



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 4, 2017 – 05:44 PM EST

PDB ID : 5VVR  
EMDB ID: : EMD-8735  
Title : Ternary complex of RNA Pol II, transcription scaffold and Rad26  
Authors : Lahiri, I.; Leschziner, A.E.  
Deposited on : unknown  
Resolution : 5.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

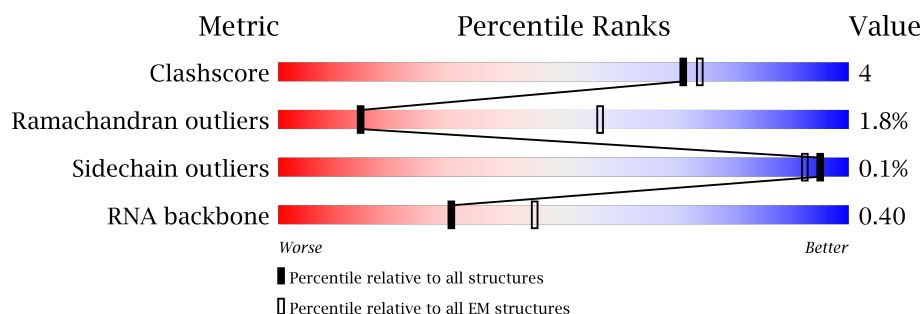
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 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	A	1733	78% 5% 16%
2	B	1224	90% 7% ..
3	C	318	77% 7% • 15%
4	D	221	76% • 21%
5	E	215	90% 9% •
6	F	155	48% • 48%
7	G	171	89% 11%
8	H	146	87% 11% •

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	122	<div><div></div><div>90%</div><div>9%</div><div></div></div>
10	J	70	<div><div></div><div>89%</div><div>11%</div><div></div></div>
11	K	120	<div><div></div><div>85%</div><div>8%</div><div>8%</div></div>
12	L	70	<div><div></div><div>53%</div><div>11%</div><div></div><div>34%</div></div>
13	M	1085	<div><div></div><div>43%</div><div></div><div>54%</div></div>
14	N	47	<div><div></div><div>62%</div><div>36%</div><div></div></div>
15	R	10	<div><div></div><div>80%</div><div>20%</div></div>
16	T	47	<div><div></div><div>51%</div><div>45%</div><div></div></div>

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 38507 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1448	Total	C	N	O	S	0	0
			11385	7168	1988	2167	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1207	Total	C	N	O	S	0	0
			9608	6062	1678	1812	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2125	1336	353	422	14		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	175	Total	C	N	O	S	0	0
			1409	870	251	286	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1760	1116	310	322	12		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	81	Total	C	N	O	S	0	0
			657	419	111	124	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	146	Total	C	N	O	S	0	0
			1161	726	195	235	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	122	Total	C	N	O	S	0	0
			997	613	182	191	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			578	366	102	104	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	111	Total	C	N	O	S	0	0
			895	575	152	166	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 13 is a protein called DNA repair and recombination protein RAD26.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	503	Total	C	N	O	S	0	0
			4087	2620	726	722	19		

- Molecule 14 is a DNA chain called DNA (NTS).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	47	Total	C	N	O	P	0	0
			965	460	176	282	47		

- Molecule 15 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	10	Total	C	N	O	P	0	0
			220	98	45	67	10		

- Molecule 16 is a DNA chain called DNA (TS).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	47	Total	C	N	O	P	0	0
			947	453	159	288	47		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	J	1	Total	Zn	0
			1	1	
17	B	1	Total	Zn	0
			1	1	
17	I	2	Total	Zn	0
			2	2	
17	C	1	Total	Zn	0
			1	1	
17	A	2	Total	Zn	0
			2	2	
17	L	1	Total	Zn	0
			1	1	

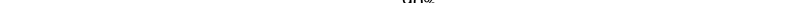
- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Mg	0
			1	1	





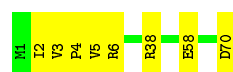


Chain I:  90% 9%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:  89% 11%



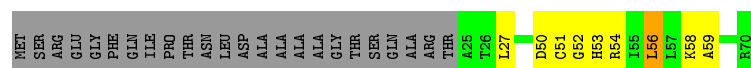
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:  85% 8% 8%



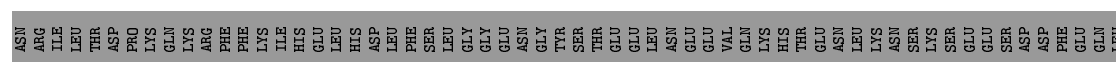
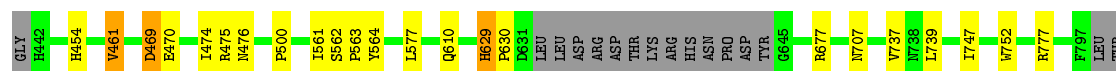
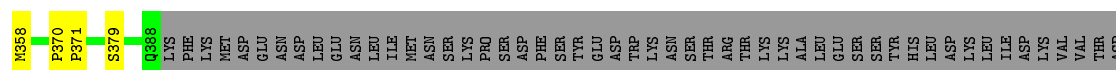
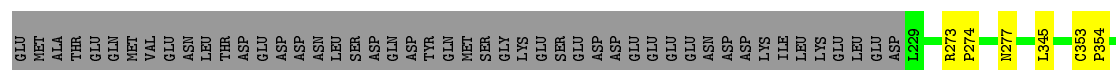
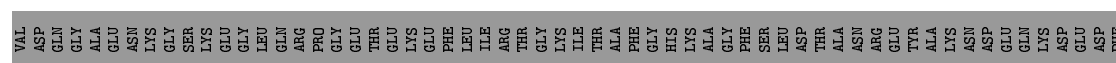
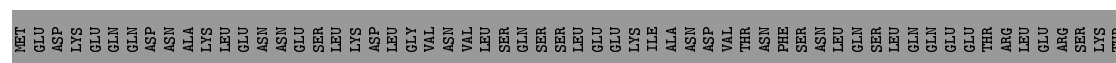
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  53% 11% 34%



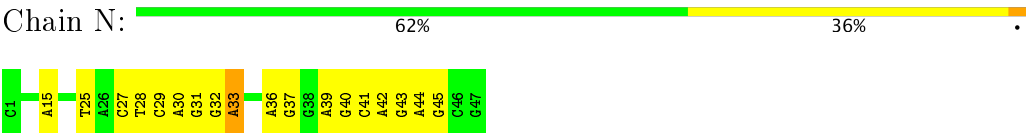
- Molecule 13: DNA repair and recombination protein RAD26

Chain M:  43% 1% 54%

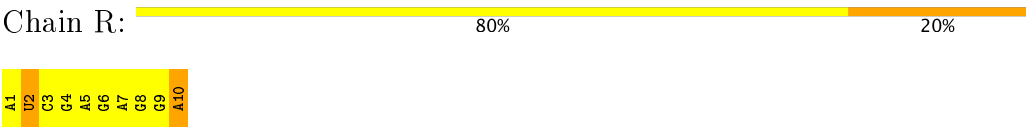


VAL	ASN	LEU	SER	GLY	VAL	SER	LYS	LEU	GLU	SER	PHE	TYR	ASN	GLY	LYS	GLU	LYS	GLU	ASN	SER	LYS	THR	GLU	ASP	ASP	ASP	GLN	TYR	ARG	LEU	ILE	GLY	GLY	LEU	LEU	GLY	GLY	GLU	SER	ASN	LEU	GLU	THR	VAL	MET	SER	HIS	ASP	SER	VAL	VAL	ASN	SER	HIS	ALA	GLY	SER	SER	SER	ALA	ASN					
ILE	ILE	THR	LYS	ILE	ALA	SER	ARG	VAL	ALA	ILE	GLU	ALA	VAL	ASN	ALA	ARG	LYS	SER	ARG	LYS	LYS	ILE	THR	LYS	LYS	GLN	TYR	ARG	GLU	ILE	ILE	THR	PRO	THR	THR	GLY	GLY	ARG	PHE	GLY	LYS	LYS	ALA	GLY	LYS	ILE	ILE	ARG	ANG	LYS	SER	HIS	ASP	SER	VAL	VAL	ASN	SER	HIS	ALA	GLY	SER	SER	SER	ALA	ASN
ILE	LEU	GLY	ASN	ILE	THR	LYS	SER	GLN	LYS	GLU	ALA	SER	LYS	GLU	LYS	ARG	GLN	GLU	ASN	TYR	ASP	ASP	GLY	ILE	THR	PHE	ALA	ARG	LYS	SER	GLU	ILE	ILE	ARG	ALA	TYR	LEU	GLN	LYS	THR	LEU	GLU	ASN	ASN	PHE	SER	SER	VAL	ILE																	
LEU	ASN	SER	ILE	GLY	VAL	SER	LEU	SER	ASP	LYS	GLU	ASP	VAL	ILE	LYS	VAL	ARG	ALA	LEU	LEU	THR	ILE	ALA	GLN	PHE	ASP	LYS	ARG	GLU	LYS	GLY	ILE	TRP	VAL	LEU	ASP	GLU	GLU	PHE	ARG	ASN	ASN	ALA	SER																						

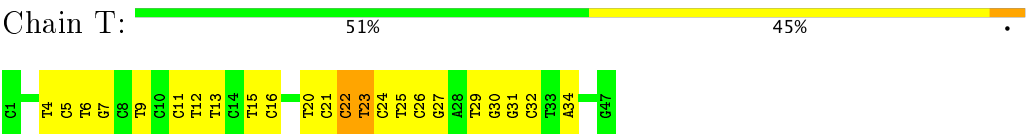
● Molecule 14: DNA (NTS)



● Molecule 15: RNA



● Molecule 16: DNA (TS)



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	19331	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	7.7	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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  >2	RMSZ	# Z  >2
1	A	0.83	0/11592	0.72	3/15682 (0.0%)
10	J	0.87	0/587	0.76	0/786
11	K	0.87	0/913	0.69	0/1232
12	L	0.78	0/366	0.91	1/485 (0.2%)
13	M	0.65	0/4180	0.71	2/5644 (0.0%)
14	N	0.59	1/1082 (0.1%)	0.82	1/1668 (0.1%)
15	R	0.59	0/247	0.80	0/384
16	T	0.72	0/1056	0.84	2/1624 (0.1%)
2	B	0.83	0/9799	0.75	5/13221 (0.0%)
3	C	0.87	0/2163	0.75	2/2930 (0.1%)
4	D	0.92	0/1419	0.68	1/1903 (0.1%)
5	E	0.87	0/1796	0.76	1/2416 (0.0%)
6	F	0.89	0/669	0.71	0/903
7	G	0.76	0/1368	0.82	2/1844 (0.1%)
8	H	0.82	0/1181	0.77	1/1602 (0.1%)
9	I	0.82	0/1016	0.75	0/1365
All	All	0.81	1/39434 (0.0%)	0.74	21/53689 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	33	DA	C3'-O3'	-5.45	1.36	1.44

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	56	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	1239	ARG	NE-CZ-NH1	7.13	123.86	120.30
2	B	405	ARG	NE-CZ-NH2	-6.49	117.06	120.30
3	C	229	TYR	CB-CG-CD1	-6.15	117.31	121.00
7	G	130	TYR	CB-CG-CD2	-6.11	117.33	121.00

There are no chirality outliers.

There are no planarity outliers.

## 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	A	11385	0	11443	57	0
2	B	9608	0	9577	60	0
3	C	2125	0	2091	15	0
4	D	1409	0	1423	4	0
5	E	1760	0	1788	12	0
6	F	657	0	673	7	0
7	G	1340	0	1357	9	0
8	H	1161	0	1124	12	0
9	I	997	0	961	7	0
10	J	578	0	591	6	0
11	K	895	0	903	7	0
12	L	364	0	389	5	0
13	M	4087	0	4145	18	0
14	N	965	0	531	29	0
15	R	220	0	110	26	0
16	T	947	0	532	41	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
18	A	1	0	0	0	0
All	All	38507	0	37638	294	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 4.

The worst 5 of 294 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)
15:R:5:A:H2'	15:R:6:G:C8	2.00	0.97
15:R:5:A:H2'	15:R:6:G:H8	1.37	0.89
11:K:49:GLU:OE1	11:K:49:GLU:HA	1.70	0.88
15:R:7:A:H2'	15:R:8:G:C8	2.09	0.88
13:M:345:LEU:HD23	13:M:345:LEU:O	1.74	0.86

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	A	1446/1733 (83%)	1312 (91%)	109 (8%)	25 (2%)	11	51
2	B	1205/1224 (98%)	1092 (91%)	86 (7%)	27 (2%)	8	44
3	C	268/318 (84%)	238 (89%)	25 (9%)	5 (2%)	9	47
4	D	171/221 (77%)	157 (92%)	14 (8%)	0	100	100
5	E	213/215 (99%)	194 (91%)	14 (7%)	5 (2%)	7	43
6	F	79/155 (51%)	76 (96%)	2 (2%)	1 (1%)	14	56
7	G	169/171 (99%)	156 (92%)	12 (7%)	1 (1%)	28	70
8	H	144/146 (99%)	126 (88%)	14 (10%)	4 (3%)	6	39
9	I	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	11	51
10	J	68/70 (97%)	60 (88%)	7 (10%)	1 (2%)	12	53
11	K	109/120 (91%)	106 (97%)	2 (2%)	1 (1%)	20	63
12	L	44/70 (63%)	34 (77%)	8 (18%)	2 (4%)	3	29
13	M	497/1085 (46%)	460 (93%)	28 (6%)	9 (2%)	10	49
All	All	4533/5650 (80%)	4113 (91%)	337 (7%)	83 (2%)	14	49

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	SER
1	A	472	LEU
1	A	568	PRO
1	A	597	LEU
2	B	44	VAL

### 5.3.2 Protein sidechains ⓘ

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	A	1264/1520 (83%)	1263 (100%)	1 (0%)	94	97
2	B	1046/1061 (99%)	1043 (100%)	3 (0%)	94	96
3	C	238/274 (87%)	238 (100%)	0	100	100
4	D	157/200 (78%)	157 (100%)	0	100	100
5	E	197/197 (100%)	197 (100%)	0	100	100
6	F	72/137 (53%)	72 (100%)	0	100	100
7	G	152/152 (100%)	151 (99%)	1 (1%)	87	93
8	H	128/128 (100%)	127 (99%)	1 (1%)	85	92
9	I	116/116 (100%)	116 (100%)	0	100	100
10	J	65/65 (100%)	65 (100%)	0	100	100
11	K	96/102 (94%)	96 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	449/978 (46%)	449 (100%)	0	100	100
All	All	4020/4987 (81%)	4014 (100%)	6 (0%)	95	97

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	679	TYR
8	H	47	PHE
2	B	860	MET
2	B	654	ARG
7	G	17	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	358	ASN
7	G	117	GLN
12	L	66	GLN
13	M	664	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	R	2	U
15	R	10	A

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 9 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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.