



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2023 – 02:10 AM EDT

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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

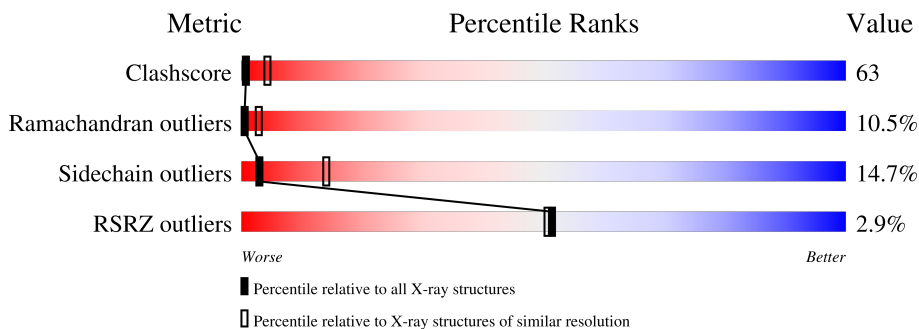
# 1 Overall quality at a glance

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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	315	18% 44% 10% 27%
1	B	315	5% 19% 43% 11% 27%
1	K	315	% 23% 38% 10% 27%
1	L	315	2% 17% 48% 8% 27%
2	C	1119	2% 25% 59% 14% .
2	M	1119	3% 24% 59% 15% .
3	D	1524	2% 20% 52% 18% . 9%

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Mol	Chain	Length	Quality of chain
3	N	1524	<p>3% 21% 52% 17% 9%</p>
4	E	99	<p>2% 29% 52% 11% 8%</p>
4	O	99	<p>4% 34% 47% 9% 5%</p>
5	F	423	<p>2% 22% 48% 10% 18%</p>
5	P	423	<p>2% 26% 44% 10% 18%</p>

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	B	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	K	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0
1	L	229	Total 1806	C 1153	N 313	O 337	S 3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

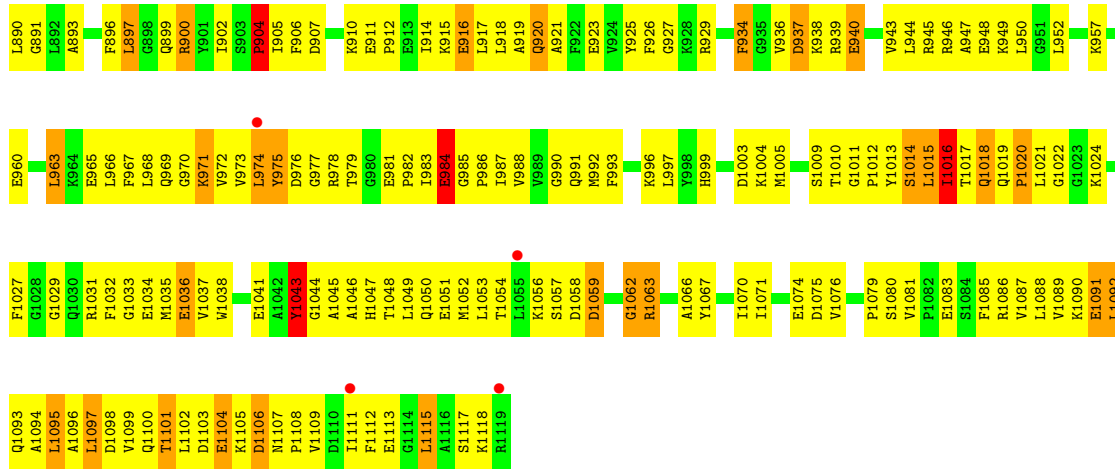




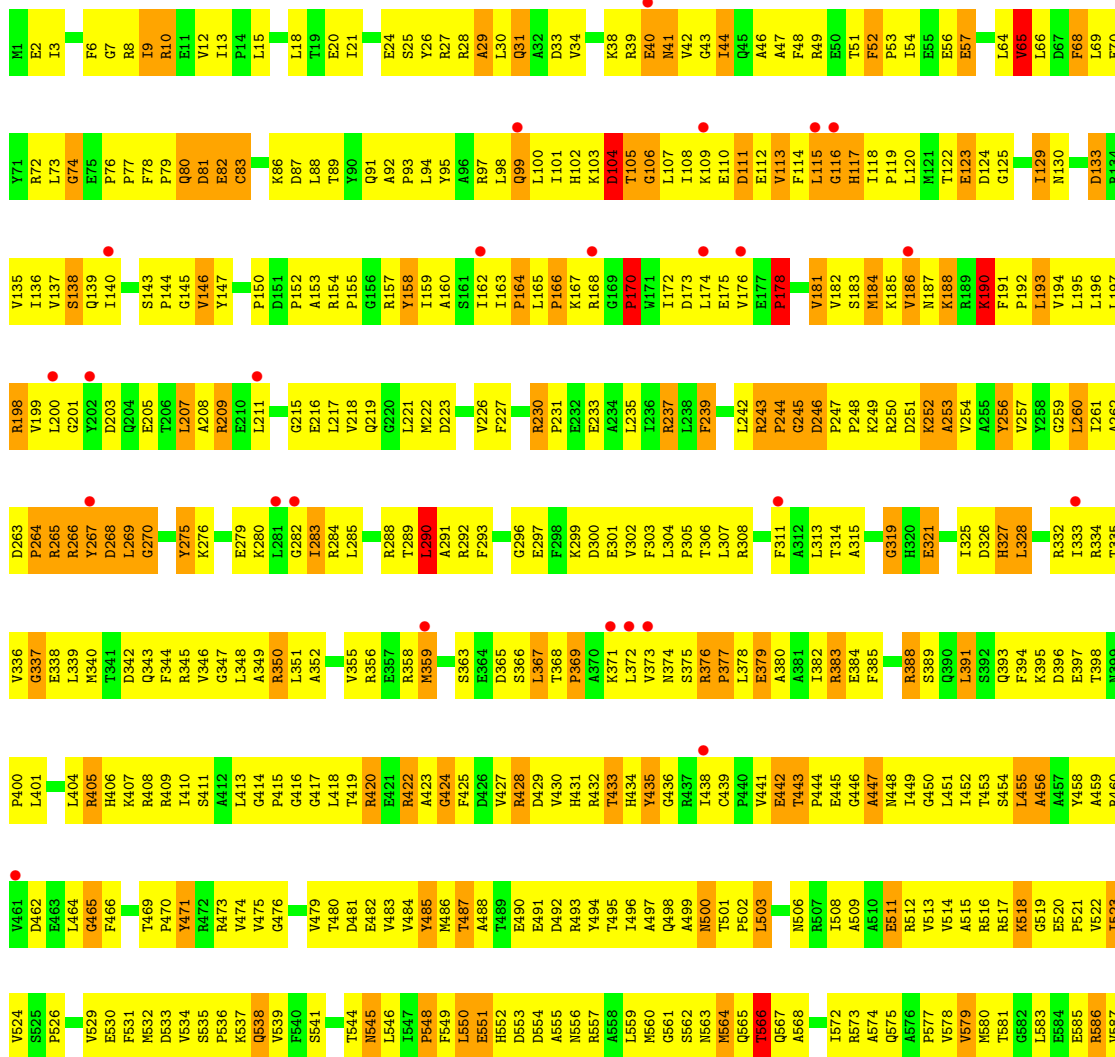


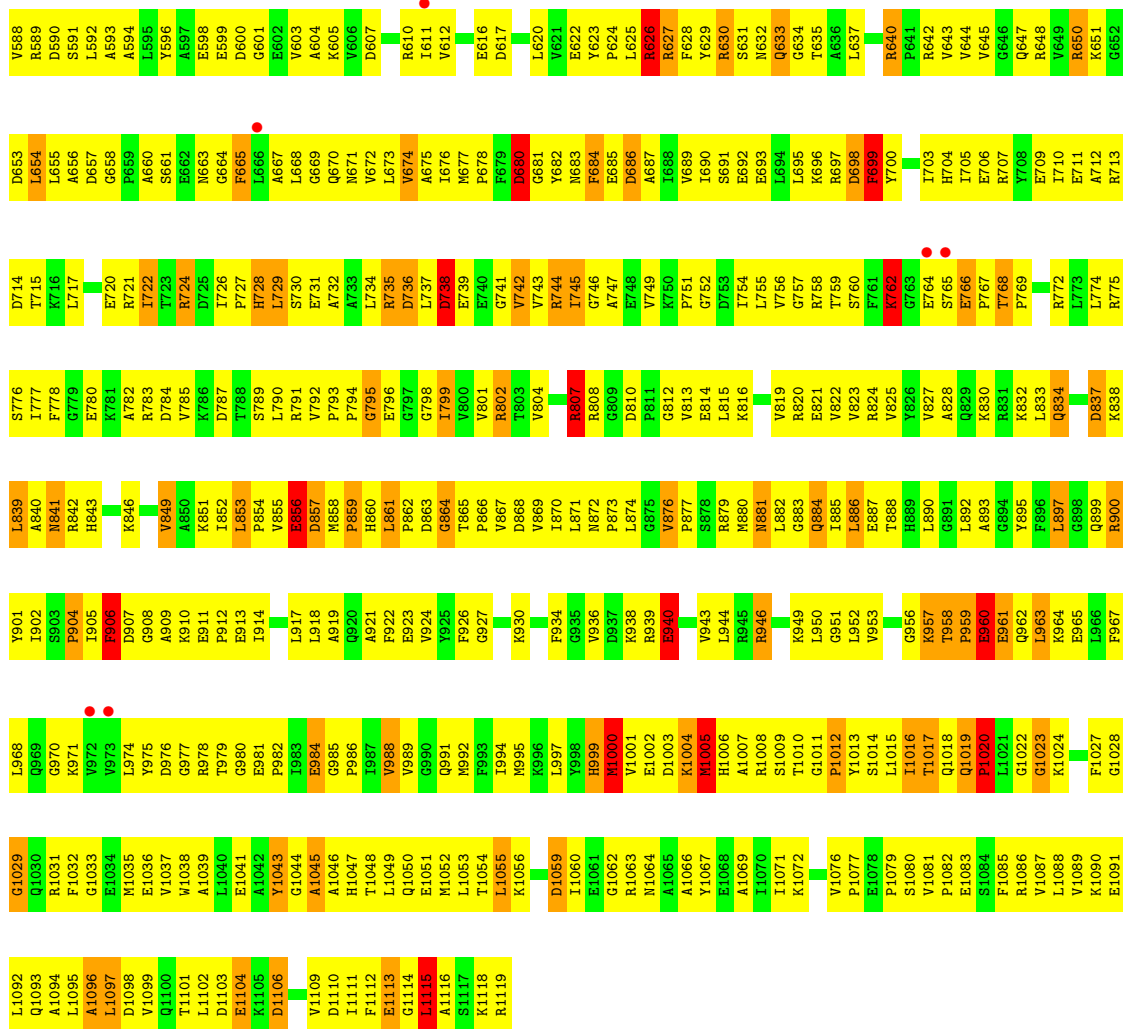
K830	R767	F699	A636	Q575	V513	M448	E379	A315	D251	R189	I128	V685	M1
R831	T768	T700	L637	A576	V514	I449	R383	G316	K252	K190	I129	L66	E2
L833	P769	S702	D638	P577	A515	G450	E384	P317	A253	F191	M130	D67	I3
Q834	E770	T701	Q639	V578	L451	A451	F385	G319	Y256	L193	A132	F68	R4
V835	E771	H703	P640	M579	R516	T452	F386	H320	Z257	V194	D133	E70	F5
G836	R772	H704	P641	M580	R517	T453	S387	H321	Y258	L195	A134	E71	R6
D837	L773	H705	R642	T681	K318	S454	S388	E321	G259	L196	R134	E72	G7
R838	L774	R707	V643	G519	G520	L455	R388	R388	R388	L197	V135	E73	R8
L839	R775	Y708	V644	E520	E521	Y458	Q390	L261	L260	R198	S137	E74	R9
A840	S776	Y709	E584	P521	P522	A459	L391	A262	A262	V199	S138	E75	R10
N841	T777	E710	G646	F521	F522	A459	S392	D263	D263	L200	Q139	E76	E11
R842	E711	W710	Q647	R586	I523	D462	S397	H327	H327	R199	V137	E77	V12
H843	A712	A712	R648	V524	I524	E463	Q393	L328	P264	L201	W137	E78	V13
H844	E713	R713	V649	S525	S525	E463	F394	G329	R285	Y202	H141	F78	I13
G844	A714	L717	R650	E528	E528	L464	K395	N330	R266	D203	P144	Q79	P16
N845	R715	L717	K651	D590	D590	G465	D396	R331	Y287	Q204	P144	Q80	P17
K846	D716	G718	G652	S591	S591	F466	E397	R332	D268	E205	G146	L18	L18
V848	W716	R721	D653	L592	L592	I467	T398	L333	E271	T206	V145	D81	T19
H849	D717	R722	L654	A594	A594	R468	N399	R334	A272	L207	Y147	E82	E20
A850	T718	T723	L655	A594	A594	T469	K399	T335	A272	A208	F148	E85	E20
K851	S719	F723	G658	Y596	Y596	P470	S403	V336	G273	R209	F148	Q22	Q22
L852	L790	R724	P659	Y596	Y596	Y471	L404	G337	R274	L219	L149	Q22	Q22
L853	R791	D725	P660	S535	S535	R472	R405	E338	Y275	E210	P150	V23	V23
R854	W792	R726	A660	P536	P536	R473	H406	L339	K276	L211	D151	E24	E24
V855	P793	P727	S661	K537	K537	V474	K407	N340	A277	P152	P152	T89	S25
E856	F793	H728	E662	D600	Q538	V475	R408	T341	E278	Y90	A153	Y26	Y26
D857	F794	L729	N663	G601	V539	G477	R409	D342	E279	G215	R154	R27	R27
H858	E796	E731	F665	E602	F540	G477	L410	R280	R280	E216	P156	R28	R28
P859	G797	E731	F666	V603	S541	V478	S411	L281	V218	G156	L217	A29	A29
H860	G798	L734	R666	A604	V542	V479	P415	G282	G282	R157	L30	L30	L30
L861	T799	R735	A667	K605	V544	T480	G416	L283	L283	Y158	Y158	Q31	Q31
P862	V800	R736	L668	V606	T544	D481	G417	L284	R284	R97	A160	A32	A32
G864	R801	L737	G669	D607	N545	E482	L418	A349	L285	L221	S161	Q88	Q88
T865	T803	D738	M671	G608	L546	V483	L418	R350	S286	M222	I100	Q99	Q99
H866	R804	E739	V672	N609	I547	V484	T419	G287	G287	E224	I162	I101	I101
V867	R805	E740	L673	R610	P548	Y485	R420	R288	V226	S225	I163	H102	H102
D868	L806	G741	V674	I611	F549	M486	G424	T289	F227	E226	P164	E40	E40
R869	R807	W742	A675	V613	L550	T487	F425	L290	A228	A228	L165	K103	K103
L870	R808	W743	M677	V614	H552	A488	V427	A291	M229	G43	K167	D104	D104
L871	G809	I745	P678	E616	H552	T489	R428	R292	P231	G43	R168	G106	G106
N872	D810	I745	E679	E616	A555	E491	V430	F293	E232	L107	G169	L107	L107
P873	P811	E748	D680	D617	N556	D492	V430	G296	E233	W171	Q45	Q45	Q45
L874	W749	W749	G881	L620	L559	R493	H431	K299	A234	I172	A46	A46	A46
G875	K750	K750	Y682	V621	M560	Y494	H431	D300	L235	D173	F48	F48	F48
V876	E814	P751	M683	E622	G561	T495	R432	D900	L236	D173	F48	F48	F48
P877	L815	G752	F684	Y623	S562	I496	T433	E301	R237	L174	E175	E175	E175
S878	L815	G752	E685	P624	S562	A497	H434	V302	L238	E175	F114	F114	F114
R879	G818	L755	E685	P624	N563	Q498	Y435	F303	P239	V176	E177	E177	E177
H880	R819	L755	V689	R626	M564	A499	G436	L304	T240	P178	F52	F52	F52
N881	R820	R758	I690	R627	Q565	N500	R437	F305	L241	H179	L54	L54	L54
L882	E821	T759	S691	F628	T566	T501	I438	T306	L241	H117	E55	E55	E55
G883	W822	S760	E921	F628	Q567	P502	C439	L307	R243	G180	E56	E56	E56
Q884	V823	S760	R630	Y629	A568	L503	G439	R308	P244	V181	E57	E57	E57
L885	R824	K762	E934	R630	E504	E504	E443	Y309	G245	S182	D58	D58	D58
L886	R825	G763	L695	M632	P570	G505	P444	L310	D246	M184	K59	K59	K59
E887	Y826	G763	L696	M632	L571	N506	P444	F311	P247	S123	D124	D124	D124
T888	S765	E765	K696	Q633	L572	R507	E445	A312	P248	H118	G125	G125	G125
H889	Q829	E766	R697	G634	R573	I508	G446	L313	K249	I118	S126	S126	S126
			D698	T635	A574	A509	A447	T314	R250	P119	K188	F127	F127



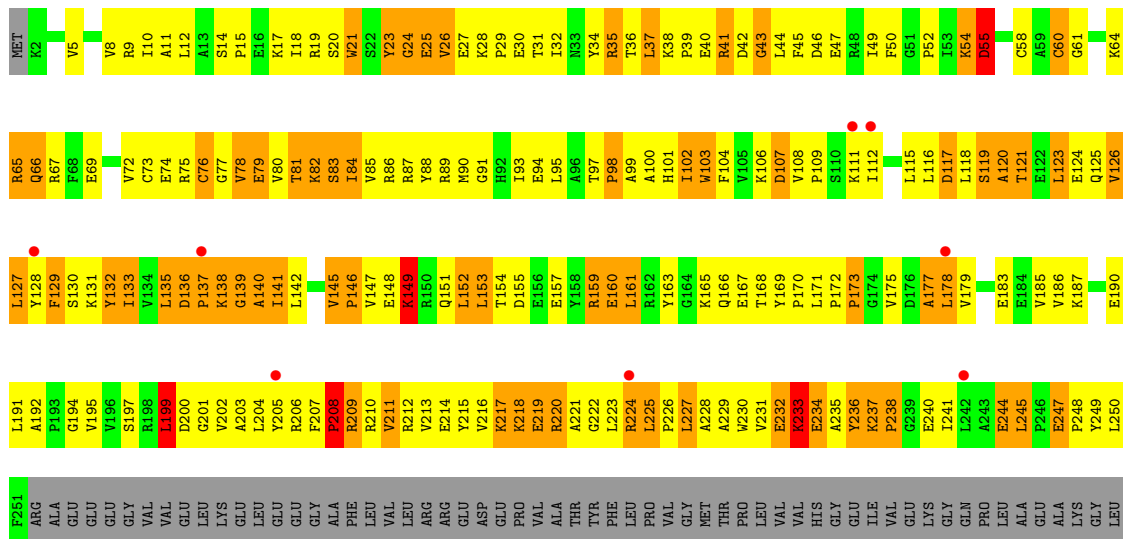
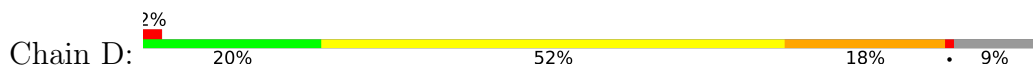


• Molecule 2: DNA-directed RNA polymerase beta chain

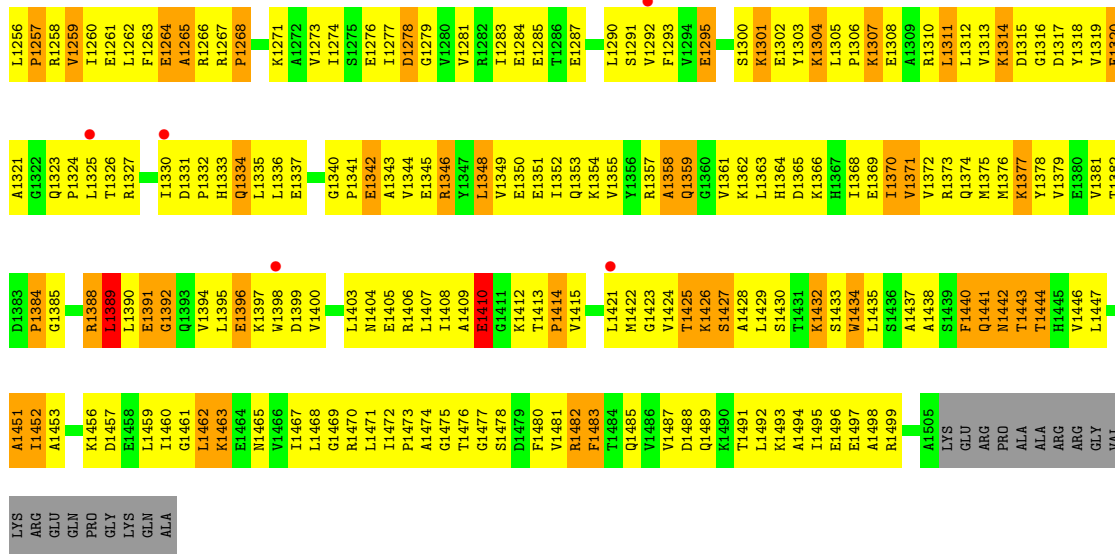




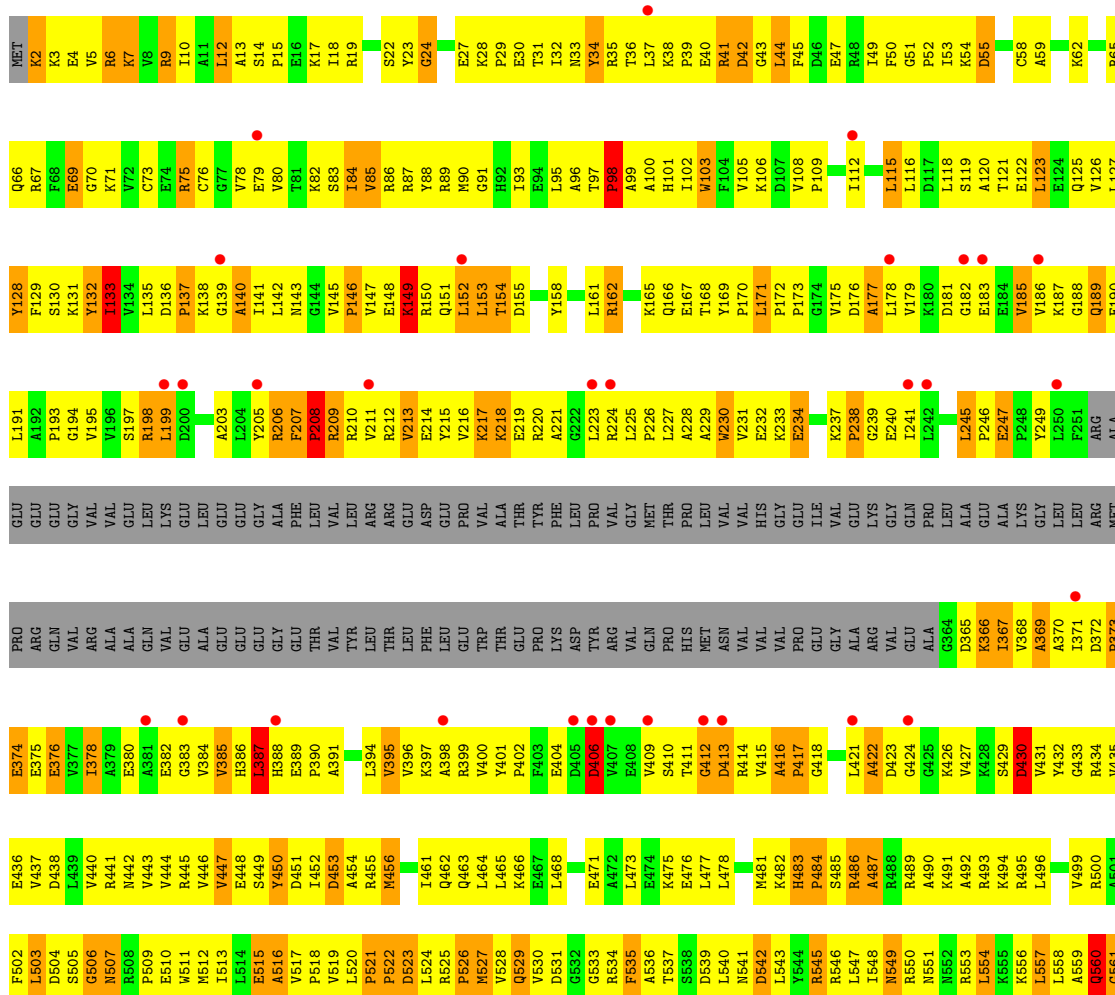
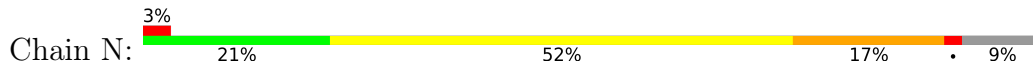
● Molecule 3: DNA-directed RNA polymerase beta' chain



C1194	S1131	Y1070	M1010	T940	I880	E811	L751	V687	D624	E564	A501	V435	I371	LEU
Q1195	L1132	F1071	F1011	F941	L861	A812	S752	W688	Y625	I368	F502	E436	D372	ARG
R1197	R1133	I1072	E1012	T944	F882	L813	F754	G688	S626	I566	L503	V437	P373	MET
Y1198	L1134	S1073	E1013	T945	A883	A814	F753	L691	G627	I567	D504	D438	E374	PRO
G1199	R1135	H1074	N1014	S945	R884	H815	A755	E692	R628	R568	S505	L439	E375	ARG
V1200	R1136	H1075	Y1015	G946	R885	H816	Q756	E693	S629	N569	G508	V440	E376	GLN
C1201	R1137	G1076	P1016	T947	V886	E817	A757	V694	V630	E570	R508	R441	E377	VAL
I1202	A1138	A1077	F1017	T948	A887	R818	E758	I695	I631	K571	P509	K442	I378	ARG
K1203	D1139	R1078	N1018	T949	E888	G819	A759	H696	V632	R572	E510	V443	I379	ALA
G1204	I1140	G1079	P1019	G950	A889	R820	R760	K697	G633	N573	M511	V444	E380	ALA
V1205	E1141	G1080	L1020	I951	H890	V821	I761	K698	V634	L574	M512	R445	A381	GLN
G1206	G1142	A1081	Y1021	D952	E891	V822	Q762	V699	P635	O575	L513	V446	E382	VAL
Y1207	L1143	D1082	V1022	D953	D892	N824	M763	V700	G636	E576	A516	V447	G383	GLU
D1208	L1144	D1083	M1023	A954	E893	A825	L764	L701	L637	A577	V517	E448	V384	ALA
L1209	Y1145	T1084	A1024	V955	K894	P826	A766	L702	K638	V578	P518	V385	V386	GLU
S1210	G1146	A1085	Q1025	V956	R895	I827	L639	N703	L639	D579	P519	H386	H387	GLU
R1211	R1147	L1086	S1026	P957	A896	H828	H767	A705	H640	A580	V519	L452	L387	GLU
M1212	V1148	R1087	G1027	E958	W897	K829	Q641	A706	Q641	L581	L520	D453	H388	GLY
A1213	L1149	T1088	A1028	E959	E898	A830	L769	P706	C642	L582	P521	A454	E389	GLU
R1214	A1150	A1089	R1029	K960	L899	G831	L770	T707	G643	D583	P522	R455	P390	THR
P1215	R1151	G1090	G1030	L964	I900	R832	S771	L708	L644	N584	D523	R456	P391	VAL
V1216	E1152	Y1092	N1031	L965	Q901	E833	P772	H709	P645	G585	V529	G457	T393	TYR
S1217	V1153	Y1093	F1032	T974	L902	T834	A773	H710	K646	R586	R524	G458	L394	LEU
I1218	E1154	L1094	Q1033	R969	D903	S835	S774	Q716	R647	R587	P526	E459	V395	THR
G1219	V1155	T1095	Q1034	K970	V904	V836	S774	G712	N648	G588	M527	A460	V396	LEU
E1219	L1156	R1096	I1035	L971	P905	G837	E776	I713	A649	A588	V528	L461	K397	PHE
A1220	R1157	K1097	R1036	L972	Q906	R838	P777	Q714	L650	P590	Q529	V462	K398	LEU
V1221	L1158	L1098	Q1037	R973	E907	L778	A779	L778	E651	N591	V530	Q463	A399	GLU
G1222	L1160	Y1099	L1038	R974	K908	R716	K780	Q717	L652	T592	D531	G469	V400	TRP
I1223	E1161	D1100	G1039	E975	N909	V842	K780	F653	F653	N593	G532	L470	Y401	THR
V1224	E1162	V1101	G1040	Q976	S910	F843	P781	P718	K654	P594	G533	L470	P402	GLU
A1225	G1163	T1102	L1041	A977	L911	V843	S782	V719	P655	G595	R534	E483	P403	PRO
L1226	R1164	H1103	R1042	L978	A918	P846	L720	L720	F656	G596	F535	L473	E404	LYS
Q1227	Y1165	E1104	G1043	T984	D913	A849	D721	V721	L657	D597	A536	E474	E408	ASP
S1228	L1167	V1106	M1045	D985	L914	L850	I785	E722	L658	R598	K475	E475	V409	ARG
I1229	M1168	V1107	Q1046	R986	V915	L850	I786	G723	K659	P599	S538	E476	S410	ARG
E1231	D1169	R1108	K1047	E987	Y916	V853	L787	Q724	K660	L600	D539	L477	T411	VAL
P1232	D1170	E1109	P1048	R988	Q917	V853	G788	S725	M661	R601	L540	L478	T412	GLN
G1233	H1171	A1110	S1049	Y989	A918	V858	L728	L728	E662	S602	M541	E479	G412	PRO
T1234	H1172	D1111	G1050	D990	F919	D859	Y790	H729	E663	L603	D542	E480	D413	HIS
L1235	L1173	C1112	E1051	Q991	L920	L860	I792	H730	P668	D605	L543	M481	R414	MET
G1236	L1174	G1113	T1052	I992	R921	Q861	T793	L731	P669	R606	Y544	K482	V415	ASN
T1237	I1175	T1114	F1053	L993	L922	D862	Q794	V732	V670	L607	R546	P484	A416	VAL
M1238	K1176	T1115	E1064	Q994	G923	V863	V795	C733	K671	S608	L547	S485	P417	VAL
R1239	A1177	M1116	V1055	L995	E925	V864	R796	E734	A672	G609	I548	R486	V420	PRO
T1240	A1178	Y1117	P1056	N996	K926	T865	K797	A735	A673	R610	I549	R487	L421	GLU
H1241	E1179	I1118	V1057	T997	T927	V866	E798	F736	R674	Q611	R550	K488	A422	GLY
L1242	E1182	S1119	R1058	E998	A928	B867	K799	N737	R675	G612	N551	R489	D423	ALA
T1243	I1183	V1120	S1059	T999	R929	Y868	K800	A738	M676	R613	N552	A490	G424	ARG
G1244	L1184	F1061	S1060	T1000	L930	M669	G801	D739	L677	F614	R553	K491	G425	VAL
V1245	V1186	F1122	P1062	L1001	L931	R872	A802	F740	E678	R615	L554	K492	K426	GLU
A1247	P1187	F1123	R1063	K1002	D932	R873	G803	D741	R679	R616	K555	R493	V427	ALA
G1248	V1188	Q1124	E1063	V1003	A933	L870	L804	G742	Q680	N617	G566	K494	K428	ALA
A1249	R1189	L1065	G1064	T1004	L934	E874	E805	D744	R681	L618	L558	R495	S429	ALA
T1253	S1190	L1066	T1066	Q1005	K935	T875	F806	Q744	D682	L619	A569	L496	D430	ALA
Q1254	P1191	V1128	V1067	A1006	Y936	S876	A807	M745	I683	G620	Q560	E497	V431	ARG
G1255	L1192	F1008	P1067	F1007	Y937	P877	T808	K621	K684	R622	G561	V498	V432	ARG
	T1193	F1068	E1069	K1009	F939	R879	E810	P750	D685	R622	A562	V499	G433	ARG
									E686	V623	P563	R500	R434	ARG



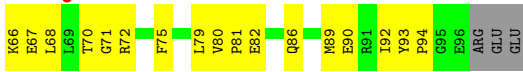
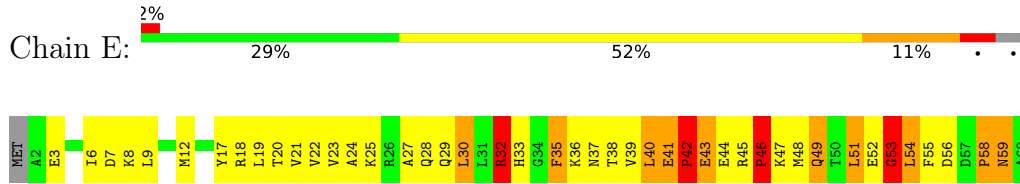
• Molecule 3: DNA-directed RNA polymerase beta' chain



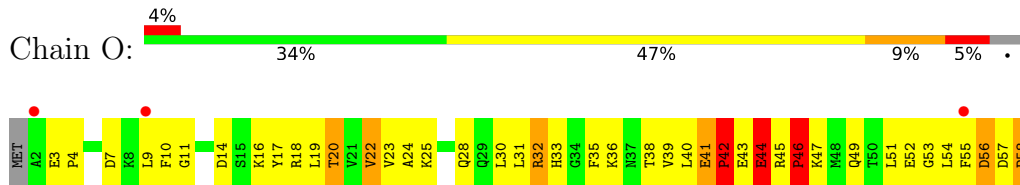
L1395	E1396	K1397	W1398	D1399	L1396	E1401	A1402	K1403	N1404	E1405	K1412	T1413	P1414	V1415	A1416	P1419	L1420	L1421	M1422	G1423	V1424	T1425	K1426	L1429	K1432	S1433	W1434	L1435	S1436	A1437	A1438	N1442	T1443	V1446	L1447	A1450	A1451	I1452	A1453	G1454	K1455	K1456	D1457	E1458	L1459	I1460	G1461	L1462	K1463	A1464	V1466											
D1331	P1332	H1333	Q1334	L1335	L1336	E1337	A1338	K1339	G1340	P1341	E1342	A1343	V1344	E1345	L1346	L1348	E1351	L1352	Q1353	K1354	V1355	Y1356	V1361	K1362	L1363	H1364	L1365	K1366	H1367	L1368	E1369	V1371	L1372	R1373	Q1374	M1375	M1376	L1377	Y1378	V1379	E1380	L1381	T1382	D1383	P1384	G1385	D1386	S1387	R1388	I1389	P1390	E1391	G1392	L1393	V1394							
K1269	A1270	K1271	A1272	V1273	L1274	S1275	E1276	L1277	D1278	L1279	P1280	A1281	L1282	L1283	E1284	L1286	E1287	K1288	L1289	S1228	L1290	S1291	F1292	F1293	V1294	E1295	G1298	G1299	L1230	Q1235	L1236	T1237	M1238	R1239	T1240	F1241	H1242	T1243	G1244	G1245	V1246	A1250	L1251	L1252	T1253	Q1254	G1255	L1256	P1257	R1258	V1259	L1260	E1261	Q1262	F1263	P1324	L1325	A1265	R1266	A1329	I1330	P1268
E1141	L1144	R1147	L1148	L1149	A1150	R1151	E1152	V1153	E1154	V1155	L1156	R1159	L1160	E1161	E1162	G1163	R1164	Y1165	Y1166	S1167	M1168	D1169	D1170	V1171	H1172	Y1173	L1174	L1175	K1176	A1177	A1178	E1179	E1182	I1183	Q1184	E1185	V1186	P1187	V1188	R1189	S1190	P1191	L1192	Q1195	R1196	R1197	Y1198	G1199	L1200	C1201	Q1202	K1203	C1204	L1140								
Y1207	D1208	L1209	S1210	M1211	A1212	R1213	P1214	L1215	I1216	I1217	V1218	E1219	A1220	V1221	G1222	L1223	V1224	A1225	Q1226	S1228	L1229	S1291	F1292	V1294	E1295	G1298	G1299	L1230	Q1235	L1236	T1237	M1238	R1239	T1240	F1241	H1242	T1243	G1244	G1245	V1246	A1250	L1251	L1252	T1253	Q1254	G1255	L1256	P1257	R1258	V1259	L1260	E1261	Q1262	F1263	P1324	L1325	A1265	R1266	A1329	I1330	P1268	
E1009	M1010	E1011	E1012	Y1015	P1016	F1017	M1018	R1018	T1018	A1019	L1020	E1021	V1022	M1023	G1027	L1032	M1031	Q1032	P1033	Q1034	L1035	Q1036	Q1037	L1038	C1039	G1040	A1041	L1042	R1043	R1044	R1045	Y1046	E1047	L1048	S1049	G1050	E1051	T1052	F1053	E1054	V1055	P1056	V1057	R1058	S1059	D1060	E1061	L1062	R1063	G1064	T1065	T1066	E1067	L1068	E1069	Y1070	S1073					
T940	F941	S942	T943	T944	S945	G946	F1017	T948	T949	M1019	C950	E951	D952	D953	A954	V955	P956	E958	E959	K960	L961	Q962	Y963	L964	E965	E966	A967	D968	R969	K970	E975	Q976	L977	Y978	E979	L983	T984	D985	R986	E987	R988	D990	Q991	K992	L992	L995	W996	T999	L1000	E1001	L1002	L986	E1009	A1006	V1007	F1008						
R818	G819	E820	A821	A822	R823	M824	A825	P826	R827	M828	L829	A830	G831	R832	E833	T834	S835	V836	G837	I839	L839	K840	Y841	W842	F843	A844	N845	P846	D847	E848	A849	L850	L851	A852	W853	T854	H855	G856	R857	D859	L860	O861	D862	L864	M865	R866	G867	E868	R869	L869	E870	E871	R872	L873	S876	P877	H878	R879				
I880	L881	F882	A883	R884	I885	V886	A887	E888	R889	V890	A891	D892	E893	K894	V895	A896	N897	E898	L899	Q901	L902	K903	V904	P905	Q906	N907	R908	N909	S910	L911	K912	D913	L914	W915	Y916	Q917	A918	F919	L920	R921	L922	G923	M924	E925	K926	T927	T865	A928	R929	L930	D932	R933	R934	L935	K936	Y937	G938	F939				
F754	A755	Q756	A757	E758	A759	E760	I761	Q762	M763	L764	S765	A766	H767	R768	L769	L770	S771	P772	E776	P777	L778	L779	A780	F781	S782	R783	D784	L785	L786	L787	Y790	L791	L792	T793	Q794	W795	R796	K797	E798	K799	K800	G801	L804	R805	F806	A807	T808	P809	E810	R811	V812	A813	L814	A814	A815	H816	S752	E817				
G697	R628	S629	I631	V632	V633	G634	P635	K636	L637	K638	L639	H640	Q641	Q642	G643	L644	P645	K646	R647	M648	E651	L652	F653	K654	P655	F656	N657	L658	K659	K660	E661	E662	E663	K664	G665	I666	P668	N669	V670	K671	A672	A673	R674	E675	R676	L677	E678	R679	Q680	R681	G620	K621	D682	L683	K684	D685	E686	V687				
A562	P563	E564	I565	I566	R567	R568	N569	E570	K571	R572	M573	L574	Q575	E576	A577	V578	D579	L582	D583	N584	G585	R586	R587	P590	V591	T592	N593	L594	G595	R598	P599	L600	E663	L601	R601	S602	L603	T604	D605	I606	G609	K610	Q611	R612	R613	Q616	M617	L618	L619	G620	K621	D682	L683	K684	D685	E686	V687					



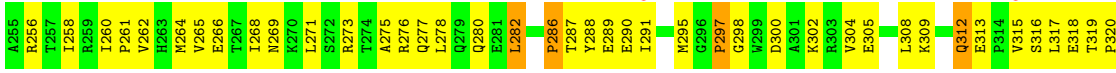
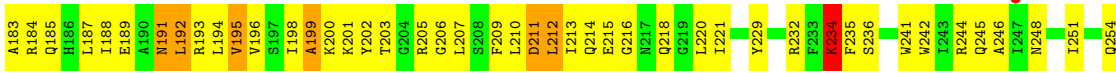
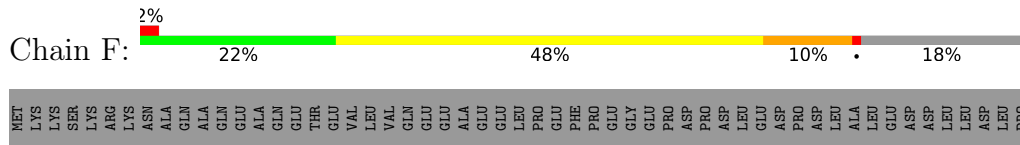
• Molecule 4: RNA polymerase omega chain



• Molecule 4: RNA polymerase omega chain

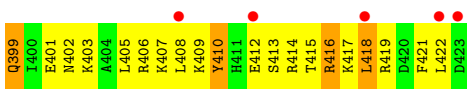
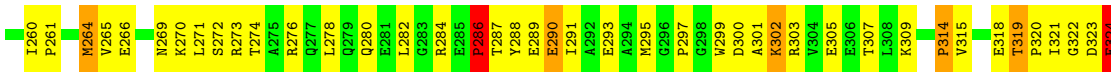
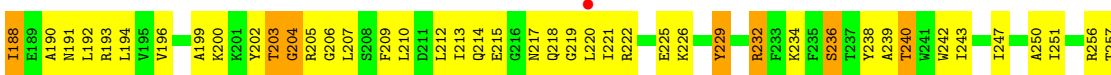
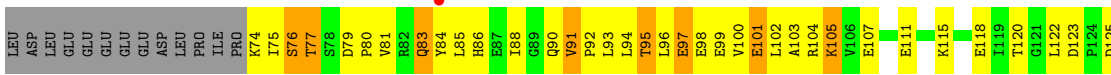
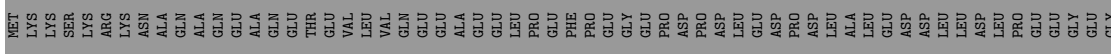


• Molecule 5: RNA polymerase sigma factor rpoD





● Molecule 5: RNA polymerase sigma factor rpoD



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 3.31Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.282 , 0.320 0.286 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.4	Xtrriage
Anisotropy	0.295	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , -23.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.499 for -h,-k,l 0.499 for h,-h-k,-l 0.064 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	53962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN

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 [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	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	1725	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	6832	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 6832 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:HD13	2:C:1016:ILE:H	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%)	0	4
1	B	227/315 (72%)	177 (78%)	37 (16%)	13 (6%)	1	11
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	7
2	C	1117/1119 (100%)	781 (70%)	226 (20%)	110 (10%)	0	3
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	2
3	N	1388/1524 (91%)	907 (65%)	332 (24%)	149 (11%)	0	3
4	E	93/99 (94%)	67 (72%)	17 (18%)	9 (10%)	0	3
4	O	93/99 (94%)	59 (63%)	20 (22%)	14 (15%)	0	1
5	F	341/423 (81%)	241 (71%)	67 (20%)	33 (10%)	0	3
5	P	341/423 (81%)	249 (73%)	57 (17%)	35 (10%)	0	3
All	All	6786/7590 (89%)	4685 (69%)	1386 (20%)	715 (10%)	0	3

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 [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
1	A	202/273 (74%)	177 (88%)	25 (12%)	4 19
1	B	202/273 (74%)	172 (85%)	30 (15%)	3 13
1	K	202/273 (74%)	173 (86%)	29 (14%)	3 15
1	L	202/273 (74%)	182 (90%)	20 (10%)	8 28
2	C	941/941 (100%)	808 (86%)	133 (14%)	3 16
2	M	941/941 (100%)	805 (86%)	136 (14%)	3 14
3	D	1170/1279 (92%)	970 (83%)	200 (17%)	2 9
3	N	1170/1279 (92%)	980 (84%)	190 (16%)	2 10
4	E	83/87 (95%)	72 (87%)	11 (13%)	4 17
4	O	83/87 (95%)	70 (84%)	13 (16%)	2 12
5	F	300/370 (81%)	264 (88%)	36 (12%)	5 20
5	P	300/370 (81%)	269 (90%)	31 (10%)	7 26
All	All	5796/6446 (90%)	4942 (85%)	854 (15%)	3 14

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

Mol	Chain	Res	Type
1	K	219	ARG
2	M	724	ARG
3	N	1412	LYS
1	L	140	MET

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Mol	Chain	Res	Type
1	K	208	LEU

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

Mol	Chain	Res	Type
2	M	632	ASN
3	N	748	HIS
2	M	843	HIS
3	N	166	GLN
3	N	1202	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	229/315 (72%)	-0.13	1 (0%) 92 93	41, 64, 87, 113	0
1	B	229/315 (72%)	0.09	16 (6%) 16 16	47, 121, 143, 143	0
1	K	229/315 (72%)	-0.06	3 (1%) 77 77	28, 63, 88, 111	0
1	L	229/315 (72%)	-0.03	7 (3%) 49 48	41, 79, 99, 116	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%) 54 52	7, 60, 125, 143	0
3	N	1392/1524 (91%)	0.05	53 (3%) 40 37	5, 65, 134, 143	0
4	E	95/99 (95%)	-0.03	2 (2%) 63 62	54, 84, 100, 106	0
4	O	95/99 (95%)	0.04	4 (4%) 36 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%) 60 59	47, 73, 110, 123	0
All	All	6818/7590 (89%)	-0.02	196 (2%) 51 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 monosaccharides 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
6	ZN	D	1525	1/1	0.85	0.29	107,107,107,107	0
6	ZN	N	1526	1/1	0.89	0.28	72,72,72,72	0
6	ZN	N	1525	1/1	0.92	0.32	108,108,108,108	0
7	MG	D	1527	1/1	0.94	0.09	19,19,19,19	0
7	MG	N	1527	1/1	0.96	0.17	29,29,29,29	0
6	ZN	D	1526	1/1	0.99	0.26	78,78,78,78	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.