



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:17 am GMT

PDB ID : 2CW0
Title : Crystal structure of Thermus thermophilus RNA polymerase holoenzyme at 3.3 angstroms resolution
Authors : Tuske, S.; Sarafianos, S.G.; Wang, X.; Hudson, B.; Sineva, E.; Mukhopadhyay, J.; Birktoft, J.J.; Leroy, O.; Ismail, S.; Clark Jr., A.D.; Dharia, C.; Napoli, A.; Laptenko, O.; Lee, J.; Borukhov, S.; Ebright, R.H.; Arnold, E.
Deposited on : 2005-06-15
Resolution : 3.30 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

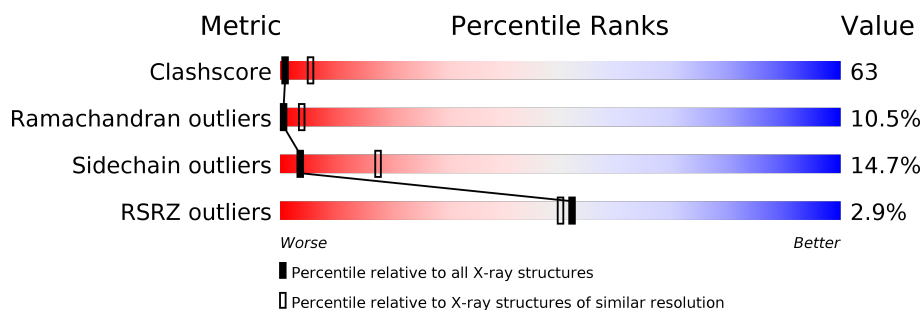
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)

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. 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	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	
3	D	1524	

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Mol	Chain	Length	Quality of chain
3	N	1524	
4	E	99	
4	O	99	
5	F	423	
5	P	423	

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
6	ZN	D	1525	-	-	-	X
6	ZN	N	1525	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 53962 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 protein called DNA-directed RNA polymerase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	B	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	K	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			
1	L	229	Total	C	N	O	S	0	0	0
			1806	1153	313	337	3			

- Molecule 2 is a protein called DNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			
2	M	1119	Total	C	N	O	S	0	0	0
			8829	5581	1577	1647	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			
3	N	1392	Total	C	N	O	S	0	0	0
			10975	6953	1941	2048	33			

- Molecule 4 is a protein called RNA polymerase omega chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			
4	O	95	Total	C	N	O	S	0	0	0
			769	488	133	144	4			

- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			
5	P	345	Total	C	N	O	S	0	0	0
			2793	1762	504	523	4			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		
6	N	2	Total	Zn	0	0
			2	2		

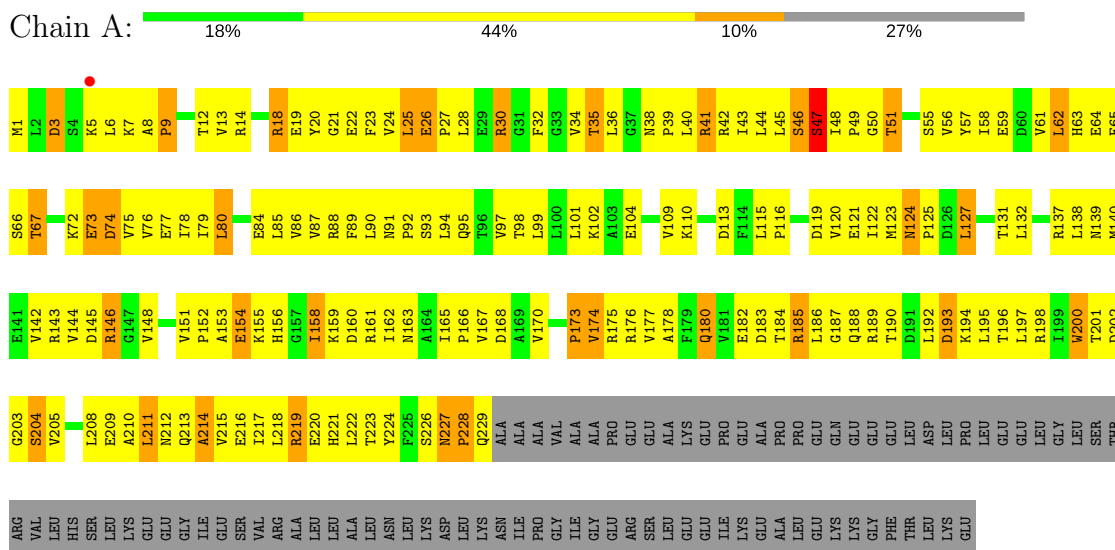
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		

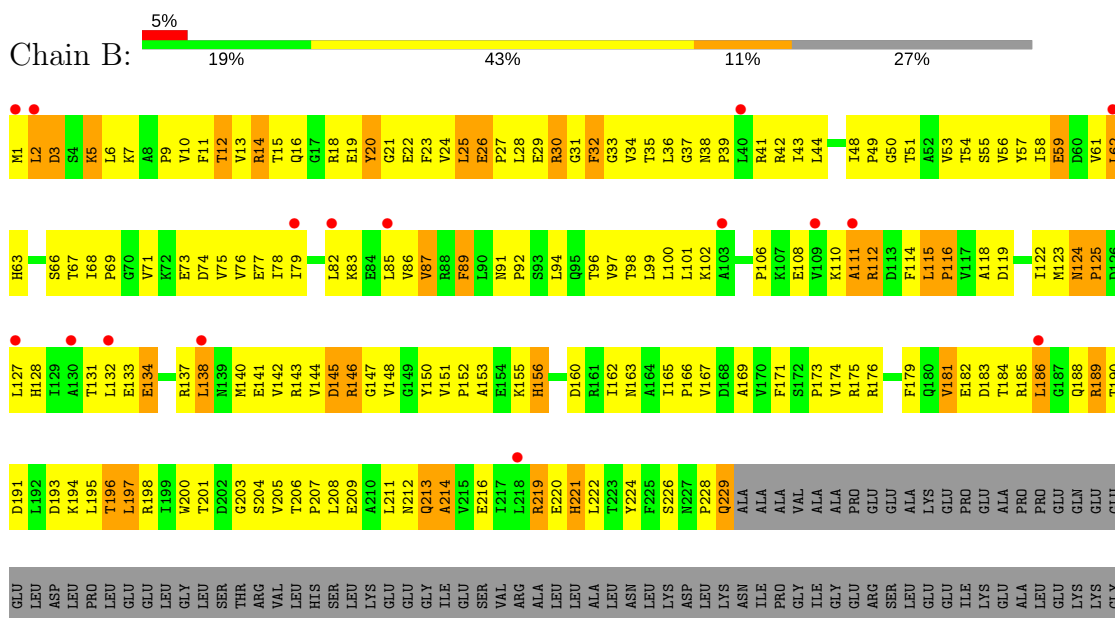
3 Residue-property plots

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: DNA-directed RNA polymerase alpha chain

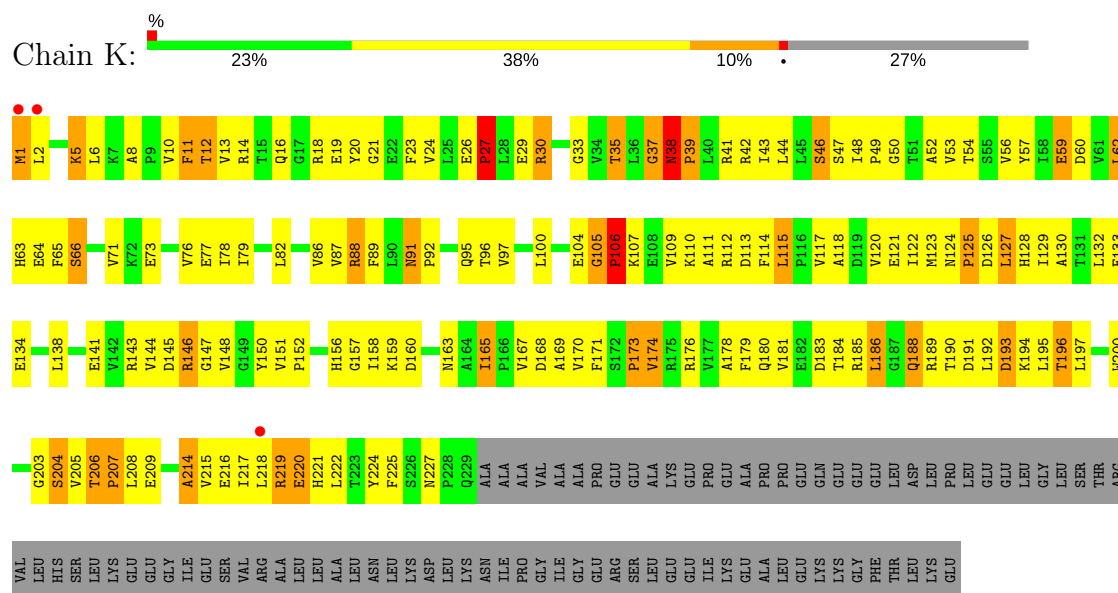


• Molecule 1: DNA-directed RNA polymerase alpha chain



PHE
THR
LEU
LYS
GLU

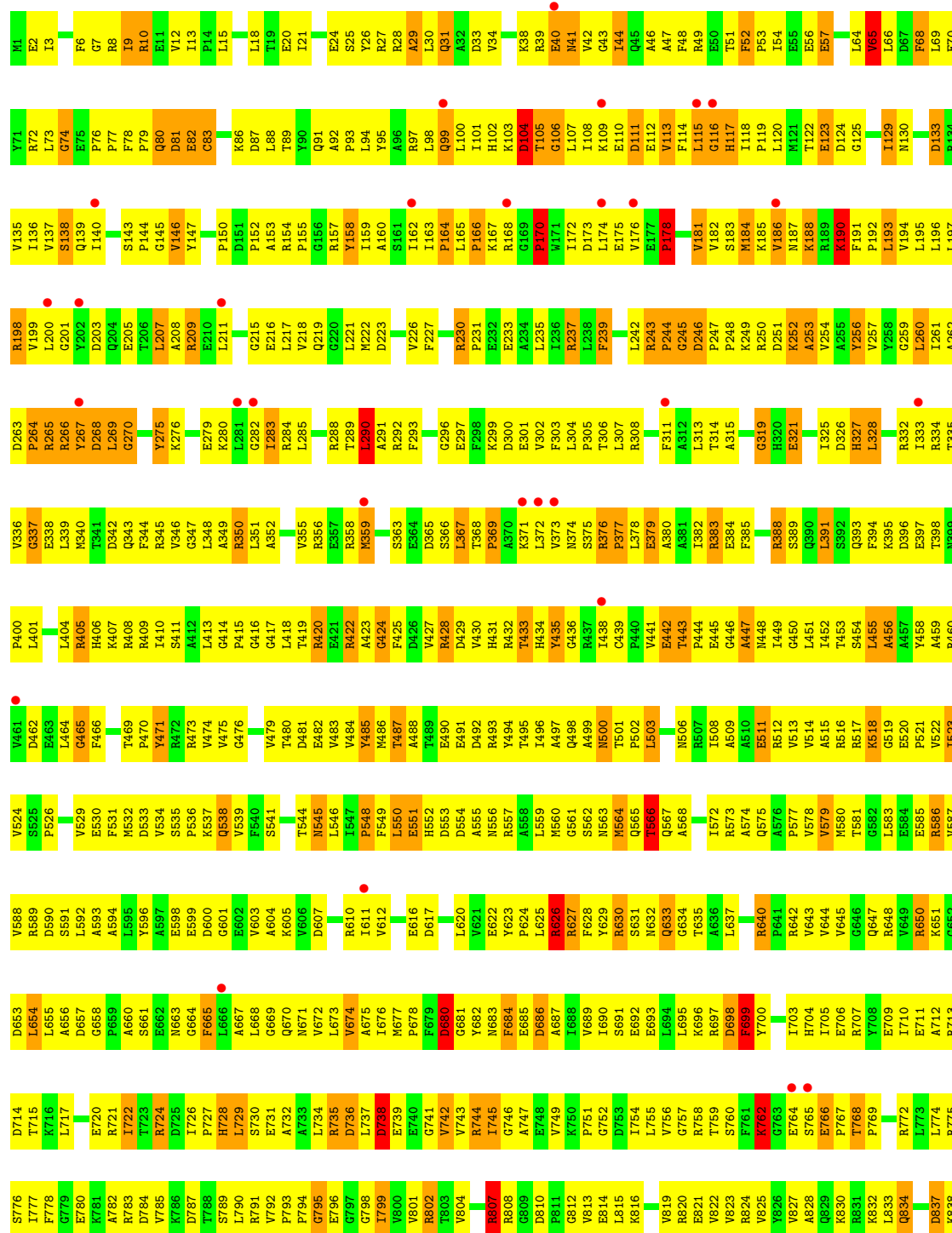
• Molecule 1: DNA-directed RNA polymerase alpha chain

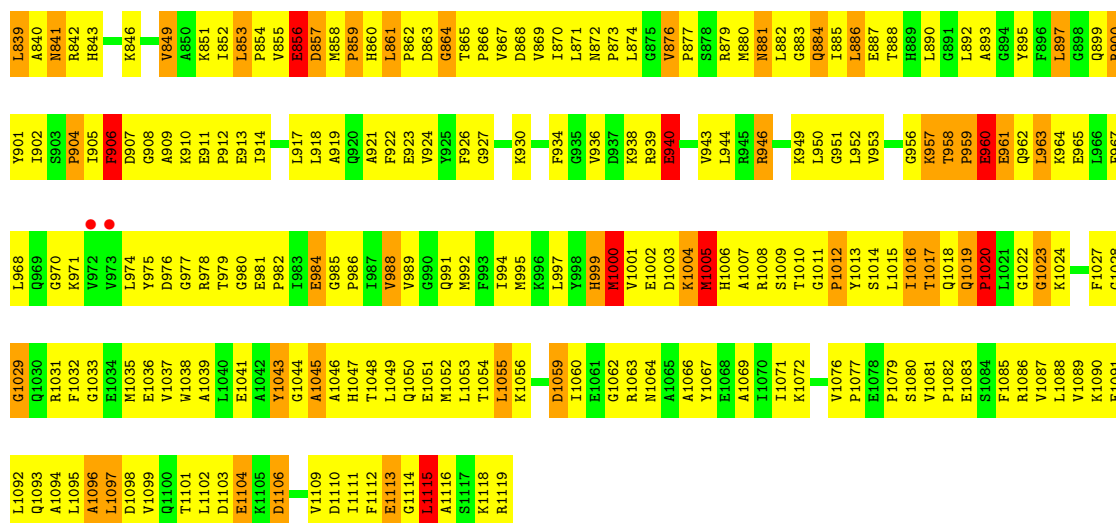




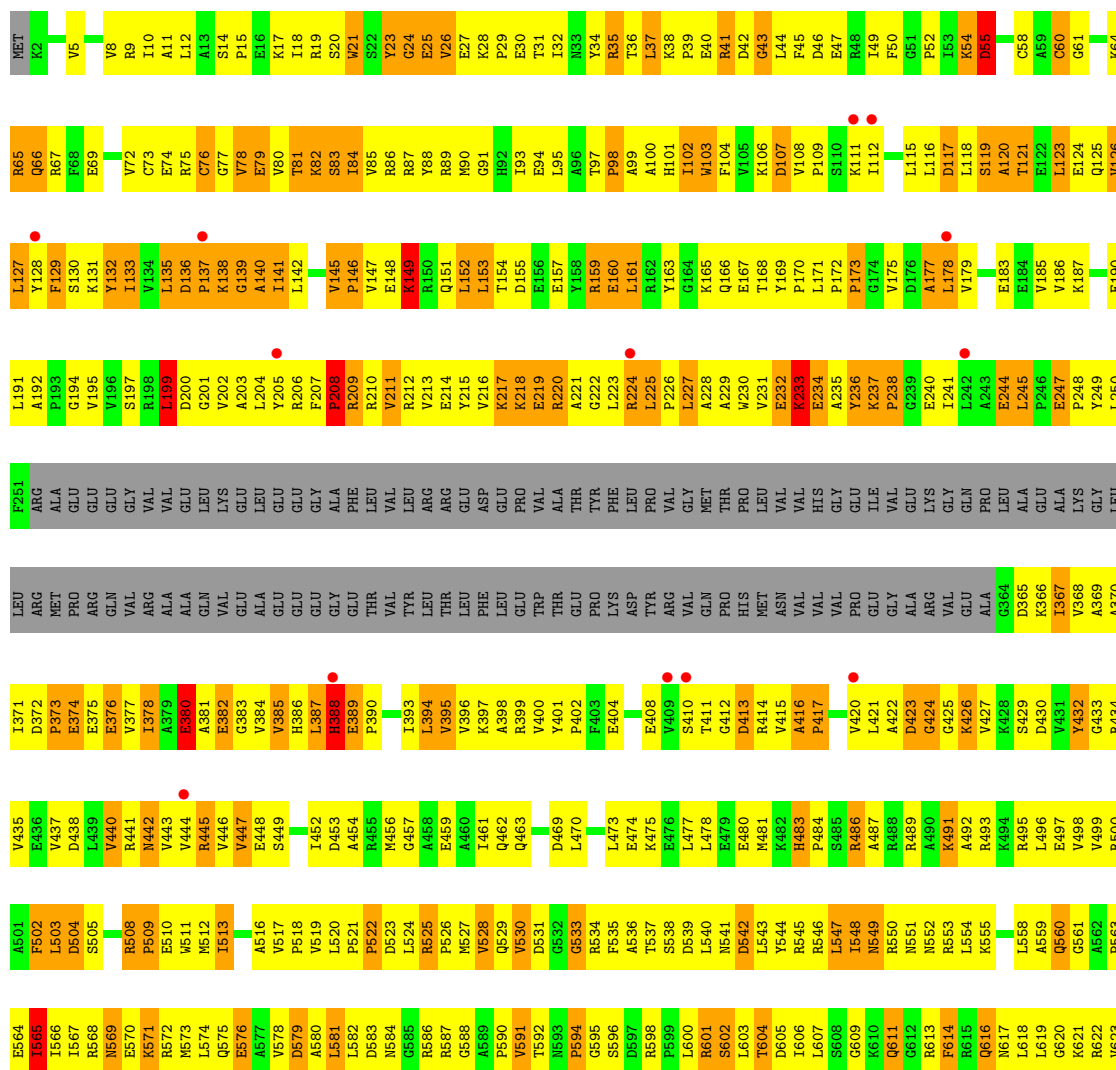
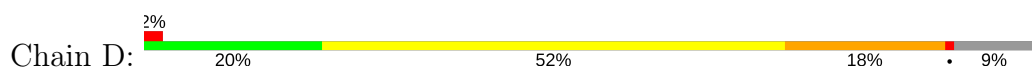


● Molecule 2: DNA-directed RNA polymerase beta chain





● Molecule 3: DNA-directed RNA polymerase beta' chain



ARG	I1452	P1384	G1322	P1257	S1131	Y1070	N1010	T940	I880	E811	L751	V687	D624
GLU	A1453	G1385	Q1323	R1288	L1132	F1071	F1011	F941	L881	A812	S752	W688	Y625
GLN			L1133	R1289	R1133	I1072	E1012		F882	L813	S753		S626
PRO	K1456	I1260	L1325	I1269	L1134	S1073	E1013	T944	A883	A814	F754	L691	G627
GLY	L1457	E1262	T1326	R1198	R1136	S1074	N1014	S945	R884	A815	A755	E692	R628
LYS	E1458	L1262	G1199	G1199	R1137	H1075	N1015	G946	R885	R816	Q756	E693	S629
GLN	L1459	F1263	V1200	C1201	R1137	G1076	P1016	I947	V886	E817	A757	V694	V630
ALA	L1460	P1268	R1327	G1203	L1138	A1077	F1017	T948	A887	R818	E758	I695	L631
	G1461			K1203	D1139	N1078	N1018	I949	R888	G819	A759	H696	V632
	L1462	R1266	P1332	C1204	L1140	K1079	P1019	E950	A889	E820	R760	K697	V633
	K1463	R1267	H1333	Y1205	E1141	G1080	P1019	I951	V890	V821	I761	K698	G634
	E1464	P1268	Q1334	G1206	G1081	A1081	Y1021		E891		Q762	V699	P635
	N1465		L1335	Y1207	A1082	G1082	Y1022	D953	D892	N824	V763	V700	D636
	V1466	K1271	L1336	D1208	L1144	D1083	M1023	A954	E893	A825	L764	L701	L637
	L1467	A1272	L1209	L1209	Y1145	N1084	A1024	V955	K894	P826	S765	L702	K638
	L1468	V1273	S1210	S1210	Q1146	A1085	Q1025	I956	K985	P827	A766	N703	L639
	G1469	I1274	R1211	R1211	R1147	L1086	S1026	P957	A896	R828	H767	R705	H640
	L1470	S1275	A1212	A1212	V1148	R1087	G1027	E958	V829	W829	W768	A705	Q641
	E1471	I1276	R1213	R1213	L1149	T1088	A1028	F859	E830	A830	L769	T706	C642
	A1472	I1277	P1214	P1214	L1150	A1089	M1028	K860	L899	G831	L770	T707	G643
	E1473	S1282	E1219	E1219	R1151		G1030	L964	I900	R832	L771	L708	L644
	L1474	I1283	V1221	V1221	E1152	Y1093	N1031		Q901	E833	P772	H709	P645
	D1475	E1284	G1222	G1222	V1153	L1094	Q1033	R969	L902	T834	A773	R710	K646
	F1476	T1286	I1223	I1223	E1154	L1095	Q1034	K970	D903	S835	S774	L711	R647
	A1477	E1287	E1224	E1224	V1155	A1096	I1035	L971	P905	V836	G775	G712	M648
	E1478	L1288	A1225	A1225	L1156			L972	P906	G837	E776	I713	A649
	D1479	S1290	Q1227	Q1227	R1159	K1097	R1036	L972	Q906	R838	P777	Q714	L650
	F1480	V1291	G1228	G1228	E1160	L1098	Q1037	L973	E907		L778	A715	E651
	L1481	I1293	I1229	I1229	L1165	V1109	L1038	I974	K908	Y841	A779	Q717	L652
	E1482	V1294	G1230	G1230	S1167	D1109	C1039	E975	N909	H842	K780	Q718	F653
	Q1483	E1295	E1231	E1231	M1168	V1107	M1045	Q976	S910	F843	Q719	P718	K654
	T1484		P1232	P1232	D1169	R1108	K1047	A977	L911	P846	S782	V719	P655
	Q1485	S1300	G1233	G1233	D1170	E1109	P1046	R988	A918		L720	L720	F656
	V1486	K1301	T1234	T1234	V1171	A1110	S1049	Y989	F919	V858	L728		E662
	L1487	E1302	Q1235	Q1235	H1172	D1111	G1050	D990	L920	D859	H729		E663
	A1488	Y1303	L1236	L1236	C1112	C1112	G091	Q991	R921	L860	I792	P730	P668
	Q1489	K1304	T1237	T1237	L1174	G1113	T1052	I992	L922	Q861	I793	L731	N669
	K1490	L1305	M1238	M1238	I1175	T1114	F1053	L993	G923	D862	Q794	V732	V670
	T1491	P1306	R1239	R1239	A1176	T1115	E1054	Q994	H924	V863	Q795	C733	K671
	L1492	K1307	F1241	F1241	A1177	N1116	P1056	L995	E925	V864	K797	E734	A672
	A1493	E1308	H1242	H1242	L1178	V1117	V1057	W996	K926	T865	A735	A735	A673
	L1494	A1309	H1243	H1243	E1179	I1118	V1057	T997	T927	V866	T736	R674	C642
	E1495	R1310	G1244	G1244	S1119	S1119	S1059	E998	A928	R867	W737	W737	R675
	S1496	L1311	G1245	G1245	V1120	V1120	S1060	T999	R929	Y868	V800	A738	M676
	A1497	L1312	V1246	V1246	F1121	F1121	F1061	T1000	L930	M869	G301	D739	L677
	R1498	K1314	A1247	A1247	L1122	D1122	P1062	E1001	L931		A902	F740	E678
	E1499	D1315	G1248	G1248	F1123	F1123	E1063	K1002	D932	R872	K1002	D741	R679
		G1316	A1249	A1249	Q1124	Q1124	G1064	V1003	A933	L873	G803	G742	Q680
		D1317			P1125	P1125	E1064	T1004	L934	E874	E805	D743	R681
		Y1318	T1253	T1253	V1188	V1188	L1065	Q1005	K935	T875	E806	Q744	D682
		E1320	Q1254	Q1254	S1190	E1127	T1066	A1006	Y836	S876	A807	W745	L683
		L1321	G1255	G1255	P1191	V1128	T1067	V1007	Y937	P877	T808		K684
		A1321	L1256	L1256	L1192	L1129	L1068	F1008	G938	G878	P750		E686

- Molecule 3: DNA-directed RNA polymerase beta' chain





[illegible]

Chain P:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	236.15Å 236.15Å 249.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.87 – 3.30	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 47.2 (29.87-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.282 , 0.320 0.286 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	92.6	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , -23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	53962	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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	A	0.46	0/1838	0.75	0/2498
1	B	0.36	0/1838	0.64	0/2498
1	K	0.46	0/1838	0.75	0/2498
1	L	0.39	0/1838	0.68	0/2498
2	C	0.45	0/8997	0.79	8/12164 (0.1%)
2	M	0.46	0/8997	0.79	8/12164 (0.1%)
3	D	0.48	0/11165	0.83	16/15088 (0.1%)
3	N	0.46	0/11165	0.81	15/15088 (0.1%)
4	E	0.42	0/783	0.80	3/1054 (0.3%)
4	O	0.42	0/783	0.80	1/1054 (0.1%)
5	F	0.40	0/2836	0.73	0/3812
5	P	0.41	0/2836	0.72	0/3812
All	All	0.45	0/54914	0.78	51/74228 (0.1%)

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
3	D	0	1
3	N	0	3
5	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1209	LEU	N-CA-C	-10.12	83.67	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	728	HIS	N-CA-C	7.66	131.69	111.00
2	C	728	HIS	N-CA-C	7.62	131.58	111.00
3	N	1209	LEU	N-CA-C	-7.26	91.39	111.00
2	M	319	GLY	N-CA-C	-7.22	95.05	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	132	TYR	Sidechain
5	F	84	TYR	Sidechain
3	N	1015	TYR	Sidechain
3	N	1318	TYR	Sidechain
3	N	132	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	A	1806	0	1861	249	0
1	B	1806	0	1861	193	0
1	K	1806	0	1861	190	0
1	L	1806	0	1861	208	0
2	C	8829	0	8933	1143	0
2	M	8829	0	8933	1183	0
3	D	10975	0	11211	1723	0
3	N	10975	0	11210	1681	0
4	E	769	0	775	94	0
4	O	769	0	775	83	0
5	F	2793	0	2873	301	0
5	P	2793	0	2873	364	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
All	All	53962	0	55027	6830	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 63.

The worst 5 of 6830 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)
3:D:1101:VAL:HG21	3:D:1424:VAL:HG22	1.21	1.20
2:C:1016:ILE:H	2:C:1016:ILE:HD13	1.06	1.16
3:D:907:GLU:HG2	3:D:1027:GLY:H	1.02	1.16
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.22	1.15
3:D:145:VAL:HG22	3:D:146:PRO:HD2	1.27	1.15

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	
1	A	227/315 (72%)	167 (74%)	39 (17%)	21 (9%)	1	5
1	B	227/315 (72%)	177 (78%)	37 (16%)	13 (6%)	2	14
1	K	227/315 (72%)	161 (71%)	39 (17%)	27 (12%)	0	2
1	L	227/315 (72%)	166 (73%)	44 (19%)	17 (8%)	1	9
2	C	1117/1119 (100%)	781 (70%)	226 (20%)	110 (10%)	1	4
2	M	1117/1119 (100%)	769 (69%)	215 (19%)	133 (12%)	0	2
3	D	1388/1524 (91%)	941 (68%)	293 (21%)	154 (11%)	0	3
3	N	1388/1524 (91%)	907 (65%)	332 (24%)	149 (11%)	0	4
4	E	93/99 (94%)	67 (72%)	17 (18%)	9 (10%)	1	5
4	O	93/99 (94%)	59 (63%)	20 (22%)	14 (15%)	0	1
5	F	341/423 (81%)	241 (71%)	67 (20%)	33 (10%)	1	5
5	P	341/423 (81%)	249 (73%)	57 (17%)	35 (10%)	0	4
All	All	6786/7590 (89%)	4685 (69%)	1386 (20%)	715 (10%)	0	4

5 of 715 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	B	3	ASP
1	B	118	ALA
1	B	160	ASP
2	C	7	GLY

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 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	
1	A	202/273 (74%)	177 (88%)	25 (12%)	5	24
1	B	202/273 (74%)	172 (85%)	30 (15%)	3	17
1	K	202/273 (74%)	173 (86%)	29 (14%)	4	18
1	L	202/273 (74%)	182 (90%)	20 (10%)	9	34
2	C	941/941 (100%)	808 (86%)	133 (14%)	4	19
2	M	941/941 (100%)	805 (86%)	136 (14%)	4	18
3	D	1170/1279 (92%)	970 (83%)	200 (17%)	2	11
3	N	1170/1279 (92%)	980 (84%)	190 (16%)	3	13
4	E	83/87 (95%)	72 (87%)	11 (13%)	4	21
4	O	83/87 (95%)	70 (84%)	13 (16%)	3	15
5	F	300/370 (81%)	264 (88%)	36 (12%)	6	26
5	P	300/370 (81%)	269 (90%)	31 (10%)	8	32
All	All	5796/6446 (90%)	4942 (85%)	854 (15%)	3	17

5 of 854 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1462	LEU
1	L	156	HIS
3	N	1326	THR
4	E	66	LYS

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Mol	Chain	Res	Type
5	F	416	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1442	ASN
1	L	38	ASN
3	N	1441	GLN
3	D	1489	GLN
1	K	95	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 6 ligands modelled in this entry, 6 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 [i](#)

There are no chain breaks in this entry.

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	A	229/315 (72%)	-0.13	1 (0%) 92 92	41, 64, 87, 113	0
1	B	229/315 (72%)	0.09	16 (6%) 17 17	47, 121, 143, 143	0
1	K	229/315 (72%)	-0.06	3 (1%) 77 75	28, 63, 88, 111	0
1	L	229/315 (72%)	-0.03	7 (3%) 49 48	41, 79, 99, 117	0
2	C	1119/1119 (100%)	-0.07	25 (2%) 62 60	12, 67, 133, 143	0
2	M	1119/1119 (100%)	-0.06	31 (2%) 53 51	6, 71, 122, 133	0
3	D	1392/1524 (91%)	-0.00	37 (2%) 55 52	7, 60, 125, 143	0
3	N	1392/1524 (91%)	0.05	53 (3%) 41 37	5, 65, 134, 143	0
4	E	95/99 (95%)	-0.03	2 (2%) 64 61	54, 84, 100, 106	0
4	O	95/99 (95%)	0.04	4 (4%) 37 34	46, 86, 117, 121	0
5	F	345/423 (81%)	-0.06	9 (2%) 56 53	48, 81, 113, 121	0
5	P	345/423 (81%)	-0.08	8 (2%) 61 58	47, 73, 110, 123	0
All	All	6818/7590 (89%)	-0.02	196 (2%) 52 50	5, 70, 129, 143	0

The worst 5 of 196 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1247	ALA	14.8
3	D	1246	VAL	9.4
2	C	211	LEU	8.7
3	N	1246	VAL	8.3
1	B	1	MET	7.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
6	ZN	D	1525	1/1	0.85	0.29	4.18	107,107,107,107	0
6	ZN	N	1525	1/1	0.92	0.32	3.59	108,108,108,108	0
6	ZN	N	1526	1/1	0.89	0.28	1.96	72,72,72,72	0
6	ZN	D	1526	1/1	0.99	0.26	1.75	78,78,78,78	0
7	MG	N	1527	1/1	0.96	0.17	-	29,29,29,29	0
7	MG	D	1527	1/1	0.94	0.09	-	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.