



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:31 PM UTC

PDB ID : 1IG8 / pdb_00001ig8
Title : Crystal Structure of Yeast Hexokinase PII with the correct amino acid sequence
Authors : Kuser, P.R.; Krauchenco, S.; Antunes, O.A.; Polikarpov, I.
Deposited on : 2001-04-17
Resolution : 2.20 Å(reported)

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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

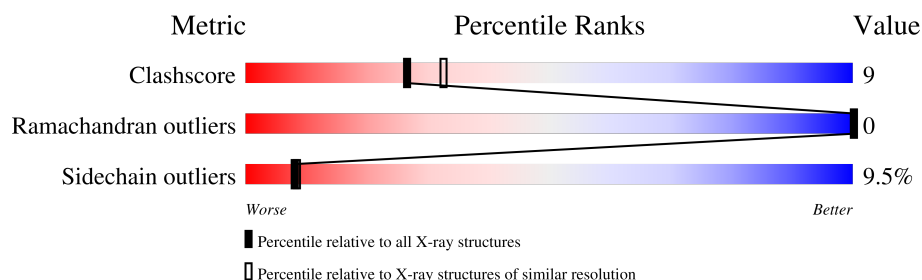
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	486	 72% 20% . . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4117 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 hexokinase PII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	469	3671	2337	607	712	15	0	0	0

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

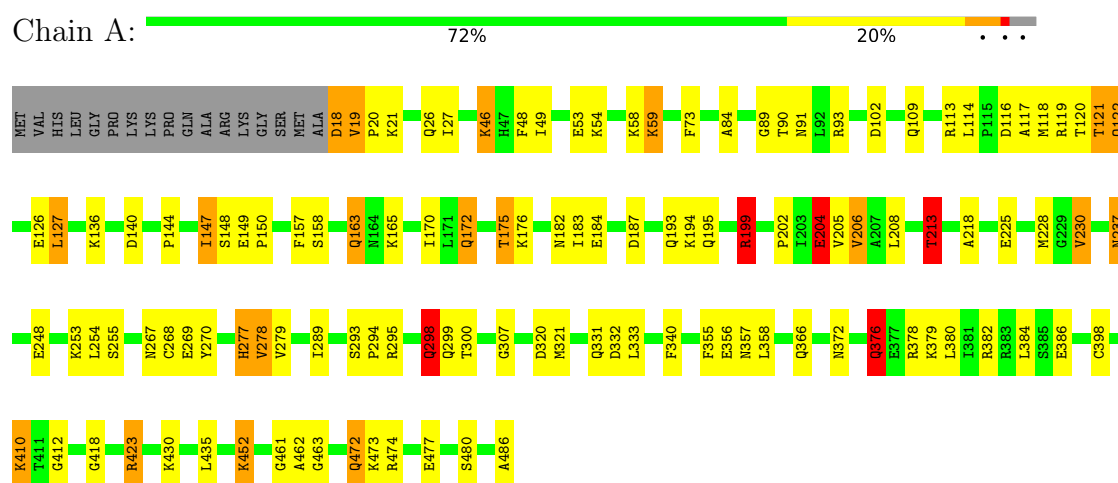
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	441	441	441	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: hexokinase PII



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	142.81Å 142.81Å 58.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	13.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (13.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4117	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: SO4

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	0.73	0/3749	1.74	59/5075 (1.2%)

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	3

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	ARG	CD-NE-CZ	15.98	146.77	124.40
1	A	199	ARG	CD-NE-CZ	12.59	142.02	124.40
1	A	474	ARG	CD-NE-CZ	12.56	141.98	124.40
1	A	278	VAL	N-CA-CB	-10.71	97.56	112.35
1	A	206	VAL	N-CA-CB	-10.15	97.13	112.67
1	A	18	ASP	CA-CB-CG	9.10	121.70	112.60
1	A	199	ARG	NE-CZ-NH2	8.06	126.45	119.20
1	A	122	GLN	CB-CG-CD	7.78	125.83	112.60
1	A	204	GLU	CA-CB-CG	7.74	129.58	114.10
1	A	278	VAL	CB-CA-C	7.37	118.91	110.88
1	A	206	VAL	CB-CA-C	7.04	117.67	110.70
1	A	48	PHE	CA-CB-CG	7.00	120.80	113.80
1	A	182	ASN	CA-CB-CG	-6.90	105.70	112.60
1	A	474	ARG	NE-CZ-NH2	-6.75	113.13	119.20
1	A	462	ALA	CA-C-N	6.68	127.36	119.94
1	A	462	ALA	C-N-CA	6.68	127.36	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLU	CB-CG-CD	6.43	123.53	112.60
1	A	149	GLU	CB-CA-C	6.24	117.31	108.76
1	A	199	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	A	163	GLN	N-CA-CB	-6.15	100.13	111.13
1	A	183	ILE	N-CA-C	-6.11	106.99	112.12
1	A	206	VAL	CA-C-O	6.07	124.19	119.46
1	A	268	CYS	CA-C-O	-5.93	114.59	120.82
1	A	157	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	398	CYS	CA-C-N	5.82	126.40	120.00
1	A	398	CYS	C-N-CA	5.82	126.40	120.00
1	A	378	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	A	320	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	376	GLN	N-CA-CB	5.71	118.52	110.12
1	A	418	GLY	CA-C-O	-5.68	118.53	122.22
1	A	298	GLN	OE1-CD-NE2	5.61	128.21	122.60
1	A	376	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	A	357	ASN	CA-CB-CG	-5.58	107.02	112.60
1	A	237	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	277	HIS	CA-CB-CG	-5.51	108.29	113.80
1	A	19	VAL	N-CA-C	5.50	120.77	108.88
1	A	356	GLU	N-CA-C	5.45	118.72	111.75
1	A	140	ASP	CA-C-O	-5.44	115.08	120.90
1	A	158	SER	CB-CA-C	5.36	117.81	111.22
1	A	102	ASP	N-CA-CB	-5.34	103.80	111.54
1	A	472	GLN	OE1-CD-NE2	5.26	127.86	122.60
1	A	289	ILE	CB-CA-C	-5.25	105.16	111.88
1	A	307	GLY	CA-C-N	5.24	127.83	120.28
1	A	307	GLY	C-N-CA	5.24	127.83	120.28
1	A	357	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	412	GLY	N-CA-C	5.24	117.19	110.96
1	A	332	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	340	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	182	ASN	N-CA-C	5.15	118.70	111.90
1	A	300	THR	CA-C-O	-5.13	115.41	120.90
1	A	320	ASP	CB-CA-C	-5.12	102.85	110.88
1	A	73	PHE	N-CA-C	-5.08	103.67	110.07
1	A	355	PHE	CA-C-N	5.07	127.78	120.38
1	A	355	PHE	C-N-CA	5.07	127.78	120.38
1	A	187	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	398	CYS	O-C-N	-5.03	116.79	122.12
1	A	84	ALA	CA-C-N	-5.02	115.97	122.94
1	A	84	ALA	C-N-CA	-5.02	115.97	122.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	140	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	THR	Mainchain
1	A	213	THR	Mainchain
1	A	279	VAL	Mainchain

5.2 Too-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 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	3671	0	3632	68	0
2	A	5	0	0	0	0
3	A	441	0	0	18	1
All	All	4117	0	3632	68	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 9.

All (68) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ($\text{\AA}$)	Clash overlap ($\text{\AA}$)
1:A:118:MET:HE1	1:A:127:LEU:HA	1.44	0.97
1:A:237:ASN:HD21	1:A:269:GLU:H	1.15	0.88
1:A:59:LYS:HE3	1:A:59:LYS:H	1.44	0.82
1:A:228:MET:HE2	1:A:230:VAL:HG13	1.63	0.81
1:A:93:ARG:HE	1:A:109:GLN:NE2	1.85	0.75
1:A:93:ARG:HE	1:A:109:GLN:HE22	1.37	0.73
1:A:228:MET:HE2	1:A:230:VAL:CG1	2.20	0.72
1:A:175:THR:HG22	1:A:176:LYS:HE2	1.73	0.70
1:A:90:THR:HG23	1:A:113:ARG:HE	1.56	0.69
1:A:193:GLN:NE2	1:A:205:VAL:H	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:GLN:HE22	1:A:205:VAL:H	1.45	0.65
1:A:461:GLY:HA2	3:A:937:HOH:O	1.98	0.64
1:A:46:LYS:HE3	1:A:46:LYS:HA	1.80	0.62
1:A:237:ASN:ND2	1:A:269:GLU:H	1.94	0.62
1:A:295:ARG:HB3	1:A:298:GLN:HG3	1.83	0.61
1:A:321:MET:HE2	1:A:380:LEU:HD21	1.83	0.60
1:A:410:LYS:HE3	3:A:872:HOH:O	2.03	0.58
1:A:193:GLN:NE2	1:A:205:VAL:HG23	2.18	0.58
1:A:237:ASN:HD21	1:A:269:GLU:N	1.95	0.57
1:A:277:HIS:HD2	3:A:505:HOH:O	1.89	0.56
1:A:293:SER:HB2	1:A:294:PRO:HD2	1.88	0.56
1:A:473:LYS:O	1:A:477:GLU:HG2	2.07	0.55
1:A:194:LYS:HG3	3:A:914:HOH:O	2.07	0.54
1:A:150:PRO:HA	1:A:202:PRO:O	2.09	0.53
1:A:218:ALA:HB2	1:A:463:GLY:HA2	1.90	0.53
1:A:147:ILE:HG12	1:A:202:PRO:HG2	1.91	0.53
1:A:27:ILE:HG12	1:A:380:LEU:HD13	1.91	0.53
1:A:299:GLN:HG2	3:A:652:HOH:O	2.09	0.52
1:A:204:GLU:HG2	3:A:747:HOH:O	2.09	0.51
1:A:120:THR:HG22	1:A:120:THR:O	2.11	0.51
1:A:49:ILE:O	1:A:53:GLU:HG3	2.11	0.51
1:A:184:GLU:HG3	3:A:673:HOH:O	2.11	0.49
1:A:26:GLN:HG3	1:A:321:MET:HE1	1.94	0.49
1:A:163:GLN:HG2	1:A:165:LYS:O	2.12	0.49
1:A:58:LYS:HG3	1:A:248:GLU:HG2	1.93	0.49
1:A:430:LYS:HE3	3:A:780:HOH:O	2.12	0.49
1:A:331:GLN:NE2	1:A:372:ASN:H	2.11	0.49
1:A:473:LYS:HD2	3:A:862:HOH:O	2.13	0.48
1:A:93:ARG:NE	1:A:109:GLN:HE22	2.07	0.48
1:A:199:ARG:HA	3:A:922:HOH:O	2.12	0.48
1:A:59:LYS:H	1:A:59:LYS:CE	2.22	0.47
1:A:18:ASP:OD2	1:A:379:LYS:HE3	2.14	0.47
1:A:382:ARG:O	1:A:386:GLU:HG3	2.14	0.47
1:A:117:ALA:HA	3:A:894:HOH:O	2.14	0.47
1:A:175:THR:HG23	1:A:176:LYS:HG3	1.98	0.46
1:A:58:LYS:HG3	1:A:248:GLU:OE1	2.15	0.46
1:A:59:LYS:HE3	1:A:59:LYS:N	2.23	0.46
1:A:213:THR:CG2	3:A:517:HOH:O	2.63	0.46
1:A:144:PRO:HA	3:A:793:HOH:O	2.16	0.46
1:A:376:GLN:H	1:A:376:GLN:CD	2.24	0.45
1:A:116:ASP:HB2	3:A:929:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLN:O	1:A:199:ARG:HG3	2.16	0.44
1:A:118:MET:CE	1:A:127:LEU:HD23	2.47	0.44
1:A:452:LYS:HB3	3:A:879:HOH:O	2.18	0.44
1:A:19:VAL:HG12	1:A:20:PRO:O	2.18	0.44
1:A:26:GLN:CB	1:A:321:MET:HE1	2.48	0.43
1:A:165:LYS:NZ	1:A:486:ALA:HB1	2.33	0.43
1:A:93:ARG:HH21	1:A:109:GLN:NE2	2.16	0.43
1:A:172:GLN:HE21	1:A:172:GLN:HB3	1.75	0.42
1:A:267:ASN:ND2	1:A:267:ASN:C	2.77	0.42
1:A:452:LYS:HE3	3:A:599:HOH:O	2.20	0.42
1:A:93:ARG:HH21	1:A:109:GLN:HE22	1.68	0.42
1:A:89:GLY:O	1:A:119:ARG:NH2	2.53	0.41
1:A:213:THR:HG21	3:A:517:HOH:O	2.20	0.41
1:A:91:ASN:OD1	1:A:113:ARG:HA	2.20	0.41
1:A:118:MET:HB3	1:A:118:MET:HE3	1.88	0.41
1:A:218:ALA:HB2	1:A:463:GLY:CA	2.51	0.41
1:A:366:GLN:HG2	3:A:875:HOH:O	2.20	0.41

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)
3:A:571:HOH:O	3:A:630:HOH:O[8_454]	2.18	0.02

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	467/486 (96%)	449 (96%)	18 (4%)	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	398/411 (97%)	360 (90%)	38 (10%)	8 8

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LYS
1	A	46	LYS
1	A	54	LYS
1	A	59	LYS
1	A	114	LEU
1	A	121	THR
1	A	122	GLN
1	A	126	GLU
1	A	127	LEU
1	A	136	LYS
1	A	147	ILE
1	A	148	SER
1	A	170	ILE
1	A	172	GLN
1	A	175	THR
1	A	199	ARG
1	A	204	GLU
1	A	206	VAL
1	A	208	LEU
1	A	213	THR
1	A	225	GLU
1	A	230	VAL
1	A	253	LYS
1	A	254	LEU
1	A	255	SER
1	A	270	TYR
1	A	278	VAL
1	A	298	GLN
1	A	333	LEU
1	A	358	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	376	GLN
1	A	384	LEU
1	A	410	LYS
1	A	423	ARG
1	A	435	LEU
1	A	452	LYS
1	A	472	GLN
1	A	480	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	122	GLN
1	A	172	GLN
1	A	182	ASN
1	A	193	GLN
1	A	237	ASN
1	A	251	GLN
1	A	267	ASN
1	A	275	ASN
1	A	277	HIS
1	A	331	GLN
1	A	357	ASN
1	A	372	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	SO4	A	501	-	4,4,4	0.60	0	6,6,6	0.72	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.