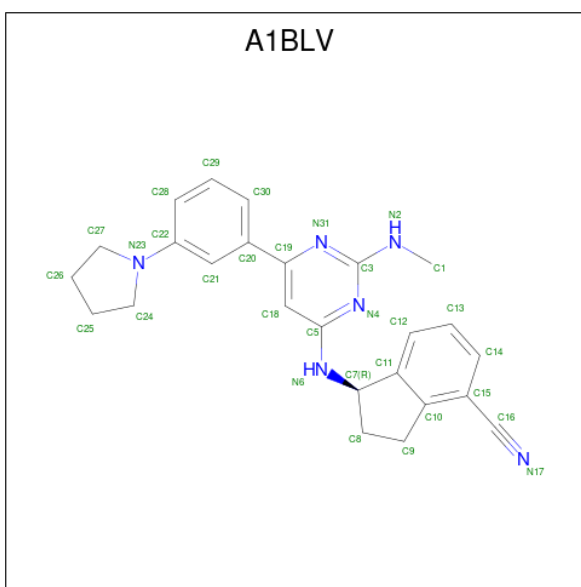
- Molecule 1 is a protein called WD repeat-containing protein 91.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	2537	1601	428	488	20	0	3	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	374	MET	-	expression tag	UNP A4D1P6
A	375	HIS	-	expression tag	UNP A4D1P6
A	376	HIS	-	expression tag	UNP A4D1P6
A	377	HIS	-	expression tag	UNP A4D1P6
A	378	HIS	-	expression tag	UNP A4D1P6
A	379	HIS	-	expression tag	UNP A4D1P6
A	380	HIS	-	expression tag	UNP A4D1P6
A	381	SER	-	expression tag	UNP A4D1P6
A	382	SER	-	expression tag	UNP A4D1P6
A	383	GLY	-	expression tag	UNP A4D1P6
A	384	ARG	-	expression tag	UNP A4D1P6
A	385	GLU	-	expression tag	UNP A4D1P6
A	386	ASN	-	expression tag	UNP A4D1P6
A	387	LEU	-	expression tag	UNP A4D1P6
A	388	TYR	-	expression tag	UNP A4D1P6
A	389	PHE	-	expression tag	UNP A4D1P6
A	390	GLN	-	expression tag	UNP A4D1P6
A	391	GLY	-	expression tag	UNP A4D1P6

- Molecule 2 is (1R)-1-({(6M)-2-(methylamino)-6-[3-(pyrrolidin-1-yl)phenyl]pyrimidin-4-yl}amino)-2,3-dihydro-1H-indene-4-carbonitrile (three-letter code: A1BLV) (formula: C₂₅H₂₆N₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			31	25	6		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	X	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	76	Total	O	0	0
			76	76		

i

Note EDS failed to run properly.

- Molecule 1: WD repeat-containing protein 91

M573	M574	M575	R601	Y604	E611	V619	I633	H634	K635	S647	Y658	S659	G660	P667	K668	G669	R670	L671	F672	T687	G709	P713	S732	K738	L743	M744	H745	LYS	ALA																				
HIS	HIS	HIS	HIS	HIS	SER	GLY	ARG	GLU	ASN	LEU	TYR	PHE	GLN	GLY	PRO	GLU	PRO	GLU	GLY	Q394	Q442	L456	R464	E481	M490	M495	V511	L519	THR	SER	SER	GLN	VAL	ASP	PHE	SER	SER	PRO	ASP	ILE	GLY	SER	LYS	GLY	M635	R641	L642	L643	G655

4 Data and refinement statistics [i](#)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.20Å 132.24Å 118.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.90 – 2.31	Depositor
% Data completeness (in resolution range)	99.5 (25.90-2.31)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.200 , 0.238	Depositor
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.190	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.029 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Total number of atoms	2645	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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

Bond lengths and bond angles in the following residue types are not validated in this section: A1BLV, UNX

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	0.55	2/2589 (0.1%)	0.78	2/3520 (0.1%)

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 outliers	#Planarity outliers
1	A	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	611	GLU	CD-OE2	6.04	1.32	1.25
1	A	660	GLY	CA-C	5.55	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	LEU	N-CA-CB	-6.18	98.03	110.40
1	A	687	THR	CA-CB-OG1	-6.00	96.39	109.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	464	ARG	Sidechain
1	A	658	TYR	Peptide
1	A	668	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	670	ARG	Sidechain

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	2537	0	2417	13	0
2	A	31	0	0	0	0
3	A	1	0	0	0	0
4	A	76	0	0	0	0
All	All	2645	0	2417	13	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 13 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:573:ASN:ND2	1:A:575:ASN:OD1	2.02	0.92
1:A:541:ARG:HD3	1:A:555[A]:GLN:NE2	2.00	0.77
1:A:541:ARG:HD3	1:A:555[A]:GLN:HE22	1.57	0.67
1:A:634:HIS:O	1:A:635:LYS:HG3	2.02	0.59
1:A:464:ARG:HD3	1:A:481:GLU:OE2	2.09	0.52

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	336/374 (90%)	326 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	266/317 (84%)	255 (96%)	11 (4%)	26	38

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	647	SER
1	A	672	PHE
1	A	743	LEU
1	A	687	THR
1	A	555[A]	GLN

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

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

Of 2 ligands modelled in this entry, 1 is unknown - leaving 1 for Mogul analysis.

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1BLV	A	801	-	35,35,35	0.38	0	43,49,49	0.58	1 (2%)

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	Torsions	Rings
2	A1BLV	A	801	-	-	0/16/32/32	0/5/5/5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	801	A1BLV	C15-C10-C11	-2.07	119.22	120.24

There are no chirality outliers.

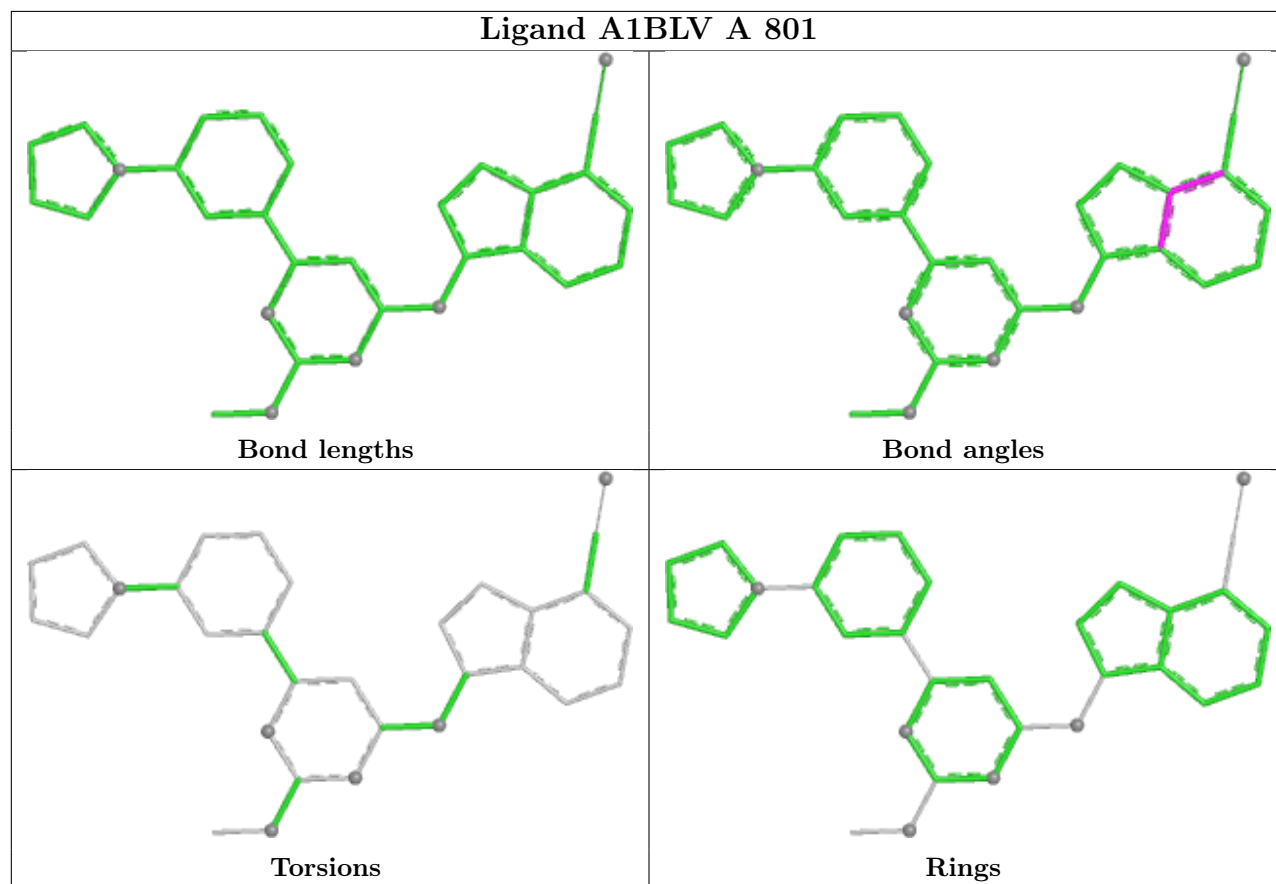
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

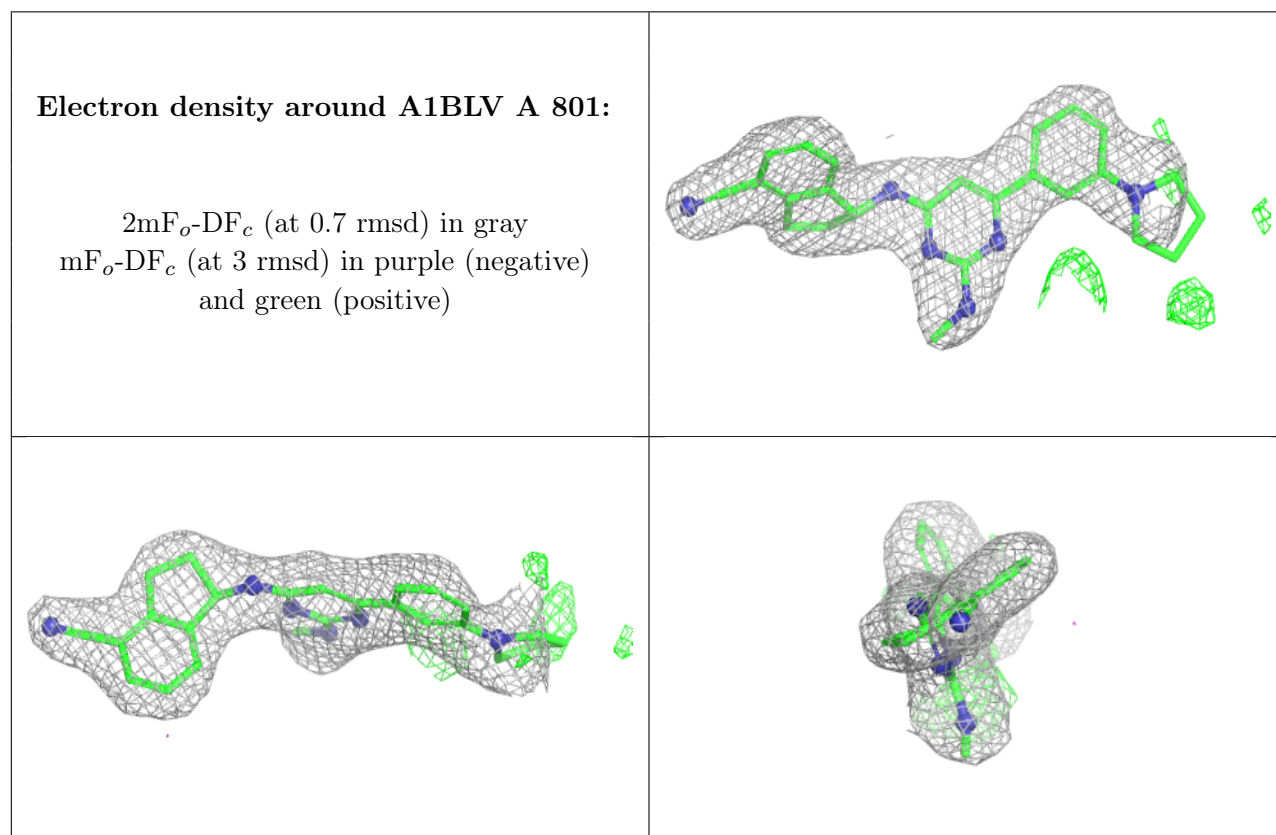
6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers

EDS failed to run properly - this section is therefore empty.