



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:49 PM BST

PDB ID : 3J8Y
EMDB ID: : EMD-6188
Title : High-resolution structure of ATP analog-bound kinesin on microtubules
Authors : Shang, Z.; Zhou, K.; Xu, C.; Csencsits, R.; Cochran, J.C.; Sindelar, C.V.
Deposited on : 2014-11-20
Resolution : 5.00 Å(reported)
Based on PDB ID : 4HNA

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

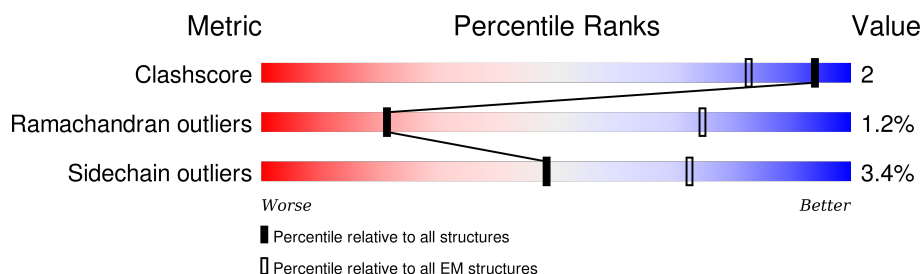
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	K	349	<div> <div>72%</div> <div>18%</div> <div>• 5%</div> </div>
2	A	451	<div> <div>67%</div> <div>24%</div> <div>• • 5%</div> </div>
3	B	445	<div> <div>71%</div> <div>22%</div> <div>• •</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9435 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	330	Total	C	N	O	S	0	0
			2582	1609	444	519	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	7	SER	CYS	CONFLICT	UNP P33176
K	168	ALA	CYS	CONFLICT	UNP P33176
K	174	SER	CYS	CONFLICT	UNP P33176
K	330	SER	CYS	CONFLICT	UNP P33176

- Molecule 2 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	430	Total	C	N	O	S	0	0
			3372	2137	573	640	22		

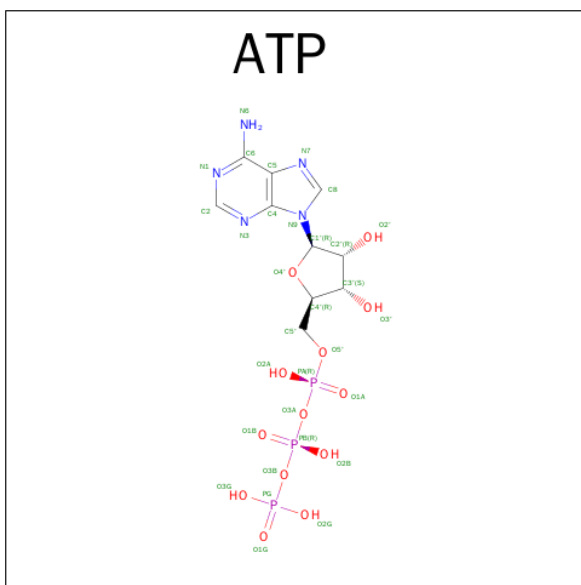
- Molecule 3 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	431	Total	C	N	O	S	0	0
			3389	2126	580	657	26		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	SER	CYS	CONFLICT	UNP F2Z5B2

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

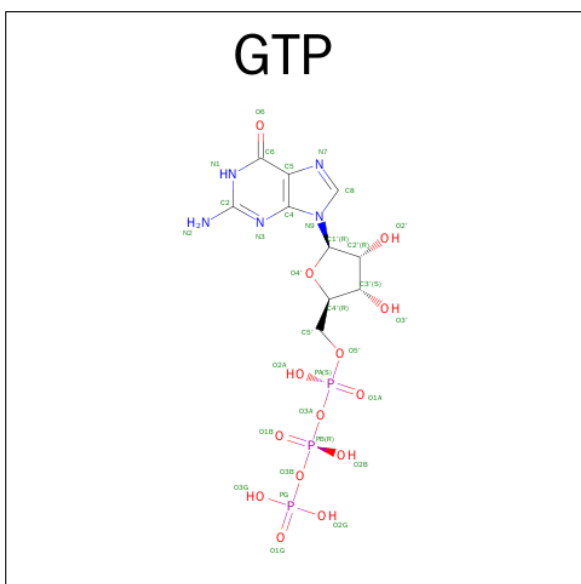


Mol	Chain	Residues	Atoms					AltConf
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

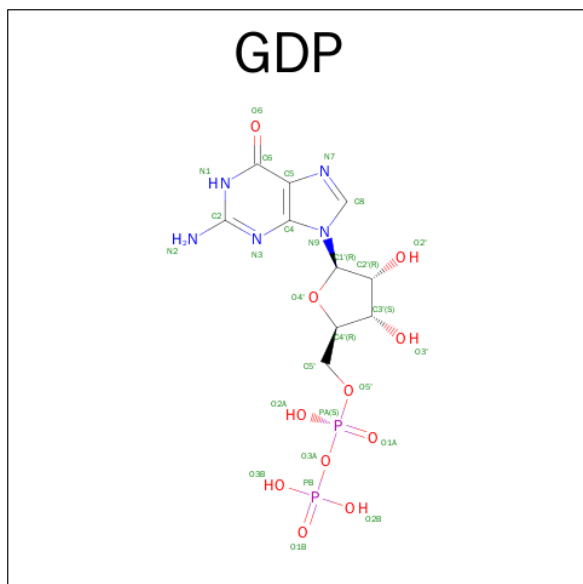
Mol	Chain	Residues	Atoms	AltConf
5	K	1	Total Mg 1 1	0

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

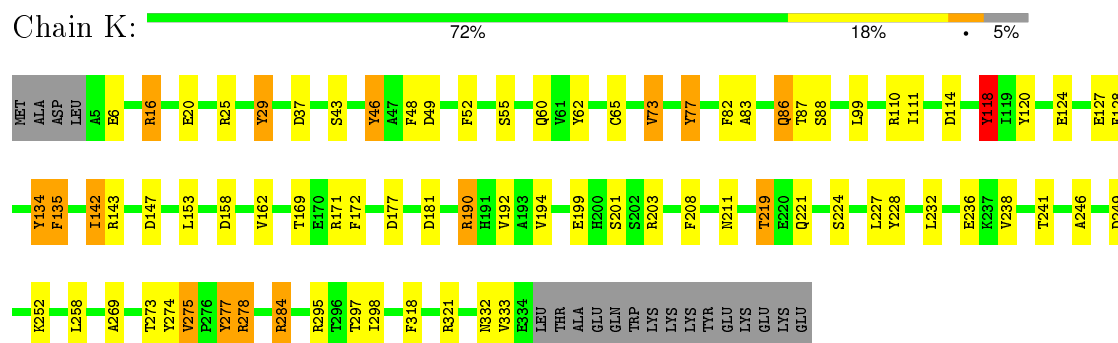
- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



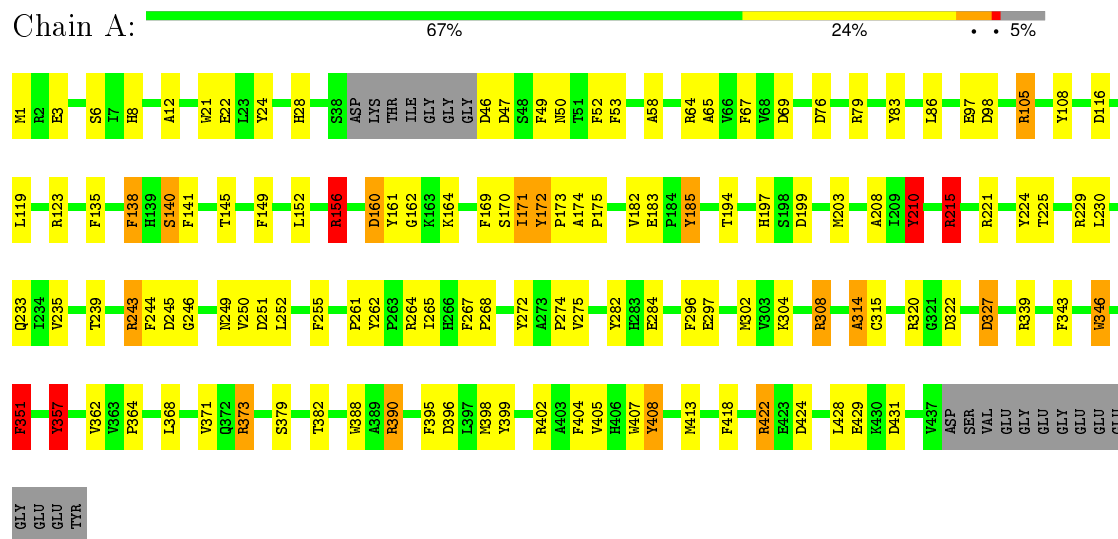
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

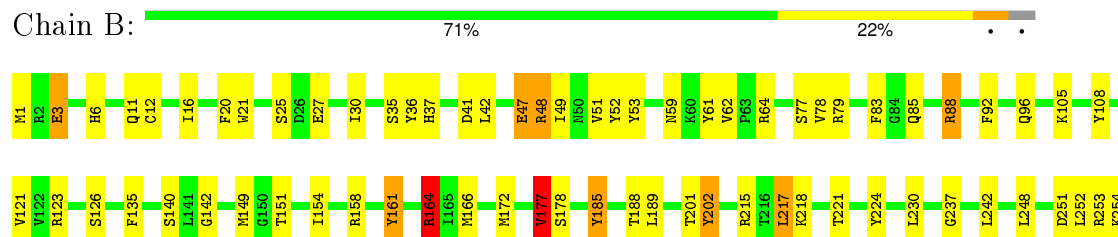
- Molecule 1: Kinesin-1 heavy chain

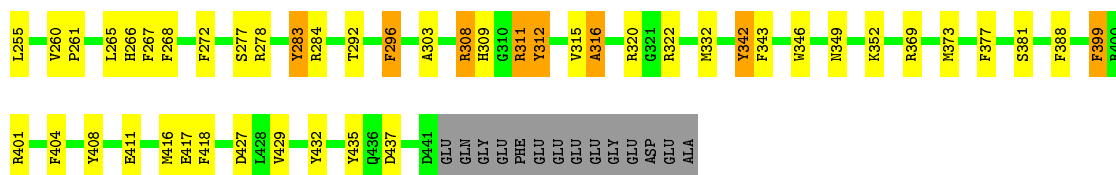


- Molecule 2: Tubulin alpha-1B chain



- Molecule 3: Tubulin beta-2B chain





4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	49961	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	done within FREALIGN	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor

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: GDP, GTP, MG, ATP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	K	1.59	13/2621 (0.5%)	2.01	73/3535 (2.1%)
2	A	1.58	19/3450 (0.6%)	2.03	99/4685 (2.1%)
3	B	1.60	16/3464 (0.5%)	1.97	102/4692 (2.2%)
All	All	1.59	48/9535 (0.5%)	2.00	274/12912 (2.1%)

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	K	0	13
2	A	0	19
3	B	0	16
All	All	0	48

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	381	SER	CA-CB	11.64	1.70	1.52
3	B	435	TYR	CE1-CZ	7.77	1.48	1.38
3	B	47	GLU	CB-CG	7.27	1.66	1.52
3	B	253	ARG	CD-NE	7.02	1.58	1.46
1	K	228	TYR	CG-CD1	6.48	1.47	1.39

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	24	TYR	CB-CG-CD1	-16.25	111.25	121.00
1	K	284	ARG	NE-CZ-NH2	-16.19	112.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	120	TYR	CB-CG-CD1	14.77	129.86	121.00
3	B	164	ARG	NE-CZ-NH1	13.35	126.97	120.30
1	K	120	TYR	CB-CG-CD2	-13.08	113.15	121.00

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	16	ARG	Sidechain
1	K	25	ARG	Sidechain
1	K	29	TYR	Sidechain
1	K	48	PHE	Sidechain
1	K	62	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	K	2582	0	2551	3	0
2	A	3372	0	3287	12	0
3	B	3389	0	3266	15	0
4	K	31	0	12	0	0
5	K	1	0	0	0	0
6	A	32	0	12	0	0
7	B	28	0	12	0	0
All	All	9435	0	9140	30	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 2.

The worst 5 of 30 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:K:142:ILE:HB	1:K:153:LEU:H	1.75	0.51
2:A:52:PHE:CD1	2:A:243:ARG:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:251:ASP:CG	3:B:252:LEU:H	2.17	0.47
3:B:315:VAL:HG11	3:B:377:PHE:CE1	2.50	0.46
3:B:399:PHE:CE1	3:B:418:PHE:HB3	2.51	0.46

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 PDB entries followed by that with respect to all EM entries.

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	K	328/349 (94%)	306 (93%)	20 (6%)	2 (1%)	30	74
2	A	428/451 (95%)	376 (88%)	46 (11%)	6 (1%)	14	58
3	B	429/445 (96%)	392 (91%)	31 (7%)	6 (1%)	14	58
All	All	1185/1245 (95%)	1074 (91%)	97 (8%)	14 (1%)	21	62

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	47	ASP
2	A	50	ASN
3	B	283	TYR
2	A	162	GLY
3	B	218	LYS

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 PDB entries followed by that with respect to all EM entries.

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	K	292/311 (94%)	282 (97%)	10 (3%)	44	76
2	A	364/379 (96%)	349 (96%)	15 (4%)	37	72
3	B	372/383 (97%)	362 (97%)	10 (3%)	52	80
All	All	1028/1073 (96%)	993 (97%)	35 (3%)	48	76

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	183	GLU
2	A	327	ASP
3	B	296	PHE
2	A	210	TYR
2	A	215	ARG

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

Mol	Chain	Res	Type
1	K	93	HIS
1	K	129	HIS
1	K	191	HIS
2	A	61	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
6	GTP	A	600	-	26,34,34	1.30	2 (7%)	29,54,54	2.41	7 (24%)
7	GDP	B	501	-	24,30,30	1.44	3 (12%)	26,47,47	2.58	8 (30%)
4	ATP	K	501	5	26,33,33	1.40	3 (11%)	26,52,52	1.29	1 (3%)

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
6	GTP	A	600	-	-	0/18/38/38	0/3/3/3
7	GDP	B	501	-	-	0/12/32/32	0/3/3/3
4	ATP	K	501	5	-	0/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	501	GDP	C5'-C4'	2.30	1.59	1.51
4	K	501	ATP	O4'-C1'	2.42	1.44	1.41
6	A	600	GTP	C2'-C3'	2.64	1.60	1.53
7	B	501	GDP	C2'-C3'	2.72	1.60	1.53
7	B	501	GDP	C2'-C1'	2.84	1.58	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	GTP	C5-C6-N1	-7.88	113.22	123.52
7	B	501	GDP	C5-C6-N1	-6.85	114.57	123.52
6	A	600	GTP	C1'-N9-C4	-3.93	122.42	126.81
7	B	501	GDP	C6-C5-C4	-3.81	116.50	120.86
6	A	600	GTP	C5'-C4'-C3'	-3.28	102.49	115.20

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.