Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 03:24 PM EDT

PDB ID	:	1IDD
Title	:	ISOCITRATE DEHYDROGENASE Y160F MUTANT APO ENZYME
Authors	:	Lee, M.E.; Dyer, D.H.; Klein, O.D.; Bolduc, J.M.; Stoddard, B.L.; Koshland Junior, D.E.
Deposited on	:	1995-01-18
Resolution	:	2.50 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 following versions of software and data (see references (i)) were used in the production of this report:

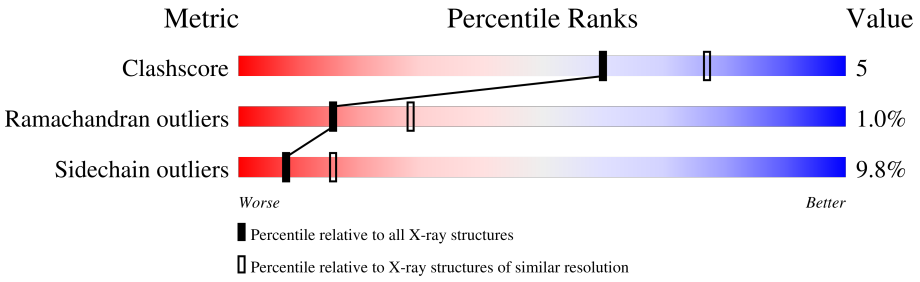
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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	416	71% 23% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3217 atoms, of which 22 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 ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	414	3217	2035	22	538	604	18	30	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	PHE	TYR	engineered mutation	UNP P08200

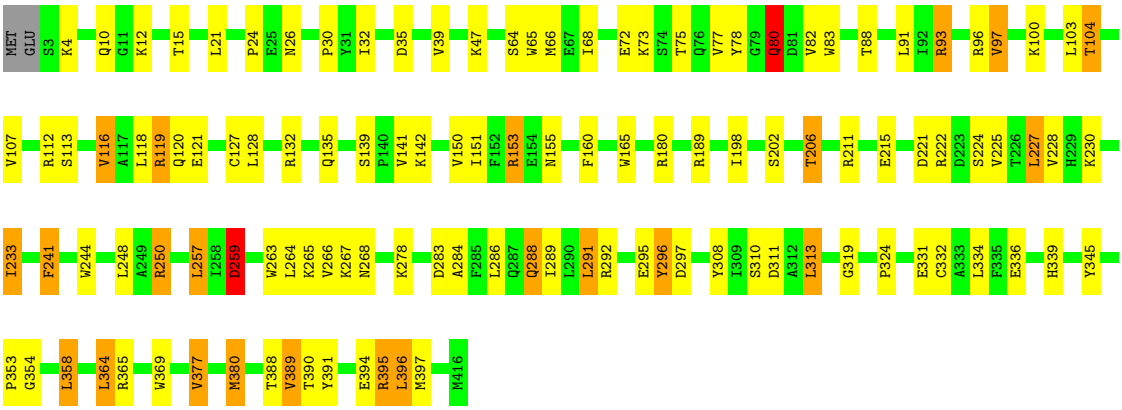
3 Residue-property plots (i)

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: ISOCITRATE DEHYDROGENASE

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 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.10Å 105.10Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.215 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3217	wwPDB-VP
Average B, all atoms (Å^2)	10.0	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	1.34	16/3256 (0.5%)	2.11	112/4403 (2.5%)

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	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	ARG	CA-CB	14.28	1.85	1.53
1	A	119	ARG	NE-CZ	12.02	1.48	1.33
1	A	119	ARG	CB-CG	11.60	1.83	1.52
1	A	119	ARG	CG-CD	9.82	1.76	1.51
1	A	221	ASP	CA-CB	7.23	1.69	1.53
1	A	119	ARG	CD-NE	7.14	1.58	1.46
1	A	310	SER	CA-CB	-6.61	1.43	1.52
1	A	395	ARG	NE-CZ	6.32	1.41	1.33
1	A	395	ARG	CA-CB	6.20	1.67	1.53
1	A	395	ARG	CG-CD	5.96	1.66	1.51
1	A	391	TYR	CA-CB	5.87	1.66	1.53
1	A	369	TRP	CG-CD2	-5.45	1.34	1.43
1	A	244	TRP	CD1-NE1	-5.38	1.28	1.38
1	A	377	VAL	CA-CB	5.31	1.65	1.54
1	A	139	SER	CA-CB	-5.29	1.45	1.52
1	A	345	TYR	CB-CG	5.11	1.59	1.51

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH1	37.44	139.02	120.30
1	A	119	ARG	NH1-CZ-NH2	-19.68	97.75	119.40
1	A	153	ARG	NE-CZ-NH2	-15.55	112.53	120.30
1	A	153	ARG	NE-CZ-NH1	14.36	127.48	120.30
1	A	119	ARG	CA-CB-CG	13.34	142.74	113.40
1	A	119	ARG	CD-NE-CZ	12.36	140.91	123.60
1	A	395	ARG	CA-CB-CG	11.76	139.28	113.40
1	A	119	ARG	O-C-N	-10.99	105.11	122.70
1	A	119	ARG	CB-CG-CD	10.51	138.92	111.60
1	A	395	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	A	222	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	221	ASP	CA-CB-CG	9.83	135.03	113.40
1	A	189	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	83	TRP	CD1-CG-CD2	9.12	113.60	106.30
1	A	390	THR	N-CA-CB	-9.08	93.04	110.30
1	A	4	LYS	N-CA-C	8.65	134.36	111.00
1	A	380	MET	CG-SD-CE	-8.65	86.36	100.20
1	A	391	TYR	CA-CB-CG	8.55	129.64	113.40
1	A	365	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	244	TRP	CE2-CD2-CG	-8.47	100.53	107.30
1	A	244	TRP	CD1-CG-CD2	8.43	113.04	106.30
1	A	119	ARG	CG-CD-NE	8.24	129.11	111.80
1	A	244	TRP	CG-CD2-CE3	8.11	141.20	133.90
1	A	150	VAL	CG1-CB-CG2	-8.01	98.08	110.90
1	A	112	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	104	THR	CA-C-N	-7.82	99.99	117.20
1	A	78	TYR	CB-CG-CD1	-7.77	116.34	121.00
1	A	83	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	198	ILE	CG1-CB-CG2	-7.72	94.43	111.40
1	A	345	TYR	CB-CG-CD1	7.66	125.60	121.00
1	A	65	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	263	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	96	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	389	VAL	N-CA-CB	-7.38	95.27	111.50
1	A	215	GLU	CA-CB-CG	7.36	129.60	113.40
1	A	103	LEU	CA-CB-CG	7.13	131.71	115.30
1	A	165	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	65	TRP	CD1-CG-CD2	7.08	111.96	106.30
1	A	165	TRP	CD1-CG-CD2	7.07	111.95	106.30
1	A	365	ARG	CA-CB-CG	6.92	128.64	113.40
1	A	319	GLY	CA-C-N	6.87	132.31	117.20
1	A	222	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	259	ASP	CA-C-N	6.68	129.56	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	319	GLY	CA-C-O	-6.63	108.67	120.60
1	A	119	ARG	N-CA-C	-6.62	93.11	111.00
1	A	278	LYS	CA-CB-CG	6.62	127.97	113.40
1	A	265	LYS	CA-CB-CG	6.61	127.93	113.40
1	A	211	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	244	TRP	CB-CG-CD1	-6.50	118.55	127.00
1	A	132	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	A	388	THR	CA-CB-CG2	6.43	121.41	112.40
1	A	397	MET	CA-CB-CG	6.43	124.23	113.30
1	A	263	TRP	CD1-CG-CD2	6.42	111.43	106.30
1	A	120	GLN	CA-C-N	6.39	131.26	117.20
1	A	119	ARG	CB-CA-C	6.38	123.15	110.40
1	A	369	TRP	CD1-CG-CD2	6.29	111.33	106.30
1	A	93	ARG	CA-CB-CG	6.27	127.19	113.40
1	A	334	LEU	CB-CG-CD2	-6.25	100.37	111.00
1	A	396	LEU	CA-CB-CG	6.21	129.57	115.30
1	A	308	TYR	CB-CG-CD2	-6.19	117.29	121.00
1	A	120	GLN	O-C-N	-6.16	112.84	122.70
1	A	142	LYS	CA-CB-CG	6.15	126.94	113.40
1	A	65	TRP	CG-CD2-CE3	6.14	139.43	133.90
1	A	364	LEU	CA-C-N	6.14	130.70	117.20
1	A	233	ILE	CA-C-N	6.13	130.68	117.20
1	A	180	ARG	CA-CB-CG	6.11	126.83	113.40
1	A	388	THR	CA-CB-OG1	-6.09	96.22	109.00
1	A	116	VAL	CA-C-N	6.06	130.54	117.20
1	A	369	TRP	CE2-CD2-CG	-6.05	102.46	107.30
1	A	250	ARG	CA-CB-CG	5.99	126.58	113.40
1	A	83	TRP	CG-CD1-NE1	-5.97	104.12	110.10
1	A	295	GLU	CA-CB-CG	5.96	126.50	113.40
1	A	227	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	112	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	119	ARG	CA-C-N	5.90	130.17	117.20
1	A	297	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	132	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	73	LYS	N-CA-CB	-5.72	100.30	110.60
1	A	21	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	332	CYS	CA-C-N	5.68	129.71	117.20
1	A	241	PHE	CA-C-N	5.65	129.63	117.20
1	A	345	TYR	O-C-N	-5.63	113.68	122.70
1	A	120	GLN	N-CA-C	5.62	126.16	111.00
1	A	395	ARG	CG-CD-NE	5.59	123.53	111.80
1	A	65	TRP	CB-CG-CD1	-5.53	119.82	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	LYS	CA-C-N	5.51	129.31	117.20
1	A	332	CYS	O-C-N	-5.47	113.95	122.70
1	A	267	LYS	CA-CB-CG	5.46	125.42	113.40
1	A	141	VAL	CA-CB-CG1	-5.44	102.74	110.90
1	A	291	LEU	CA-CB-CG	5.43	127.80	115.30
1	A	395	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
1	A	78	TYR	CB-CG-CD2	5.43	124.26	121.00
1	A	296	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	225	VAL	CG1-CB-CG2	-5.36	102.32	110.90
1	A	96	ARG	CA-CB-CG	-5.32	101.69	113.40
1	A	12	LYS	CA-CB-CG	5.31	125.09	113.40
1	A	283	ASP	CA-CB-CG	5.29	125.05	113.40
1	A	96	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	10	GLN	N-CA-C	-5.24	96.86	111.00
1	A	263	TRP	CG-CD2-CE3	5.23	138.61	133.90
1	A	311	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	292	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	83	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	A	257	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	82	VAL	CA-C-N	-5.10	105.97	117.20
1	A	151	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	A	116	VAL	O-C-N	-5.04	114.64	122.70
1	A	180	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	32	ILE	N-CA-C	-5.01	97.46	111.00
1	A	266	VAL	CA-C-N	5.01	128.22	117.20
1	A	118	LEU	CA-C-O	-5.00	109.59	120.10
1	A	288	GLN	CA-C-N	5.00	128.20	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	TYR	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	3195	22	3222	29	0
All	All	3195	22	3222	29	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 5.

All (29) 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:119:ARG:CD	1:A:119:ARG:CG	1.76	1.61
1:A:119:ARG:CG	1:A:119:ARG:CB	1.83	1.56
1:A:119:ARG:CB	1:A:119:ARG:CA	1.85	1.52
1:A:119:ARG:HH11	1:A:153:ARG:HH22	1.31	0.76
1:A:75:THR:HB	1:A:80:GLN:HA	1.68	0.75
1:A:119:ARG:CB	1:A:119:ARG:HA	2.15	0.67
1:A:202:SER:O	1:A:206:THR:HG23	1.95	0.66
1:A:284:ALA:O	1:A:288:GLN:HG2	1.96	0.65
1:A:68:ILE:HD12	1:A:88:THR:HG23	1.81	0.62
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.82	0.61
1:A:119:ARG:CD	1:A:119:ARG:HG3	2.18	0.56
1:A:93:ARG:HH12	1:A:331:GLU:HG3	1.73	0.54
1:A:113:SER:HB3	1:A:116:VAL:HB	1.90	0.54
1:A:127:CYS:HB2	1:A:155:ASN:ND2	2.26	0.51
1:A:119:ARG:HH11	1:A:153:ARG:NH2	2.07	0.50
1:A:30:PRO:HA	1:A:66:MET:O	2.13	0.49
1:A:35:ASP:OD1	1:A:72:GLU:HB3	2.13	0.48
1:A:257:LEU:HD23	1:A:264:LEU:HD12	1.95	0.48
1:A:206:THR:HB	1:A:241:PHE:CD1	2.49	0.47
1:A:119:ARG:CG	1:A:119:ARG:HB3	2.23	0.47
1:A:394:GLU:C	1:A:396:LEU:H	2.18	0.46
1:A:119:ARG:CD	1:A:119:ARG:HG2	2.18	0.46
1:A:30:PRO:HD2	1:A:97:VAL:O	2.17	0.45
1:A:324:PRO:HB3	1:A:358:LEU:HB3	2.00	0.43
1:A:354:GLY:O	1:A:358:LEU:HB2	2.18	0.43
1:A:93:ARG:NH1	1:A:331:GLU:HG3	2.34	0.42
1:A:119:ARG:CG	1:A:119:ARG:HB2	2.23	0.42
1:A:250:ARG:HH11	1:A:250:ARG:HD2	1.73	0.41
1:A:100:LYS:HE3	1:A:336:GLU:OE1	2.21	0.41

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	412/416 (99%)	382 (93%)	26 (6%)	4 (1%)	15 28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ASP
1	A	395	ARG
1	A	80	GLN
1	A	24	PRO

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	336/338 (99%)	303 (90%)	33 (10%)	8 15

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	26	ASN
1	A	39	VAL
1	A	64	SER
1	A	77	VAL
1	A	80	GLN
1	A	91	LEU

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Mol	Chain	Res	Type
1	A	97	VAL
1	A	104	THR
1	A	107	VAL
1	A	121	GLU
1	A	128	LEU
1	A	135	GLN
1	A	160	PHE
1	A	206	THR
1	A	224	SER
1	A	227	LEU
1	A	228	VAL
1	A	230	LYS
1	A	233	ILE
1	A	248	LEU
1	A	259	ASP
1	A	268	ASN
1	A	286	LEU
1	A	291	LEU
1	A	313	LEU
1	A	339	HIS
1	A	353	PRO
1	A	358	LEU
1	A	364	LEU
1	A	377	VAL
1	A	380	MET
1	A	389	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	327	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.