



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:59 PM GMT

PDB ID : 1XOI  
Title : Human Liver Glycogen Phosphorylase A complexed with Chloroindoloyl glycine amide  
Authors : Wright, S.W.; Rath, V.L.; Gibbs, E.M.; Treadway, J.L.  
Deposited on : 2004-10-06  
Resolution : 2.10 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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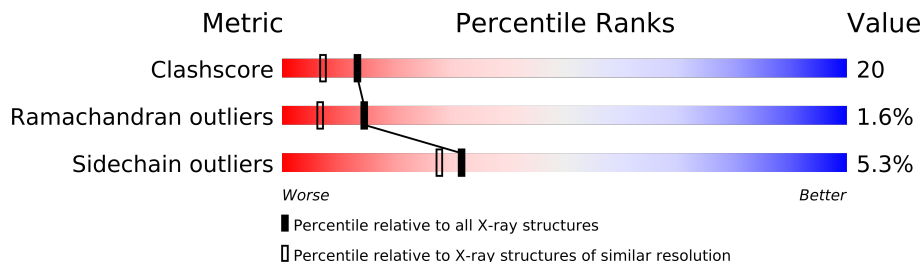
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	846	
1	B	846	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 13762 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

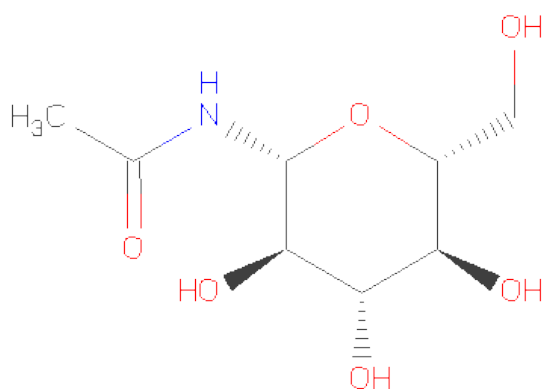
- Molecule 1 is a protein called Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	804	Total	C	N	O	S	0	0	0
			6508	4180	1107	1192	29			
1	B	804	Total	C	N	O	S	0	0	0
			6508	4180	1107	1192	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	ALA	GLY	CONFLICT	UNP P06737
B	1323	ALA	GLY	CONFLICT	UNP P06737

- Molecule 2 is SUGAR (1-N-ACETYL-BETA-D-GLUCOSAMINE) (three-letter code: NBG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



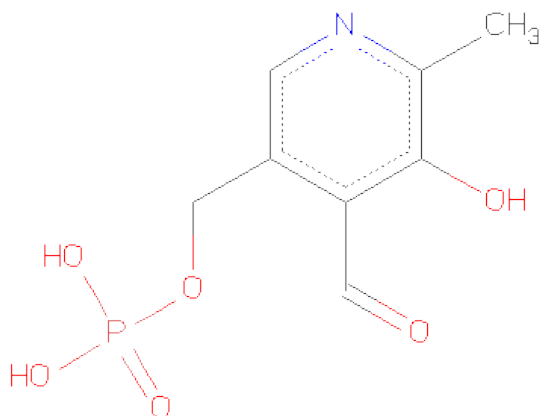
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		

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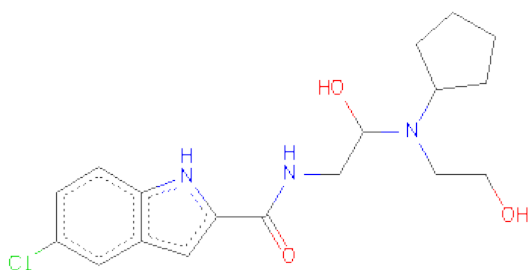
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is 5-CHLORO-1H-INDOLE-2-CARBOXYLICACID{[CYCLOPENTYL-(2-HYDROXY-ETHYL)-CARBAMOYL]-METHYL}-AMIDE (three-letter code: 288) (formula:  $C_{18}H_{24}ClN_3O_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			25	18	1	3	3		
4	B	1	Total	C	Cl	N	O	0	0
			25	18	1	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	323	Total	O	0	0
			323	323		
5	B	313	Total	O	0	0
			313	313		

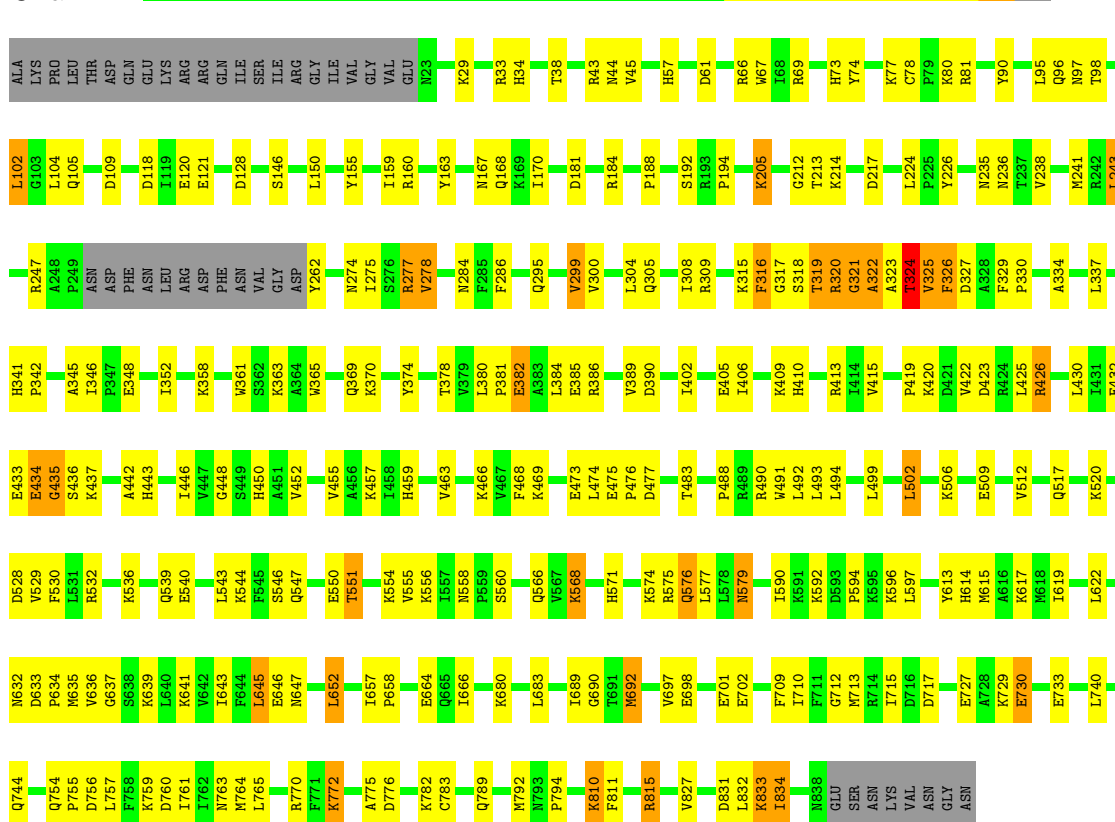
### 3 Residue-property plots

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.

Note EDS was not executed.

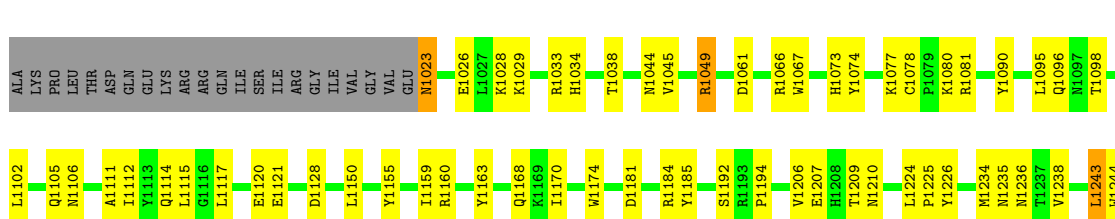
- Molecule 1: Glycogen phosphorylase, liver form

Chain A:



- Molecule 1: Glycogen phosphorylase, liver form

Chain B:



K1759	L1640	L1543	K1437	P1342	R1247
D1760	K1641	L1543		A1345	A1248
	V1642	S1546	A1442	I1346	P1249
M1763	I1643	Q1547	H1443	E1348	ASN
M1764	L1644	E1550	I1446	I1352	PHE
R1770	L1645	T1551	V1447		ASN
F1771	E1646		G1448		LEU
K1772	M1647	V1555	S1449		ASP
		I1557	A1451		ARG
A1775	S1651	K1556	H1450		PHE
D1776	L1652	I1557	V1452		ASN
	I1657	N1558			VAL
C1783	P1658	P1559	V1455		GLY
		S1560	A1456		ASP
K1786	I1666	S1561	K1457		Y1262
		M1562	I1458		
Q1789	S1674		H1459		
		Q1566			
M1792	K1680	V1567	I1462		N1274
N1793		K1568	V1463		I1275
P1794	L1683				S1276
		H1571	K1466		R1277
L1802	I1689		V1467		V1278
	G1690	K1574	F1468		
K1810	T1691	R1575	K1469		F1286
	M1692	Q1576			
D1814	V1697	L1577	E1473		Q1295
R1815	I1578	N1579	L1474		V1299
	E1698		E1475		V1300
K1818			P1476		
	E1701	K1592	D1477		L1304
P1829	E1702	D1593			
S1830	F1709	P1594	P1488		I1308
D1831	I1710	K1595			
K1833		K1596	W1491		K1312
I1834	I1715	L1597	L1492		A1313
S1835		F1598	L1493		S1314
L1836		V1599	L1494		K1315
S1837	E1727	P1600			F1316
N1838	A1728	R1601	L1499		G1317
	K1729				S1318
	E1730	G1607	L1502		T1319
					R1320
GLU					G1321
SER	E1733	Y1613	K1506		A1322
ASN	A1734	H1614			A1323
LYS	L1735	M1615	E1509		T1324
VAL	P1736				V1325
ASN		I1619	V1512		F1326
GLY		T1620			D1327
ASN	L1740	K1621	D1528		A1328
		L1622	V1529		F1329
	Q1744		F1530		P1330
			L1531		
P1752		N1632	R1532		A1334
K1753		D1633			
Q1754		P1634	K1536		L1337
P1755		M1635			
D1756		V1636			L1337
L1757			Q1539		G1435
F1758		K1639	E1540		H1341

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.91Å 123.91Å 123.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	99.00 – 2.10	Depositor
% Data completeness (in resolution range)	92.6 (99.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.5	Depositor
R, $R_{free}$	0.206 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 288, NBG, PLP

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	0.36	0/6653	0.61	0/8998
1	B	0.37	0/6653	0.62	1/8998 (0.0%)
All	All	0.36	0/13306	0.61	1/17996 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1323	ALA	N-CA-C	-5.38	96.46	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6508	0	6518	278	0
1	B	6508	0	6518	264	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
3	A	15	0	7	1	0
3	B	15	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	25	0	22	0	0
4	B	25	0	22	3	0
5	A	323	0	0	51	0
5	B	313	0	0	35	0
All	All	13762	0	13124	536	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 536 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1434:GLU:H	1:B:1434:GLU:CD	1.62	0.98
1:A:96:GLN:HE21	1:A:105:GLN:HE22	1.10	0.98
1:A:236:ASN:HB3	1:A:834:ILE:HB	1.46	0.97
1:A:434:GLU:CD	1:A:434:GLU:H	1.65	0.96
1:B:1168:GLN:HE21	1:B:1647:ASN:H	1.03	0.96

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	800/846 (95%)	748 (94%)	39 (5%)	13 (2%)	14	7
1	B	800/846 (95%)	749 (94%)	38 (5%)	13 (2%)	14	7
All	All	1600/1692 (95%)	1497 (94%)	77 (5%)	26 (2%)	14	7

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	PHE
1	A	318	SER
1	B	1317	GLY
1	B	1320	ARG

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Mol	Chain	Res	Type
1	B	1322	ALA

### 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	702/739 (95%)	663 (94%)	39 (6%)	30	25
1	B	702/739 (95%)	666 (95%)	36 (5%)	33	29
All	All	1404/1478 (95%)	1329 (95%)	75 (5%)	32	28

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	692	MET
1	B	1078	CYS
1	B	1730	GLU
1	A	730	GLU
1	A	833	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	614	HIS
1	B	1073	HIS
1	B	1576	GLN
1	A	754	GLN
1	B	1032	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	PLP	A	860	-	14,15,16	1.87	5 (35%)	20,22,23	1.19	2 (10%)
2	NBG	A	861	-	15,15,15	1.48	3 (20%)	21,21,21	1.35	2 (9%)
4	288	A	862	-	27,27,27	2.24	3 (11%)	37,37,37	1.84	5 (13%)
3	PLP	B	1860	-	14,15,16	1.70	1 (7%)	20,22,23	1.20	2 (10%)
2	NBG	B	1861	-	15,15,15	1.77	3 (20%)	21,21,21	1.30	2 (9%)
4	288	B	1862	-	27,27,27	2.26	2 (7%)	37,37,37	1.82	4 (10%)

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
3	PLP	A	860	-	-	0/6/6/8	0/1/1/1
2	NBG	A	861	-	-	0/5/26/26	0/1/1/1
4	288	A	862	-	1/1/4/5	1/16/27/27	0/1/3/3
3	PLP	B	1860	-	-	0/6/6/8	0/1/1/1
2	NBG	B	1861	-	-	0/5/26/26	0/1/1/1
4	288	B	1862	-	1/1/4/5	1/16/27/27	0/1/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1862	288	O17-C15	-10.36	1.21	1.41
4	A	862	288	O17-C15	-9.81	1.22	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1860	PLP	C3-C2	-4.93	1.37	1.40
3	A	860	PLP	C3-C2	-4.69	1.37	1.40
2	B	1861	NBG	C2-C1	4.46	1.57	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1862	288	O17-C15-C14	6.76	119.34	107.77
4	A	862	288	O17-C15-C14	6.71	119.26	107.77
4	B	1862	288	C14-C15-N16	6.53	120.42	110.73
4	A	862	288	C14-C15-N16	6.17	119.88	110.73
2	A	861	NBG	C5-O5-C1	4.56	118.83	112.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	862	288	C15
4	B	1862	288	C15

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1862	288	N16-C15-C14-N12
4	A	862	288	N16-C15-C14-N12

There are no ring outliers.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.