



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 21, 2017 – 12:43 AM EDT

PDB ID : 5M3M
EMDB ID: : EMD-4148
Title : Free monomeric RNA polymerase I at 4.0Å resolution
Authors : Neyer, S.; Kunz, M.; Geiss, C.; Hantsche, M.; Hodirnau, V.-V.; Seybert, A.;
Engel, C.; Scheffer, M.P.; Cramer, P.; Frangakis, A.S.
Deposited on : unknown
Resolution : 4.00 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

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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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-20029824

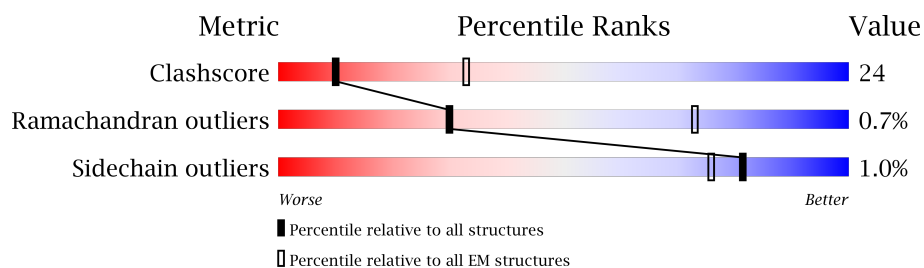
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.



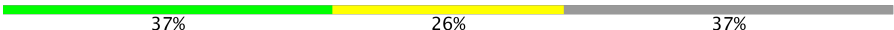

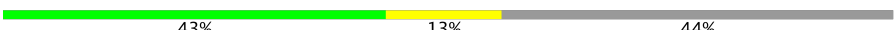

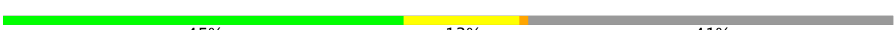
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1664	44% 43% 12%
2	B	1203	49% 48% .
3	C	335	41% 49% 9%
4	E	215	44% 54% .
5	F	155	32% 31% 37%
6	H	146	48% 42% 10%
7	I	125	46% 46% 7%
8	J	70	44% 54% .
9	K	142	33% 38% 29%

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Mol	Chain	Length	Quality of chain
10	L	70	
11	M	415	
12	N	233	
13	D	137	
14	G	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SO4	B	1301	-	-	X	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 33233 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1462	Total	C	N	O	S	0	0
			11558	7304	2006	2187	61		

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1166	Total	C	N	O	S	0	0
			9266	5864	1617	1734	51		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	98	Total	C	N	O	S	0	0
			807	512	142	150	3		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	116	Total	C	N	O	S	0	0
			883	550	148	176	9		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	97	Total	C	N	O		0	0
			771	490	124	157			

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	131	Total	C	N	O	S	0	0
			1035	660	171	200	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	58	Total	C	N	O		0	0
			459	289	78	92			

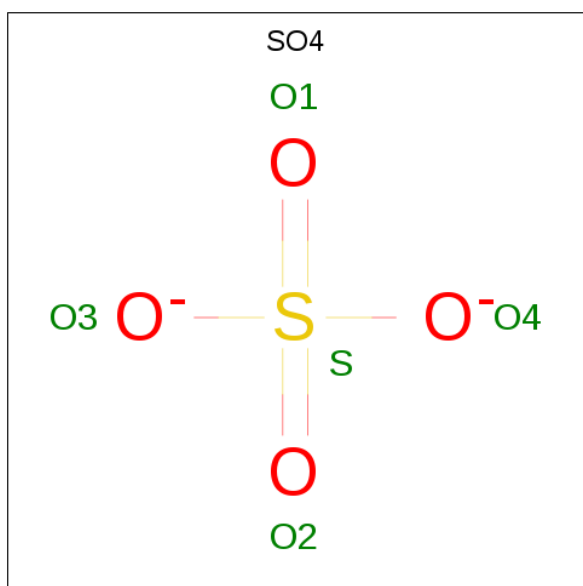
- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	192	Total	C	N	O	S	0	0
			1518	979	261	273	5		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

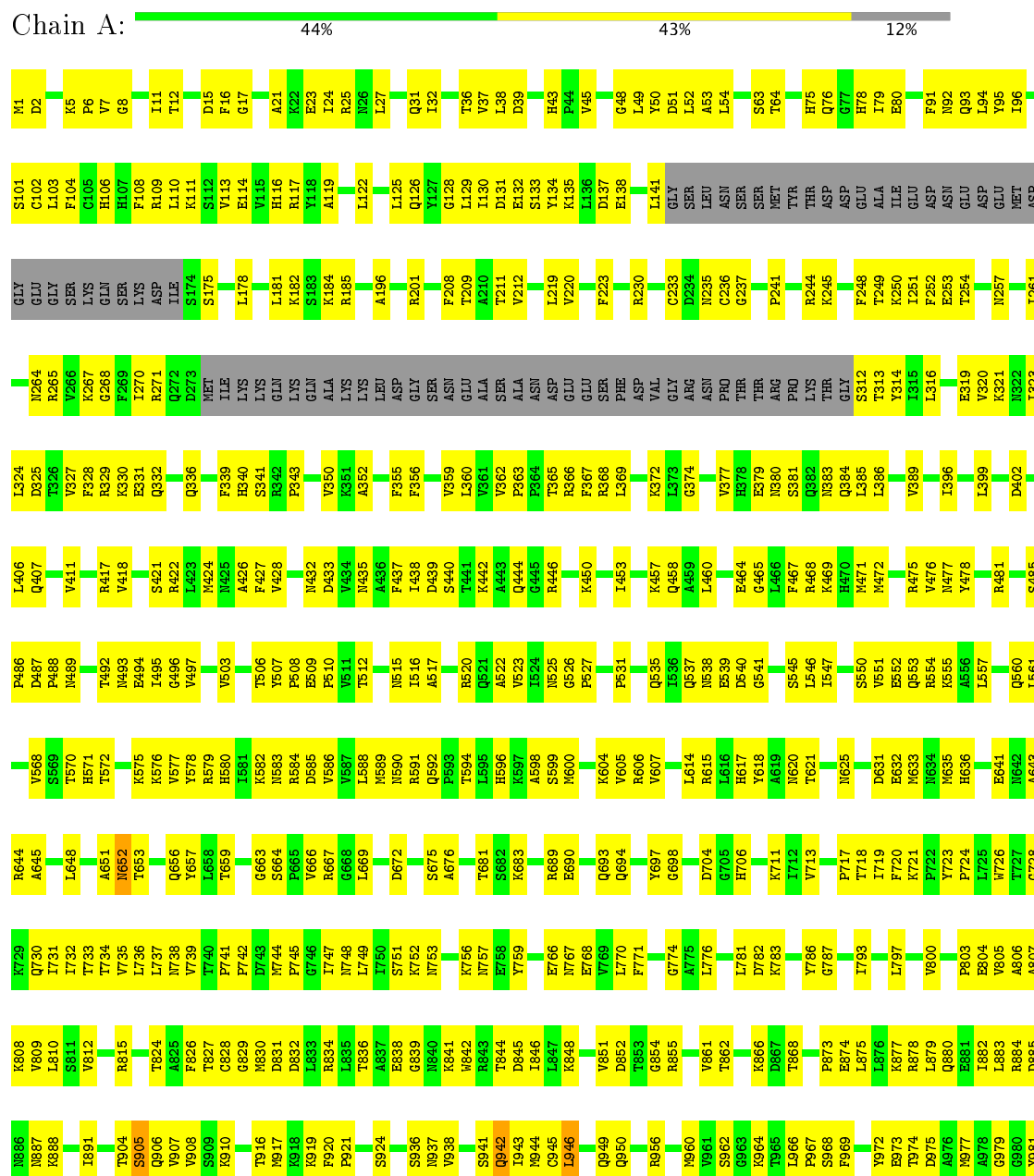


Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	O	S	0
			5	4	1	

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 the various outlier classes 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 I subunit RPA190

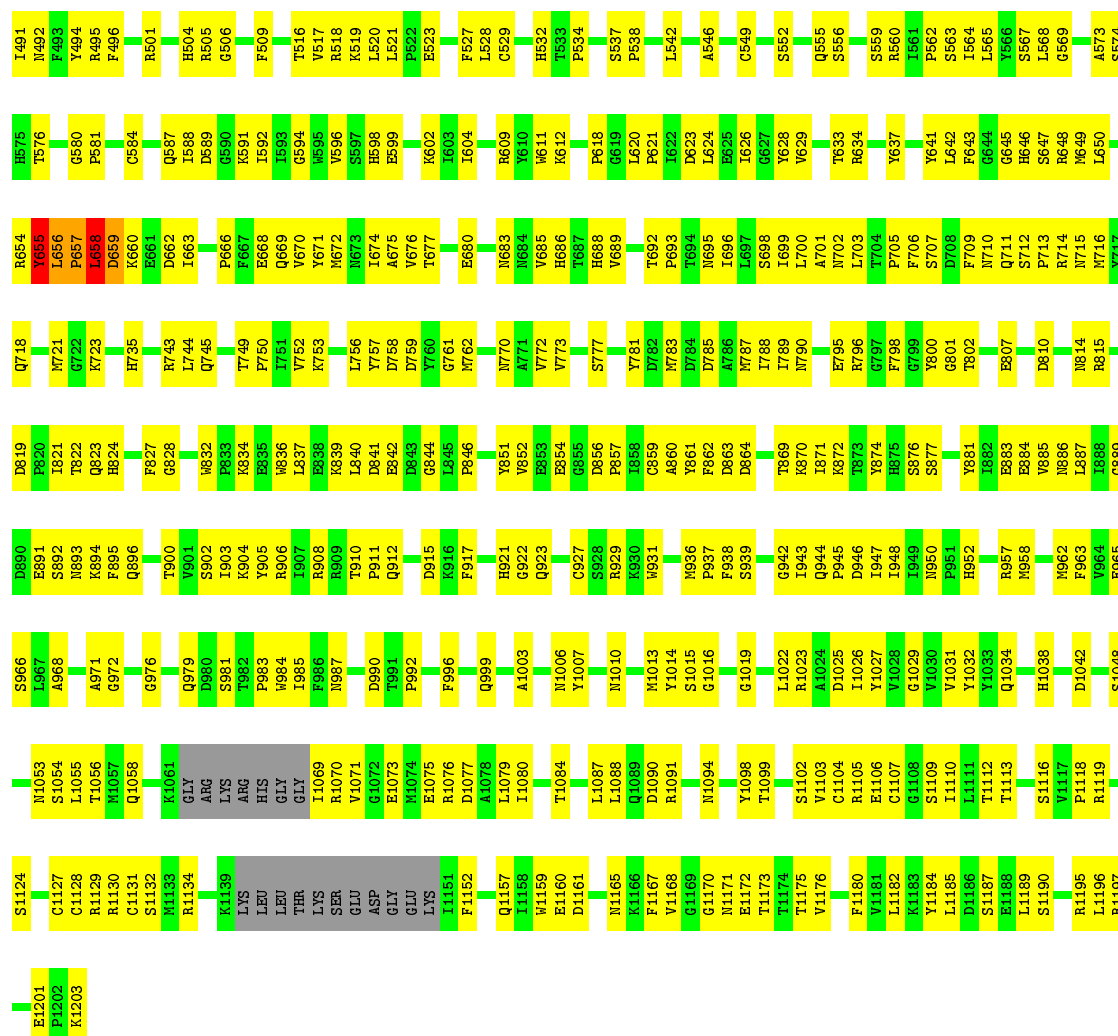


V982	K963	Y1074	F1166	Q1250	Q1314	VAL	V1442	V1520	S1609	F1610	M1611	K1612	V1524	M1529	V1443	Q1443	VAL	SER
K984	G985	K1078	L1172	A1251	M1315	TYP	Q1446	T1521	M1611	K1612	VAL	V1524	V1524	M1529	Q1447	Q1443	ASP	SER
F986	Y987	K1079	K1173	F1254	V1316	TRP	R1446	V1521	M1611	K1612	VAL	V1524	V1524	M1529	Q1447	Q1443	ASP	SER
S988	Y988	P1082	M1174	C1255	M1319	PRO	S1448	M1530	F1617	T1617	GLU	V1530	M1530	M1529	S1449	Q1443	ASP	SER
Y996	M1000	L1085	R1176	S1257	F1321	GLU	I1450	E1533	K1624	L1627	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
G1005	L1006	A1094	E1183	I1258	H1322	ASP	I1451	F1535	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
L1007	I1007	A1094	V1185	K1260	H1323	GLU	S1452	F1535	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
D1008	T1009	S1098	G1186	V1261	L1324	ILE	H1453	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
A1010	VAL	L1085	I1187	L1262	L1325	THR	H1454	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
LYS	THR	L1085	I1187	L1262	L1325	MET	H1455	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
SER	ARG	L1085	I1187	L1262	L1325	ARG	F1456	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
ARG	SER	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
SER	SER	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
G1017	VAL	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
Q1020	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
L1023	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
T1024	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
K1025	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
H1031	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
Y1034	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
R1039	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
D1040	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
A1041	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
D1042	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
G1043	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
M1049	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
Y1050	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
G1051	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
D1053	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
A1054	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
I1055	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
D1056	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
I1057	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
T1058	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
K1059	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
E1060	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
S1061	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
H1062	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
F1066	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER
L1070	THR	L1085	I1187	L1262	L1325	THR	I1457	I1536	A1625	L1628	T1617	M1530	M1530	M1529	S1449	Q1443	ASP	SER

• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

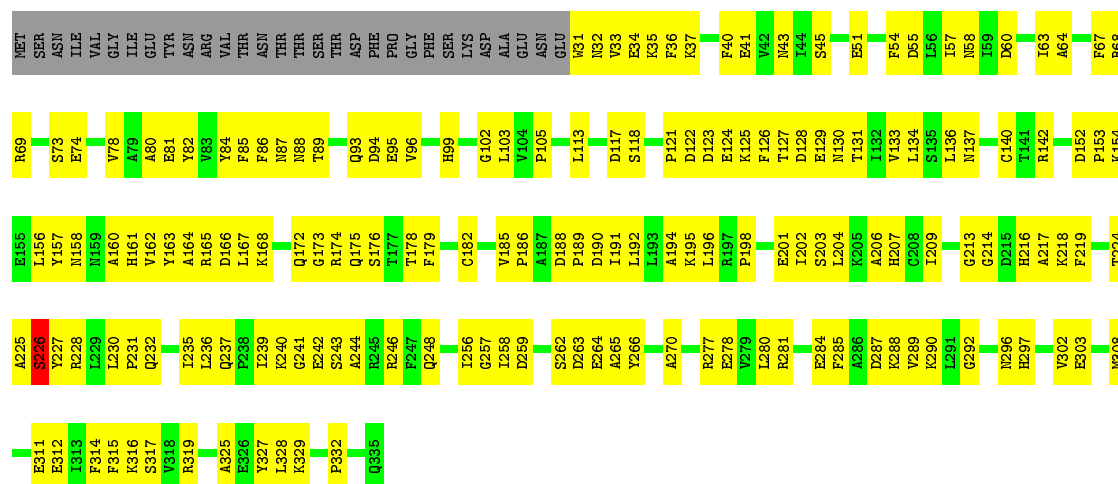
Chain B:  49% 48%

MET	SER	LYS	VAL	ILE	PRO	PRO	GLY	GLN	ALA	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR
F74	D75	G76	H80	SER	GLU	ASP	GLU	ILE	SER	ASN	S88	G92	G92	G92	G92	G92	G92	G92	G92
L161	P162	V163	M164	S167	M168	R169	C170	H171	L172	M173	K174	M175	M175	M175	M175	M175	M175	M175	M175
S245	T247	T247	V249	Y252	L253	D254	D255	G256	Q257	R261	F262	S263	S263	S263	S263	S263	S263	S263	S263
Q328	S329	L330	G331	R335	A340	S341	P342	D343	Q344	S345	D346	V349	E352	V353	R356	V358	L359	V360	H361
N411	T417	L421	T424	Q427	V428	D431	R434	R436	G438	G439	N441	D442	K443	K443	K443	K443	K443	K443	K443
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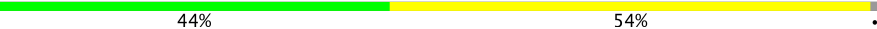


- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 41% 49% 9%



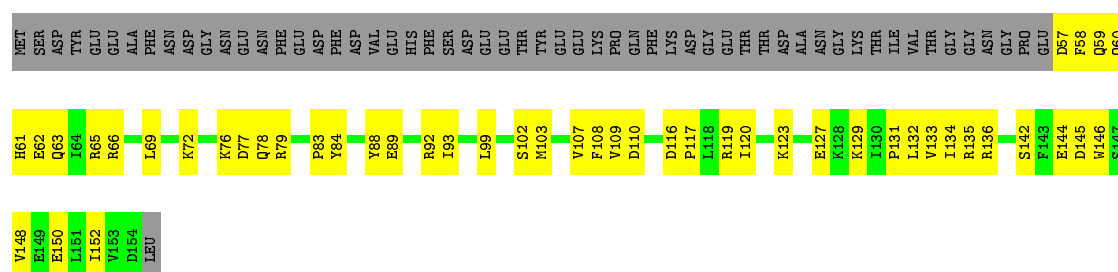
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 



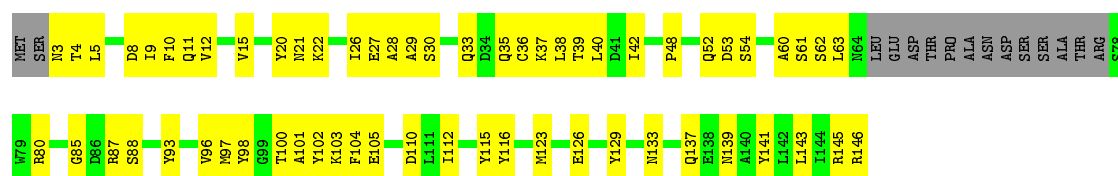
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 



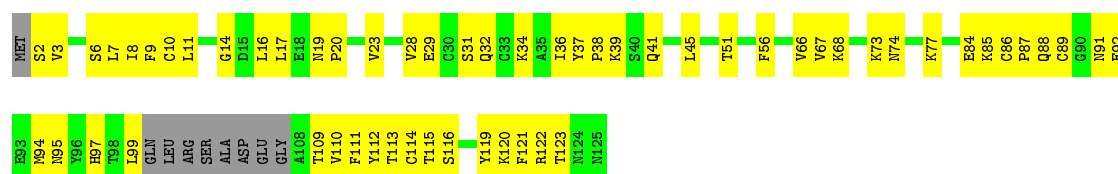
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



- Molecule 7: DNA-directed RNA polymerase I subunit RPA12

Chain I: 

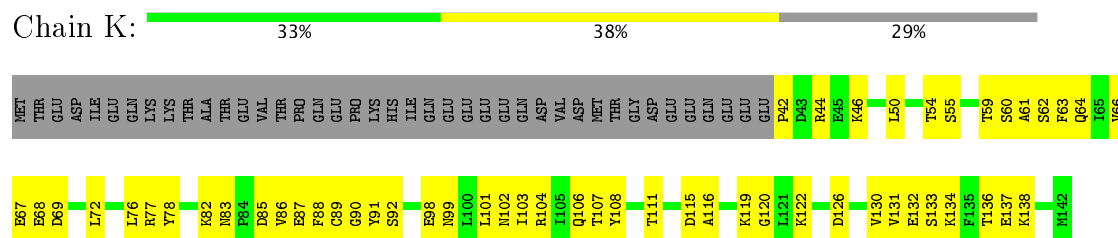


- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

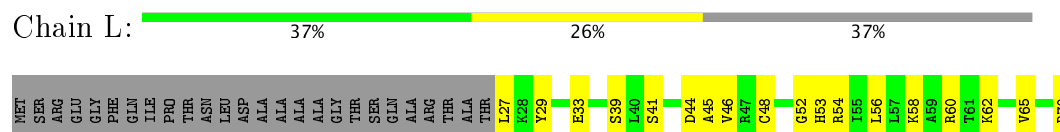
Chain J: 



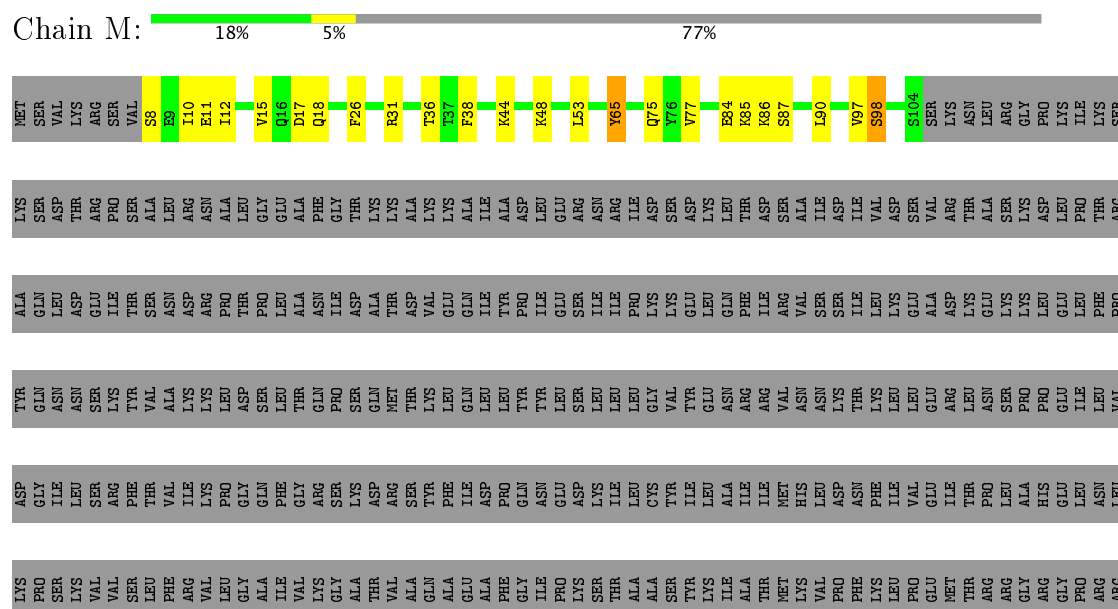
- Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2



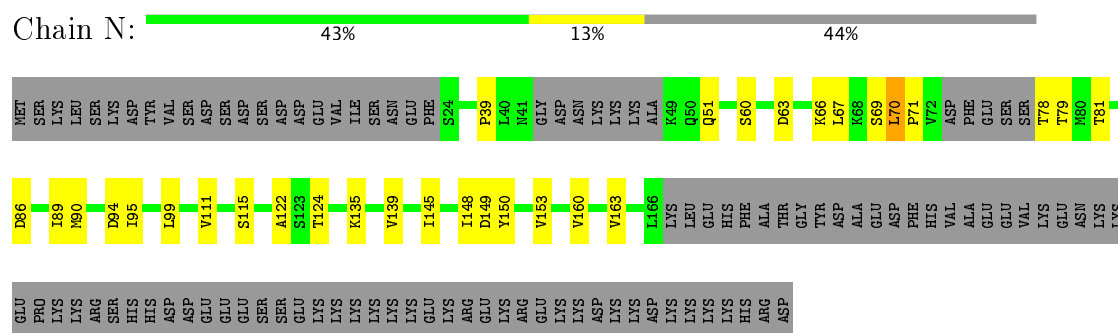
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: DNA-directed RNA polymerase I subunit RPA49

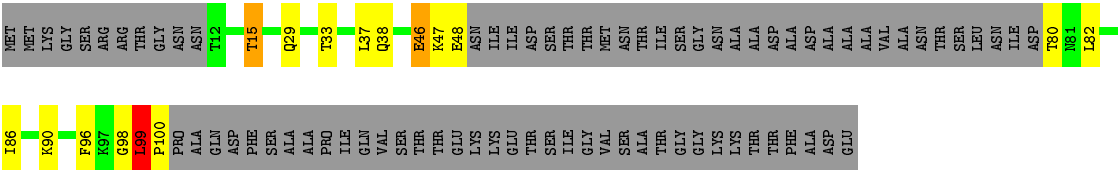


- Molecule 12: DNA-directed RNA polymerase I subunit RPA34

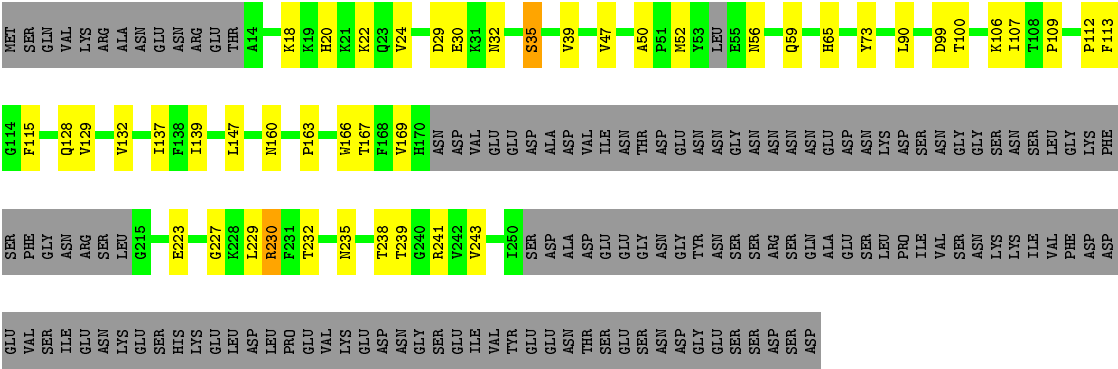


- Molecule 13: DNA-directed RNA polymerase I subunit RPA14





● Molecule 14: DNA-directed RNA polymerase I subunit RPA43



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (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: ZN, SO4

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	0.40	0/11770	0.51	0/15895
10	L	0.40	0/354	0.53	0/468
11	M	0.40	0/786	0.55	0/1057
12	N	0.39	0/1052	0.55	0/1418
13	D	0.40	0/465	0.58	0/630
14	G	0.37	0/1555	0.66	3/2113 (0.1%)
2	B	0.45	0/9471	0.53	0/12805
3	C	0.45	0/2475	0.51	0/3354
4	E	0.40	0/1771	0.50	0/2383
5	F	0.37	0/821	0.48	0/1106
6	H	0.46	0/1070	0.54	0/1449
7	I	0.38	0/895	0.49	0/1205
8	J	0.50	0/578	0.53	0/775
9	K	0.45	0/804	0.55	0/1083
All	All	0.42	0/33867	0.53	3/45741 (0.0%)

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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	241	ARG	NE-CZ-NH1	11.80	126.20	120.30
14	G	241	ARG	NE-CZ-NH2	-11.62	114.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	G	241	ARG	CD-NE-CZ	6.08	132.12	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1649	VAL	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	11558	0	11642	651	0
2	B	9266	0	9151	558	0
3	C	2423	0	2412	156	0
4	E	1735	0	1764	98	0
5	F	807	0	827	45	0
6	H	1052	0	1021	47	0
7	I	883	0	879	60	0
8	J	569	0	585	36	0
9	K	793	0	790	56	0
10	L	352	0	374	20	0
11	M	771	0	755	11	0
12	N	1035	0	1069	29	0
13	D	459	0	462	8	0
14	G	1518	0	1528	31	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	B	5	0	0	8	0
All	All	33233	0	33259	1613	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 24.

The worst 5 of 1613 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)
2:B:656:LEU:O	12:N:153:VAL:HG11	1.62	0.97
3:C:225:ALA:O	3:C:226:SER:HB2	1.63	0.95
1:A:1501:ILE:HG22	1:A:1502:PRO:HD2	1.49	0.94
2:B:894:LYS:HG2	10:L:54:ARG:HH21	1.33	0.94
5:F:66:ARG:HA	5:F:69:LEU:HD12	1.50	0.93

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	1448/1664 (87%)	1364 (94%)	75 (5%)	9 (1%)	28	70
2	B	1158/1203 (96%)	1110 (96%)	41 (4%)	7 (1%)	28	70
3	C	303/335 (90%)	283 (93%)	19 (6%)	1 (0%)	44	80
4	E	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
5	F	96/155 (62%)	94 (98%)	2 (2%)	0	100	100
6	H	127/146 (87%)	124 (98%)	3 (2%)	0	100	100
7	I	112/125 (90%)	108 (96%)	4 (4%)	0	100	100
8	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
9	K	99/142 (70%)	95 (96%)	4 (4%)	0	100	100
10	L	42/70 (60%)	38 (90%)	4 (10%)	0	100	100
11	M	95/415 (23%)	86 (90%)	7 (7%)	2 (2%)	8	48
12	N	125/233 (54%)	108 (86%)	13 (10%)	4 (3%)	5	39
13	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	4	36
14	G	186/326 (57%)	171 (92%)	13 (7%)	2 (1%)	17	60
All	All	4122/5236 (79%)	3894 (94%)	201 (5%)	27 (1%)	30	68

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	946	LEU
2	B	657	PRO
2	B	658	LEU
2	B	659	ASP
3	C	226	SER

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	1292/1465 (88%)	1288 (100%)	4 (0%)	94	97
2	B	1022/1053 (97%)	1020 (100%)	2 (0%)	94	97
3	C	269/296 (91%)	268 (100%)	1 (0%)	93	96
4	E	194/197 (98%)	194 (100%)	0	100	100
5	F	88/137 (64%)	88 (100%)	0	100	100
6	H	115/128 (90%)	115 (100%)	0	100	100
7	I	103/110 (94%)	103 (100%)	0	100	100
8	J	64/65 (98%)	64 (100%)	0	100	100
9	K	91/130 (70%)	91 (100%)	0	100	100
10	L	39/57 (68%)	39 (100%)	0	100	100
11	M	88/371 (24%)	79 (90%)	9 (10%)	8	37
12	N	124/220 (56%)	120 (97%)	4 (3%)	44	74
13	D	55/116 (47%)	49 (89%)	6 (11%)	7	35
14	G	170/291 (58%)	158 (93%)	12 (7%)	17	53
All	All	3714/4636 (80%)	3676 (99%)	38 (1%)	81	90

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	N	124	THR
13	D	29	GLN

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Mol	Chain	Res	Type
14	G	230	ARG
12	N	145	ILE
13	D	38	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	248	ASN
2	B	547	HIS
6	H	35	GLN
2	B	254	ASN
2	B	427	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 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	$\# Z > 2$
16	SO4	B	1301	-	4,4,4	0.14	0	6,6,6	0.33	0

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
16	SO4	B	1301	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1301	SO4	8	0

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.