



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2023 – 12:13 AM EDT

PDB ID : 1R8Y
Title : Crystal Structure of Mouse Glycine N-Methyltransferase (Monoclinic Form)
Authors : Pakhomova, S.; Luka, Z.; Wagner, C.; Newcomer, M.E.
Deposited on : 2003-10-28
Resolution : 3.00 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

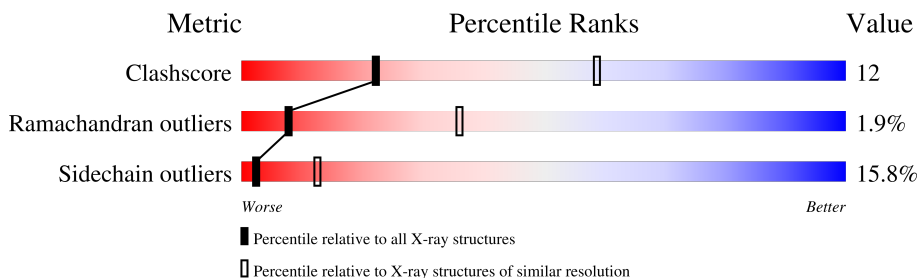
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 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	292	
1	B	292	
1	C	292	
1	D	292	
1	E	292	
1	F	292	
1	G	292	
1	H	292	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BME	B	2057	-	-	X	-

2 Entry composition

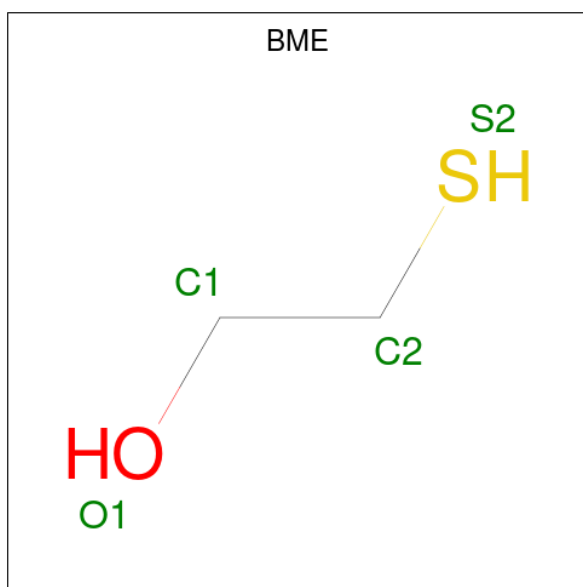
There are 3 unique types of molecules in this entry. The entry contains 17606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	281	2192	1391	380	408	13	0	0	0
1	B	282	2201	1399	382	407	13	0	0	0
1	C	283	2175	1382	378	402	13	0	0	0
1	D	286	2226	1417	382	414	13	0	0	0
1	E	286	2216	1408	385	410	13	0	0	0
1	F	282	2137	1357	370	397	13	0	0	0
1	G	283	2217	1409	385	410	13	0	0	0
1	H	282	2188	1391	379	405	13	0	0	0

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 4 2 1 1	0	0
2	A	1	Total C O S 4 2 1 1	0	0
2	B	1	Total C O S 4 2 1 1	0	0
2	D	1	Total C O S 4 2 1 1	0	0
2	D	1	Total C O S 4 2 1 1	0	0
2	D	1	Total C O S 4 2 1 1	0	0
2	E	1	Total C O S 4 2 1 1	0	0
2	F	1	Total C O S 4 2 1 1	0	0
2	G	1	Total C O S 4 2 1 1	0	0
2	G	1	Total C O S 4 2 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	4	Total O 4 4	0	0
3	D	3	Total O 3 3	0	0

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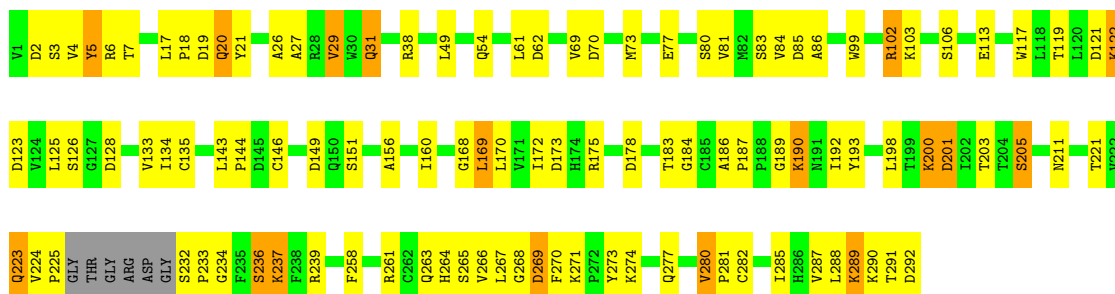
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	2	Total O 2 2	0	0
3	F	3	Total O 3 3	0	0
3	G	2	Total O 2 2	0	0



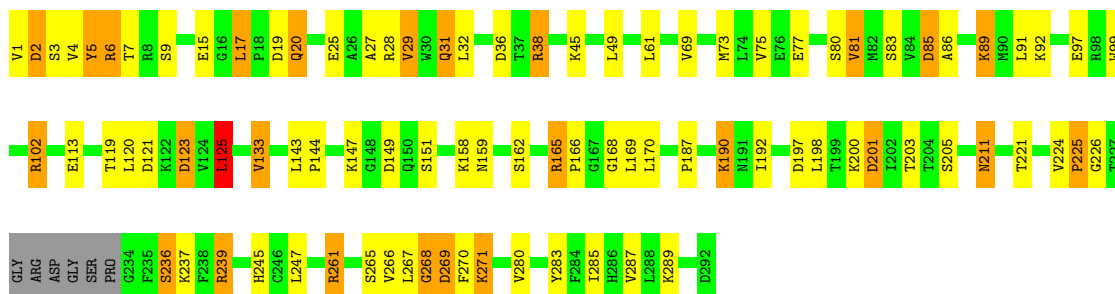
- Molecule 1: glycine N-methyltransferase

Chain D: 61% 31% 6%



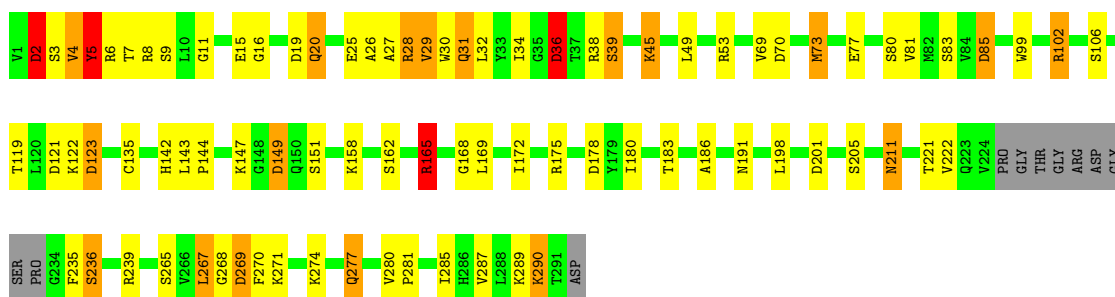
- Molecule 1: glycine N-methyltransferase

Chain E: 67% 22% 9%



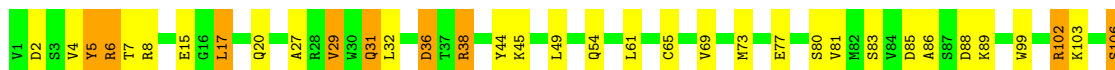
- Molecule 1: glycine N-methyltransferase

Chain F: 67% 22% 6%



- Molecule 1: glycine N-methyltransferase

Chain G: 62% 27% 7%





- Molecule 1: glycine N-methyltransferase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.98Å 108.30Å 119.01Å 90.00° 93.71° 90.00°	Depositor
Resolution (Å)	13.00 – 3.00	Depositor
% Data completeness (in resolution range)	74.2 (13.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.222 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	17606	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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

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	1/2244 (0.0%)	0.98	12/3047 (0.4%)
1	B	0.83	3/2253 (0.1%)	0.93	8/3058 (0.3%)
1	C	0.74	0/2228	0.90	7/3029 (0.2%)
1	D	0.83	0/2280	0.96	9/3096 (0.3%)
1	E	0.79	0/2269	0.94	9/3081 (0.3%)
1	F	0.77	0/2189	0.92	9/2978 (0.3%)
1	G	0.85	1/2269 (0.0%)	0.99	13/3076 (0.4%)
1	H	0.79	1/2240 (0.0%)	0.95	6/3043 (0.2%)
All	All	0.81	6/17972 (0.0%)	0.95	73/24408 (0.3%)

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
1	C	0	2
1	E	0	1
1	G	0	1
1	H	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	SER	CA-CB	5.91	1.61	1.52
1	H	1	VAL	CB-CG1	5.46	1.64	1.52
1	G	152	GLU	CD-OE1	5.41	1.31	1.25
1	B	37	THR	CA-CB	5.29	1.67	1.53
1	A	37	THR	CA-CB	5.18	1.66	1.53

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ASP	CB-CG-OD2	8.89	126.30	118.30
1	G	198	LEU	CA-CB-CG	7.98	133.65	115.30
1	D	128	ASP	CB-CG-OD2	7.56	125.11	118.30
1	C	269	ASP	CB-CG-OD2	7.45	125.00	118.30
1	H	128	ASP	CB-CG-OD2	7.43	124.99	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	ARG	Peptide
1	C	36	ASP	Peptide
1	C	38	ARG	Peptide
1	E	1	VAL	Peptide
1	G	38	ARG	Peptide

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	2192	0	2106	72	0
1	B	2201	0	2121	78	0
1	C	2175	0	2063	41	0
1	D	2226	0	2156	64	0
1	E	2216	0	2134	58	0
1	F	2137	0	1985	46	0
1	G	2217	0	2158	47	0
1	H	2188	0	2103	53	0
2	A	8	0	10	3	0
2	B	4	0	5	5	0
2	D	12	0	15	1	0
2	E	4	0	5	0	0
2	F	4	0	5	0	0
2	G	8	0	10	2	0
3	C	4	0	0	1	0
3	D	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	2	0	0	3	0
3	F	3	0	0	1	0
3	G	2	0	0	0	0
All	All	17606	0	16876	402	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 12.

The worst 5 of 402 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:H:4:VAL:HG12	1:H:5:TYR:H	1.15	1.09
1:A:264:HIS:ND1	1:A:288:LEU:HD21	1.71	1.05
1:A:37:THR:O	1:A:38:ARG:HG3	1.62	0.99
1:C:20:GLN:HG2	3:C:293:HOH:O	1.66	0.96
1:E:20:GLN:HG2	3:E:5247:HOH:O	1.67	0.94

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	277/292 (95%)	250 (90%)	22 (8%)	5 (2%)	8	37
1	B	278/292 (95%)	250 (90%)	23 (8%)	5 (2%)	8	37
1	C	279/292 (96%)	253 (91%)	20 (7%)	6 (2%)	6	31
1	D	282/292 (97%)	258 (92%)	21 (7%)	3 (1%)	14	50
1	E	282/292 (97%)	253 (90%)	24 (8%)	5 (2%)	8	37
1	F	278/292 (95%)	245 (88%)	24 (9%)	9 (3%)	4	22
1	G	279/292 (96%)	250 (90%)	24 (9%)	5 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	278/292 (95%)	252 (91%)	22 (8%)	4 (1%)	11	43
All	All	2233/2336 (96%)	2011 (90%)	180 (8%)	42 (2%)	8	36

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	20	GLN
1	B	20	GLN
1	B	39	SER
1	C	5	TYR

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	230/246 (94%)	195 (85%)	35 (15%)	3	14
1	B	230/246 (94%)	193 (84%)	37 (16%)	2	12
1	C	222/246 (90%)	191 (86%)	31 (14%)	3	16
1	D	236/246 (96%)	197 (84%)	39 (16%)	2	11
1	E	231/246 (94%)	191 (83%)	40 (17%)	2	10
1	F	211/246 (86%)	178 (84%)	33 (16%)	2	13
1	G	235/246 (96%)	197 (84%)	38 (16%)	2	12
1	H	228/246 (93%)	193 (85%)	35 (15%)	2	13
All	All	1823/1968 (93%)	1535 (84%)	288 (16%)	2	12

5 of 288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	122	LYS
1	H	287	VAL
1	G	190	LYS
1	H	38	ARG

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Mol	Chain	Res	Type
1	C	237	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	211	ASN
1	H	150	GLN
1	H	264	HIS
1	H	159	ASN
1	G	245	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
2	BME	A	1282	1	3,3,3	0.94	0	1,2,2	2.02	1 (100%)
2	BME	A	1262	1	3,3,3	0.57	0	1,2,2	0.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BME	E	5246	1	3,3,3	0.36	0	1,2,2	0.76	0
2	BME	D	4246	1	3,3,3	0.29	0	1,2,2	0.45	0
2	BME	G	7246	1	3,3,3	0.78	0	1,2,2	1.23	0
2	BME	D	4185	1	3,3,3	0.78	0	1,2,2	2.00	1 (100%)
2	BME	D	4262	1	3,3,3	0.31	0	1,2,2	0.35	0
2	BME	B	2057	1	3,3,3	0.47	0	1,2,2	0.61	0
2	BME	G	7282	1	3,3,3	0.47	0	1,2,2	1.11	0
2	BME	F	6282	1	3,3,3	0.34	0	1,2,2	0.63	0

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	BME	A	1282	1	-	1/1/1/1	-
2	BME	A	1262	1	-	1/1/1/1	-
2	BME	E	5246	1	-	1/1/1/1	-
2	BME	D	4246	1	-	0/1/1/1	-
2	BME	G	7246	1	-	1/1/1/1	-
2	BME	D	4185	1	-	1/1/1/1	-
2	BME	D	4262	1	-	0/1/1/1	-
2	BME	B	2057	1	-	0/1/1/1	-
2	BME	G	7282	1	-	0/1/1/1	-
2	BME	F	6282	1	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1282	BME	O1-C1-C2	2.02	118.80	110.83
2	D	4185	BME	O1-C1-C2	2.00	118.74	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1262	BME	O1-C1-C2-S2
2	D	4185	BME	O1-C1-C2-S2
2	E	5246	BME	O1-C1-C2-S2
2	A	1282	BME	O1-C1-C2-S2

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Mol	Chain	Res	Type	Atoms
2	G	7246	BME	O1-C1-C2-S2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1282	BME	1	0
2	A	1262	BME	2	0
2	D	4185	BME	1	0
2	B	2057	BME	5	0
2	G	7282	BME	2	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 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.