



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:49 PM UTC

PDB ID : 4NCK / pdb_00004nck
Title : Crystal Structure of Pyrococcus furiosus Rad50 R797G mutation
Authors : Classen, S.; Williams, G.J.; Arvai, A.S.; Williams, R.S.
Deposited on : 2013-10-24
Resolution : 1.99 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) : 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

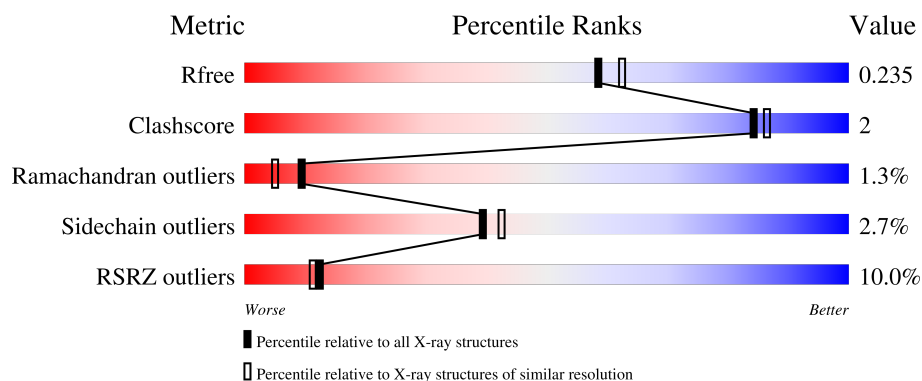
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	339	10% 83% 9% 8%
1	B	339	8% 85% 6% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9552 atoms, of which 4562 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.

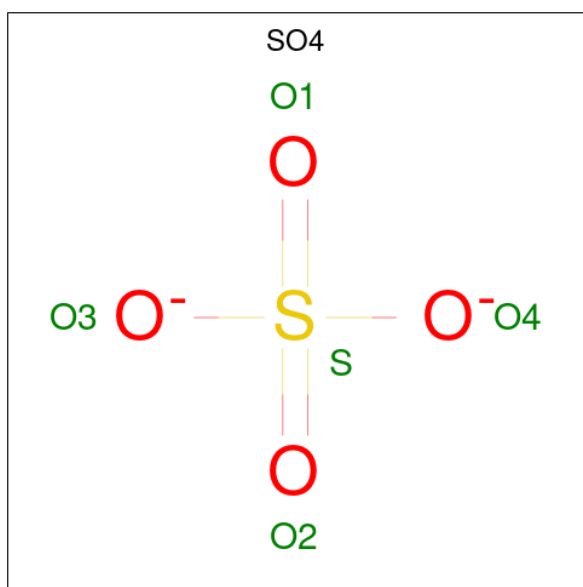
- Molecule 1 is a protein called DNA double-strand break repair Rad50 ATPase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	313	Total	C	H	N	O	S	0	5	0
			4625	1512	2284	389	435	5			
1	B	309	Total	C	H	N	O	S	0	2	0
			4596	1491	2278	390	432	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	721	GLY	-	linker	UNP P58301
A	722	GLY	-	linker	UNP P58301
A	723	SER	-	linker	UNP P58301
A	724	GLY	-	linker	UNP P58301
A	725	GLY	-	linker	UNP P58301
A	797	GLY	ARG	engineered mutation	UNP P58301
B	721	GLY	-	linker	UNP P58301
B	722	GLY	-	linker	UNP P58301
B	723	SER	-	linker	UNP P58301
B	724	GLY	-	linker	UNP P58301
B	725	GLY	-	linker	UNP P58301
B	797	GLY	ARG	engineered mutation	UNP P58301

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



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

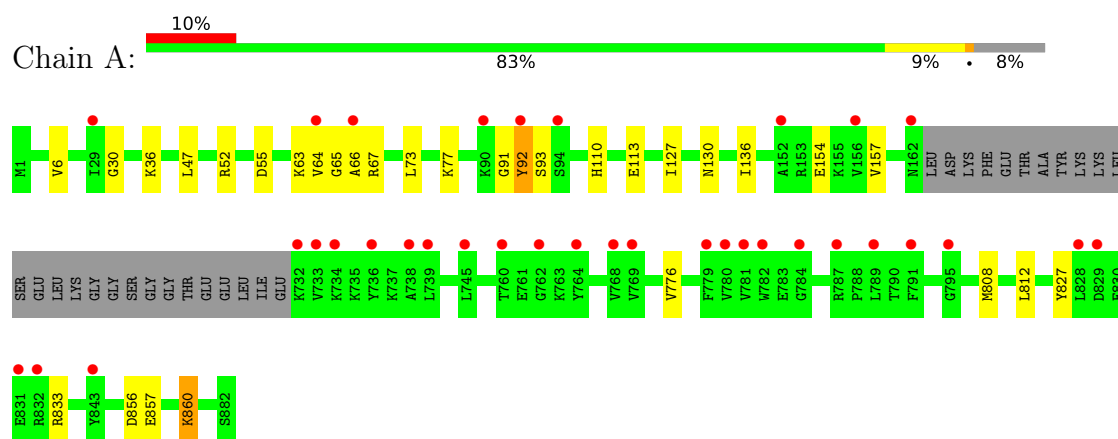
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	200	Total	O	0	0
			200	200		
5	B	124	Total	O	0	0
			124	124		

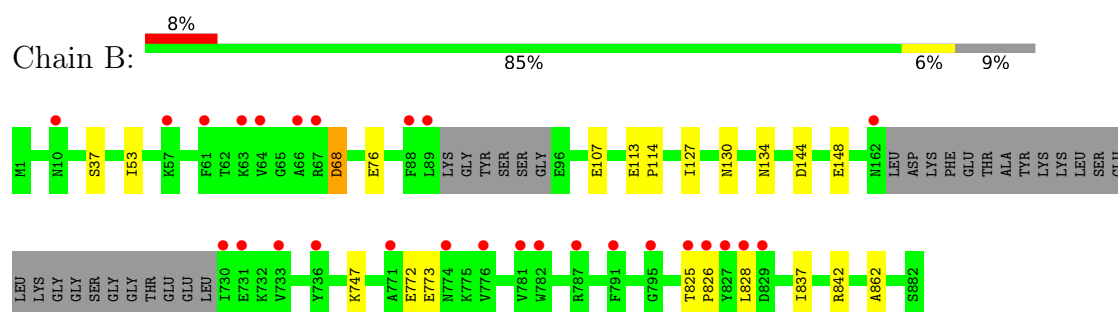
3 Residue-property plots [i](#)

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: DNA double-strand break repair Rad50 ATPase



- Molecule 1: DNA double-strand break repair Rad50 ATPase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.67Å 68.06Å 202.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.24 – 1.99 48.24 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.24-1.99) 99.3 (48.24-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.00Å)	Xtriage
Refinement program	PHENIX dev_1233	Depositor
R, R_{free}	0.181 , 0.230 0.185 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 74.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9552	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: SO4, CL, MG

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	0.76	0/2390	0.87	1/3233 (0.0%)
1	B	0.69	0/2358	0.81	1/3194 (0.0%)
All	All	0.72	0/4748	0.84	2/6427 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	GLU	N-CA-C	6.43	117.98	110.97
1	A	812	LEU	N-CA-C	5.02	116.83	111.36

There are no chirality outliers.

There are no planarity outliers.

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	2341	2284	2290	16	0
1	B	2318	2278	2268	7	0
2	B	5	0	0	0	0
3	B	1	0	0	0	0
4	B	1	0	0	0	0
5	A	200	0	0	1	2
5	B	124	0	0	3	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4990	4562	4558	21	2

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 2.

All (21) 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:B:144:ASP:OD2	5:B:1045:HOH:O	2.12	0.67
1:A:6:VAL:HG23	1:A:73[A]:LEU:HD23	1.83	0.58
1:B:76:GLU:OE2	5:B:1032:HOH:O	2.18	0.57
1:A:157:VAL:HA	1:A:808:MET:HE1	1.85	0.56
1:A:77:LYS:NZ	5:A:924:HOH:O	2.35	0.53
1:A:6:VAL:HG23	1:A:73[A]:LEU:CD2	2.40	0.50
1:A:30:GLY:O	1:A:36:LYS:HE3	2.12	0.50
1:A:93:SER:OG	1:B:68:ASP:OD1	2.25	0.47
1:B:837:ILE:HG23	1:B:862:ALA:HB2	1.96	0.47
1:A:91:GLY:O	1:A:92:TYR:CB	2.62	0.47
1:A:63:LYS:O	1:A:65:GLY:N	2.48	0.47
1:A:52:ARG:NH2	1:A:55:ASP:OD2	2.49	0.45
1:A:857:GLU:OE1	1:A:860:LYS:NZ	2.31	0.45
1:A:833:ARG:NE	1:A:856:ASP:OD2	2.49	0.45
1:B:113:GLU:OE1	5:B:1030:HOH:O	2.21	0.43
1:A:30:GLY:O	1:A:36:LYS:CE	2.67	0.42
1:A:110:HIS:CD2	1:B:114:PRO:HG2	2.55	0.41
1:B:130:ASN:ND2	1:B:134:ASN:HD22	2.18	0.41
1:A:154:GLU:HA	1:A:776:VAL:HG23	2.01	0.41
1:A:127:ILE:HD11	1:A:136:ILE:CD1	2.50	0.41
1:A:47:LEU:HD21	1:A:73[B]:LEU:HD21	2.03	0.40

All (2) 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)
5:A:946:HOH:O	5:B:1085:HOH:O[1_655]	2.16	0.04
5:A:930:HOH:O	5:B:1087:HOH:O[1_655]	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	314/339 (93%)	303 (96%)	7 (2%)	4 (1%)	9	5
1	B	305/339 (90%)	293 (96%)	8 (3%)	4 (1%)	9	5
All	All	619/678 (91%)	596 (96%)	15 (2%)	8 (1%)	9	5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	92	TYR
1	B	773	GLU
1	B	826	PRO
1	A	66	ALA
1	A	67	ARG
1	B	772	GLU
1	B	828	LEU

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	225/293 (77%)	221 (98%)	4 (2%)	51	58
1	B	229/293 (78%)	221 (96%)	8 (4%)	32	32
All	All	454/586 (78%)	442 (97%)	12 (3%)	39	44

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	GLU
1	A	130	ASN
1	A	827	TYR
1	A	860	LYS
1	B	37	SER
1	B	53	ILE
1	B	68	ASP
1	B	107	GLU
1	B	127	ILE
1	B	747	LYS
1	B	825	THR
1	B	842	ARG

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	855	HIS
1	B	134	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	B	901	-	4,4,4	0.23	0	6,6,6	0.12	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

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	313/339 (92%)	0.40	35 (11%) 10 9	19, 52, 119, 147	5 (1%)
1	B	309/339 (91%)	0.49	27 (8%) 16 15	29, 65, 113, 145	2 (0%)
All	All	622/678 (91%)	0.45	62 (9%) 12 11	19, 61, 117, 147	7 (1%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	7.5
1	A	769	VAL	5.9
1	B	730	ILE	4.5
1	A	782	TRP	4.5
1	A	736	TYR	3.9
1	A	781	VAL	3.9
1	A	92	TYR	3.8
1	A	732	LYS	3.7
1	B	736	TYR	3.6
1	B	162	ASN	3.6
1	A	64	VAL	3.4
1	A	66	ALA	3.2
1	A	156	VAL	3.2
1	B	66	ALA	3.1
1	B	63	LYS	3.1
1	B	64	VAL	3.1
1	B	733	VAL	3.0
1	A	739	LEU	2.9
1	A	828	LEU	2.9
1	B	828	LEU	2.9
1	A	843	TYR	2.9
1	A	791	PHE	2.9
1	A	787	ARG	2.8
1	A	795	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	88	PHE	2.7
1	A	29	ILE	2.7
1	B	826	PRO	2.6
1	A	162	ASN	2.6
1	A	779	PHE	2.5
1	A	831	GLU	2.5
1	B	787	ARG	2.5
1	B	10	ASN	2.4
1	B	791	PHE	2.4
1	B	827	TYR	2.3
1	A	90	LYS	2.3
1	A	760	THR	2.3
1	A	745	LEU	2.3
1	B	782	TRP	2.3
1	B	825	THR	2.3
1	A	94	SER	2.2
1	B	57	LYS	2.2
1	B	795	GLY	2.2
1	B	774	ASN	2.2
1	A	734	LYS	2.2
1	A	780	VAL	2.2
1	A	152	ALA	2.2
1	A	738	ALA	2.2
1	B	67	ARG	2.2
1	B	61	PHE	2.1
1	B	776	VAL	2.1
1	B	781	VAL	2.1
1	A	829	ASP	2.1
1	A	762	GLY	2.1
1	A	832	ARG	2.1
1	B	731	GLU	2.1
1	A	789	LEU	2.1
1	B	829	ASP	2.1
1	A	784	GLY	2.1
1	A	768	VAL	2.1
1	A	764	TYR	2.0
1	A	733	VAL	2.0
1	B	771	ALA	2.0

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

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($\text{\AA}^2$)	Q<0.9
2	SO4	B	901	5/5	0.79	0.16	118,119,120,121	0
4	MG	B	903	1/1	0.93	0.32	80,80,80,80	0
3	CL	B	902	1/1	0.95	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.