



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:48 PM GMT

PDB ID : 1VAO  
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE  
Authors : Mattevi, A.  
Deposited on : 1997-04-10  
Resolution : 2.50 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](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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

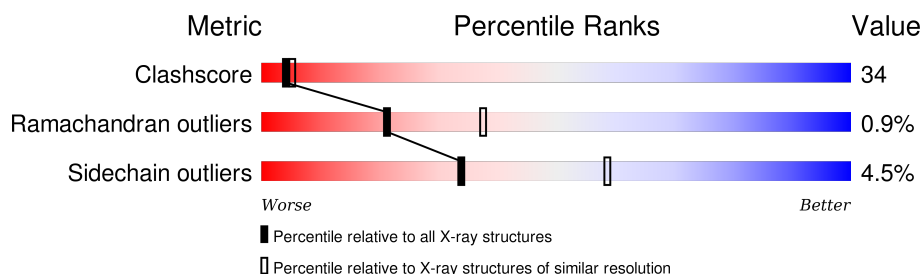
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9134 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 VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			
1	B	550	Total	C	N	O	S	36	0	0
			4351	2793	744	790	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

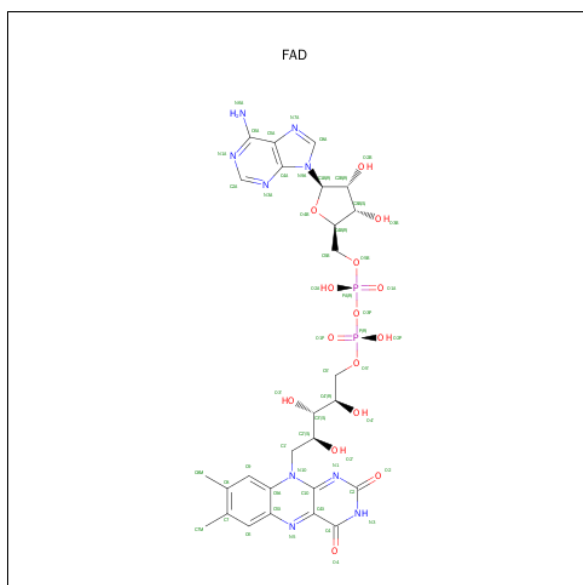


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 53 27 9 15 2	0	0
4	B	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 5 is water.

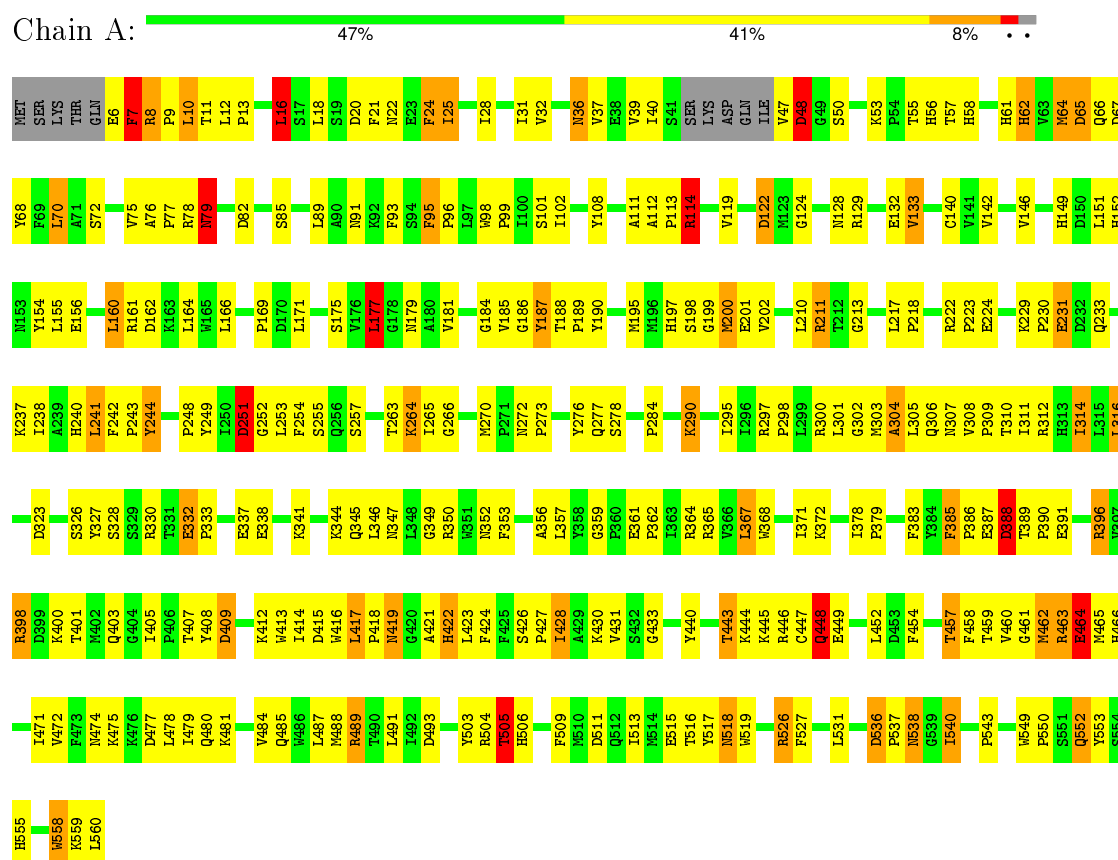
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0
5	B	150	Total O 150 150	0	0

### 3 Residue-property plots

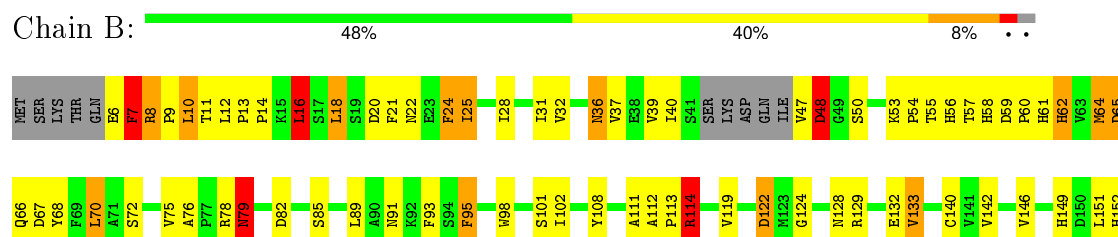
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: VANILLYL-ALCOHOL OXIDASE



#### • Molecule 1: VANILLYL-ALCOHOL OXIDASE



Q480	K481	R482	K483	V484	Q485	V486	L487	V488	R489	T490	L491	T492	D493	M500	Y503	R504	R506	F509	N510	D511	Q512	I513	N514	E515	T516	N517	N518	N519	N526	F527	L531	D536	P537	N538	Q539	I540	P543	N549	P550	S551	Q552	Y553	H555	N558	K559	L560						
Q404	I405	P406	T407	V408	D409	K412	W413	I414	D415	W416	L417	P418	N419	G420	A421	H422	L423	F424	I428	A429	K430	V431	S432	G433	Y440	T443	K444	K445	R446	C447	Q449	E449	F454	T457	F458	T459	V460	G461	M462	R463	E464	M465	H466	I471	V472	N474	K475	K476	D477	L478	I479	
S328	S329	R330	T331	E332	P333	E337	E338	K341	K344	Q345	L346	N347	L348	G349	R350	N351	N352	F353	A356	L357	T358	G359	P360	E361	P362	T363	R364	R365	T366	K368	L371	K372	P379	F383	T384	P386	E387	D388	T389	P390	R396	V397	R398	D399	K400	T401	N402	Q403				
P243	Y244	G245	F246	G247	P248	Y249	I250	D251	G252	L253	P254	S255	I261	T263	K264	I265	G266	M270	P271	N272	P273	Y276	Q277	S278	T288	P289	Y290	M295	I296	T296	R297	P298	L299	R300	L301	G302	P303	A304	L305	Q306	P307	V308	P309	T310	L311	R312	R313	L314	L315	L316	K324	Y327
R153	Y154	L155	E156	L160	R161	D162	K163	L164	W165	L166	P169	D170	L171	S175	V176	L177	G178	N179	A180	V181	G184	V185	G186	T187	T188	P189	Y190	M195	I196	H197	S198	G199	M200	E201	V202	L210	R211	R222	P223	E224	K229	P230	E231	D232	Q233	I238	K239	H240	L241	F242		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.24Å 130.24Å 133.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	98.9 (30.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.88	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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: CL, FAD, ACT

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	0.76	3/4470 (0.1%)	1.68	89/6075 (1.5%)
1	B	0.76	3/4470 (0.1%)	1.68	89/6075 (1.5%)
All	All	0.76	6/8940 (0.1%)	1.68	178/12150 (1.5%)

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	2	0
1	B	2	0
All	All	4	0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	PHE	CE1-CZ	7.54	1.51	1.37
1	B	7	PHE	CE1-CZ	7.50	1.51	1.37
1	A	7	PHE	CD1-CE1	7.35	1.53	1.39
1	B	7	PHE	CD1-CE1	7.35	1.53	1.39
1	A	7	PHE	CD2-CE2	6.36	1.51	1.39

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	ARG	NE-CZ-NH2	-19.95	110.33	120.30
1	A	526	ARG	NE-CZ-NH2	-19.88	110.36	120.30
1	B	526	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	A	526	ARG	NE-CZ-NH1	13.87	127.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	ARG	NE-CZ-NH1	12.01	126.31	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	7	PHE	CA
1	A	332	GLU	CA
1	B	7	PHE	CA
1	B	332	GLU	CA

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	4351	0	4288	307	1
1	B	4351	0	4288	286	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	29	6	0
4	B	53	0	29	5	0
5	A	166	0	0	19	0
5	B	150	0	0	11	0
All	All	9134	0	8640	580	1

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 34.

The worst 5 of 580 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)
4:B:600:FAD:H51A	4:B:600:FAD:H8A	1.22	1.16
4:A:600:FAD:H8A	4:A:600:FAD:H51A	1.23	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:HD21	1:B:253:LEU:HD21	1.11	1.07
1:A:211:ARG:HG3	1:B:519:TRP:CZ3	1.99	0.98
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.46	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ARG:NH2	1:A:330:ARG:NH2[2_765]	2.15	0.05

## 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	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	21	37
1	B	546/560 (98%)	503 (92%)	38 (7%)	5 (1%)	21	37
All	All	1092/1120 (98%)	1006 (92%)	76 (7%)	10 (1%)	21	37

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	B	48	ASP
1	A	199	GLY
1	A	388	ASP
1	B	199	GLY

### 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	470/482 (98%)	449 (96%)	21 (4%)	34	59
1	B	470/482 (98%)	449 (96%)	21 (4%)	34	59
All	All	940/964 (98%)	898 (96%)	42 (4%)	34	59

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	TYR
1	B	64	MET
1	B	464	GLU
1	A	505	THR
1	B	7	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	552	GLN
1	B	66	GLN
1	B	520	ASN
1	B	56	HIS
1	B	79	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
4	FAD	A	600	1	48,58,58	0.97	2 (4%)	54,89,89	1.56	6 (11%)
2	ACT	A	601	-	1,3,3	3.81	1 (100%)	0,3,3	0.00	-
4	FAD	B	600	1	48,58,58	0.97	2 (4%)	54,89,89	1.55	6 (11%)
2	ACT	B	601	-	1,3,3	3.87	1 (100%)	0,3,3	0.00	-

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
4	FAD	A	600	1	-	0/30/50/50	0/6/6/6
2	ACT	A	601	-	-	0/0/0/0	0/0/0/0
4	FAD	B	600	1	-	0/30/50/50	0/6/6/6
2	ACT	B	601	-	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	FAD	O5B-C5B	-3.38	1.31	1.44
4	B	600	FAD	O5B-C5B	-3.36	1.31	1.44
4	A	600	FAD	C4-N3	3.37	1.39	1.33
4	B	600	FAD	C4-N3	3.37	1.39	1.33
2	A	601	ACT	CH3-C	3.81	1.54	1.48

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C4X-C4-N3	-5.25	116.42	123.59
4	B	600	FAD	C4X-C4-N3	-5.22	116.46	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	FAD	C4X-C10-N10	-2.61	118.98	120.52
4	B	600	FAD	C4X-C10-N10	-2.58	119.00	120.52
4	B	600	FAD	O4B-C4B-C5B	-2.02	102.09	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	FAD	6	0
4	B	600	FAD	5	0

## 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 ⓘ

### 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.