



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 01:35 am BST

PDB ID : 2R93
Title : Elongation complex of RNA polymerase II with a hepatitis delta virus-derived RNA stem loop
Authors : Lehmann, E.; Brueckner, F.; Cramer, P.
Deposited on : 2007-09-12
Resolution : 4.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

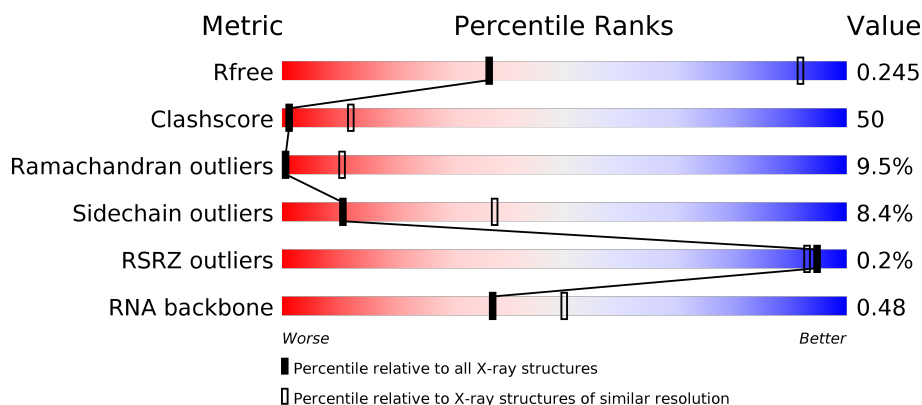
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



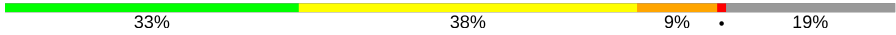


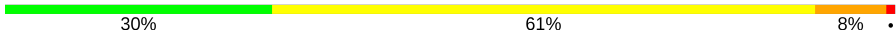
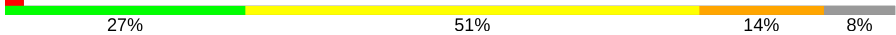
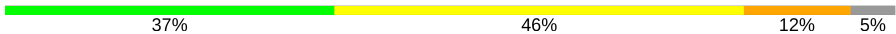
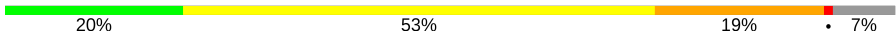
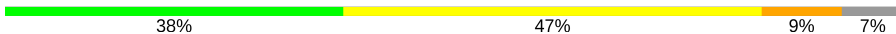

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)
RNA backbone	3102	1048 (5.00-3.00)

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 on 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	R	18	<div> <div>28%</div> <div>28%</div> <div>17%</div> <div>6%</div> <div>22%</div> </div>
2	A	1733	<div> <div>29%</div> <div>44%</div> <div>8%</div> <div>•</div> <div>18%</div> </div>
3	B	1224	<div> <div>28%</div> <div>51%</div> <div>11%</div> <div>•</div> <div>9%</div> </div>
4	C	318	<div> <div>26%</div> <div>48%</div> <div>8%</div> <div>•</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	221	
6	E	215	
7	F	155	
8	G	171	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31500 atoms, of which 0 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 RNA chain called RNA (5'-R(*UP*GP*AP*UP*UP*CP*UP*CP*UP*AP*UP*CP*GP*GP*AP*AP*UP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	14	Total	C	N	O	P	0	0	0
			289	132	49	96	12			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1422	Total	C	N	O	S	0	0	0
			11194	7054	1959	2119	62			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1112	Total	C	N	O	S	0	0	0
			8841	5596	1550	1640	55			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	135	Total	C	N	O	S	0	0	0
			1084	683	183	214	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	116	Total	C	N	O	S	0	0	0
			944	581	172	181	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	112	Total	C	N	O	S	0	0	0
			904	580	154	168	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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


- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	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 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.

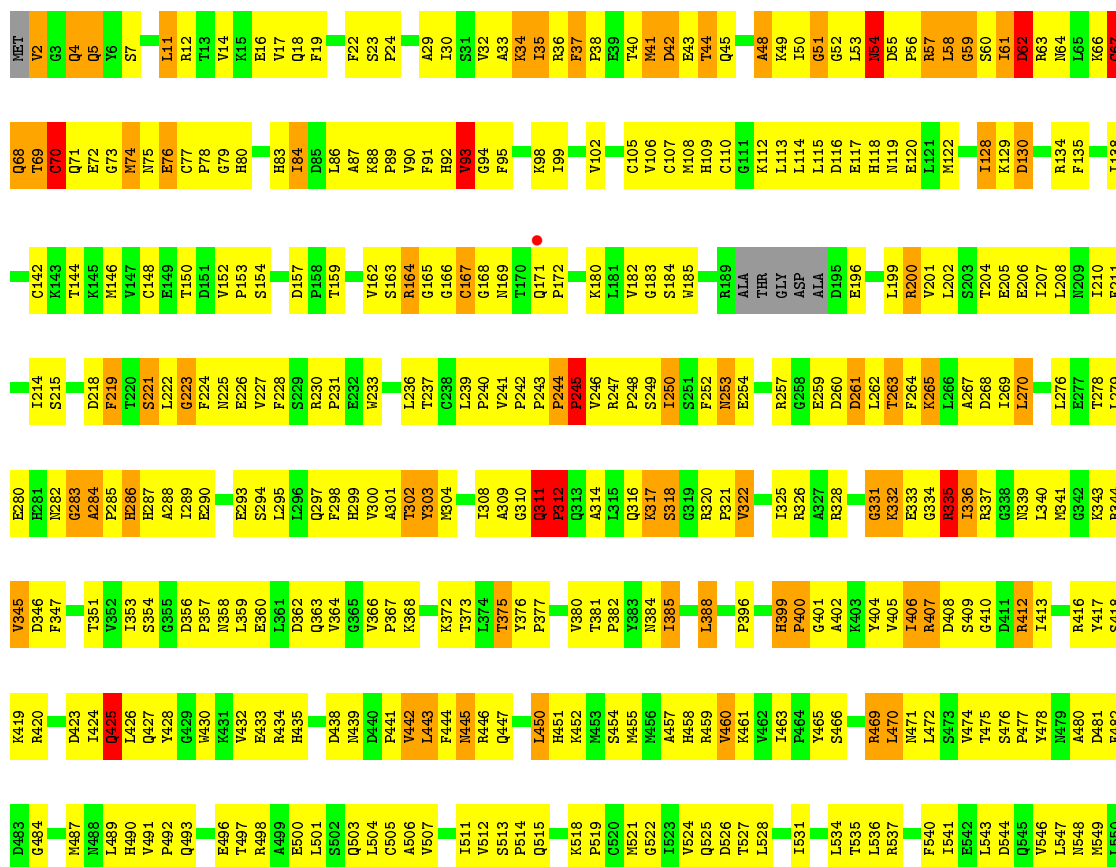
- Molecule 1: RNA (5'-R(*UP*GP*AP*UP*UP*CP*UP*CP*UP*AP*UP*CP*GP*GP*AP*AP*UP*C)-3')

Chain R: 



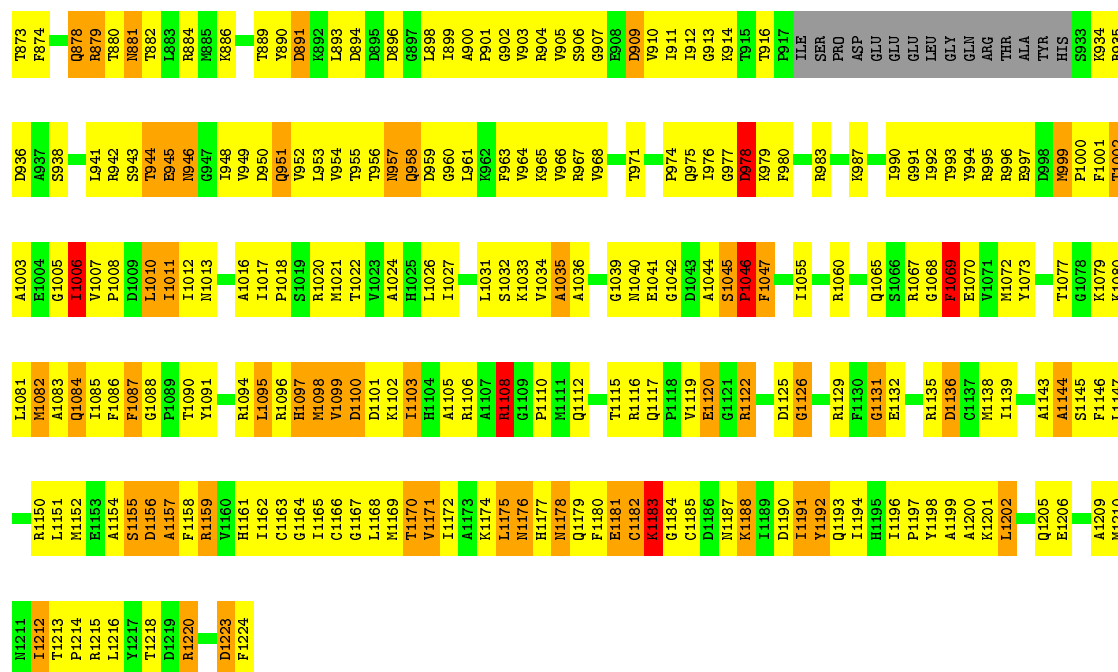
- Molecule 2: DNA-directed RNA polymerase II subunit RPB1

Chain A: 

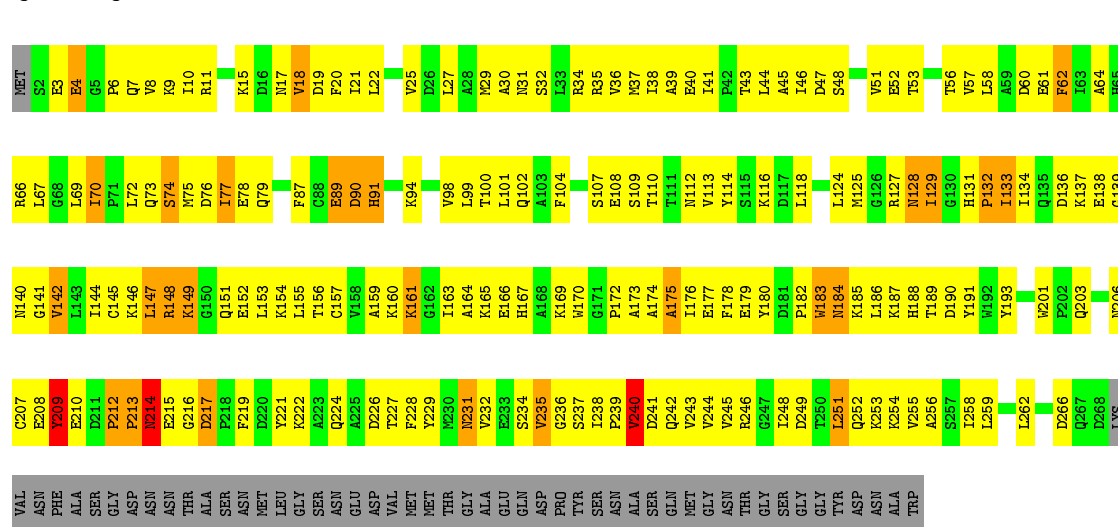


SER	GLU	GLY	F1402	M1330	K1261	L1192	E1121	S1056	D985	L908	Y836	A763	K595	J626	Y551
PRO	ALA	GLY	E1403	S1331	K1262	L1193	P1122	V1057	I986	D909	I837	C764	E596	G627	M552
SER	THR	VAL	E1404	F1332	I1263	M1194	G1123	V1058	Y987	P910	Q838	V765	A697	G628	
THR	THR	THR	T1405	I1333	E1264		H1124	H1059	L988		R839	G766	Q698	I629	I560
SER	SER	PRO	V1406	I1334	N1265	D1198	H1125	P1060	L993	E914	R840	Q767	A699	I630	P561
PRO	PRO	TYR		I1335	T1266		D1127	G1061			L841	Q768	H631	H631	T562
THR	GLY	SER	L1409	M1336	M1267	A1201	Q1130	M1062	N996	I919	V842	R774	L701	V632	P563
SER	PHE	ASN	F1410	E1337	L1268	M1202		M1063	I997		K843	I775	L702	V633	A564
PRO	GLY	GLU	E1411				L1133	V1064	L997	I920	A844	I776	H706	I634	I565
SER	VAL	SER	G1412				I1134	G1065	L998	G921	L845	A777		I635	
THR	THR	GLY	G1413					V1066		D922	E846	F777		E636	K567
SER	SER	LEU					I1138	L1067	R1001	D847	D847	G778	T709	K637	P568
PRO	PRO	ASN	A1416					A1068	G1002	L848	I848	F779	L710	G638	K569
THR	GLY	ASN	E1417				T1141	A1069	K1003	M849	M849	V780	R711	P639	P570
SER	PHE	ALA	L1418					S1071	M1004	V850	V850	I781	E712	L571	L571
PRO	PRO	ASP	D1419				L1139	G1070	E1005	H851	H851	R782	S713	M572	
SER	PRO	LEU	R1280					V1066		L929	Y852	T783	F714	S573	S573
THR	THR	ASP	A1347				K1144	L1074	I1007	D930	D853	L784		G574	G574
SER	VAL	VAL	L1348				S1145	G1213	I1007	D930	D853	L784		K575	K575
PRO	SER	VAL	V1349				T1146	P1075	Q1008	E931	M854	P785		Q576	Q576
PRO	PRO	LYS	K1350				T1147	A1076	M1009		T855	F787		N648	N648
THR	THR	ASP	E1351				I1148			D939	T856	H787		I577	I577
SER	TYR	GLU	S1425				S1149	M1079	Q1010	R940	R857	R720	R720	Q650	L578
PRO	PRO	LEU	E1426				S1150	R1011	Q1011	K941	R857	S788		K651	S579
SER	PRO	MET	N1427				E1151	L1081	R1012		M858	K789			
THR	THR	PHE	V1428				I1152	ASN	D1013	L942	S859		L722	V580	V580
SER	SER	SER	I1429				Y1153	THR	V1015	R944	G861	P794	L723	M654	L588
PRO	PRO	PRO	L1430				T1154	PHE	T1016		A862	E795	E724		
THR	ALA	LEU	G1431					HIS	L1017	V946	V946	S796	A725	L657	Q589
SER	TYR	VAL	Q1432					PHE	F1018		V863	K797	R726	L658	R590
PRO	SER	ASP	M1433					ALA	C1019	M954	F866	F799	D727	H659	F591
PRO	PRO	ASP	R1366					GLY			L867	V600	K728	N660	D592
SER	PRO	SER	H1367				S1160	VAL	L1022		L868	E801	A729	G661	T595
THR	THR	GLY	V1299				V1161	VAL			P957	E801		F662	T596
SER	PRO	SER	K1300				I1162	ALA	L1026	P958	G869	N802	L732	S663	T596
PRO	PRO	ASP	E1303				I1163	SER	R1025		D870	S803		T664	L597
THR	ALA	ALA	M1304				P1164	K1092	L1027	N959	D871	Y804		L598	
PRO	PRO	GLY	L1371				E1165	K1093	A1027	I960	G872	L805		I666	S599
SER	PRO	ASP	D1166					V1094	T1028	R961	M873	R806		P600	P600
THR	THR	ASP						T1095	R1029	R962	D874	G807		D668	K601
PRO	PRO	ASP	I1169				I1170	S1096	R1030	I963	A875	L808	L740	T669	D602
SER	TYR	ALA	I1170					G1097	L1031	I964		T809	M741	M603	M603
PRO	PRO	GLY							Q1032	Q965				G673	G604
THR	THR	GLY	H1173				F1174	R1100	Q1033	R966	I886	E812	V743	P674	I612
SER	PRO	ALA	L1174				S1175	K1102	E1034	A967	G887	F813	K744	T675	I613
SER	PRO	THR	V1242				L1176	E1103	Y1035	Q968	G887	F814	Q745	M676	L606
PRO	PRO	GLY	V1243					L1104	R1036	Q969	S889	F815	M746	I607	I607
PRO	PRO	GLY	M1244					L1037	L1037	T970	S889	H816	V747	I679	I608
PRO	PRO	GLY	P1245				ASP	L1038	F971	H972		A817	M748	T680	
PRO	PRO	GLY	LYS				GLU	K1039	T1038	H972		H816		E681	I612
PRO	PRO	GLY	SER				GLU	L1106	Q1040	I973		H816		T682	I613
PRO	PRO	GLY	LEU				ALA	V1107	A1041	D974		M818		I683	F614
PRO	PRO	GLY	ASP				GLU		F1042		K695	R821		V616	G615
PRO	PRO	GLY	ASP				GLN	M1111		H975	R896			V617	V616
PRO	PRO	GLY	ALA				GLN	K1112	V1045	T976	Y897	I825	S753	A684	V616
PRO	PRO	GLY	GLU				PHE	T1113	L1046	T976	R898	D826	S754	E685	I616
PRO	PRO	GLY	THR				THR	P1114	S1047	K977	R898	T827	F755	A686	E618
PRO	PRO	GLY	GLU				GLU	S1116	ASP	S979	D900	N757	K687	K619	K619
PRO	PRO	GLY	ASP				Q1187	L1116	L1048	D980	L901	V829	I758	K620	K620
PRO	PRO	GLY	E1255				Q1188	T1117	L1049	L981	L902	K830	I758	V690	T821
PRO	PRO	GLY	E1255				S1189	T1118	L1049	L981	L902	K830	I758	V690	T821
PRO	PRO	GLY	M1259				P1190	V1119	L1049	L981	L902	K830	I758	V690	T821
PRO	PRO	GLY	L1260				W1191	L1120	Q1052	L981	L902	K830	I758	V690	T821
PRO	PRO	GLY	L1260				W1191	L1120	Q1052	L981	L902	K830	I758	V690	T821



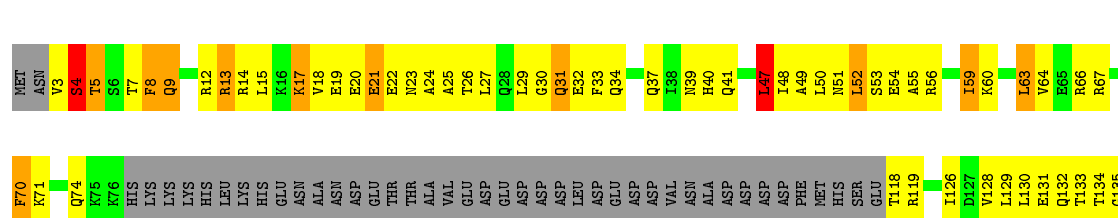


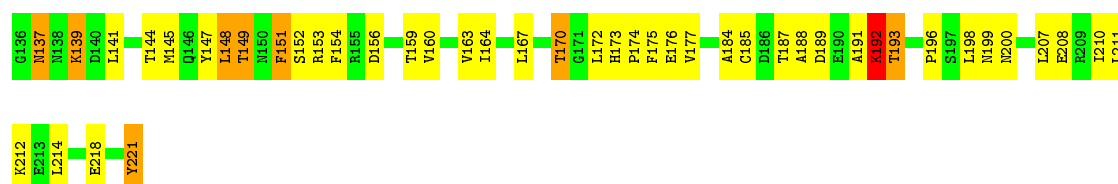
Chain C:



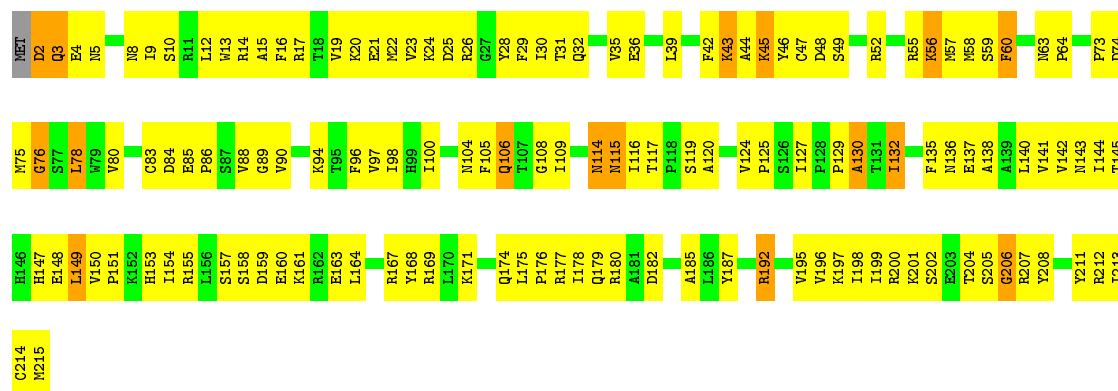
• Molecule 5: DNA-directed RNA polymerase II subunit RPB4

Chain D:

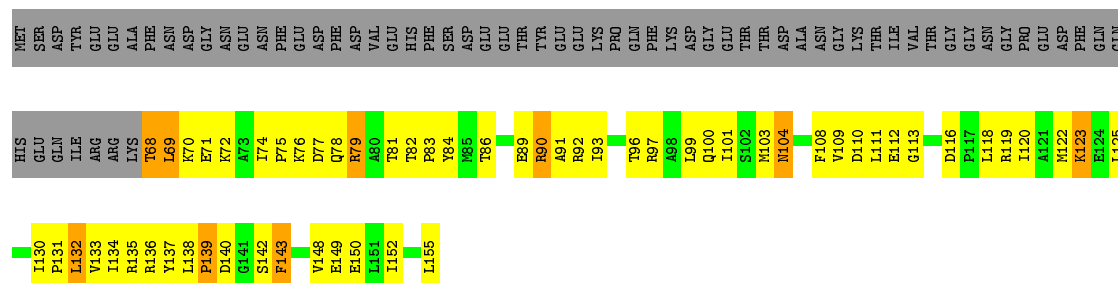




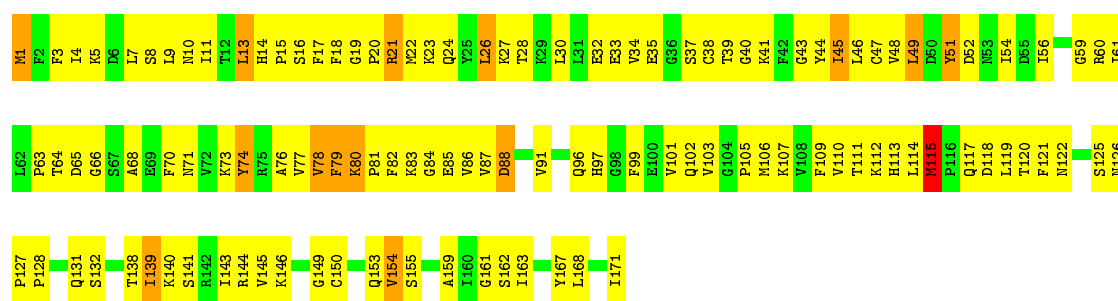
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC1



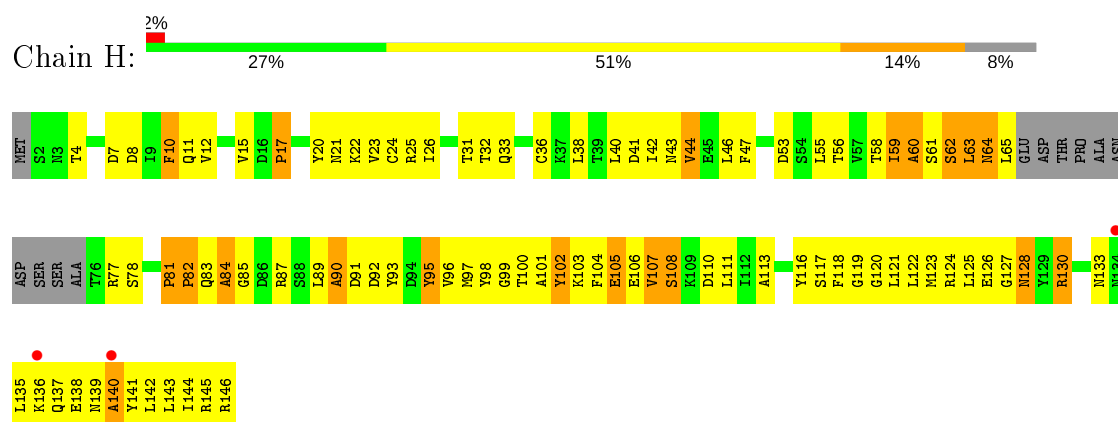
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC2



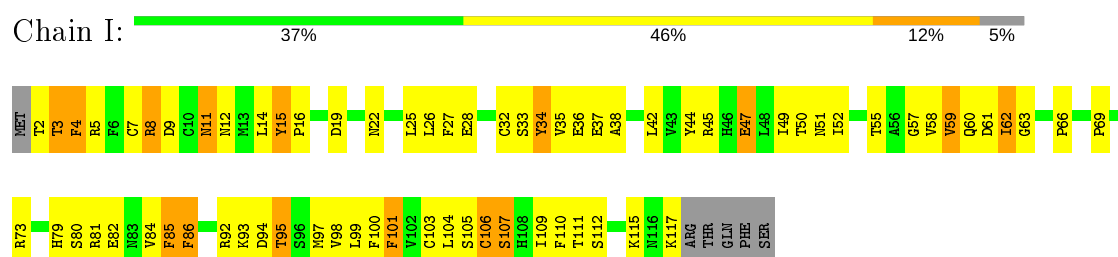
• Molecule 8: DNA-directed RNA polymerase II subunit RPB7



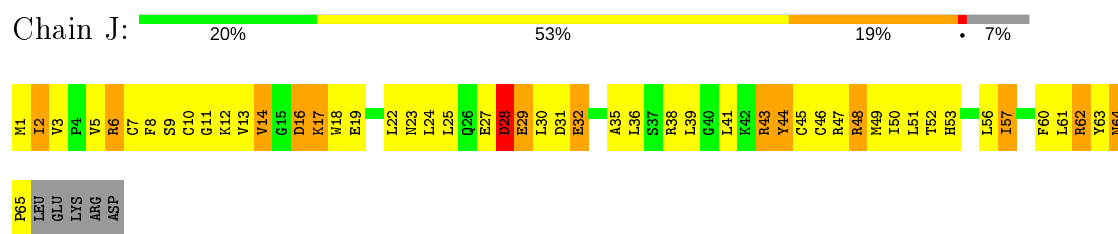
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



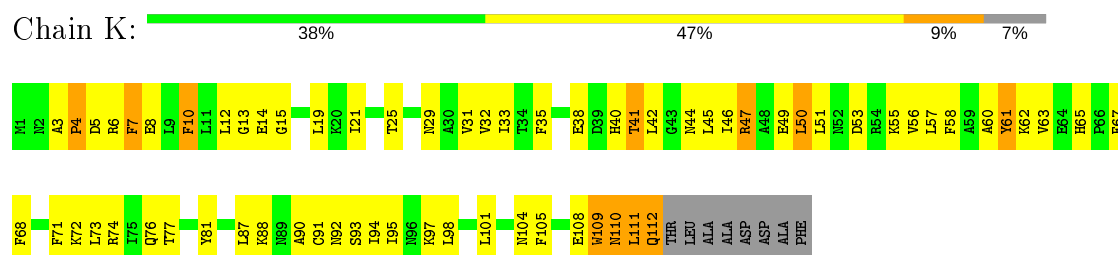
• Molecule 10: DNA-directed RNA polymerase II subunit RPB9



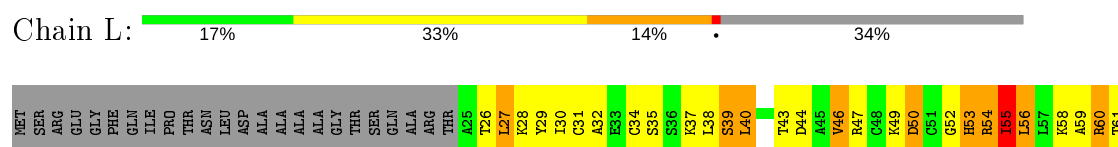
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 12: DNA-directed RNA polymerase II subunit RPB11



• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



K62	
R63	
L64	
V65	
A69	
R70	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	223.34Å 394.88Å 284.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.00 48.28 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.00) 97.2 (48.28-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 4.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.216 , 0.241 0.224 , 0.245	Depositor DCC
R_{free} test set	2129 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	103.2	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.010 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	31500	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	R	0.87	0/321	1.11	3/496 (0.6%)
2	A	0.42	0/11394	0.71	6/15407 (0.0%)
3	B	0.41	0/9013	0.68	0/12152
4	C	0.42	0/2139	0.72	1/2899 (0.0%)
5	D	0.40	0/1444	0.66	0/1935
6	E	0.38	0/1788	0.64	0/2406
7	F	0.53	0/723	0.92	2/974 (0.2%)
8	G	0.44	0/1368	0.72	0/1844
9	H	0.38	0/1102	0.64	0/1492
10	I	0.36	0/962	0.64	0/1295
11	J	0.47	0/541	0.72	0/727
12	K	0.44	0/922	0.65	0/1244
13	L	0.48	0/366	0.72	0/485
All	All	0.42	0/32083	0.70	12/43356 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	F	70	LYS	N-CA-C	-10.69	82.14	111.00
7	F	69	LEU	CA-CB-CG	9.42	136.97	115.30
1	R	7	U	O4'-C1'-N1	7.69	114.35	108.20
2	A	1176	LEU	N-CA-C	7.45	131.12	111.00
2	A	1176	LEU	CA-CB-CG	7.44	132.41	115.30

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	R	289	0	153	11	0
2	A	11194	0	11279	1192	0
3	B	8841	0	8875	1024	0
4	C	2101	0	2056	260	0
5	D	1434	0	1460	119	0
6	E	1752	0	1776	150	0
7	F	712	0	737	108	0
8	G	1340	0	1357	159	0
9	H	1084	0	1057	128	0
10	I	944	0	901	98	0
11	J	532	0	543	90	0
12	K	904	0	911	106	0
13	L	364	0	387	49	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31500	0	31492	3165	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 50.

The worst 5 of 3165 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)
7:F:68:THR:HG21	7:F:69:LEU:N	1.59	1.16
7:F:69:LEU:HD23	7:F:71:GLU:CB	1.77	1.14
7:F:69:LEU:HD23	7:F:71:GLU:HB2	1.17	1.12
2:A:58:LEU:HD12	2:A:59:GLY:N	1.65	1.11
2:A:34:LYS:NZ	2:A:57:ARG:HH12	1.50	1.09

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 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	
2	A	1412/1733 (82%)	1032 (73%)	252 (18%)	128 (9%)	1	12
3	B	1096/1224 (90%)	781 (71%)	206 (19%)	109 (10%)	0	9
4	C	265/318 (83%)	169 (64%)	66 (25%)	30 (11%)	0	6
5	D	174/221 (79%)	133 (76%)	27 (16%)	14 (8%)	1	14
6	E	212/215 (99%)	166 (78%)	32 (15%)	14 (7%)	1	17
7	F	85/155 (55%)	70 (82%)	11 (13%)	4 (5%)	2	23
8	G	169/171 (99%)	128 (76%)	32 (19%)	9 (5%)	2	21
9	H	131/146 (90%)	78 (60%)	33 (25%)	20 (15%)	0	3
10	I	114/122 (93%)	76 (67%)	26 (23%)	12 (10%)	0	8
11	J	63/70 (90%)	37 (59%)	16 (25%)	10 (16%)	0	3
12	K	110/120 (92%)	88 (80%)	15 (14%)	7 (6%)	1	18
13	L	44/70 (63%)	20 (46%)	12 (27%)	12 (27%)	0	0
All	All	3875/4565 (85%)	2778 (72%)	728 (19%)	369 (10%)	0	10

5 of 369 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	42	ASP
2	A	48	ALA
2	A	54	ASN
2	A	57	ARG
2	A	62	ASP

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	
2	A	1245/1520 (82%)	1136 (91%)	109 (9%)	10	35
3	B	964/1061 (91%)	882 (92%)	82 (8%)	10	37
4	C	235/274 (86%)	219 (93%)	16 (7%)	16	44
5	D	160/200 (80%)	138 (86%)	22 (14%)	3	20
6	E	196/197 (100%)	187 (95%)	9 (5%)	27	54
7	F	78/137 (57%)	72 (92%)	6 (8%)	13	40
8	G	152/152 (100%)	133 (88%)	19 (12%)	4	22
9	H	119/128 (93%)	115 (97%)	4 (3%)	37	61
10	I	110/116 (95%)	104 (94%)	6 (6%)	21	50
11	J	60/65 (92%)	53 (88%)	7 (12%)	5	24
12	K	97/102 (95%)	89 (92%)	8 (8%)	11	38
13	L	40/57 (70%)	37 (92%)	3 (8%)	13	41
All	All	3456/4009 (86%)	3165 (92%)	291 (8%)	11	37

5 of 291 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	473	MET
3	B	957	ASN
10	I	15	TYR
3	B	502	ILE
3	B	724	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	518	HIS
3	B	1065	GLN
10	I	90	GLN
3	B	706	GLN
3	B	842	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	12/18 (66%)	4 (33%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	6	C
1	R	7	U
1	R	13	G
1	R	17	U

There are no RNA pucker outliers to report.

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 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	68:THR	C	69:LEU	N	4.50

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	R	14/18 (77%)	0.66	0 100 100	128, 147, 176, 188	0
2	A	1422/1733 (82%)	-0.40	2 (0%) 95 94	57, 116, 171, 200	0
3	B	1112/1224 (90%)	-0.36	2 (0%) 95 93	61, 126, 184, 200	0
4	C	267/318 (83%)	-0.42	0 100 100	73, 111, 159, 176	0
5	D	178/221 (80%)	-0.35	0 100 100	88, 133, 179, 192	0
6	E	214/215 (99%)	-0.37	0 100 100	93, 154, 191, 199	0
7	F	88/155 (56%)	-0.54	0 100 100	61, 93, 130, 153	0
8	G	171/171 (100%)	-0.41	0 100 100	88, 116, 155, 163	0
9	H	135/146 (92%)	0.13	3 (2%) 62 52	131, 161, 187, 196	0
10	I	116/122 (95%)	-0.20	0 100 100	110, 161, 191, 196	0
11	J	65/70 (92%)	-0.53	0 100 100	79, 109, 145, 149	0
12	K	112/120 (93%)	-0.45	0 100 100	76, 115, 140, 158	0
13	L	46/70 (65%)	0.02	0 100 100	107, 170, 191, 193	0
All	All	3940/4583 (85%)	-0.36	7 (0%) 95 93	57, 122, 182, 200	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	471	LYS	3.5
2	A	1455	PRO	2.9
2	A	171	GLN	2.3
9	H	136	LYS	2.2
9	H	134	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
14	ZN	I	204	1/1	0.89	0.04	190,190,190,190	0
14	ZN	L	105	1/1	0.96	0.06	156,156,156,156	0
14	ZN	A	1506	1/1	0.97	0.07	119,119,119,119	0
15	MG	A	1	1/1	0.97	0.15	68,68,68,68	0
14	ZN	A	1508	1/1	0.99	0.14	79,79,79,79	0
14	ZN	B	1307	1/1	0.99	0.20	78,78,78,78	0
14	ZN	C	302	1/1	0.99	0.13	71,71,71,71	0
14	ZN	J	101	1/1	0.99	0.24	86,86,86,86	0
14	ZN	I	203	1/1	0.99	0.18	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.