



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:02 AM UTC

PDB ID : 6SCI / pdb_00006sci
Title : Structure of AdhE form 1
Authors : Lovering, A.L.; Bragginton, E.
Deposited on : 2019-07-24
Resolution : 1.95 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

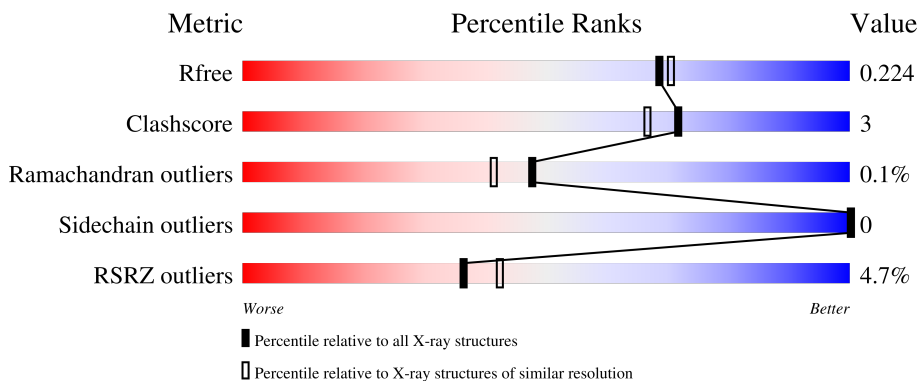
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
R_{free}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	455	 4% 83% 6% 11%
1	B	455	 5% 82% 6% 12%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6351 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 Aldehyde-alcohol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	3112	1987	526	583	16	0	3	0
1	B	402	3112	1987	528	581	16	0	3	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	MET	-	initiating methionine	UNP P0A9Q7
A	450	ASP	-	cloning artifact	UNP P0A9Q7
A	892	PRO	-	expression tag	UNP P0A9Q7
A	893	TRP	-	expression tag	UNP P0A9Q7
A	894	GLY	-	expression tag	UNP P0A9Q7
A	895	ALA	-	expression tag	UNP P0A9Q7
A	896	GLY	-	expression tag	UNP P0A9Q7
A	897	GLY	-	expression tag	UNP P0A9Q7
A	898	LEU	-	expression tag	UNP P0A9Q7
A	899	GLU	-	expression tag	UNP P0A9Q7
A	900	VAL	-	expression tag	UNP P0A9Q7
A	901	LEU	-	expression tag	UNP P0A9Q7
A	902	PHE	-	expression tag	UNP P0A9Q7
A	903	GLN	-	expression tag	UNP P0A9Q7
B	449	MET	-	initiating methionine	UNP P0A9Q7
B	450	ASP	-	cloning artifact	UNP P0A9Q7
B	892	PRO	-	expression tag	UNP P0A9Q7
B	893	TRP	-	expression tag	UNP P0A9Q7
B	894	GLY	-	expression tag	UNP P0A9Q7
B	895	ALA	-	expression tag	UNP P0A9Q7
B	896	GLY	-	expression tag	UNP P0A9Q7
B	897	GLY	-	expression tag	UNP P0A9Q7
B	898	LEU	-	expression tag	UNP P0A9Q7
B	899	GLU	-	expression tag	UNP P0A9Q7
B	900	VAL	-	expression tag	UNP P0A9Q7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	901	LEU	-	expression tag	UNP P0A9Q7
B	902	PHE	-	expression tag	UNP P0A9Q7
B	903	GLN	-	expression tag	UNP P0A9Q7

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

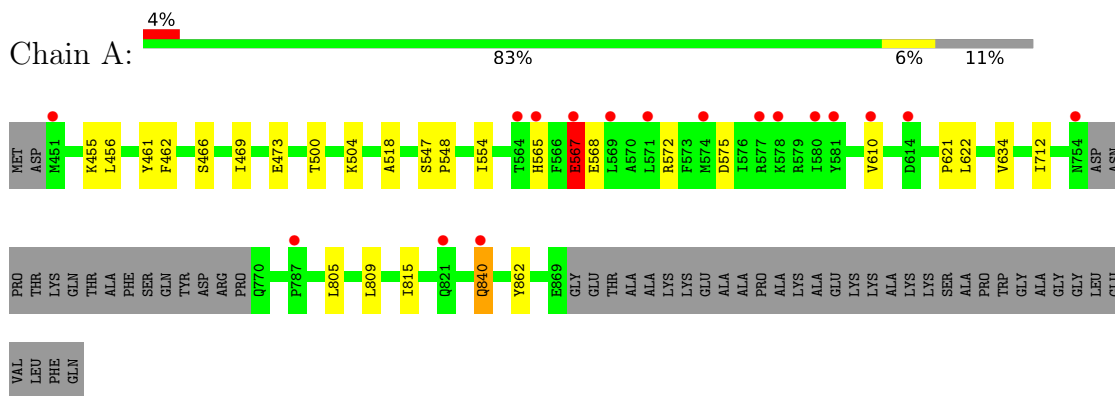
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	66	Total O 66 66	0	0
3	B	59	Total O 59 59	0	0

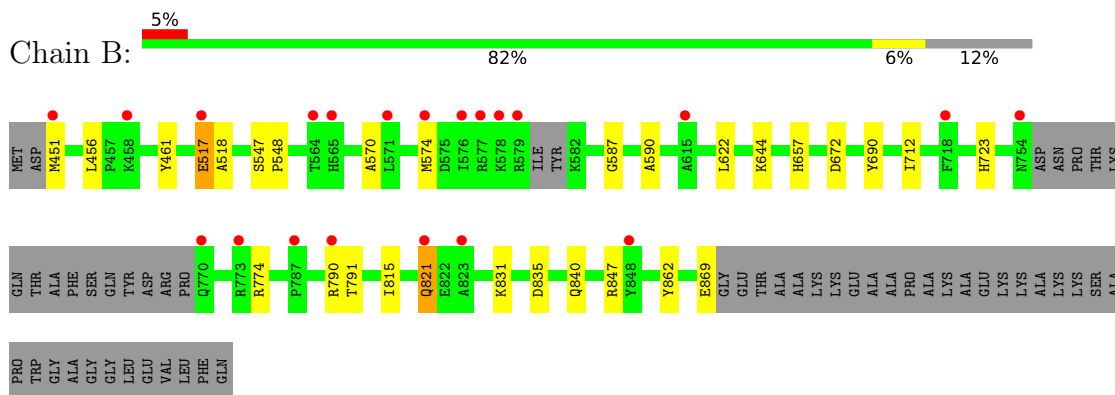
3 Residue-property plots [i](#)

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 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.

- Molecule 1: Aldehyde-alcohol dehydrogenase



- Molecule 1: Aldehyde-alcohol dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.03Å 96.73Å 122.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.25 – 1.95 57.25 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (57.25-1.95) 99.6 (57.25-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.182 , 0.217 0.190 , 0.224	Depositor DCC
R_{free} test set	3028 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtrriage
Anisotropy	0.184	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6351	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: FE

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	0.36	0/3186	0.58	2/4320 (0.0%)
1	B	0.35	0/3185	0.64	7/4314 (0.2%)
All	All	0.35	0/6371	0.61	9/8634 (0.1%)

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	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	821	GLN	CA-CB-CG	12.12	138.34	114.10
1	B	517	GLU	CA-CB-CG	8.81	131.71	114.10
1	A	567	GLU	CA-CB-CG	8.29	130.68	114.10
1	B	821	GLN	CB-CA-C	7.52	124.14	109.33
1	B	821	GLN	N-CA-CB	-7.19	98.79	111.08
1	A	840	GLN	N-CA-C	-6.98	103.44	112.23
1	B	517	GLU	CB-CG-CD	-6.82	101.01	112.60
1	B	821	GLN	CB-CG-CD	-6.82	101.01	112.60
1	B	517	GLU	N-CA-CB	5.57	118.96	109.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	821	GLN	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	3112	0	3103	22	0
1	B	3112	0	3120	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	66	0	0	0	0
3	B	59	0	0	0	0
All	All	6351	0	6223	41	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 3.

All (41) 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:565:HIS:HB3	1:A:567:GLU:OE1	1.56	1.03
1:A:805:LEU:O	1:A:809:LEU:HD13	1.81	0.80
1:A:461:TYR:OH	1:A:473:GLU:OE1	2.00	0.78
1:A:565:HIS:HB2	1:A:568:GLU:HG3	1.67	0.76
1:A:565:HIS:CB	1:A:567:GLU:OE1	2.35	0.70
1:A:575:ASP:HB3	1:A:840:GLN:HG2	1.77	0.64
1:B:790:ARG:CG	1:B:791:THR:H	2.14	0.61
1:A:455:LYS:NZ	1:B:461:TYR:OH	2.36	0.58
1:B:790:ARG:CD	1:B:791:THR:H	2.17	0.58
1:A:500:THR:O	1:A:504:LYS:HG3	2.06	0.55
1:B:790:ARG:HD3	1:B:791:THR:H	1.72	0.55
1:A:456:LEU:HD21	1:A:712:ILE:HG23	1.90	0.54
1:A:518:ALA:O	1:A:547[A]:SER:OG	2.25	0.54
1:B:570:ALA:HA	1:B:622:LEU:HD11	1.90	0.53
1:A:469:ILE:HB	1:B:451:MET:HE3	1.90	0.53
1:B:574:MET:HG2	1:B:840:GLN:NE2	2.25	0.52
1:A:610:VAL:HG22	1:A:621:PRO:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:ARG:HD3	1:B:791:THR:N	2.24	0.52
1:A:568:GLU:O	1:A:572:ARG:HG3	2.11	0.51
1:B:790:ARG:HG2	1:B:791:THR:H	1.74	0.51
1:B:456:LEU:HD21	1:B:712:ILE:HG23	1.93	0.50
1:B:847:ARG:NH1	1:B:869:GLU:OE2	2.36	0.49
1:B:815:ILE:HB	1:B:862:TYR:HA	1.95	0.48
1:B:831:LYS:HE3	1:B:835:ASP:OD2	2.15	0.47
1:A:815:ILE:HB	1:A:862:TYR:HA	1.97	0.46
1:B:547[A]:SER:HB2	1:B:548:PRO:HD3	1.99	0.45
1:B:518:ALA:O	1:B:547[A]:SER:OG	2.31	0.45
1:A:466:SER:CB	1:B:451:MET:HG3	2.47	0.44
1:B:517:GLU:HB2	1:B:518:ALA:H	1.39	0.44
1:B:672:ASP:CG	1:B:774:ARG:HH22	2.25	0.44
1:A:575:ASP:OD2	1:A:840:GLN:NE2	2.51	0.44
1:B:644:LYS:HB3	1:B:690:TYR:CE1	2.52	0.44
1:A:554:ILE:HD12	1:A:622:LEU:HD13	2.01	0.43
1:B:657:HIS:CD2	1:B:723:HIS:CE1	3.08	0.42
1:A:547[A]:SER:HB2	1:A:548:PRO:HD3	2.02	0.42
1:B:790:ARG:CG	1:B:791:THR:N	2.80	0.42
1:B:587:GLY:HA2	1:B:590:ALA:O	2.20	0.42
1:A:466:SER:HB3	1:B:451:MET:HG3	2.01	0.41
1:A:547[B]:SER:HB3	1:A:548:PRO:HD3	2.02	0.41
1:A:565:HIS:HB2	1:A:568:GLU:CG	2.46	0.41
1:A:462:PHE:HA	1:A:634:VAL:O	2.20	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	403/455 (89%)	393 (98%)	9 (2%)	1 (0%)	43 36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	399/455 (88%)	391 (98%)	8 (2%)	0	100	100
All	All	802/910 (88%)	784 (98%)	17 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	567	GLU

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	325/363 (90%)	325 (100%)	0	100	100
1	B	327/363 (90%)	327 (100%)	0	100	100
All	All	652/726 (90%)	652 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	840	GLN
1	B	770	GLN
1	B	781	HIS
1	B	840	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	404/455 (88%)	0.13	17 (4%) 40 47	14, 30, 59, 83	3 (0%)
1	B	402/455 (88%)	0.14	21 (5%) 33 38	14, 31, 60, 82	3 (0%)
All	All	806/910 (88%)	0.13	38 (4%) 36 42	14, 30, 60, 83	6 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	ILE	5.7
1	B	451	MET	5.6
1	A	840	GLN	4.4
1	B	578	LYS	4.0
1	A	571	LEU	3.7
1	B	579	ARG	3.6
1	A	581	TYR	3.5
1	A	569	LEU	3.4
1	B	615	ALA	3.4
1	B	718	PHE	3.3
1	A	567	GLU	3.3
1	B	787	PRO	3.2
1	A	574	MET	3.0
1	B	773	ARG	2.9
1	B	576	ILE	2.9
1	A	565	HIS	2.8
1	A	451	MET	2.8
1	A	787	PRO	2.8
1	B	574	MET	2.8
1	B	770	GLN	2.7
1	A	564	THR	2.6
1	B	565	HIS	2.6
1	B	821	GLN	2.6
1	B	577	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	790	ARG	2.5
1	A	821	GLN	2.5
1	A	614	ASP	2.4
1	B	823	ALA	2.3
1	B	517	GLU	2.3
1	B	571	LEU	2.3
1	B	848	TYR	2.2
1	A	754	ASN	2.2
1	B	754	ASN	2.2
1	A	577	ARG	2.1
1	B	564	THR	2.1
1	A	578	LYS	2.0
1	B	458	LYS	2.0
1	A	610	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	A	1001	1/1	0.99	0.02	21,21,21,21	0
2	FE	B	1001	1/1	0.99	0.02	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.