



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:32 PM GMT

PDB ID : 1B7H
Title : OLIGO-PEPTIDE BINDING PROTEIN COMPLEXED WITH LYSYL-NO
RLEUCYL-LYSINE
Authors : Davies, T.G.; Tame, J.R.H.
Deposited on : 1998-11-16
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

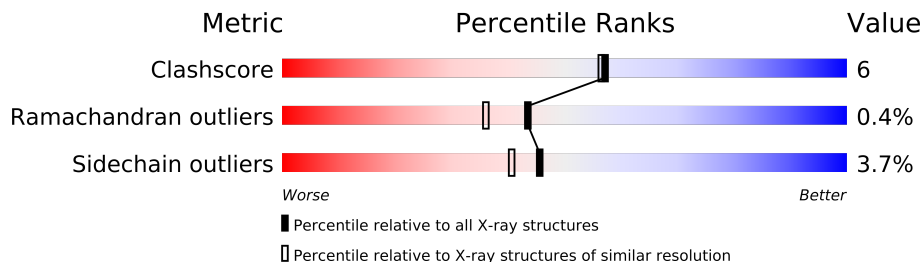
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. 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	517	
2	B	3	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4467 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 PERIPLASMIC OLIGO-PEPTIDE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	9	0	0
			4165	2666	700	794	5			

- Molecule 2 is a protein called LYS-NLE-LYS PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			27	18	5	4			

- Molecule 3 is URANIUM ATOM (three-letter code: U1) (formula: U).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	U	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	270	Total	O	0	0
			270	270		
4	B	3	Total	O	0	0
			3	3		

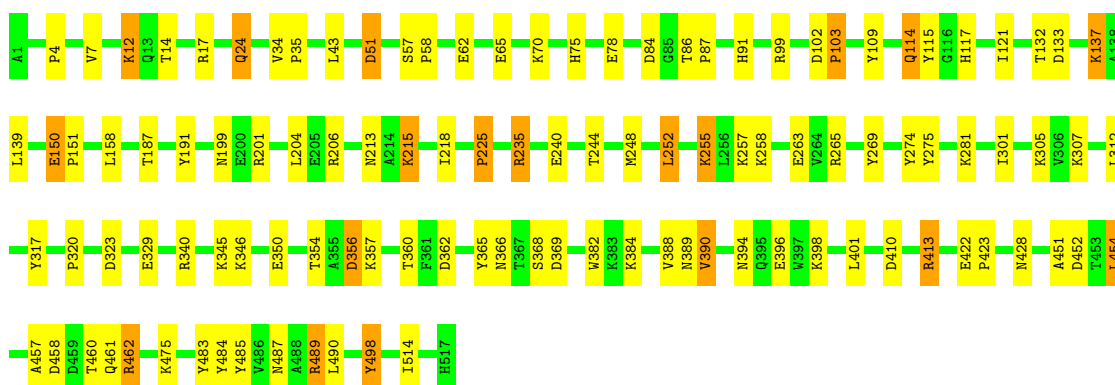
3 Residue-property plots

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: PERIPLASMIC OLIGO-PEPTIDE BINDING PROTEIN

Chain A: 



• Molecule 2: LYS-NLE-LYS PEPTIDE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2 A	Depositor
Cell constants a, b, c, α , β , γ	104.01Å 74.08Å 69.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.0 (20.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4467	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: U1, NLE

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	0.83	4/4276 (0.1%)	1.78	63/5830 (1.1%)
2	B	1.12	0/17	1.73	0/16
All	All	0.83	4/4293 (0.1%)	1.78	63/5846 (1.1%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLU	CD-OE1	-7.33	1.17	1.25
1	A	150	GLU	CG-CD	6.48	1.61	1.51
1	A	329	GLU	CG-CD	6.37	1.61	1.51
1	A	384	LYS	CD-CE	-5.70	1.37	1.51

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ARG	NE-CZ-NH1	30.58	135.59	120.30
1	A	413	ARG	NE-CZ-NH2	-28.36	106.12	120.30
1	A	201	ARG	CD-NE-CZ	26.06	160.09	123.60
1	A	356	ASP	CB-CG-OD1	-23.11	97.50	118.30
1	A	356	ASP	CB-CG-OD2	22.51	138.56	118.30
1	A	489	ARG	NE-CZ-NH1	19.86	130.23	120.30
1	A	235	ARG	CD-NE-CZ	11.90	140.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	GLN	CA-CB-CG	11.12	137.87	113.40
1	A	51	ASP	CB-CG-OD2	10.62	127.86	118.30
1	A	410	ASP	CB-CG-OD2	10.60	127.84	118.30
1	A	410	ASP	CB-CG-OD1	-9.91	109.39	118.30
1	A	102	ASP	CB-CG-OD2	8.37	125.83	118.30
1	A	12	LYS	CA-CB-CG	8.28	131.61	113.40
1	A	452	ASP	CB-CG-OD1	8.13	125.62	118.30
1	A	340	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	A	489	ARG	CD-NE-CZ	7.70	134.37	123.60
1	A	484	TYR	CB-CG-CD1	-7.62	116.43	121.00
1	A	265	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	99	ARG	NE-CZ-NH1	-7.47	116.57	120.30
1	A	329	GLU	OE1-CD-OE2	7.46	132.25	123.30
1	A	457	ALA	N-CA-CB	-7.05	100.24	110.10
1	A	317	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	A	102	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	A	235	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	A	201	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	17	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	A	369	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	133	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	489	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	51	ASP	CB-CG-OD1	-6.35	112.59	118.30
1	A	99	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	84	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	422	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	A	485	TYR	CA-CB-CG	6.15	125.09	113.40
1	A	489	ARG	NH1-CZ-NH2	-6.14	112.65	119.40
1	A	275	TYR	CA-CB-CG	-6.07	101.86	113.40
1	A	345	LYS	CD-CE-NZ	6.07	125.67	111.70
1	A	362	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	62	GLU	OE1-CD-OE2	5.89	130.37	123.30
1	A	109	TYR	CB-CG-CD1	5.87	124.52	121.00
1	A	498	TYR	CB-CG-CD1	5.83	124.50	121.00
1	A	366	ASN	N-CA-CB	5.80	121.03	110.60
1	A	281	LYS	CA-CB-CG	5.79	126.15	113.40
1	A	103	PRO	N-CA-CB	5.79	110.25	103.30
1	A	475	LYS	CD-CE-NZ	5.76	124.94	111.70
1	A	329	GLU	CG-CD-OE1	-5.70	106.91	118.30
1	A	133	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	274	TYR	CZ-CE2-CD2	-5.63	114.74	119.80
1	A	452	ASP	CB-CG-OD2	-5.62	113.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	TYR	CB-CG-CD2	5.59	124.36	121.00
1	A	320	PRO	N-CA-CB	5.47	109.87	103.30
1	A	91	HIS	CA-CB-CG	-5.44	104.35	113.60
1	A	201	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	462	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	158	LEU	CB-CA-C	-5.25	100.22	110.20
1	A	390	VAL	N-CA-CB	-5.25	99.96	111.50
1	A	485	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	A	461	GLN	CG-CD-OE1	-5.11	111.39	121.60
1	A	109	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	317	TYR	CB-CG-CD1	5.07	124.04	121.00
1	A	396	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	191	TYR	CB-CG-CD1	5.04	124.03	121.00
1	A	12	LYS	CB-CA-C	5.02	120.45	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	GLN	Mainchain

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	4165	0	4076	53	0
2	B	27	0	38	2	0
3	A	2	0	0	0	0
4	A	270	0	0	11	0
4	B	3	0	0	0	0
All	All	4467	0	4114	53	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 6.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:199:ASN:CB	4:A:779:HOH:O	1.87	1.19
1:A:451:ALA:CA	4:A:754:HOH:O	1.78	1.16
1:A:451:ALA:HA	4:A:754:HOH:O	1.29	1.15
1:A:199:ASN:CA	4:A:779:HOH:O	1.93	1.14
1:A:215:LYS:HE3	4:A:777:HOH:O	0.82	1.00
1:A:451:ALA:O	4:A:754:HOH:O	1.80	0.99
1:A:199:ASN:HA	4:A:779:HOH:O	1.62	0.89
1:A:199:ASN:HB3	4:A:779:HOH:O	1.58	0.87
1:A:252:LEU:HA	1:A:255:LYS:HE2	1.58	0.84
1:A:401:LEU:HD22	2:B:2:NLE:HD2	1.67	0.76
1:A:451:ALA:C	4:A:754:HOH:O	1.96	0.74
1:A:215:LYS:CE	4:A:777:HOH:O	1.66	0.65
1:A:255:LYS:H	1:A:255:LYS:NZ	1.95	0.64
1:A:150:GLU:HB3	1:A:151:PRO:HD2	1.82	0.61
1:A:255:LYS:H	1:A:255:LYS:HZ3	1.49	0.60
1:A:218:ILE:HD11	1:A:514:ILE:HG12	1.84	0.59
1:A:137:LYS:HG3	1:A:139:LEU:HD23	1.87	0.56
1:A:252:LEU:HA	1:A:255:LYS:CE	2.35	0.55
1:A:24:GLN:O	1:A:398:LYS:HE3	2.09	0.53
1:A:199:ASN:ND2	4:A:779:HOH:O	2.41	0.52
1:A:218:ILE:CD1	1:A:514:ILE:HG12	2.39	0.52
1:A:307:LYS:HE3	1:A:483:TYR:OH	2.09	0.51
1:A:382:TRP:HB3	1:A:388:VAL:HG22	1.92	0.51
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.48	0.49
1:A:365:TYR:O	1:A:394:ASN:HA	2.13	0.49
1:A:458:ASP:OD2	1:A:460:THR:HB	2.12	0.49
1:A:117:HIS:ND1	1:A:454:LEU:HD11	2.27	0.49
1:A:244:THR:HG23	1:A:490:LEU:HB2	1.95	0.49
1:A:401:LEU:HD22	2:B:2:NLE:CD	2.40	0.49
1:A:4:PRO:O	1:A:7:VAL:HG13	2.13	0.49
1:A:360:THR:HA	1:A:389:ASN:O	2.13	0.48
1:A:43:LEU:O	1:A:187:THR:HB	2.14	0.47
1:A:323:ASP:O	1:A:423:PRO:HD3	2.15	0.47
1:A:235:ARG:HD3	1:A:240:GLU:OE1	2.14	0.47
1:A:248:MET:CE	1:A:248:MET:HA	2.44	0.47
1:A:354:THR:OG1	1:A:357:LYS:N	2.48	0.47
1:A:114:GLN:HA	1:A:121:ILE:HG21	1.97	0.46
1:A:263:GLU:O	1:A:490:LEU:HA	2.15	0.46
1:A:346:LYS:HE2	1:A:350:GLU:OE2	2.15	0.46
1:A:301:ILE:HA	1:A:305:LYS:HG3	1.97	0.45
1:A:137:LYS:HB3	1:A:137:LYS:HE2	1.57	0.45
1:A:269:TYR:HB2	1:A:487:ASN:HB2	1.99	0.45
1:A:489:ARG:HD2	1:A:498:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:LEU:HD21	1:A:204:LEU:HD22	2.01	0.42
1:A:206:ARG:HD3	1:A:213:ASN:OD1	2.19	0.42
1:A:57:SER:HB3	1:A:58:PRO:HD2	2.00	0.42
1:A:51:ASP:HB3	1:A:57:SER:OG	2.20	0.42
1:A:34:VAL:HB	1:A:35:PRO:HD3	2.02	0.42
1:A:269:TYR:CG	1:A:487:ASN:HB2	2.55	0.41
1:A:240:GLU:O	1:A:240:GLU:HG2	2.19	0.41
1:A:12:LYS:HD2	1:A:14:THR:HG23	2.03	0.41
1:A:65:GLU:OE2	1:A:75:HIS:NE2	2.48	0.41
1:A:86:THR:HA	1:A:87:PRO:HD3	1.85	0.40

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	515/517 (100%)	492 (96%)	21 (4%)	2 (0%)	43 36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO
1	A	368	SER

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	455/455 (100%)	438 (96%)	17 (4%)	45 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	2/2 (100%)	2 (100%)	0	100	100
All	All	457/457 (100%)	440 (96%)	17 (4%)	45	40

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	78	GLU
1	A	103	PRO
1	A	132	THR
1	A	137	LYS
1	A	215	LYS
1	A	225	PRO
1	A	252	LEU
1	A	255	LYS
1	A	257	LYS
1	A	258	LYS
1	A	312	LEU
1	A	356	ASP
1	A	390	VAL
1	A	413	ARG
1	A	454	LEU
1	A	462	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	279	ASN
1	A	280	GLN
1	A	304	ASN
1	A	338	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NLE	B	2	2	7,7,8	6.84	3 (42%)	5,7,9	1.87	1 (20%)

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	NLE	B	2	2	-	0/4/6/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NLE	O-C	17.43	1.23	1.11
2	B	2	NLE	CA-C	3.60	1.55	1.48
2	B	2	NLE	CB-CA	-3.15	1.50	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NLE	C-CA-N	-3.64	110.19	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

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.