



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 11:24 pm BST

PDB ID : 3EQL
Title : Crystal structure of the T. Thermophilus RNA polymerase holoenzyme in complex with antibiotic myxopyronin
Authors : Vassilyev, D.G.; Vassilyeva, M.N.; Artsimovitch, I.
Deposited on : 2008-09-30
Resolution : 2.70 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:

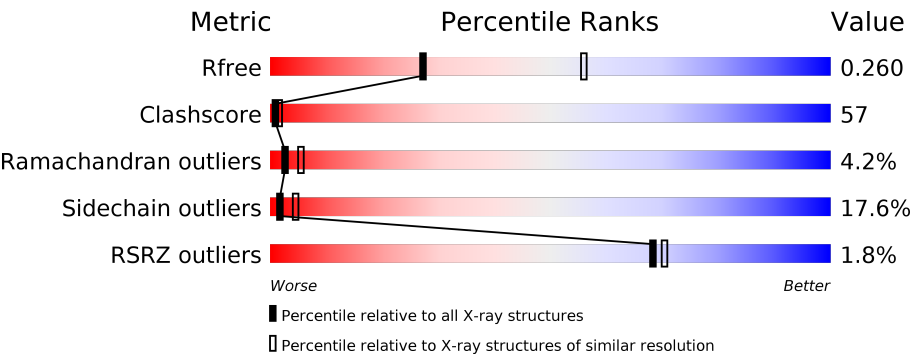
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	A	315	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	
2	M	1119	

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Mol	Chain	Length	Quality of chain
3	D	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%24%51%11%•13%</div></div>
3	N	1524	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%25%49%11%•13%</div></div>
4	E	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%21%61%11%••</div></div>
4	O	99	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%22%60%12%••</div></div>
5	F	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%25%45%11%•18%</div></div>
5	P	423	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%27%44%9%•18%</div></div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 57340 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 subunit alpha.

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 subunit beta.

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 subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			
3	N	1321	Total	C	N	O	S	0	0	0
			10407	6585	1845	1944	33			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			
4	O	95	Total	C	N	O	S	0	0	0
			770	491	133	142	4			

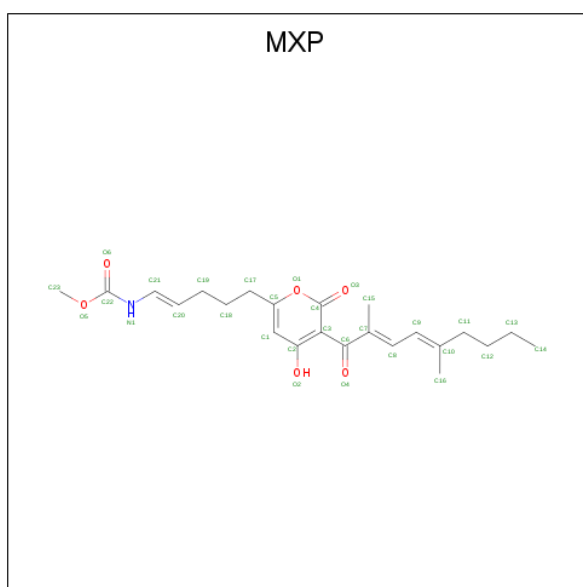
- Molecule 5 is a protein called RNA polymerase sigma factor rpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	4			
5	P	345	Total	C	N	O	S	0	0	0
			2771	1744	504	519	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 Myxopyronin B (three-letter code: MXP) (formula: C₂₃H₃₁NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			30	23	1	6		
7	N	1	Total	C	N	O	0	0
			30	23	1	6		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

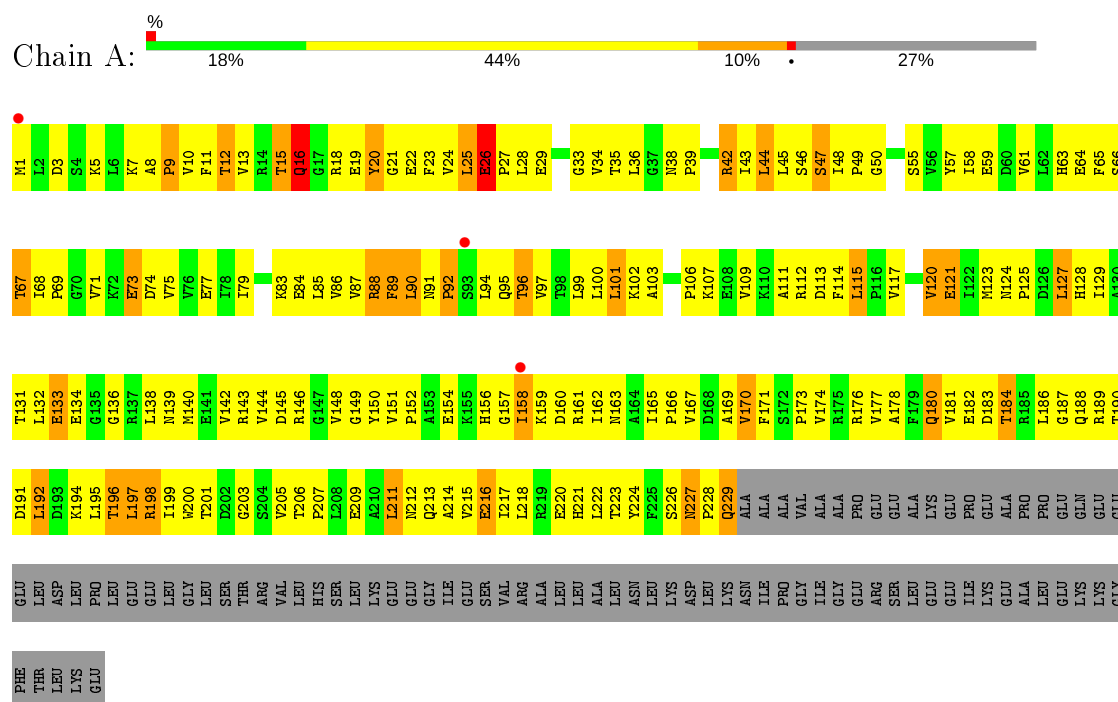
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	141	Total O 141 141	0	0
9	B	149	Total O 149 149	0	0
9	C	704	Total O 704 704	0	0
9	D	927	Total O 927 927	0	0
9	E	82	Total O 82 82	0	0
9	F	305	Total O 305 305	0	0
9	K	152	Total O 152 152	0	0
9	L	148	Total O 148 148	0	0
9	M	680	Total O 680 680	0	0
9	N	864	Total O 864 864	0	0
9	O	84	Total O 84 84	0	0
9	P	260	Total O 260 260	0	0

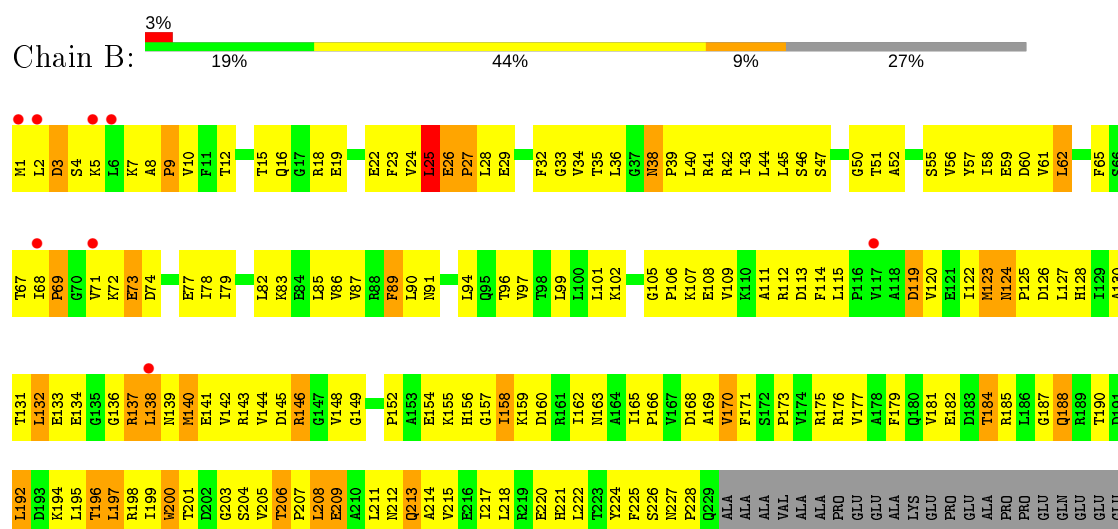
3 Residue-property plots

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 subunit alpha

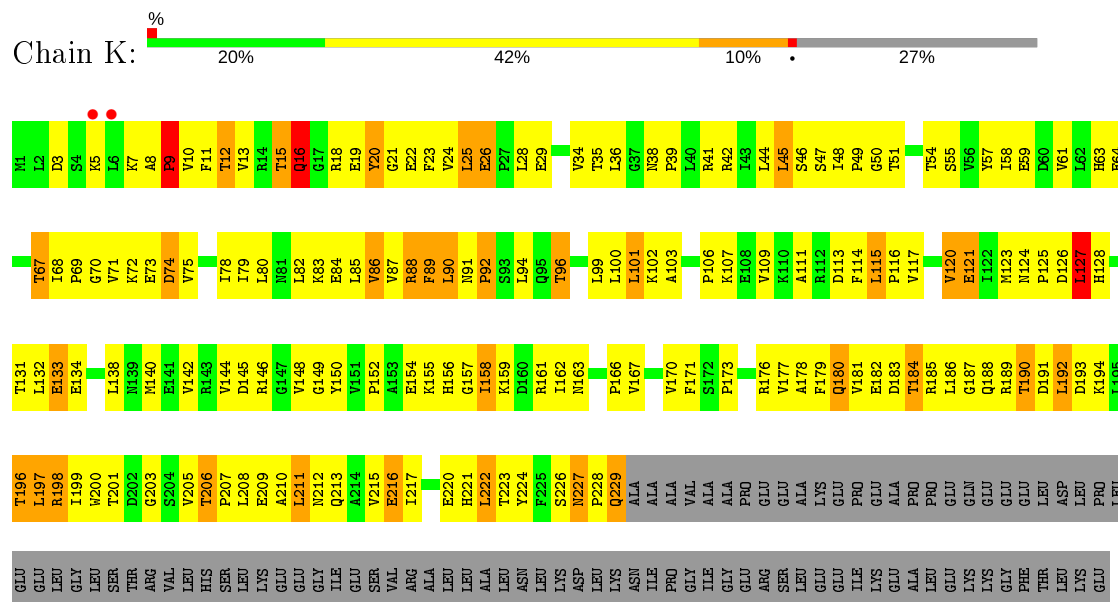


• Molecule 1: DNA-directed RNA polymerase subunit alpha

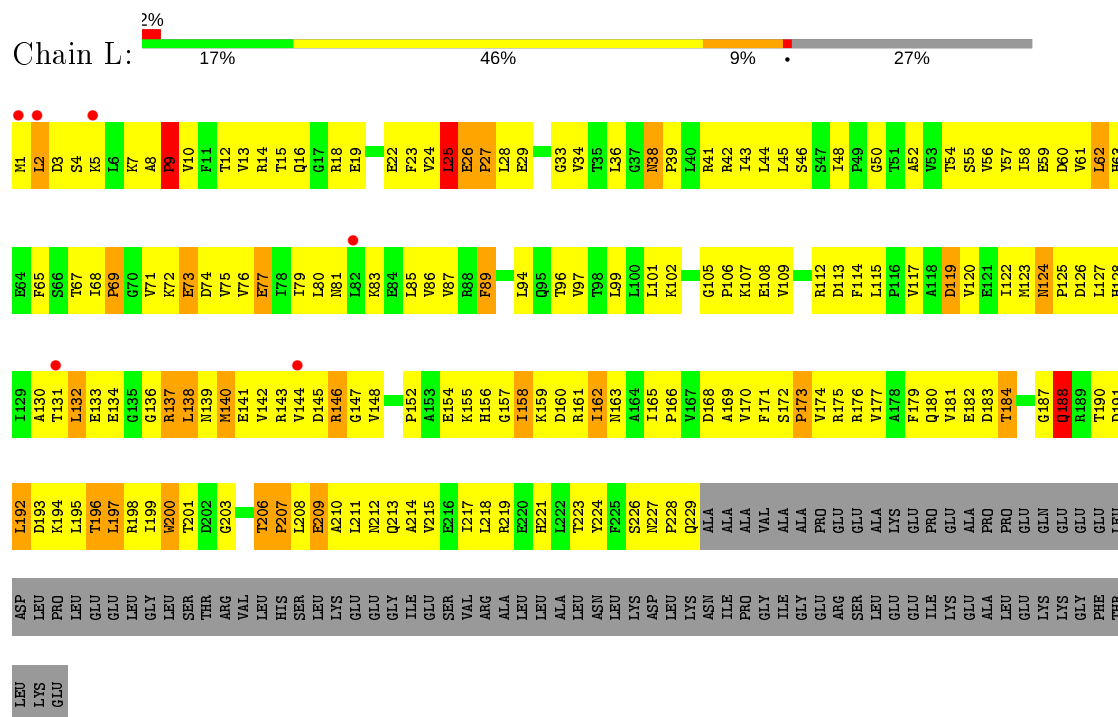


LEU	ASP	LEU	PRQ	LEU	GLU	GLU	GLY	SER	THR	ARG	VAL	LEU	HIS	SER	LEU	LYS	GLU	GLY	LEU	ALA	LEU	LEU	ALA	LEU	ASN	LEU	LYS	ASP	LEU	LYS	ASN	ILE	PRQ	GLY	ILE	GLY	ARG	SER	LEU	GLU	GLU	ILE	LYS	GLY	PHE
THR	LEU	LYS	GLU																																										

• Molecule 1: DNA-directed RNA polymerase subunit alpha



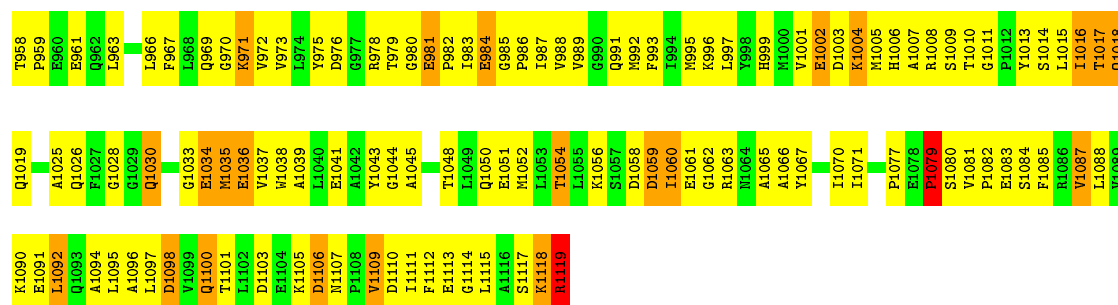
• Molecule 1: DNA-directed RNA polymerase subunit alpha



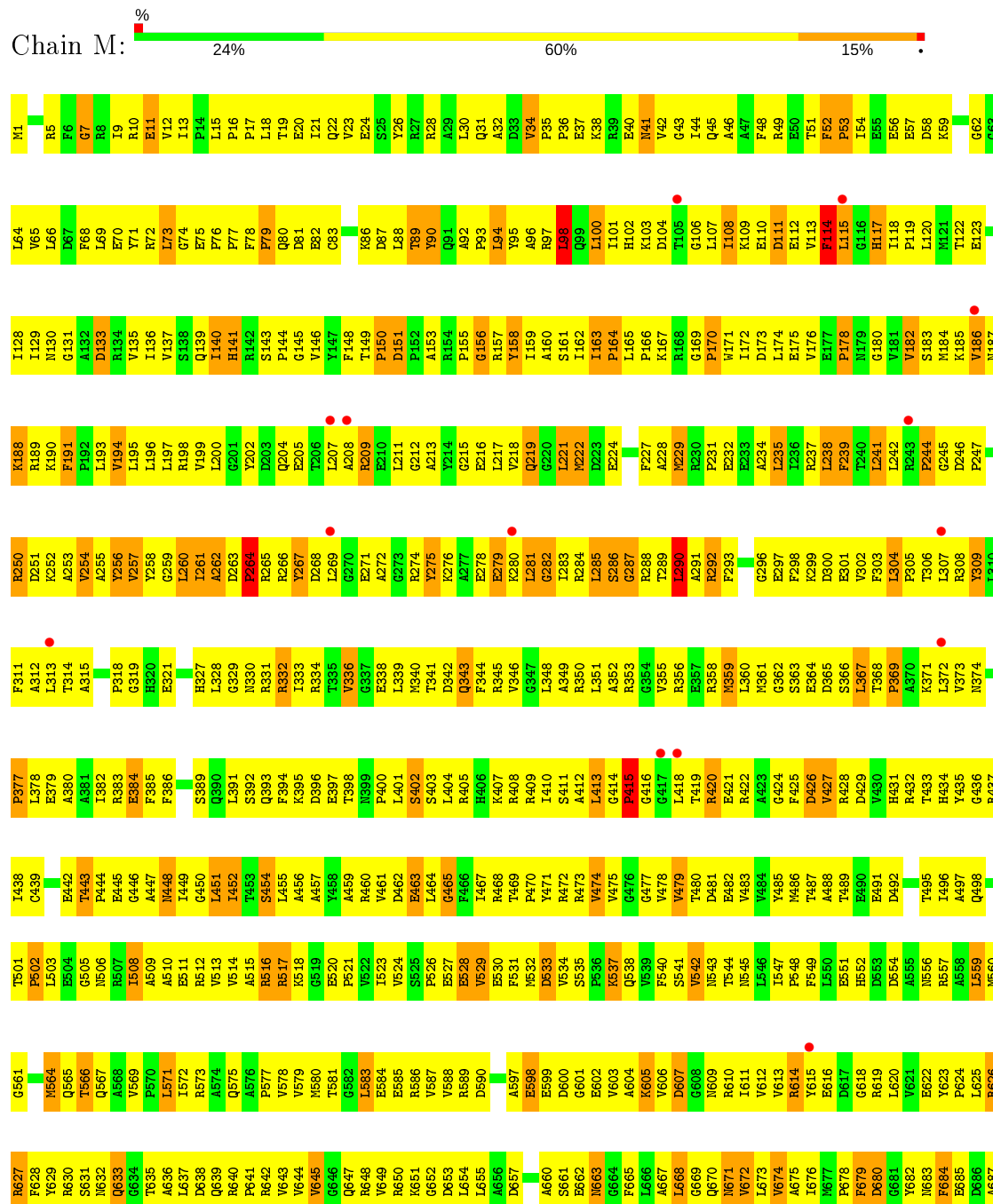
• Molecule 2: DNA-directed RNA polymerase subunit beta

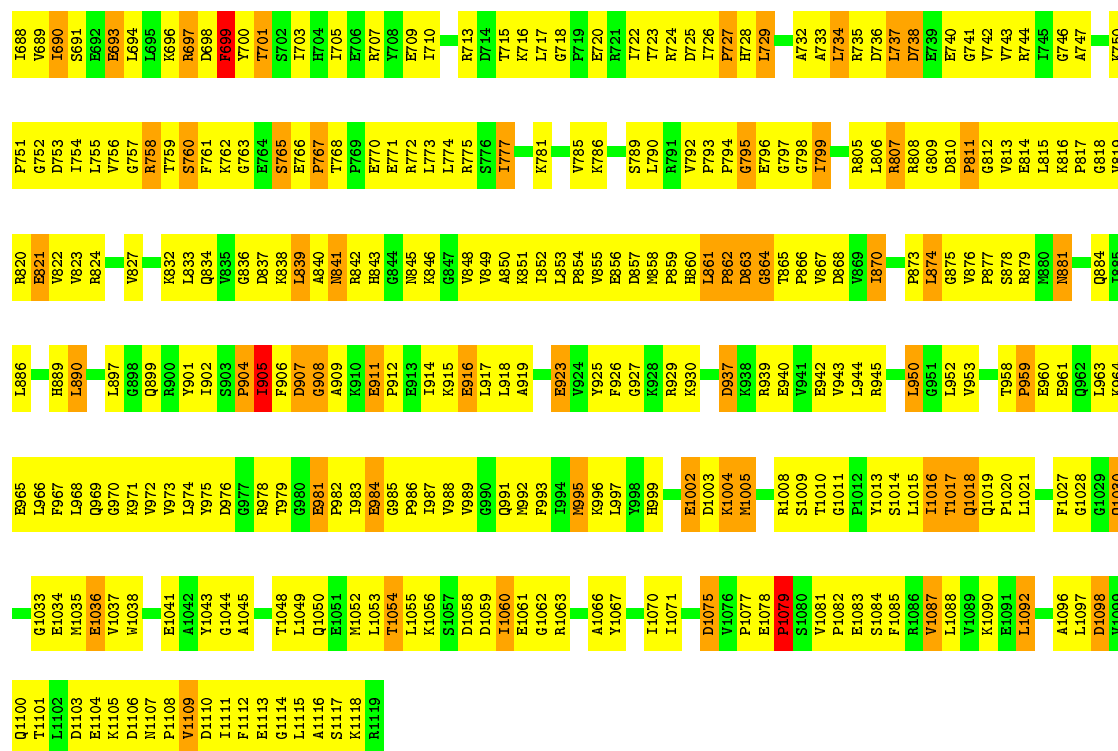


E887	E821	G752	I690	Y629	M564	A497	H434	V373	R308	P247	K185	T122	G62	H1
E888	V822	D753	S691	R630	M564	Q498	V435	R374	Y309	P247	V186	E123	G63	E2
E889	S631	L754	E693	S831	Q565	T501	R436	R375	L310	R250	M187	D124	L64	I3
L890	R824	L755	E692	N632	T566	P502	R437	R376	F311	D251	K188	G125	V65	K4
	V827	V756	L694	Q633	Q567	P502	L438	R377	A312	K252	R189	S126	L66	R5
F886	A828	G757	L695	G634	A568	L503	Q439	L378	L313	A253	K190	G127	D67	F6
L897		R758	K896	T635	V659	E504	R440	E379	T314	V254	F191	I128	P68	G7
G898	R831	T759	R697	A836	P570	G505	V441	A380	V317	A255	F192	I129	L69	R8
R909	K832	S760	D698	L637	L571	I508	E442	A381	P318	Y256	L193	M130	E70	I9
R900	L833	K762	F699	D638	S172	A509	T443	R382	P318	V257	F194	G131	Y71	R10
Y901	R900	R763	R900	Q639	R573	A510	P444	R383	G132	Y258	L195	A132	R72	E11
I902	Q834	G764	T702	R640	A574	E511	E445	E321	E321	G259	L196	D133	L73	V12
S903	V835	S765	S701	R641	Q575	R512	G446	F384	V322	L260	L197	G134	G74	I13
P904	G836	S766	I703	R642	A576	R513	A447	F385			R198	V135	E75	F14
I905	D837	E766	H704	V643	P577	V514	I448	F386	I325		V199	I136	P76	L15
F906	R838	T767	R705	V578	S577	V515	I449				L200	V137	P77	L16
D907	L839	K768	E706	V645	V579	A515	L451				G201	S138	F78	P17
G908	A840	R769	R707	G646	M580	R516	L450				Y202	G203	F79	L18
A909	N841	E770	Y708	Q647	T581	R517	T452				D203	H140	Q80	T19
R910	R842	E771	E709	R648	G582	K518	T453				Q204	H141	D81	E20
E911	H843	R772	I710	V649	L583	I523	S454				E205	R142	S82	I21
P912	G844	L773	E711	R650	E584	E530	L455				T206	S143	R84	Q22
E913	N845	L774	A712	K651	E585	P536	A456				L207	P144	R84	V23
R914	K846	R775	R713	G652	R586	Q537	A457				A208	G145	E85	E24
I915	G847	S776	D714	D653	V587	P526	Y458				R209	V146	K86	S25
K915	R848	I777	T715	L654	V588	E527	A459				A272	Y147	D87	Y26
E916	V849		K716	L655		E528					E210	F148		Y26
L917	A850	E780	L717	A656	S591	V529	V461				L211	R274	L88	R28
L918	G851	G718	D657	G718	L592	E530	D462				G212	T149	T89	R28
I919	R852	V785	P719	G658		F531	E463				A213	P150	Y90	A29
R920	L853	K786	R720	P659	A597	M532	L464				G215	D151	Q91	L30
A921	P854		E721	A660	E598	D533	G465				E216	P155	A92	Q31
F922	R855	S789	I722	S661	E599	V534	F466				L217	G156	P93	A32
E923	E856	L790	R723	N662	D600	S535	L467				K280	R157	L94	D33
V924	R857	R791	R724	G663	G601	P536	R468				L281	G156	Y95	V34
Y925	M858	V792	D725	G664	E602	K537	T469				G347	Y158	A96	P35
F926	P859		I726	F665	V603	Q538	P470				I283	I159	R97	P36
Q927	H860	G795	P727	L666	A604	V539	Y471				N222	A160	L98	E37
	L861		H728	A667	R605	F540	R472				D223	S185	Q99	K38
R928	R862	G798	L729	L668	V606	S541	R473				V226	I162	L100	R39
R929	D863	I799	S730	G669	D607	V542	V474				G227	I163	I101	E40
K930	G864		E731	Q670	G608	N543	V475				A228	P164	H102	N41
	T865	R802	A732	N671	N609	T544	G476				N229	L165	V42	G43
P866	V867	L734	A733	V672	R610	N545	G477				R230	P166	D104	G43
D868	R806	L806	L734	L673	I611	L946	V478				P231	G169	T105	I44
V869	R807	D736	R735	V674	V612	S547	V479				E232	P170	G106	Q45
I870	R808	A675	R614	R614	V613	P548	T480				A234	W171	L107	A46
	G809	L737	D738	I676	R615	F549	D481				D295	I172	I108	A47
P873	D810	V671	A732	N671	V615	L550	V483				G296	D173	K109	F48
L874	P811	E740	E739	D680	R619	H551	V484				F298	L174	E110	R49
G875	G812	G741	E740	D681	L620	H552	V485				R237	E175	E112	T51
V876	V813	V742	V742	G681	V621	D553	R426				L238	V176	V113	F52
P877	E814	E814	V743	N683	E622	D554	M486				F239	E177	F114	F53
S878	L815	F684	R744	N556	G623	A555	T487				T240	P178	L115	I54
R879	K816	I745	I745	E685	P624	R557	A488				L241	G179	G116	E45
L880											F303	G180	H117	E56
G881											L242	V181	I118	E57
L952											R244	V182	P119	D58
V953											G245	S183	L120	K59
	Q884										D246	M184	M121	

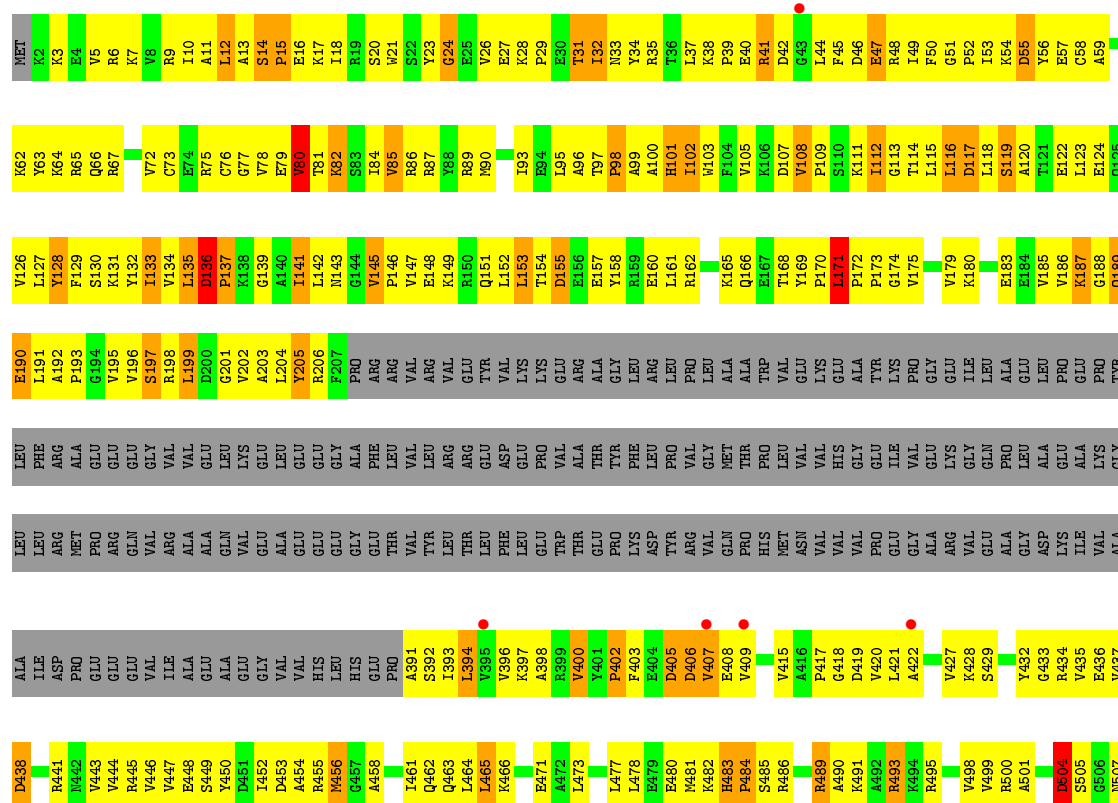


• Molecule 2: DNA-directed RNA polymerase subunit beta





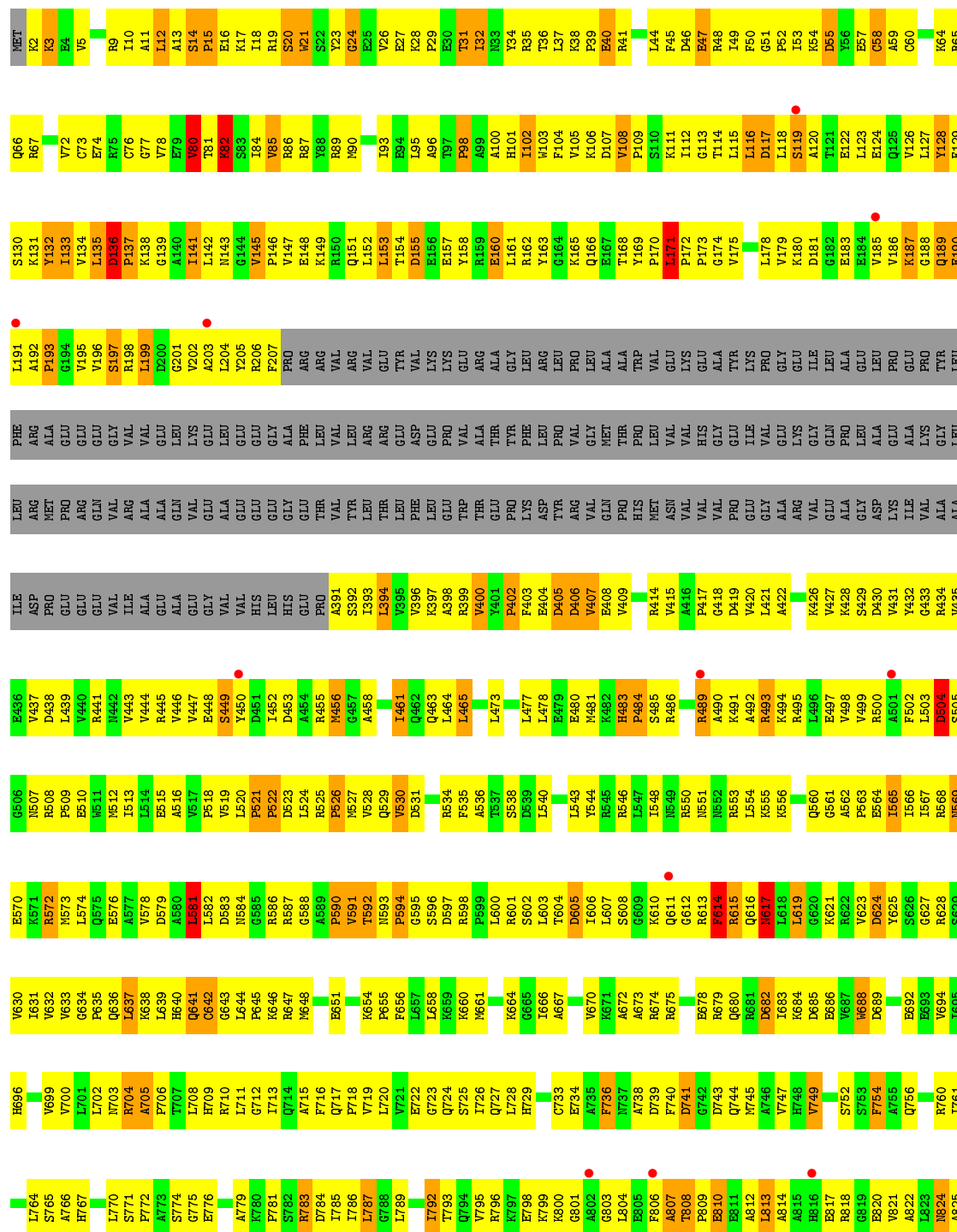
• Molecule 3: DNA-directed RNA polymerase subunit beta'

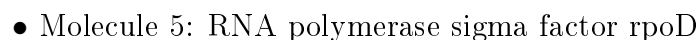
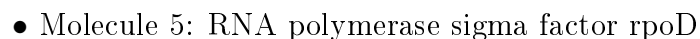


G1411	E1350	I1283	V1221	E1154	S1091	F1030	V955	I895	V821	A757	V694	V632	K571	R508
K1412	E1351	E1284	G1222	V1155	G1092	I1031	V956	E888	A822	E758	I695	V633	R572	P509
T1413	I1352	E1285	I1223	E1156	Y1093	Q1032	I956	E889	L823	A759	G696	G634	M570	E510
P1414	Q1353	T1286	V1224	R1159	L1094	Q1033	P957	A899	R824	R760	G697	P635	L574	M511
V1415	K1354			L1160	T1095	Q1034	E958	V890	A825	I761	K698	Q636	Q575	M512
A1416	V1355		S1228	E1161	K1096	I1035	E959	E891	A826	Q762	V699	L637	E576	I513
H1417	I1356	L1280	I1229		K1097	R1036	K960	E892	I827	A763		K638	A577	L514
K1418	R1357	S1291	G1230	R1164	L1098	Q1037		E893	K828	L764	L702	L639	A578	E516
P1419	F1293	V1282	G1231	Y1165	Y1099	L1038	Y963	K894	R829	S765	R703	H640		A516
L1420	Q1358	E1287	E1231	L1166	D1100	D1039	L964	V895	A830	A766	R704	Q641	L581	P517
L1421	G1360	E1294	G1232	S1167	V1101	G1040	E965	A896	G831	H767	A705	C642	L582	P518
M1422	T1361	E1295	T1234	M1168	T1102	G1041		K897	E832	N768	P706	G643	D583	V519
G1423	K1362	E1299	Q1235		K1103	R1042	D968	E898	E833	L769	T707	L644	N584	L520
V1424	L1363	S1300	L1236	V1171	E1104	G1043		L899	T834	L770	L708	P645	P521	P521
T1425	K1364	K1301	T1237	L1172	I1105	L1044	L972	I900	S835	S771	H709	R646	P522	P522
K1426	D1365	E1302	M1238	L1173	V1106	M1045		Q901	V836	A766	R710	R647	D523	D523
S1427	K1366	K1303	R1239	L1174	V1107	Q1046	E975	L902	G837	A773	G642	M648	G588	L524
A1428	H1367	K1304	T1240	L1175	K1108	K1047			R838	S774	G712	A649	A589	R525
L1429	F1241	L1305	R1241	K1176	E1109	P1048	M880	Q906	L839	G775	I713	L650	P590	P526
E1430	E1368	P1306	H1242	A1177	A1110	S1049		E907	K840	E776	G714	E551	M527	M527
T1431	I1370	K1307	T1243		D1111	G1050	L983	E908	H841	P777	A715		T592	T592
K1432	E1308	E1308	G1244	E1179	G1112	E1051	T984		H842	L778	F716	K654	N593	Q529
S1433	V1372	A1309	G1245		G1113	T1052	D985		F843		Q717	P655	P594	V530
V1434	R1373	R1310	V1246	I1183	T1114	F1053		L911	F843			K656	G595	D531
	G1374	L1311	A1247		T1115		E887	I912	A844	F781	P718	L657	G596	G532
S1438	M1375	L1312	G1248	V1186	N1116	P1056	R888	I914	R845	R783	L720	L658	D597	G583
F1440	K1376	V1313	A1249	P1187	I1117	V1057	Y989	L916	D847	D784	G721	K659	P598	R534
Q1441	L1314	E1250	L1250	P1188	I1118	R1058		V916	E848	E722	E722	K660	P599	F535
N1442	D1315	D1251	D1251	R1189	S1119	S1059	Q991		A849	T786	G723	M661	L600	L600
T1443	V1378	G1316	I1252	L1190	V1120	S1060	I992	L920	L850	L787	Q724	E662	R601	T537
T1444	E1380	D1317	T1253	P1191	P1121	F1061	L993	L921	L851	G788	S725	E663	S602	S602
	V1381	V1318	Q1254	L1192	L1122	R1062	Q994	L922	A852	L789	I726	K664	L603	D539
T1447	T1382	I1319	G1255	L1193	F1123	E1063	L995	G923	H853		Q727	G665	T604	L540
L1448	D1383	E1320	L1256	C1194	G1124	G1064	M996	E925	L728		L728	I666	D605	L543
E1449	P1384	A1321	P1257	Q1195	P1125	L1065	T997	R926	L729		P730	A667	L606	Y544
A1450	G1385	Q1322	R1258	T1196	D1126	T1066	E998	I926	R859	V795	L731	V670	S608	R545
A1451	D1386	G1323	V1259	R1197	E1127	V1067	T999	T927	L860	R796	G732	K671	G609	R546
	S1387	P1324	I1260	Y1198	V1128	L1068	T1000	A928	Q861	K797	C733	A672	K610	L547
K1455	R1388	L1325	E1261	G1199	T1129	E1069	E1001	R929	D862	E798		A673	Q611	L548
K1456	L1389	T1326	L1262	V1200	R1130	Y1070	K1002	L930	H864	K799		R674	G612	N549
D1457	L1390	R1327	E1263	C1201	L1132	F1071	V1003	D932	T865	Q801	F736	R675	R613	R550
			E1264	Q1202	L1133	I1072			R866	A802	A738	M676	F614	N551
E1458			A1265	K1203	R1133	S1073	A1006		R867	G803	D739	L677	R615	
L1460	V1394	I1330	R1266	C1204	L1134	S1074	V1007	K935	E807	L804	F740	E678	Q616	L584
G1461	L1395		A1267	Y1205		H1075	F1008	Y936	Y868		D741	R679	N617	K555
L1462	E1396	Q1384	P1268	G1206	R1137	G1076	K1009	G938					L618	L588
K1463	K1397	L1336	K1269	Y1207	D1139	A1077	N1010	G938	K871	F806	Q680	R681	L619	A559
E1464	W1398	E1337	A1270	D1208	I1140	R1078		F941	R872	T808	D743	D682	G620	Q560
N1465	V1399	A1338	K1271	L1209	K1271	K1079	N1018	T942	L873	A807	Q744	I683	K621	G561
V1466	V1400	K1339	A1272	S1210	E1141	G1080	P1019	T943	E874	P809	M745	D683	R622	A562
I1467	E1401	G1340	V1273	M1211	A1142	G1081	L1020	T944	T875	E810	A746	D684	G623	G561
L1468	A1402	P1341	I1274	A1212	G1143	A1082	Y1021	T944	S876	E811	F747	D685	K622	A562
G1469	E1342	E1342	S1275	R1213	L1144	D1083	M1022	S945	P877	A812	H748	E686	G624	P563
R1470	N1403	L1403	E1276	P1214	V1145	T1084	M1023	G946	G878	L813	P749	V687	Y625	E564
K1471	A1404	K1343	I1277	P1214	K1146	A1085	A1024	I947	R879	A814	P750	W688	S626	I566
L1472	R1405	E1345	D1278	S1216	R1147	L1086	Q1025	T948	R890			D689	G627	I566
P1473	L1407	R1346	G1279	I1217		L1087	S1026	I949	L881	E817	S753	A690	R628	I567
A1474	I1408	Y1347	V1280	G1218	R1151	R1088	G1027	G950	F882	R818	F754	L691	S629	R568
G1475	L1348	E1152	E1281	E1152	A1152	A1089	A1028	I951	A883	A755	R755	E592	V630	N569
T1476	T1476	V1349	R1282	A1220	V1153	D1090	R1029	D952	R894	E820	Q756	E593	I631	E570



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





T383	R259	S327	I188
R394	I260	F328	E189
E395	P281	Y329	A190
R396	V262	G330	N191
I397	H263	D331	L192
R398	M264	F332	R193
Q399	V265	I333	L194
I400	E266	F334	V195
E401	T267	D335	K200
I402	I268	E336	T203
R403	N269	H337	G204
A404	K270	L338	R205
I405	L271	P339	G206
R406		S340	L207
R407	T274	P341	S208
L408	R276	V342	F209
R409	A275	D343	L210
Y410	Q277		D211
R411	L278	S348	L212
E412	Q279	L349	I213
S413	Q280	L350	Q214
	E281	S351	E215
R416	L282	E352	G216
	G283	E353	N217
R419	R284	L354	Q218
D420	E285	E355	G219
F421	P286	R356	L220
L422	T287	A357	I221
D423	Y288	L358	R222
	E289	S359	A223
	E290	K360	V224
	I291	L361	E225
	A292	S362	K226
		E363	
	M295	R364	R232
	G296	E365	F233
	P297	A366	K234
	G298	M367	F235
	W299	V368	S236
	D300	L369	
		K370	
	R303	L371	
	V304	R372	T240
	E305	K373	E241
	E306	G374	W242
		L375	I243
	K309	I376	R244
	I310	D377	Q245
	A311	G378	A246
	Q312	ARG	I247
		GLU	N248
	V315	HIS	R249
	S316	THR	A250
	L317	LEU	I251
	E318	E384	Q254
		E385	A255
	I321		R256
		F390	T257
	K325	G391	I258
	D326	V392	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	235.00Å 235.00Å 254.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.70 39.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-2.70) 90.4 (39.96-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.270 0.238 , 0.260	Depositor DCC
R_{free} test set	18510 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l 0.048 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	57340	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.84	2/1838 (0.1%)	1.04	9/2498 (0.4%)
1	B	0.74	1/1838 (0.1%)	0.95	9/2498 (0.4%)
1	K	0.81	2/1838 (0.1%)	1.00	8/2498 (0.3%)
1	L	0.75	1/1838 (0.1%)	0.96	10/2498 (0.4%)
2	C	0.73	0/8997	0.94	14/12164 (0.1%)
2	M	0.73	0/8997	0.94	14/12164 (0.1%)
3	D	0.75	2/10582 (0.0%)	0.97	15/14294 (0.1%)
3	N	0.75	1/10582 (0.0%)	0.97	18/14294 (0.1%)
4	E	0.73	0/784	1.23	5/1057 (0.5%)
4	O	0.71	0/784	1.08	3/1057 (0.3%)
5	F	0.65	0/2812	0.85	3/3781 (0.1%)
5	P	0.65	0/2812	0.86	2/3781 (0.1%)
All	All	0.74	9/53702 (0.0%)	0.96	110/72584 (0.2%)

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	N	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	C-O	-11.04	1.02	1.23
1	K	26	GLU	C-O	-10.57	1.03	1.23
1	B	26	GLU	C-O	-10.23	1.03	1.23
1	L	26	GLU	C-O	-9.82	1.04	1.23
1	A	16	GLN	CB-CG	5.82	1.68	1.52

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	94	PRO	CA-N-CD	-18.30	85.89	111.50
1	B	138	LEU	CA-CB-CG	12.41	143.84	115.30
1	L	138	LEU	CA-CB-CG	12.19	143.33	115.30
4	O	94	PRO	CA-N-CD	-9.89	97.65	111.50
1	K	26	GLU	CA-C-N	9.51	143.72	117.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	184	0
1	B	1806	0	1861	197	0
1	K	1806	0	1861	212	0
1	L	1806	0	1861	198	0
2	C	8829	0	8933	1145	0
2	M	8829	0	8933	1073	0
3	D	10407	0	10633	1296	0
3	N	10407	0	10633	1283	0
4	E	770	0	784	121	0
4	O	770	0	784	113	0
5	F	2771	0	2844	316	0
5	P	2771	0	2844	312	0
6	D	2	0	0	0	0
6	N	2	0	0	0	0
7	D	30	0	31	18	0
7	N	30	0	31	18	0
8	D	1	0	0	0	0
8	N	1	0	0	0	0
9	A	141	0	0	28	0
9	B	149	0	0	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	704	0	0	215	0
9	D	927	0	0	239	0
9	E	82	0	0	29	0
9	F	305	0	0	77	0
9	K	152	0	0	41	0
9	L	148	0	0	34	0
9	M	680	0	0	180	0
9	N	864	0	0	235	0
9	O	84	0	0	26	0
9	P	260	0	0	71	0
All	All	57340	0	53894	6054	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 57.

The worst 5 of 6054 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:610:LYS:HD3	7:D:1527:MXP:C15	1.49	1.41
3:N:610:LYS:HD3	7:N:1527:MXP:C15	1.55	1.37
3:N:136:ASP:HB3	3:N:137:PRO:HD3	1.27	1.15
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.27	1.13
3:D:610:LYS:HD3	7:D:1527:MXP:H15B	1.19	1.10

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%)	200 (88%)	24 (11%)	3 (1%)	12 30
1	B	227/315 (72%)	195 (86%)	29 (13%)	3 (1%)	12 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	227/315 (72%)	201 (88%)	22 (10%)	4 (2%)	8	21
1	L	227/315 (72%)	199 (88%)	25 (11%)	3 (1%)	12	30
2	C	1117/1119 (100%)	905 (81%)	154 (14%)	58 (5%)	2	3
2	M	1117/1119 (100%)	904 (81%)	153 (14%)	60 (5%)	2	3
3	D	1317/1524 (86%)	1098 (83%)	170 (13%)	49 (4%)	3	7
3	N	1317/1524 (86%)	1089 (83%)	176 (13%)	52 (4%)	3	6
4	E	93/99 (94%)	77 (83%)	12 (13%)	4 (4%)	2	5
4	O	93/99 (94%)	77 (83%)	10 (11%)	6 (6%)	1	2
5	F	341/423 (81%)	285 (84%)	37 (11%)	19 (6%)	2	3
5	P	341/423 (81%)	287 (84%)	36 (11%)	18 (5%)	2	3
All	All	6644/7590 (88%)	5517 (83%)	848 (13%)	279 (4%)	3	5

5 of 279 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	B	29	GLU
2	C	7	GLY
2	C	178	PRO
2	C	231	PRO

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%)	161 (80%)	41 (20%)	1	3
1	B	202/273 (74%)	163 (81%)	39 (19%)	1	3
1	K	202/273 (74%)	159 (79%)	43 (21%)	1	3
1	L	202/273 (74%)	166 (82%)	36 (18%)	2	4
2	C	941/941 (100%)	755 (80%)	186 (20%)	1	3
2	M	941/941 (100%)	757 (80%)	184 (20%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1112/1279 (87%)	935 (84%)	177 (16%)	2	6
3	N	1112/1279 (87%)	934 (84%)	178 (16%)	2	6
4	E	84/88 (96%)	68 (81%)	16 (19%)	1	4
4	O	84/88 (96%)	68 (81%)	16 (19%)	1	4
5	F	295/370 (80%)	252 (85%)	43 (15%)	3	7
5	P	295/370 (80%)	254 (86%)	41 (14%)	3	8
All	All	5672/6448 (88%)	4672 (82%)	1000 (18%)	2	4

5 of 1000 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	57	ASP
1	L	112	ARG
3	N	1415	VAL
5	F	117	SER
1	K	20	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	86	HIS
1	L	128	HIS
3	N	1465	ASN
5	F	312	GLN
1	K	139	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
7	MXP	D	1527	-	25,30,30	2.87	11 (44%)	27,38,38	3.35	8 (29%)
7	MXP	N	1527	-	25,30,30	3.15	12 (48%)	27,38,38	3.56	11 (40%)

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
7	MXP	D	1527	-	-	7/27/28/28	0/1/1/1
7	MXP	N	1527	-	-	7/27/28/28	0/1/1/1

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	1527	MXP	C9-C10	7.23	1.41	1.34
7	D	1527	MXP	C9-C10	6.34	1.40	1.34
7	D	1527	MXP	O1-C5	6.19	1.43	1.35
7	N	1527	MXP	O1-C5	6.18	1.43	1.35
7	N	1527	MXP	C1-C5	5.45	1.45	1.35

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	1527	MXP	O4-C6-C7	12.36	138.42	120.83
7	D	1527	MXP	O4-C6-C7	11.53	137.24	120.83
7	D	1527	MXP	C8-C9-C10	-6.76	116.93	127.30
7	N	1527	MXP	C8-C9-C10	-6.57	117.22	127.30
7	D	1527	MXP	C23-O5-C22	6.10	122.86	115.66

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

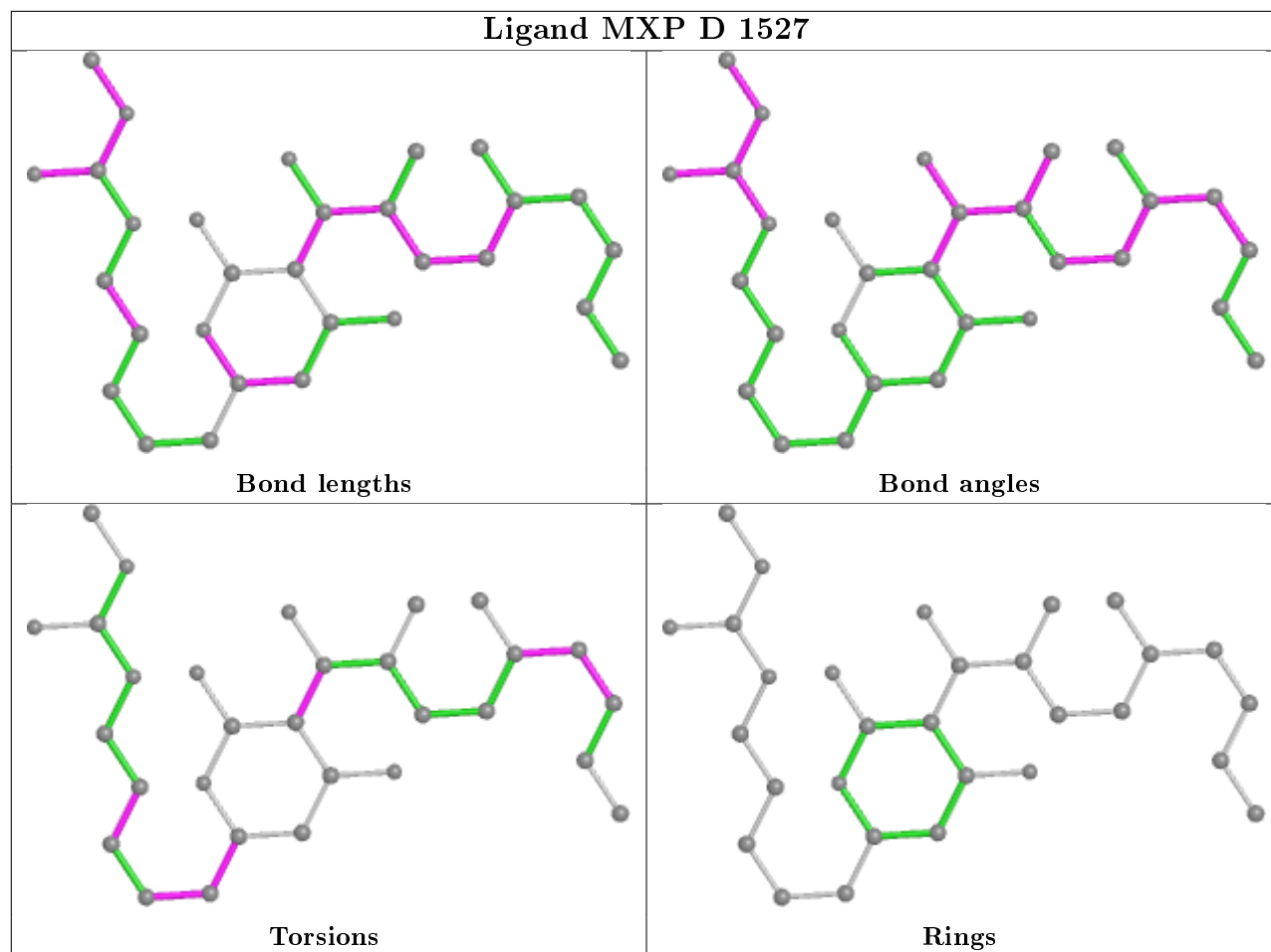
Mol	Chain	Res	Type	Atoms
7	N	1527	MXP	C5-C17-C18-C19
7	D	1527	MXP	C5-C17-C18-C19
7	D	1527	MXP	C10-C11-C12-C13
7	D	1527	MXP	C2-C3-C6-O4
7	N	1527	MXP	C10-C11-C12-C13

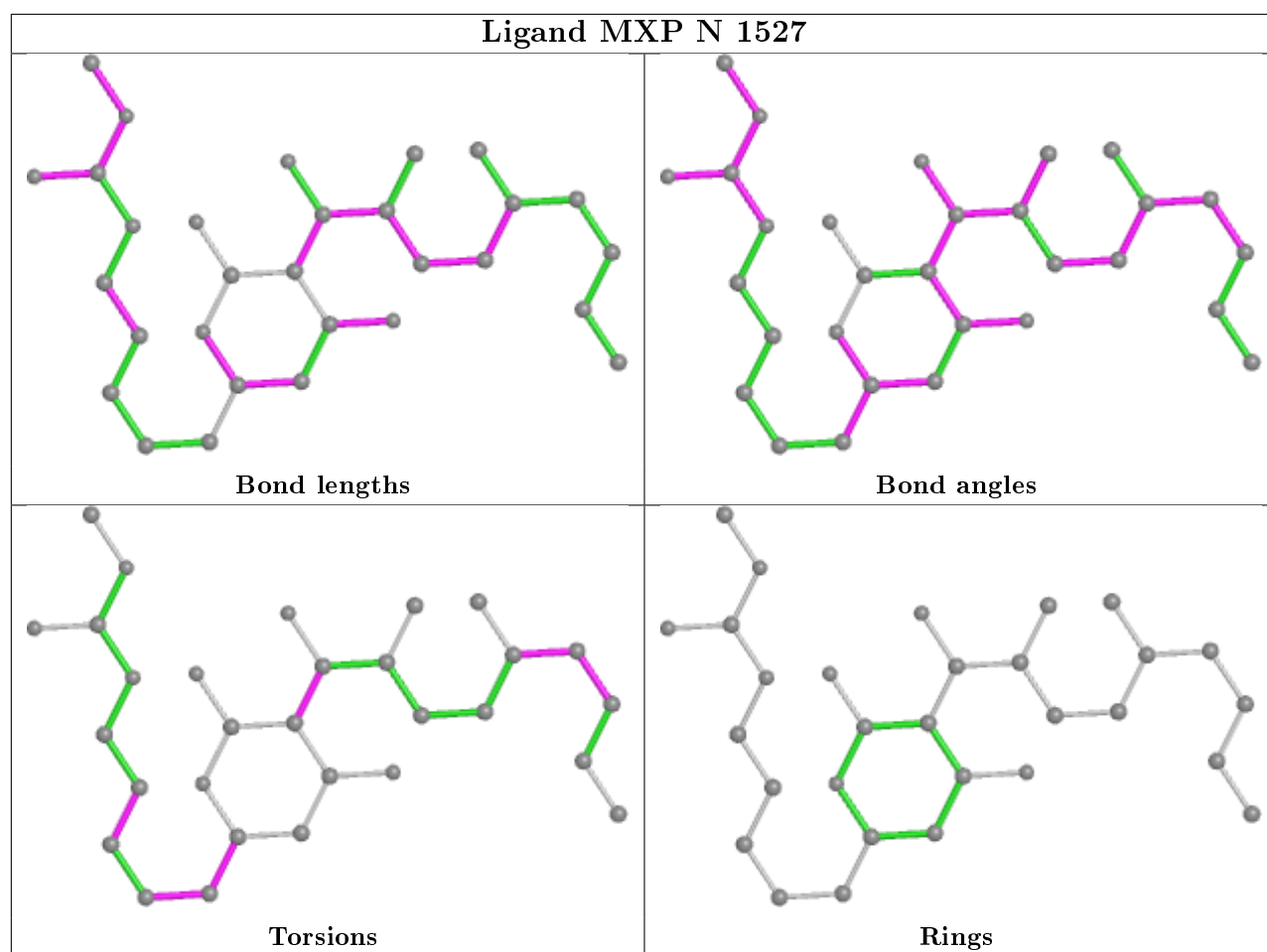
There are no ring outliers.

2 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1527	MXP	18	0
7	N	1527	MXP	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	-0.06	3 (1%) 77 78	28, 50, 78, 101	0
1	B	229/315 (72%)	-0.06	8 (3%) 44 44	36, 71, 86, 104	0
1	K	229/315 (72%)	-0.08	2 (0%) 84 85	25, 52, 81, 93	0
1	L	229/315 (72%)	-0.05	6 (2%) 56 57	47, 73, 86, 104	0
2	C	1119/1119 (100%)	-0.06	27 (2%) 59 60	14, 62, 88, 96	0
2	M	1119/1119 (100%)	-0.09	14 (1%) 77 78	11, 60, 86, 101	0
3	D	1321/1524 (86%)	-0.08	20 (1%) 73 76	10, 53, 85, 107	0
3	N	1321/1524 (86%)	-0.10	21 (1%) 72 74	11, 54, 85, 109	0
4	E	95/99 (95%)	-0.13	2 (2%) 63 65	30, 64, 90, 95	0
4	O	95/99 (95%)	-0.19	2 (2%) 63 65	29, 61, 83, 100	0
5	F	345/423 (81%)	-0.10	5 (1%) 75 77	27, 68, 89, 100	0
5	P	345/423 (81%)	-0.07	9 (2%) 56 57	23, 68, 91, 103	0
All	All	6676/7590 (87%)	-0.09	119 (1%) 68 70	10, 59, 87, 109	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1241	PHE	8.6
3	N	1240	THR	6.2
3	N	1243	THR	6.1
2	C	186	VAL	6.0
2	M	186	VAL	5.8

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](#)

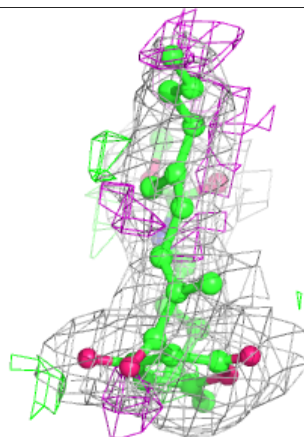
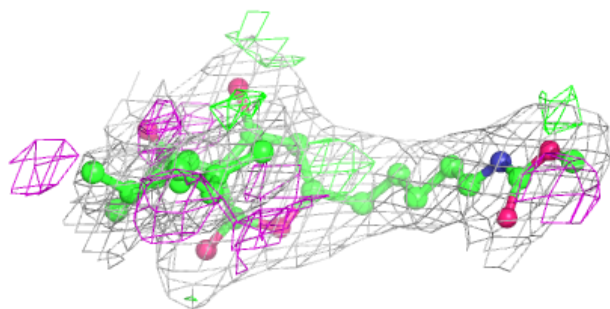
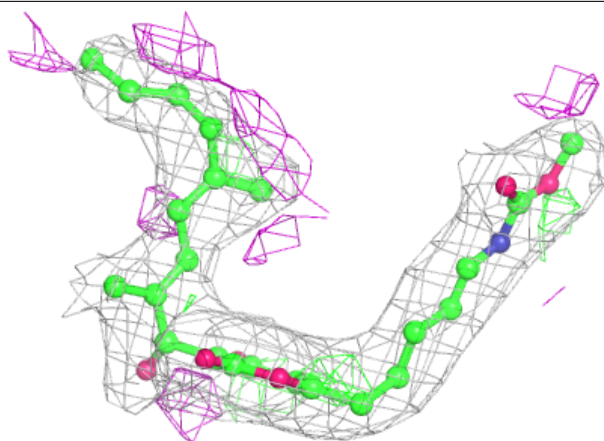
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MXP	D	1527	30/30	0.96	0.19	13,20,27,34	0
7	MXP	N	1527	30/30	0.96	0.17	17,30,38,40	0
6	ZN	N	1526	1/1	0.97	0.18	66,66,66,66	0
8	MG	N	1528	1/1	0.97	0.07	41,41,41,41	0
6	ZN	D	1525	1/1	0.97	0.14	62,62,62,62	0
8	MG	D	1528	1/1	0.98	0.09	35,35,35,35	0
6	ZN	D	1526	1/1	0.99	0.21	48,48,48,48	0
6	ZN	N	1525	1/1	0.99	0.17	58,58,58,58	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

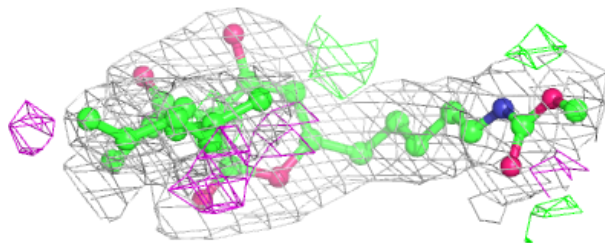
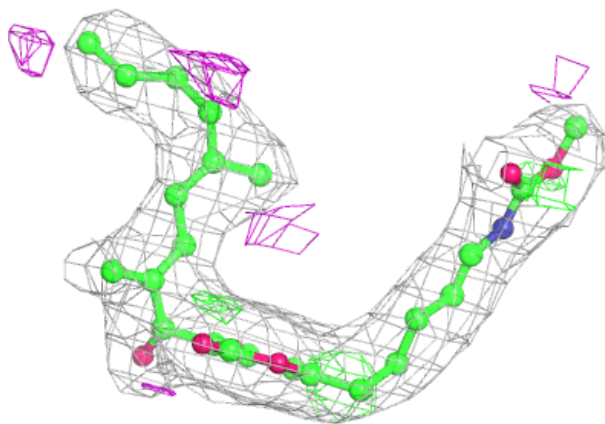
Electron density around MXP D 1527:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MXP N 1527:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.