Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 01:44 AM EDT

PDB ID	:	2SIL
Title	:	THE STRUCTURES OF SALMONELLA TYPHIMURIUM LT2 NEURAMINIDASE AND ITS COMPLEX WITH A TRANSITION STATE ANALOGUE AT 1.6 ANGSTROMS RESOLUTION
Authors	:	Taylor, G.L.; Crennell, S.J.; Garman, E.F.; Vimr, E.R.; Laver, W.G.
Deposited on	:	1994-07-13
Resolution	:	1.60 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 (i) 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 (i)) were used in the production of this report:

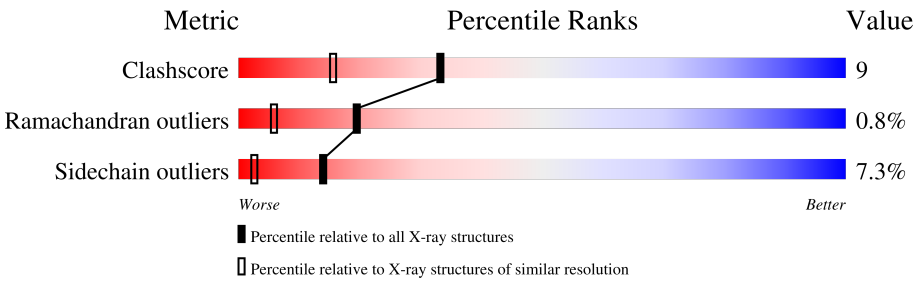
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	381	68% 25% 5% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3149 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 SIALIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	2954	1847	513	584	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	329	ASP	ALA	CONFLICT	UNP P29768

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	195	195	195	0	0

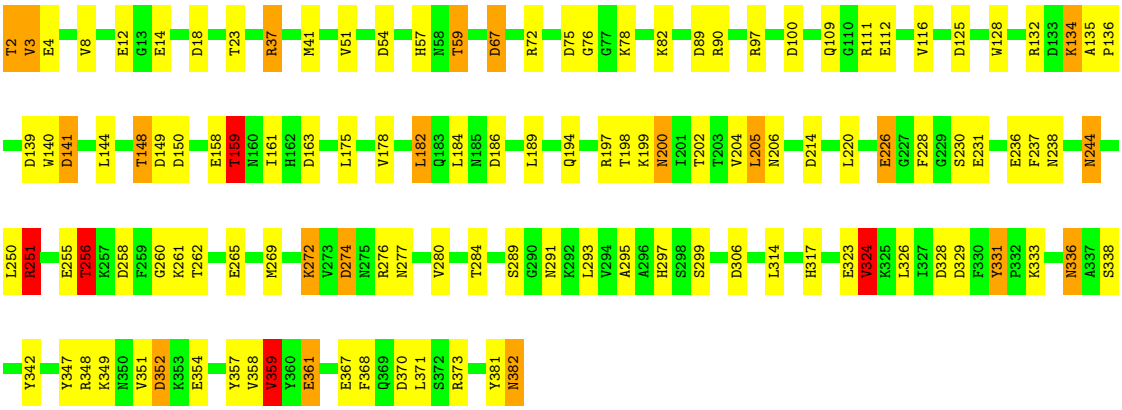
3 Residue-property plots (i)

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: SIALIDASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.50Å 82.50Å 91.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3149	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	1.58	16/3012 (0.5%)	2.07	82/4079 (2.0%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	ASN	C-OXT	71.80	2.59	1.23
1	A	367	GLU	CD-OE2	7.37	1.33	1.25
1	A	158	GLU	CD-OE2	6.44	1.32	1.25
1	A	265	GLU	CD-OE1	6.36	1.32	1.25
1	A	4	GLU	CD-OE2	6.30	1.32	1.25
1	A	323	GLU	CD-OE2	6.14	1.32	1.25
1	A	199	LYS	CE-NZ	6.06	1.64	1.49
1	A	14	GLU	CD-OE2	5.91	1.32	1.25
1	A	231	GLU	CD-OE2	5.76	1.31	1.25
1	A	236	GLU	CD-OE2	-5.45	1.19	1.25
1	A	361	GLU	CD-OE2	5.36	1.31	1.25
1	A	112	GLU	CD-OE1	5.27	1.31	1.25
1	A	226	GLU	CD-OE2	5.23	1.31	1.25
1	A	354	GLU	CD-OE2	5.19	1.31	1.25
1	A	12	GLU	CD-OE2	5.14	1.31	1.25
1	A	255	GLU	CD-OE2	-5.05	1.20	1.25

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ARG	NE-CZ-NH1	-34.69	102.95	120.30
1	A	90	ARG	NE-CZ-NH2	31.14	135.87	120.30
1	A	90	ARG	NE-CZ-NH1	-29.74	105.43	120.30
1	A	251	ARG	NE-CZ-NH2	28.77	134.69	120.30
1	A	37	ARG	NE-CZ-NH1	28.65	134.62	120.30
1	A	37	ARG	NE-CZ-NH2	-24.41	108.10	120.30
1	A	251	ARG	CD-NE-CZ	22.01	154.42	123.60
1	A	90	ARG	CD-NE-CZ	16.50	146.69	123.60
1	A	72	ARG	NE-CZ-NH1	13.19	126.90	120.30
1	A	72	ARG	NE-CZ-NH2	-12.23	114.18	120.30
1	A	111	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	274	ASP	CB-CG-OD2	-10.70	108.67	118.30
1	A	159	THR	N-CA-CB	-10.67	90.03	110.30
1	A	141	ASP	CB-CG-OD1	10.48	127.73	118.30
1	A	90	ARG	CG-CD-NE	-9.95	90.90	111.80
1	A	214	ASP	CB-CG-OD1	9.67	127.00	118.30
1	A	67	ASP	CB-CG-OD2	-9.45	109.79	118.30
1	A	18	ASP	CB-CG-OD1	8.97	126.37	118.30
1	A	329	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	89	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	18	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	A	67	ASP	CB-CG-OD1	7.75	125.27	118.30
1	A	149	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	148	THR	N-CA-CB	-7.44	96.17	110.30
1	A	116	VAL	CG1-CB-CG2	7.43	122.79	110.90
1	A	139	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	370	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	A	357	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	A	274	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	116	VAL	CB-CA-C	-7.14	97.83	111.40
1	A	328	ASP	CB-CG-OD1	7.06	124.66	118.30
1	A	324	VAL	CB-CA-C	-7.02	98.07	111.40
1	A	141	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	A	280	VAL	CA-CB-CG1	6.95	121.33	110.90
1	A	289	SER	N-CA-CB	6.93	120.89	110.50
1	A	328	ASP	CB-CG-OD2	-6.93	112.07	118.30
1	A	373	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	352	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	116	VAL	CA-CB-CG2	6.57	120.76	110.90
1	A	347	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	A	59	THR	CB-CA-C	-6.46	94.15	111.60
1	A	348	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	163	ASP	CB-CG-OD1	6.43	124.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	256	THR	CA-CB-OG1	6.42	122.47	109.00
1	A	54	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	358	VAL	CA-CB-CG1	6.23	120.25	110.90
1	A	54	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	75	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	359	VAL	CG1-CB-CG2	6.18	120.79	110.90
1	A	150	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	3	VAL	N-CA-C	-6.11	94.49	111.00
1	A	125	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	A	100	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	256	THR	N-CA-CB	6.04	121.77	110.30
1	A	280	VAL	CG1-CB-CG2	6.00	120.50	110.90
1	A	163	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	159	THR	OG1-CB-CG2	5.87	123.50	110.00
1	A	202	THR	CA-CB-CG2	-5.83	104.25	112.40
1	A	148	THR	OG1-CB-CG2	5.81	123.37	110.00
1	A	370	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	237	PHE	CB-CG-CD1	5.79	124.86	120.80
1	A	347	TYR	CB-CG-CD1	5.77	124.46	121.00
1	A	276	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	256	THR	CB-CA-C	-5.66	96.33	111.60
1	A	276	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	2	THR	CB-CA-C	5.57	126.64	111.60
1	A	214	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	342	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	306	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	A	186	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	A	326	LEU	CB-CG-CD1	-5.36	101.89	111.00
1	A	358	VAL	CG1-CB-CG2	5.34	119.45	110.90
1	A	357	TYR	CB-CG-CD1	5.30	124.18	121.00
1	A	329	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	97	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	331	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	23	THR	CA-CB-CG2	-5.07	105.30	112.40
1	A	186	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	72	ARG	CG-CD-NE	-5.04	101.21	111.80
1	A	111	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	238	ASN	C-N-CA	-5.03	109.12	121.70
1	A	220	LEU	CB-CA-C	-5.02	100.67	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	251	ARG	Sidechain

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	2954	0	2883	50	0
2	A	195	0	0	2	0
All	All	3149	0	2883	50	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 9.

All (50) 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:A:256:THR:HG21	1:A:260:GLY:H	1.15	1.06
1:A:256:THR:HG21	1:A:260:GLY:N	1.89	0.86
1:A:41:MET:HE3	1:A:359:VAL:HG13	1.59	0.85
1:A:200:ASN:H	1:A:200:ASN:HD22	1.21	0.83
1:A:2:THR:HB	1:A:76:GLY:HA3	1.60	0.83
1:A:159:THR:HG23	1:A:161:ILE:H	1.45	0.80
1:A:200:ASN:H	1:A:200:ASN:ND2	1.74	0.79
1:A:37:ARG:HD2	1:A:361:GLU:OE2	1.84	0.77
1:A:204:VAL:HG12	1:A:205:LEU:HD13	1.68	0.75
1:A:349:LYS:HE2	1:A:352:ASP:HA	1.70	0.74
1:A:256:THR:HG23	1:A:262:THR:O	1.89	0.73
1:A:159:THR:CG2	1:A:161:ILE:H	2.02	0.71
1:A:3:VAL:HB	1:A:78:LYS:HG2	1.73	0.70
1:A:3:VAL:HB	1:A:78:LYS:CG	2.26	0.65
1:A:134:LYS:HE2	1:A:135:ALA:H	1.61	0.64
1:A:41:MET:HE3	1:A:359:VAL:CG1	2.26	0.63
1:A:8:VAL:O	1:A:82:LYS:HE2	2.00	0.61
1:A:317:HIS:CD2	1:A:324:VAL:HG13	2.36	0.61
1:A:132:ARG:NH1	2:A:626:HOH:O	2.35	0.60
1:A:134:LYS:HE2	1:A:135:ALA:N	2.18	0.59
1:A:336:ASN:HD22	1:A:338:SER:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:HD22	1:A:371:LEU:HD13	1.87	0.56
1:A:256:THR:HG22	1:A:258:ASP:H	1.70	0.55
1:A:159:THR:HG21	2:A:631:HOH:O	2.05	0.54
1:A:57:HIS:HE1	1:A:67:ASP:OD2	1.91	0.53
1:A:140:TRP:CG	1:A:141:ASP:N	2.80	0.50
1:A:226:GLU:HB2	1:A:228:PHE:CE2	2.47	0.49
1:A:250:LEU:HD23	1:A:274:ASP:HB2	1.93	0.49
1:A:284:THR:OG1	1:A:297:HIS:HD2	1.96	0.47
1:A:336:ASN:HD22	1:A:336:ASN:C	2.18	0.47
1:A:204:VAL:HG12	1:A:205:LEU:CD1	2.42	0.46
1:A:336:ASN:ND2	1:A:338:SER:H	2.12	0.46
1:A:269:MET:HA	1:A:272:LYS:HG2	1.98	0.46
1:A:200:ASN:HD22	1:A:200:ASN:N	2.00	0.46
1:A:197:ARG:HH11	1:A:206:ASN:ND2	2.14	0.45
1:A:244:ASN:C	1:A:244:ASN:HD22	2.20	0.45
1:A:182:LEU:HD22	1:A:184:LEU:HD23	1.99	0.45
1:A:41:MET:HE2	1:A:51:VAL:HG22	1.98	0.45
1:A:297:HIS:HE1	1:A:299:SER:OG	2.00	0.45
1:A:295:ALA:HB3	1:A:317:HIS:HB2	2.00	0.44
1:A:198:THR:CB	1:A:200:ASN:HD21	2.31	0.43
1:A:244:ASN:HD22	1:A:251:ARG:HH21	1.66	0.43
1:A:244:ASN:ND2	1:A:251:ARG:HH21	2.16	0.43
1:A:3:VAL:HB	1:A:78:LYS:HG3	1.99	0.42
1:A:135:ALA:HA	1:A:136:PRO:HA	1.84	0.42
1:A:41:MET:HE2	1:A:51:VAL:CG2	2.50	0.42
1:A:200:ASN:ND2	1:A:200:ASN:N	2.50	0.42
1:A:331:TYR:CE1	1:A:333:LYS:HD3	2.55	0.41
1:A:382:ASN:OXT	1:A:382:ASN:C	2.59	0.40
1:A:41:MET:HE1	1:A:368:PHE:CD2	2.56	0.40

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	379/381 (100%)	366 (97%)	10 (3%)	3 (1%)	19 6

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	VAL
1	A	230	SER
1	A	351	VAL

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	327/327 (100%)	303 (93%)	24 (7%)	14 2

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	THR
1	A	109	GLN
1	A	128	TRP
1	A	134	LYS
1	A	144	LEU
1	A	148	THR
1	A	159	THR
1	A	175	LEU
1	A	182	LEU
1	A	189	LEU
1	A	194	GLN
1	A	200	ASN
1	A	205	LEU
1	A	244	ASN
1	A	256	THR
1	A	261	LYS
1	A	272	LYS
1	A	277	ASN

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Mol	Chain	Res	Type
1	A	291	ASN
1	A	293	LEU
1	A	324	VAL
1	A	336	ASN
1	A	359	VAL
1	A	381	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	81	ASN
1	A	124	ASN
1	A	194	GLN
1	A	200	ASN
1	A	206	ASN
1	A	232	ASN
1	A	244	ASN
1	A	275	ASN
1	A	277	ASN
1	A	297	HIS
1	A	304	ASN
1	A	317	HIS
1	A	336	ASN
1	A	382	ASN

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)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.