



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:44 PM BST

PDB ID : 3J1N
EMDB ID: : EMD-5407
Title : Cryo-EM map of a yeast minimal preinitiation complex interacting with the Mediator Head module
Authors : Asturias, F.J.; Imasaki, T.
Deposited on : 2012-03-29
Resolution : 16.00 Å(reported)
Based on PDB ID : 1WCM

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 : unknown
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

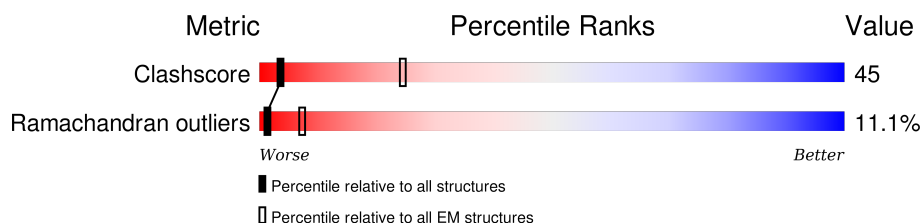
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 16.00 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

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	A	1455	60% 31% 6% •
2	B	1224	62% 23% • 11%
3	C	268	66% 29% 5% •
4	D	218	55% 24% • 19%
5	E	215	79% 18% •
6	F	84	63% 37%
7	G	171	74% 23% •
8	H	146	59% 28% • 9%
9	I	122	75% 20% • •
10	J	70	53% 36% • 7%
11	K	120	83% 10% • 5%

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Mol	Chain	Length	Quality of chain
12	L	70	<div><div></div><div></div><div></div><div></div></div> <div><div>31%</div><div>27%</div><div>7%</div><div>34%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 19237 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	1412	Total	C	N	O	0	0
			6964	4140	1412	1412		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	1094	Total	C	N	O	0	0
			5397	3209	1094	1094		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	266	Total	C	N	O	0	0
			1317	785	266	266		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	177	Total	C	N	O	0	0
			878	524	177	177		

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPABC1.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	214	Total	C	N	O	0	0
			1062	634	214	214		

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPABC2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	84	Total	C	N	O	0	0
			417	249	84	84		

- 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	0	0
			841	499	171	171		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPABC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	133	Total	C	N	O	0	0
			659	393	133	133		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	118	Total	C	N	O	0	0
			587	351	118	118		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPABC5.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	65	Total	C	N	O	0	0
			321	191	65	65		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	114	Total	C	N	O	0	0
			565	337	114	114		

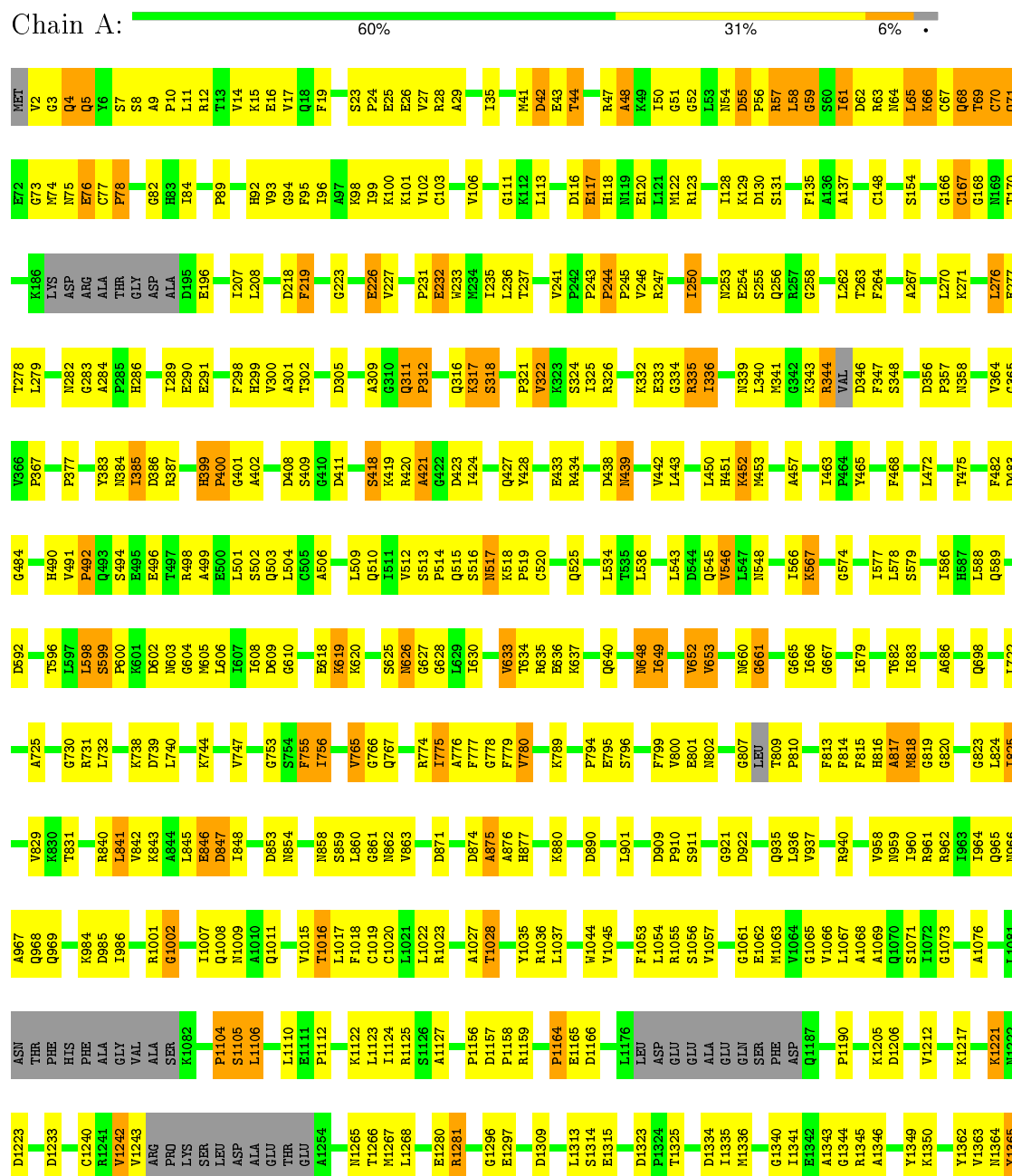
- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPABC4.

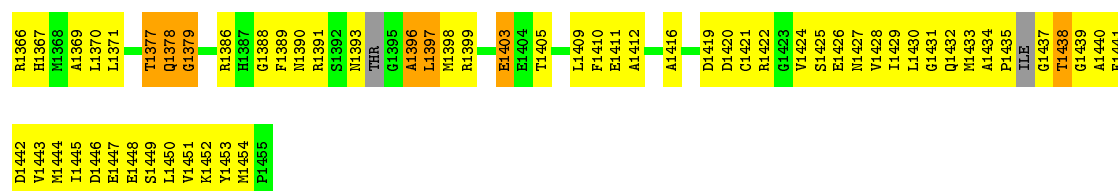
Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	46	Total	C	N	O	0	0
			229	137	46	46		

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.

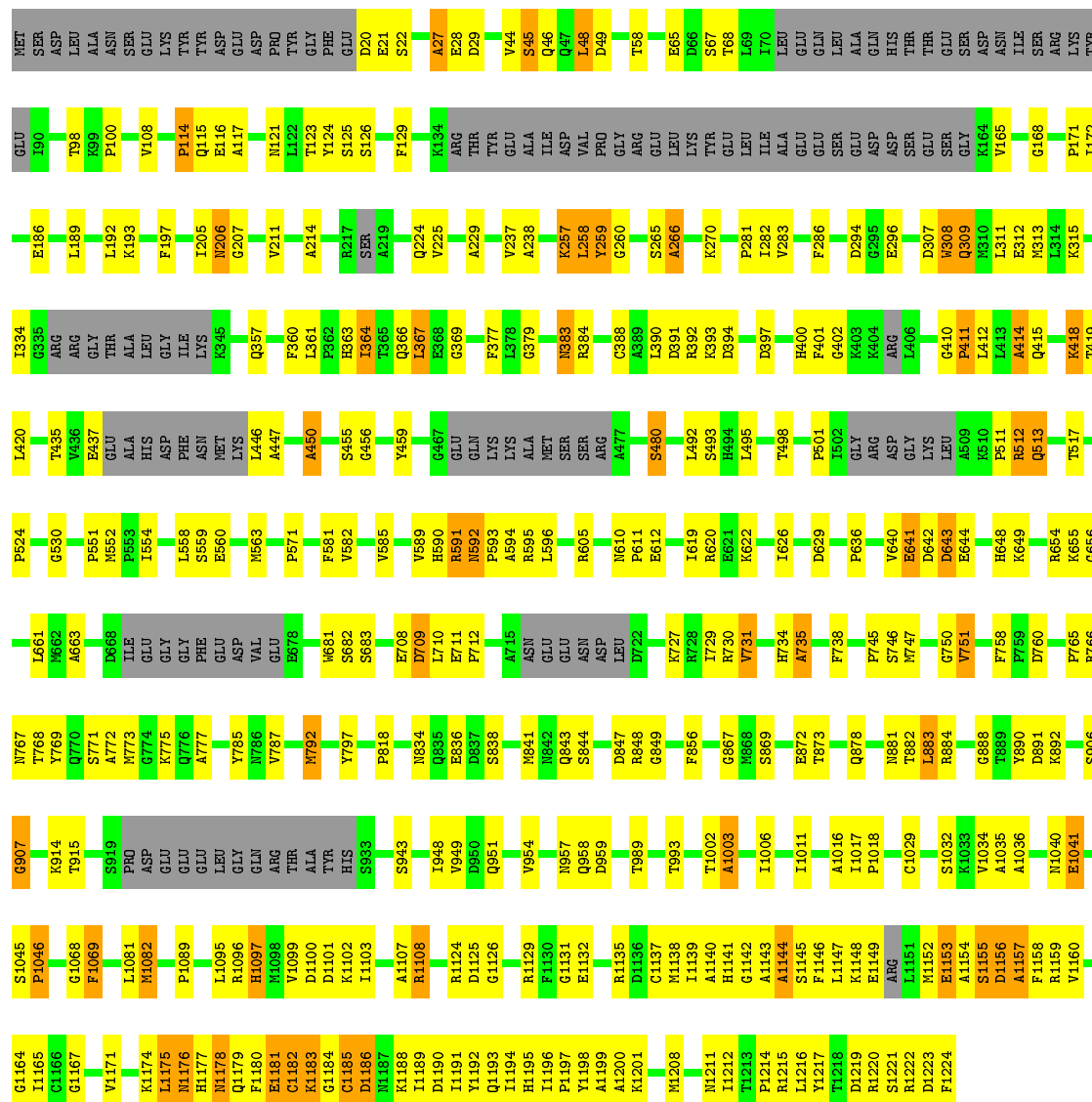
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

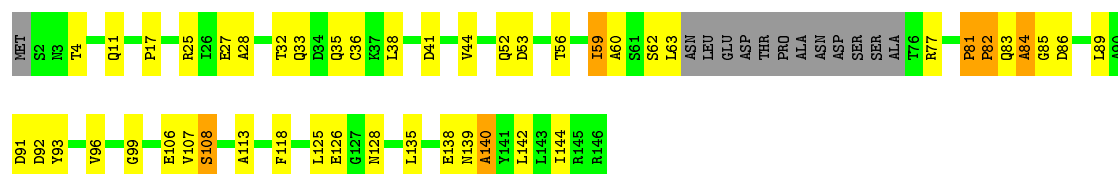
Chain B: 62% 23% 11%



• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

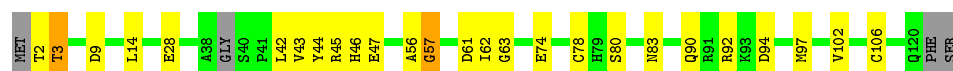
Chain C: 66% 29% 5%





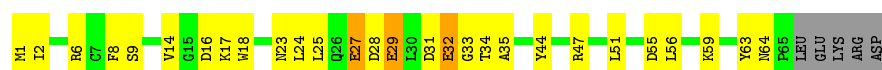
- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 75% 20% • •



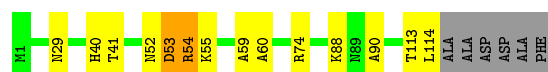
- Molecule 10: DNA-directed RNA polymerase II subunit RPABC5

Chain J: 53% 36% • 7%



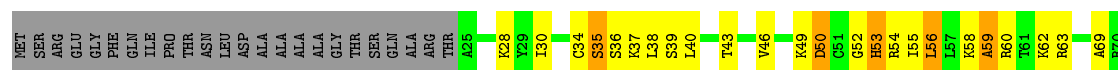
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K: 83% 10% • 5%



- Molecule 12: DNA-directed RNA polymerase II subunit RPABC4

Chain L: 31% 27% 7% 34%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	51000	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Each CCD frame	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	50000	Depositor
Image detector	Tietz F415 4kx4k CCD camera	Depositor

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 >2	RMSZ	# Z >2
1	A	0.41	0/6953	0.77	3/9659 (0.0%)
10	J	0.45	0/320	0.88	0/444
11	K	0.40	0/564	0.70	0/785
12	L	0.52	0/228	0.82	0/317
2	B	0.39	0/5384	0.74	1/7473 (0.0%)
3	C	0.44	0/1316	0.81	0/1833
4	D	0.36	0/876	0.75	1/1219 (0.1%)
5	E	0.34	0/1061	0.66	0/1479
6	F	0.48	0/416	0.80	0/579
7	G	0.45	0/840	0.80	0/1166
8	H	0.34	0/657	0.69	0/913
9	I	0.43	0/585	0.82	0/814
All	All	0.41	0/19200	0.76	5/26681 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1403	GLU	N-CA-C	5.38	125.52	111.00
2	B	1185	CYS	N-CA-C	-5.30	96.70	111.00
1	A	452	LYS	N-CA-C	-5.21	96.93	111.00
4	D	7	THR	N-CA-C	5.14	124.88	111.00
1	A	344	ARG	N-CA-C	-5.04	97.38	111.00

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	6964	0	3039	671	0
2	B	5397	0	2399	433	0
3	C	1317	0	590	53	0
4	D	878	0	387	63	0
5	E	1062	0	453	43	0
6	F	417	0	180	123	0
7	G	841	0	354	181	0
8	H	659	0	296	30	0
9	I	587	0	235	31	0
10	J	321	0	137	15	0
11	K	565	0	260	6	0
12	L	229	0	107	12	0
All	All	19237	0	8437	1250	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 45.

The worst 5 of 1250 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)
6:F:143:PHE:CB	7:G:68:ALA:CA	1.76	1.61
1:A:344:ARG:CA	2:B:1129:ARG:HA	1.27	1.60
6:F:143:PHE:CA	7:G:68:ALA:HB1	1.11	1.58
2:B:1148:LYS:HA	2:B:1200:ALA:CB	1.22	1.57
1:A:1444:MET:CB	7:G:10:ASN:CB	1.82	1.57

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	1390/1455 (96%)	938 (68%)	290 (21%)	162 (12%)	0	9
2	B	1068/1224 (87%)	727 (68%)	220 (21%)	121 (11%)	0	10
3	C	264/268 (98%)	159 (60%)	66 (25%)	39 (15%)	0	5
4	D	173/218 (79%)	122 (70%)	34 (20%)	17 (10%)	1	14
5	E	212/215 (99%)	148 (70%)	49 (23%)	15 (7%)	1	22
6	F	82/84 (98%)	64 (78%)	14 (17%)	4 (5%)	3	31
7	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	1	22
8	H	129/146 (88%)	84 (65%)	30 (23%)	15 (12%)	0	9
9	I	114/122 (93%)	77 (68%)	30 (26%)	7 (6%)	2	26
10	J	63/70 (90%)	37 (59%)	10 (16%)	16 (25%)	0	1
11	K	112/120 (93%)	89 (80%)	18 (16%)	5 (4%)	3	33
12	L	44/70 (63%)	19 (43%)	14 (32%)	11 (25%)	0	2
All	All	3820/4163 (92%)	2595 (68%)	801 (21%)	424 (11%)	1	11

5 of 424 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	48	ALA
1	A	54	ASN
1	A	55	ASP
1	A	57	ARG

5.3.2 Protein sidechains [i](#)

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

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](#)

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.