



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 06:49 AM EDT

PDB ID : 3DXJ  
Title : Crystal structure of thermus thermophilus rna polymerase holoenzyme in complex with the antibiotic myxopyronin  
Authors : Das, K.; Arnold, E.  
Deposited on : 2008-07-24  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

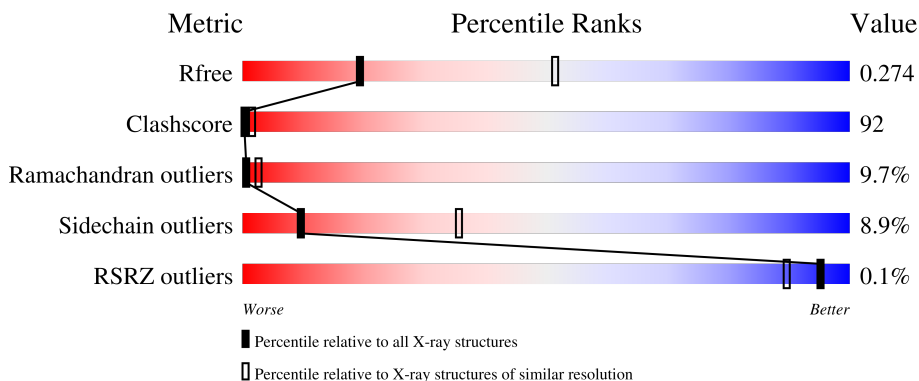
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	B	315	
1	K	315	
1	L	315	
2	C	1119	

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Mol	Chain	Length	Quality of chain			
2	M	1119	17%	69%	13%	•
3	D	1524	15%	69%	14%	••
3	N	1524	15%	68%	15%	••
4	E	99	19%	61%	14%	••
4	O	99	23%	57%	15%	••
5	F	423	9%	57%	16%	• 17%
5	P	423	9%	55%	18%	• 17%

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
10	NE6	D	1529	X	-	-	-
10	NE6	N	1528	X	-	-	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 56149 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; CHAIN A, B, K, L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	231	Total	C	N	O	S	0	0	0
			1816	1159	315	339	3			
1	B	243	Total	C	N	O	S	0	0	0
			1902	1212	328	359	3			
1	K	231	Total	C	N	O	S	0	0	0
			1816	1159	315	339	3			
1	L	243	Total	C	N	O	S	0	0	0
			1902	1212	328	359	3			

- Molecule 2 is a protein called BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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 BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1504	Total	C	N	O	S	0	0	0
			11864	7518	2091	2219	36			
3	N	1504	Total	C	N	O	S	0	0	0
			11864	7518	2091	2219	36			

- Molecule 4 is a protein called BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O.

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			

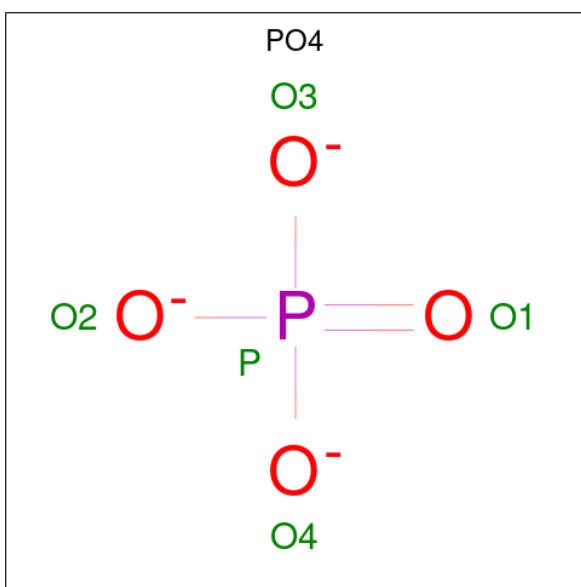
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLU	VAL	variant	UNP Q8RQE7
E	92	ILE	LEU	variant	UNP Q8RQE7
E	95	GLY	VAL	variant	UNP Q8RQE7
O	61	GLU	VAL	variant	UNP Q8RQE7
O	92	ILE	LEU	variant	UNP Q8RQE7
O	95	GLY	VAL	variant	UNP Q8RQE7

- Molecule 5 is a protein called RNA polymerase principal sigma factor (RpoD); CHAIN F, P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	349	Total	C	N	O	S	0	0	0
			2829	1785	513	527	4			
5	P	349	Total	C	N	O	S	0	0	0
			2829	1785	513	527	4			

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

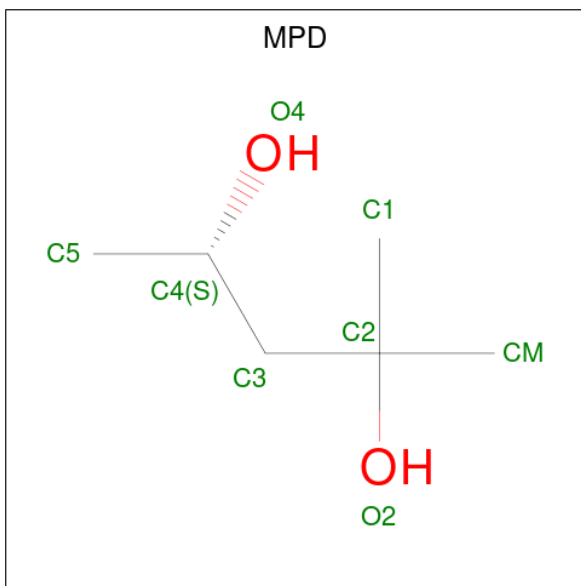


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

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

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

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).

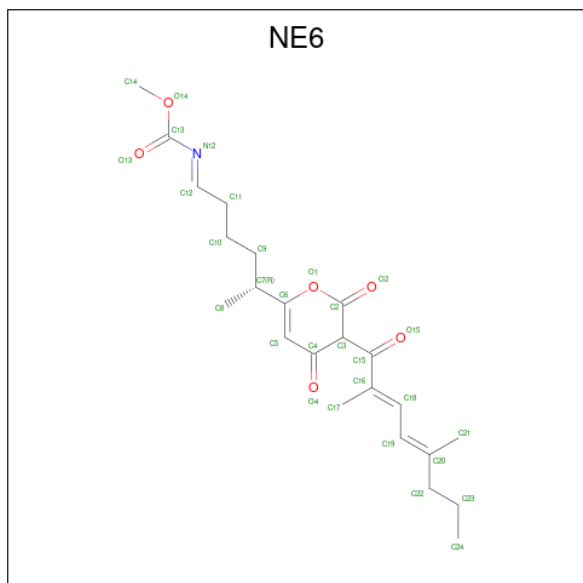


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			8	6	2		
8	C	1	Total	C	O	0	0
			8	6	2		
8	M	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is methyl [(1E,5R)-5-{(3S)-3-[(2E,4E)-2,5-dimethylocta-2,4-dienoyl]-2,4-dihydro-3,4-dihydro-2H-pyran-6-yl}hexylidene]carbamate (three-letter code: NE6) (formula: C<sub>23</sub>H<sub>31</sub>NO<sub>6</sub>).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O 1 1	0	0
11	B	1	Total O 1 1	0	0
11	C	7	Total O 7 7	0	0
11	D	10	Total O 10 10	0	0
11	F	1	Total O 1 1	0	0

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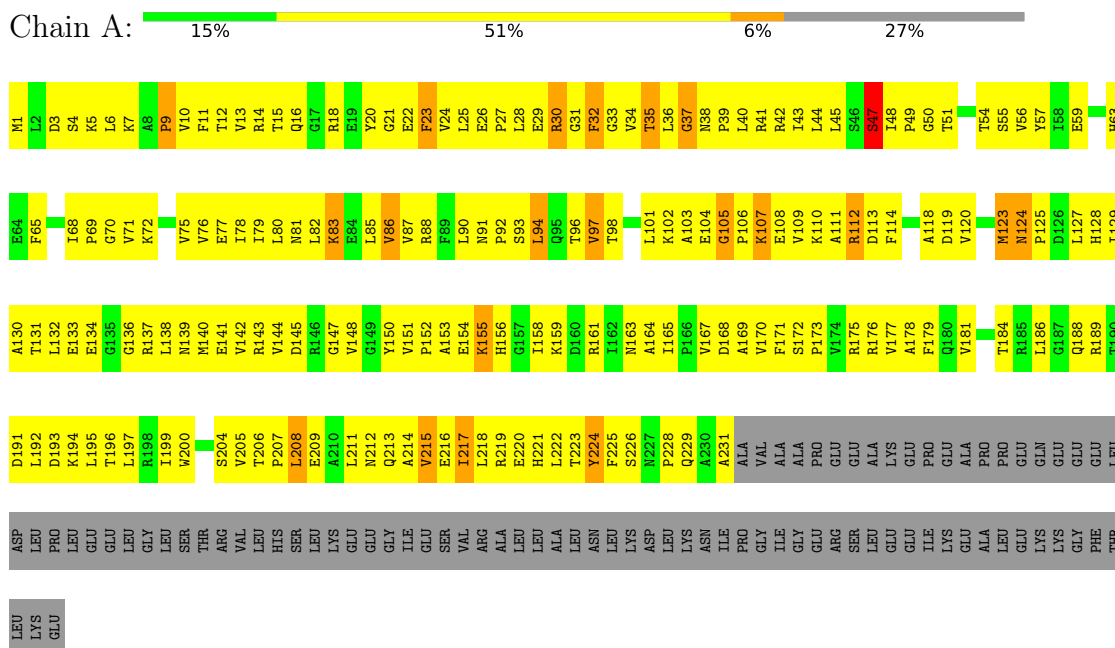
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
11	M	5	Total 5	O 5	0	0
11	N	4	Total 4	O 4	0	0
11	O	1	Total 1	O 1	0	0



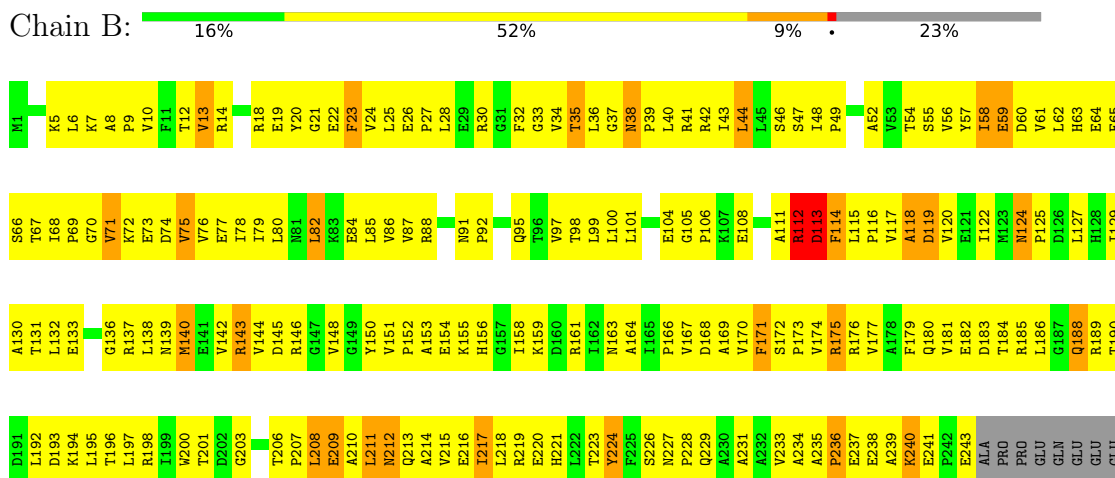
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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; CHAIN A, B, K, L

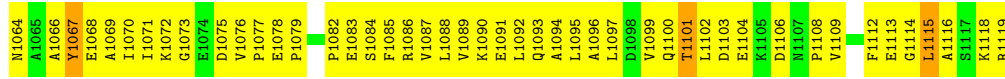


- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

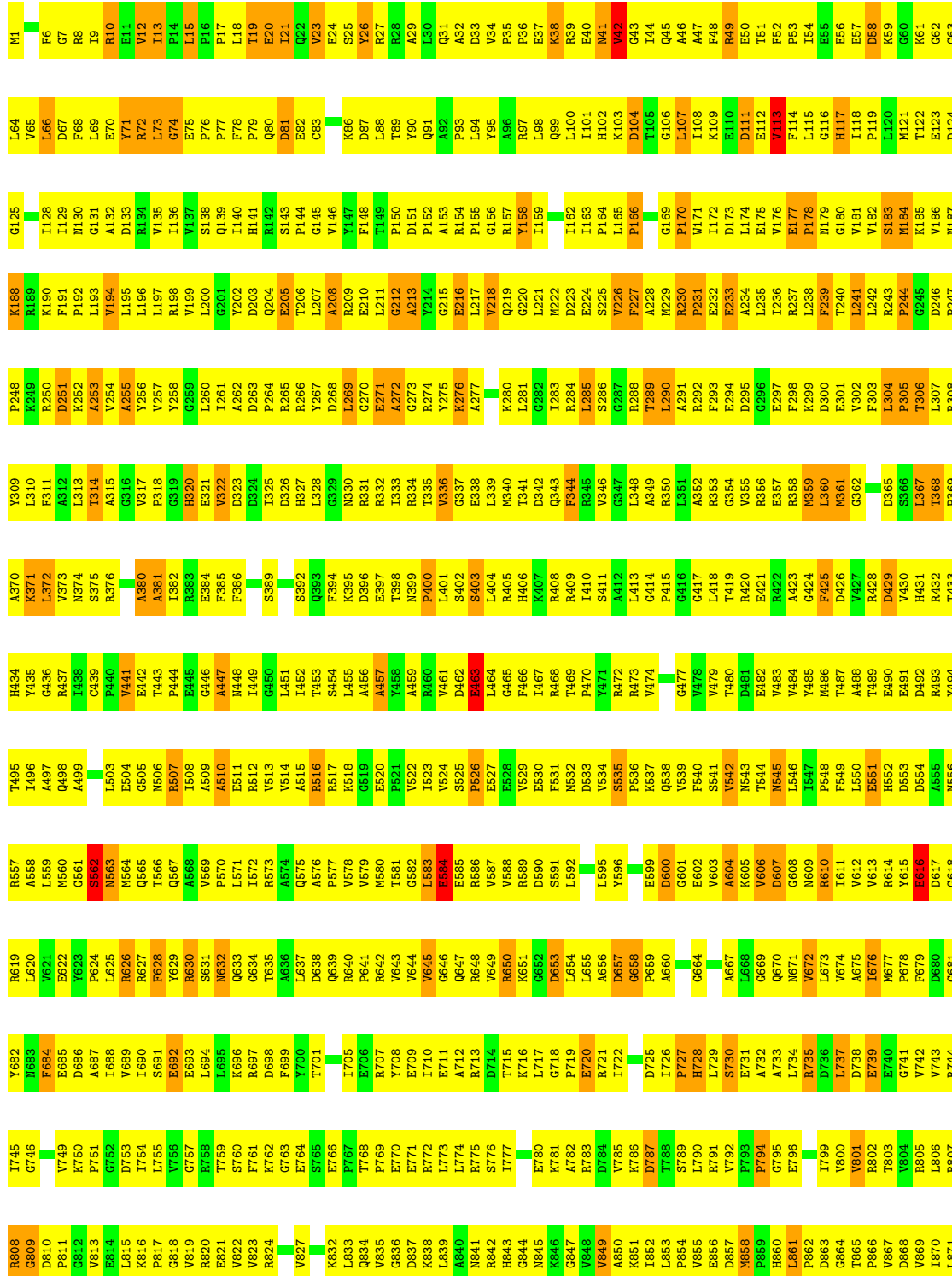








● Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M



N872	N873	L874	G875	V876	P877	S878	R879	M880	N881	Q884	L885	L886	E887	T888	H889	L890	G891	L892	A893	G894	Y895	F896	L897	G898	Q899	R900	Y901	I902	S903	P904	I905	F906	D907	G908	A909	K910	E911	P912	E913	I914	K915	E916	L917	L918	A919	P920	A921	F922	E923	V924	Y925	F926	G927	K928	R929	K930	G931	E932
G933	F934	D937	K938	R939	E940	V941	E942	V943	L944	R945	R946	A947	E948	K949	V953	K957	T958	E959	E960	E961	Q962	L963	K964	E965	L966	F967	L968	Q969	G970	K971	L974	D975	G976	G977	R978	T979	G980	E981	V982	V983	G984	L985	L986	L987	L988	L989	L990	L991	F992	F993	K994	L995	L996	L997	H998	L999		
H1000	V1001	D1002	M1003	M1004	H1005	H1006	A1007	L1008	S1009	T1010	G1011	Y1012	S1014	L1015	T1016	T1017	Q1018	Q1019	P1020	G1021	G1022	G1023	Q1026	F1027	G1028	G1029	G1030	L1031	F1032	G1033	M1034	M1035	L1036	V1037	W1038	A1039	L1040	E1041	A1042	A1043	A1044	A1045	A1046	H1047	T1048	L1049	P1050	L1051	M1052	L1053	L1054	L1055	M1056	F1057	D1058	I1059	I1060	E1061
G1062	R1063	M1064	A1065	A1066	Y1067	E1068	A1069	I1070	I1071	K1072	L1073	D1074	V1075	P1076	P1077	E1078	S1079	S1080	V1081	P1082	E1083	S1084	F1085	R1086	V1087	L1088	V1089	K1090	E1091	L1092	Q1093	A1094	L1095	A1096	L1097	D1098	V1099	Q1100	T1101	L1102	D1103	E1104	K1105	D1106	M1107	P1108	V1109	D1110	F1111	F1112	E1113	G1114	L1115	A1116	S1117	K1118	R1119	

● Molecule 3: BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N

Chain D: 15% 69% 14%

MET	K2	K3	K4	R5	R6	K7	V8	R9	I10	A11	L12	A13	S14	P15	E16	K17	I18	R19	S20	W21	E22	Y23	Y24	E25	G26	E27	K28	P29	E30	T31	I32	N33	Y34	R35	T36	L37	K38	P39	E40	R41	D42	C43	L44	F45	D46	E47	R48	P49	I49	F50	G51	I53	K54	D55	Y56	E57	C58	A59	C60	
G61	K62	Y63	E64	R65	Q66	R67	F68	E69	G70	K71	V72	C73	E74	R75	C76	G77	V78	E79	S20	T81	K82	S83	I84	V85	R86	R87	Y88	R89	M90	G91	H92	I93	E94	L95	A96	T97	P98	A99	A100	H101	I102	W103	F104	V106	K106	D107	T108	R108	P109	S110	K111	I112	G113	T114	L115	D116	D117	L118	S119	A120
T121	E122	L123	E124	R125	V126	L127	Y128	F129	S130	K131	L132	I133	V134	L135	D136	C137	G138	E139	T81	Y205	R206	F207	I84	V145	P146	V147	E148	K149	R150	Q151	L152	I93	T154	D155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	V169	P170	L171	P172	G173	V175	L176	A177	L178	D181	G182		
E183	E184	V185	L186	K187	G188	Q189	E190	L191	A192	P193	G194	V195	R198	L199	D200	A203	R204	Y205	R206	F207	N143	G144	V145	P146	V147	E148	K149	R150	Q151	L152	I93	T154	D155	E156	E157	Y158	R159	E160	L161	R162	Y163	G164	K165	Q166	E167	T168	V169	P170	L171	P172	G173	V175	L176	A177	L178	D181	G182			
E247	P248	Y249	L250	F251	R252	A253	E254	E255	G256	G257	L258	V259	E260	L261	K262	E263	E264	F265	G266	A268	F269	V270	L271	V272	L273	R274	Y281	Y282	F283	R284	A221	G222	V286	R287	M288	L289	P290	L291	V292	V293	H294	G295	E296	L297	V298	E299	K300	G301	Q302	P303	L304	A305	E306	A307						
K308	G309	L310	L311	R312	K313	P314	R315	Q316	V317	R318	A319	V322	E323	A324	E325	E326	P327	T330	V331	E332	F333	L334	L335	E336	L337	E338	F401	F402	F403	W340	E341	P342	K343	D344	Y345	R346	V347	Q348	P349	H350	K351	N352	V353	V354	V355	P356	E357	G358	A359	V361	K366	K367	L368	L369	A370					
L371	D372	P373	E374	E375	E376	V377	L378	A379	E380	V384	V385	H386	L387	H388	S449	E450	P390	A391	S392	L393	L394	V395	M456	C457	A458	A398	R399	V400	Q401	P402	F403	E404	D406	V407	E408	Y409	S410	T411	G412	D413	R414	V415	A416	F417	G418	L421	M481	K482	H483	P484	S485	R486	R487	A488	R489	A490	V431	Y432	A493	G433
R434	V435	E436	V437	D438	L439	V440	R441	R442	V443	V444	R445	V446	V447	E448	S449	D451	L452	D453	A454	R455	M456	C457	A458	E459	A460	L461	Q462	Q463	Q464	L465	L466	E467	L468	D469	L470	E471	A472	L473	L474	E475	E476	L477	L478	E479	E480	M481	K482	H483	P484	S485	R486	R487	A488	R489	A490	V431	Y432	A493	G433	
K494	R495	L496	E497	V498	V499	R500	R501	F502	L503	P504	S505	G506	N507	R508	P509	E510	K511	N512	L513	L514	E515	A516	V517	P518	V519	L520	P521	P522	D523	L524	R525	P526	N527	V528	Q529	L530	F531	F532	A533	V534	F535	R536	A537	S538	D539	L540	N541	D542	L543	V544	R545	R546	L547	A548	N549	R550	N551	L552	A553	R554
L554	K555	L556	L557	L558	A559	O560	G561	A562	P563	E564	L565	L566	L567	R568	N569	K570	E571	K572	L573	L574	E575	E576	A577	V578	D579	A580	L581	L582	G583	L584	P585	N586	R587	P590	L591	S592	L593	R594	S595	S596	D597	R598	P599	L600	L601	S602	L603	T604	D605	L606	L607	R608	G609	L610	K611	G612	R613	A673	F614	
R615	Q616	N617	L618	L619	G620	K621	R622	G623	D624	G625	L626	G627	R628	S629	V630	I631	V632	K633	G634	P635	Q636	L637	K638	L639	H640	Q641	C642	G643	G644	L645	P646	K647	R648	L649	L650	E651	L652	F653	K654	G655	S656	L657	D658	R659	L660	L661	S662	L663	T664	D665	L666	A667	P668	N669	V670	K671	A672	R673	F674	

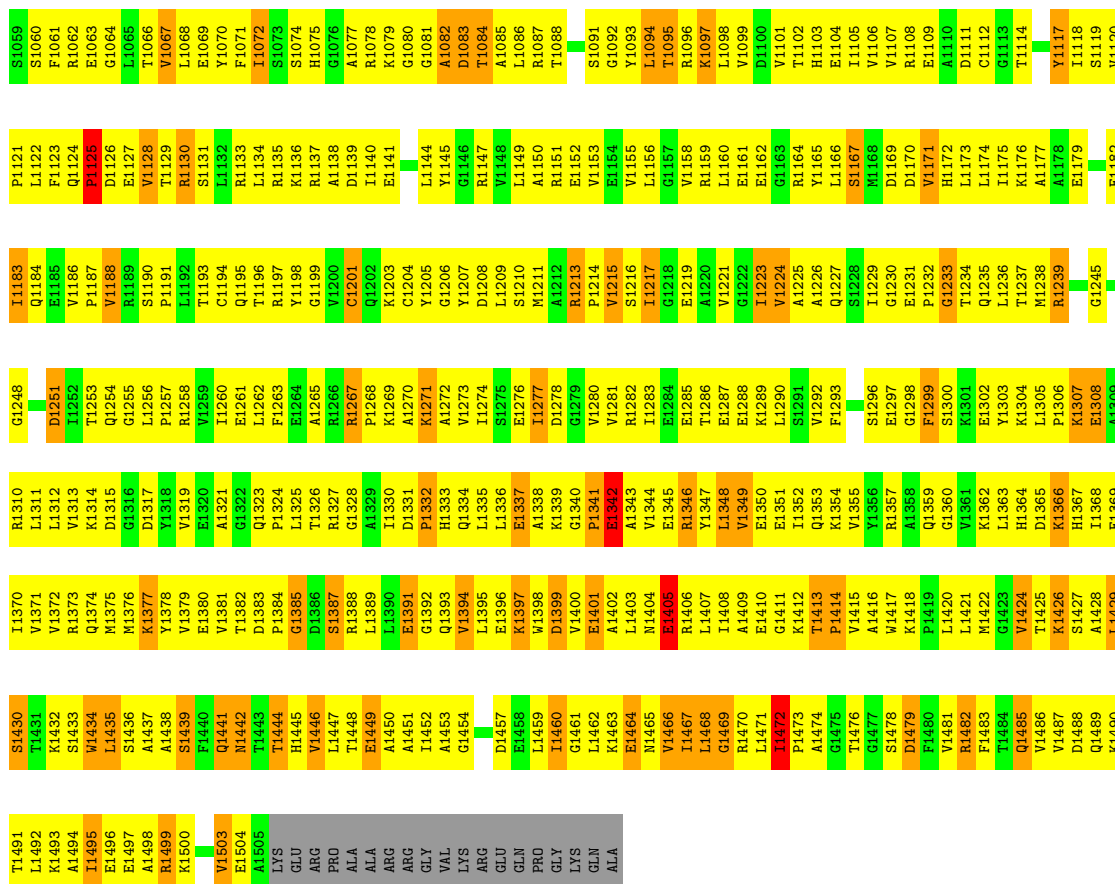
A1484	V1372	L1236	L1173	T1114	P1048	E987	F919	D859	K799	M737	R675
I1495	R1373	T1237	L1174	T1115	S1049	R988	L920	L860	K800	A738	M676
E1496	Q1374	R1238	I1175	N1116	G1050	R989	R921	Q861	G801	D739	L677
A1497	M1375	R1239	K1176	N1117	E1051	D990	L922	D862	A802	F740	E678
R1498	K1376	V1313	A1177	I1118	F1052	Q991	G923	V863	G803	D741	R679
R1499	M1377	G1245	A1178	I1119	T1053	I992	M924	H864	L804	G742	Q680
K1500	Y1378	V1246	E1179	S1119	E1054	L993	E925	T865	E805	D743	R681
E1501	V1379	A1249	A1180	V1120	V1055	Q994	K926	V866	F806	Q744	D682
A1502	Q1380	I1252	E1182	L1122	P1056	L995	T927	H868	A807	M745	L683
E1503	V1381	L1263	I1183	F1123	V1057	W996	A928	T808	T808	A746	K684
A1504	T1382	Q1264	Q1184	L1124	R1058	R997	R909	V747	V747	V747	D685
A1505	D1383	G1265	E1185	Q1124	S1059	E998	L930	E810	E810	H748	E686
LVS	P1384	G1285	V1186	D1126	S1060	T999	L931	H871	H749	H749	V687
GLU	P1385	L1266	P1187	E1127	F1061	T1000	D932	R872	F750	F750	M688
ARG	T1325	L1267	V1188	V1128	R1062	E1001	A933	L873	L751	L751	D689
PRO	T1326	P1257	V1189	E1129	L1066	K1002	L934	K874	A814	S752	A690
ALA	R1327	P1258	R1190	R1130	T1066	V1003	K935	T875	A815	S753	L691
ALA	L1390	V1259	S1190	R1131	V1067	A1006	Y936	S876	H816	F754	E692
ARG	L1391	I1260	P1191	S1131	V1068	Y1007	Y937	R877	E817	A755	E693
ARG	G1392	E1261	L1192	R1132	L1068	F1008	G938	R878	R818	Q756	V694
GLY	Q1393	L1262	T1193	R1133	E1069	F1009	F939	R879	G819	A757	L695
VAL	V1394	F1263	L1194	L1134	Y1070	K1009	T940	E880	E820	E758	H696
LVS	L1395	E1264	Q1195	R1135	F1071	M1010	F941	L881	V821	A759	G697
ARG	L1396	K1269	T1196	K1136	S1072	F1011	S942	F882	K822	R760	K698
GLU	K1397	A1270	R1197	R1137	I1073	E1012	T943	A883	L823	I761	V699
GLN	M1398	I1274	Y1198	A1138	S1074	E1013	T944	R884	N824	V769	V700
PRO	D1399	I1275	G1199	D1139	H1075	N1014	S945	I885	A825	L764	L701
ALA	V1400	I1276	K1203	I1140	G1076	N1015	G946	R886	G826	S765	L702
GLM	E1401	T1277	L1204	A1142	A1077	F1016	I947	A887	I827	A766	N703
GLM	A1402	I1278	C1204	A1143	R1078	F1017	T948	E888	R767	H767	R704
GLM	L1403	D1279	G1143	G1143	K1079	N1018	I949	A889	V829	N768	A705
ALA	M1404	G1279	G1206	G1144	G1080	P1019	Q950	V890	A830	L770	P706
E1405	E1405	V1280	I1207	L1145	G1081	L1020	I951	E891	G831	L771	T707
R1406	R1406	R1281	D1208	Y1146	A1082	Y1021	D952	D892	R832	S771	L708
L1407	L1407	I1282	L1209	R1147	D1083	D1022	D953	E893	E833	P772	H709
I1408	I1408	I1283	S1210	V1148	T1084	M1023	A954	K894	T834	A773	R710
A1409	A1409	E1284	M1211	L1149	A1085	A1024	V955	V895	S835	S774	L711
E1410	E1410	E1285	A1212	A1150	L1086	Q1025	I956	A896	V836	G775	G712
G1411	G1411	T1286	R1213	R1151	R1087	S1026	P957	W897	G837	E776	I713
K1412	K1412	E1287	P1214	E1152	T1088	G1027	E958	E898	R838	P777	Q714
T1413	T1413	E1288	V1215	V1153	A1089	A1029	E959	L899	L839	L778	A715
G1414	P1414	K1289	S1216	E1154	D1090	R1029	K960	I900	K840	A779	F716
V1415	V1415	L1290	I1217	V1155	S1091	G1030	K961	Q901	Y841	K760	Q717
A1416	A1416	S1291	G1218	L1156	I1092	M1031	Q962	L902	R842	P781	L720
W1417	W1417	V1292	E1219	G1157	Y1093	P1032	Y963	D903	F843	S782	V721
D1479	K1418	F1293	E1220	V1158	L1094	Q1033	L964	P904	R844	R783	P730
F1480	P1419	V1294	V1221	R1159	T1095	Q1034	E965	P905	N845	D784	G721
V1481	L1420	E1295	G1222	L1160	R1096	I1035	E966	Q906	R846	I785	Q724
R1482	L1421	S1296	I1223	E1161	K1097	R1036	A967	E907	D847	I786	S725
F1483	M1422	E1297	E1162	V1162	L1098	Q1037	D968	K908	E848	L787	I726
T1484	G1423	G1298	G1163	V1099	V1099	L1038	R969	N909	A849	G788	Q727
Q1485	V1424	F1299	Q1227	D1100	D1100	C1039	K970	S910	L850	L728	L728
V1486	T1425	S1300	I1228	V1101	V1101	G1040	L971	L911	L851	Y791	H729
V1487	K1426	K1301	N1229	L1166	T1102	L1041	L972	K912	A852	I792	P730
D1488	A1427	K1366	S1167	H1103	H1103	R1042	Q973	D913	R853	T793	L731
O1489	A1428	H1367	M1168	E1104	E1104	G1043	L983	L914	A854	Q794	V732
K1490	L1429	K1304	D1169	I1105	I1105	L1044	L984	V915	H855	V795	C733
T1491	S1430	L1305	D1170	V1106	V1106	Q1045	P984	Y916	G856	R796	E734
L1492	P1306	P1306	T1234	I1171	I1171	Q1046	D985	Q1047	Q157	K797	A735
K1493	K1307	K1307	H1172	R1108	R1108	K1047	R986	A918	V858	E798	F736

• Molecule 3: BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N

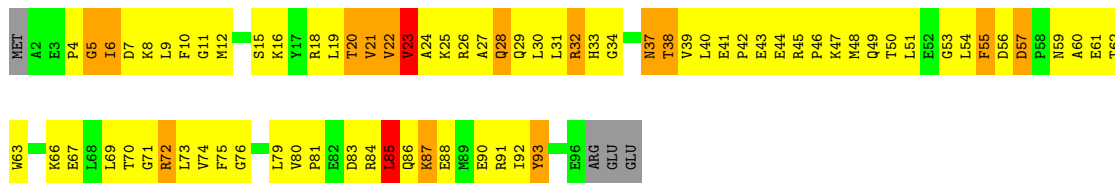
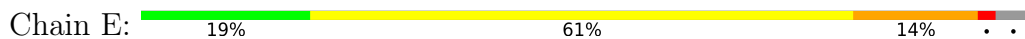


ME1	Y56	C58	C60	G61	G62	Y63
K2	E57	C58	C60	G61	G62	Y63
K3	E57	C58	C60	G61	G62	Y63
E4	E57	C58	C60	G61	G62	Y63
V5	E57	C58	C60	G61	G62	Y63
R6	E57	C58	C60	G61	G62	Y63
R6	E57	C58	C60	G61	G62	Y63
K7	E57	C58	C60	G61	G62	Y63
V8	E57	C58	C60	G61	G62	Y63
R9	E57	C58	C60	G61	G62	Y63
I10	E57	C58	C60	G61	G62	Y63
A13	E57	C58	C60	G61	G62	Y63
S14	E57	C58	C60	G61	G62	Y63
P15	E57	C58	C60	G61	G62	Y63
E16	E57	C58	C60	G61	G62	Y63
ARG	E57	C58	C60	G61	G62	Y63
PRO	E57	C58	C60	G61	G62	Y63
ALA	E57	C58	C60	G61	G62	Y63
ALA	E57	C58	C60	G61	G62	Y63
ALA	E57	C58	C60	G61	G62	Y63
ARG	E57	C58	C60	G61	G62	Y63
ARG	E57	C58	C60	G61	G62	Y63
GLY	E57	C58	C60	G61	G62	Y63
VAL	E57	C58	C60	G61	G62	Y63
LVS	E57	C58	C60	G61	G62	Y63
ARG	E57	C58	C60	G61	G62	Y63
GLU	E57	C58	C60	G61	G62	Y63
GLN	E57	C58	C60	G61	G62	Y63
PRO	E57	C58	C60	G61	G62	Y63
GLY	E57	C58	C60	G61	G62	Y63
T31	E57	C58	C60	G61	G62	Y63
T32	E57	C58	C60	G61	G62	Y63
T33	E57	C58	C60	G61	G62	Y63
N33	E57	C58	C60	G61	G62	Y63
Y34	E57	C58	C60	G61	G62	Y63
R35	E57	C58	C60	G61	G62	Y63
R36	E57	C58	C60	G61	G62	Y63
L37	E57	C58	C60	G61	G62	Y63
K38	E57	C58	C60	G61	G62	Y63
P39	E57	C58	C60	G61	G62	Y63
E40	E57	C58	C60	G61	G62	Y63
R41	E57	C58	C60	G61	G62	Y63
D42	E57	C58	C60	G61	G62	Y63
G43	E57	C58	C60	G61	G62	Y63
L44	E57	C58	C60	G61	G62	Y63
F45	E57	C58	C60	G61	G62	Y63
D46	E57	C58	C60	G61	G62	Y63
E47	E57	C58	C60	G61	G62	Y63
R48	E57	C58	C60	G61	G62	Y63
T49	E57	C58	C60	G61	G62	Y63
F50	E57	C58	C60	G61	G62	Y63
G51	E57	C58	C60	G61	G62	Y63
P52	E57	C58	C60	G61	G62	Y63
I53	E57	C58	C60	G61	G62	Y63
Y56	E57	C58	C60	G61	G62	Y63
E57	E57	C58	C60	G61	G62	Y63
C58	E57	C58	C60	G61	G62	Y63
A59	E57	C58	C60	G61	G62	Y63
C60	E57	C58	C60	G61	G62	Y63
G61	E57	C58	C60	G61	G62	Y63
G62	E57	C58	C60	G61	G62	Y63
L1492	E57	C58	C60	G61	G62	Y63
K1493	E57	C58	C60	G61	G62	Y63

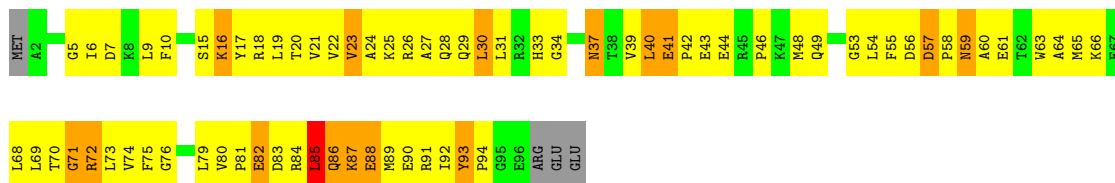
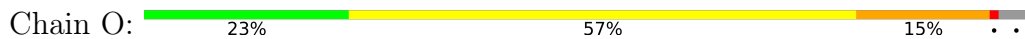
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E998	T999	L931	K871	P809	V747	E678	M617	K556	L496	E436	L371	L310	Y249	K187	K65
T1000	A933	D932	K872	E810	H748	Q679	L618	L557	E497	V437	D372	R312	L250	G188	Q66
E1001	L934	A933	K873	E811	V749	Q680	L619	L558	V498	D438	F251	R313	F251	Q189	Y128
K1002	K935	K935	K874	L813	P750	L751	R622	A559	V499	L439	E374	K314	R252	E190	E69
V1003	Y836	Y836	K875	L814	L751	L751	R623	Q560	R500	V440	E375	P314	A253	L191	G70
T1004	Y937	Y937	D865	A815	F754	D865	V623	G561	A501	R441	E376	R315	E254	A192	K71
Q1005	G938	G938	D866	H816	A755	D866	D624	A562	F802	M442	V377	Q316	E255	V195	V72
A1006	F939	F939	E886	H817	A756	E886	Y625	P563	L503	V443	L378	V317	E256	I133	C73
V1007	T940	T940	V687	E818	Q756	V687	S626	E564	S504	V444	A379	R318	G257	V196	E74
F1008	F941	F941	A690	G819	Q757	A690	R628	I566	S505	R445	V258	A319	V258	S197	R75
K1009	S942	S942	L691	E820	A759	L691	S629	I567	G506	V446	A381	A320	E260	P136	C76
V1010	T943	T943	E892	V821	R760	E892	V630	R568	R508	V447	V447	Q321	E261	P137	G77
F1011	T944	T944	E893	A822	I761	E893	L631	N569	P909	S449	V385	V322	L261	D200	V78
M1018	L823	L823	V694	E830	Q762	V694	V632	E570	E510	V450	L387	E323	K262	G201	E79
E1012	S945	S945	I695	N824	M763	I695	G633	K571	P518	D451	L387	E324	E263	V202	V80
E1013	G946	G946	G634	A825	L764	G634	H640	K572	M512	W511	H388	E325	L264	A140	V81
N1014	T948	T948	G697	E826	S765	G697	P635	M573	L513	A458	E389	E326	E265	A203	T82
Y1015	I949	I949	K698	L827	A766	K698	Q636	L574	L514	A454	P390	E327	E266	Y205	K82
P1016	G950	G950	K699	I827	H767	K699	Q636	L574	L515	A454	A391	G328	G267	R206	S83
F1017	V890	V890	L637	V899	H767	V899	L637	Q575	E515	R455	S392	G329	G267	R207	I84
M1018	E829	E829	K638	V700	A516	K638	G638	E576	M456	M456	S393	T330	F269	P208	V85
P1019	A830	A830	L701	L701	L769	L701	L639	A577	V517	G457	L394	V331	F289	R208	R86
D952	G831	G831	L702	N703	L770	L702	H640	A578	P518	A458	L394	Y332	L270	R209	R87
D953	E892	E892	N703	N703	L770	N703	H641	D579	V519	A459	V396	L333	V271	R210	Y88
A954	F772	F772	R704	R704	P772	R704	C642	A580	L520	A460	V396	L333	L272	V211	R89
V955	K884	K884	R704	R704	P772	R704	C642	A580	L520	A460	K397	T334	R273	R212	M90
I956	B995	B995	A649	A649	A773	A649	G643	L581	P521	L461	A399	L335	R274	R213	G91
S957	A896	A896	H709	H709	G775	H709	L644	L582	E528	Q462	R399	F336	E275	V213	H92
E958	G837	G837	R710	R710	G775	R710	P645	D583	S523	Q463	V400	L337	D276	Y215	I93
S1026	E898	E898	L711	L711	G775	L711	K646	N584	L524	L464	Y401	E338	E277	V216	E94
G1027	L899	L899	G712	G712	A779	G712	R647	G585	R525	L465	F402	A339	P278	K217	I95
K961	I900	I900	I713	I713	A779	I713	M648	R586	P526	K466	F403	T340	V279	K218	A96
Q962	K901	K901	Q714	Q714	K780	Q714	A649	R587	M527	E467	E404	E341	A280	E219	T97
L963	L902	L902	A715	A715	L781	A715	L650	P590	V528	L468	D405	P342	T281	E219	P98
L964	G903	G903	F716	F716	S782	F716	L652	E651	Q529	D469	D406	K343	Y282	R220	A99
E965	V904	V904	Q717	Q717	R783	Q717	L652	V591	V530	L470	V407	F283	F283	A221	A99
E966	P905	P905	L720	L720	D784	L720	F653	T592	D531	E471	E408	R346	G222	L223	H101
A967	Q906	Q906	L785	L785	I785	L785	K654	N593	G532	A472	V409	V347	R224	L102	H101
D968	E907	E907	P655	P655	I786	P655	P655	P894	G533	L473	S410	Q348	V285	L102	H102
R969	K908	K908	Q724	Q724	L787	Q724	F656	G595	R534	E474	T411	P349	V286	L225	W103
K970	N909	N909	S725	S725	G788	S725	L657	S596	F535	K475	G412	H350	G287	P226	F104
L1038	S910	S910	I726	I726	L789	I726	L658	D597	A536	E476	D413	K351	L227	L227	F105
L972	L911	L911	Q727	Q727	Y790	Q727	K659	R598	T537	L477	R414	K352	T289	A228	K106
Q973	K912	K912	L728	L728	Y791	L728	K660	P599	S538	L478	V415	V353	P290	A229	D107
I974	V915	V915	H729	H729	I792	H729	M661	L800	D539	E479	A416	V354	L281	W230	V108
L983	Y916	Y916	P730	P730	T793	P730	E662	R601	L540	E480	P417	V355	V292	V230	P109
T984	Q917	Q917	L731	L731	Q794	L731	E663	S602	N541	R481	G418	P356	H294	K233	S110
D885	A918	A918	C733	C733	V795	C733	K664	L603	D542	K482	D419	E357	G295	A235	K111
R886	F919	F919	I666	I666	K797	I666	G665	T604	L543	H483	V420	G358	E296	Y236	G113
E887	L820	L820	A667	A667	E798	A667	P667	D605	Y544	P484	L421	A359	L297	K237	T114
R888	R921	R921	P668	P668	E799	P668	P668	L606	R645	S488	A422	K360	V298	D176	L115
Y889	G922	G922	F736	F736	K900	F736	N669	L607	R546	R486	D423	V361	E299	G239	L116
E1051	G923	G923	N737	N737	K900	N737	N669	S608	L547	A487	K428	E362	E299	E240	D117
T1052	M924	M924	A738	A738	G801	A738	V670	G609	L548	R488	K300	A363	K300	E240	D117
F1053	E925	E925	F739	F739	A802	F739	K671	K610	N549	R489	S429	G364	G302	L242	S119
L993	K926	K926	F740	F740	G803	F740	A673	G612	N551	A490	D430	D365	P303	A243	K180
Q994	T927	T927	D743	D743	L804	D743	R674	G812	N551	K491	V431	K366	E306	E244	T121
L995	A928	A928	F806	F806	E805	F806	R675	R613	N552	A492	V432	L367	E306	L245	D181
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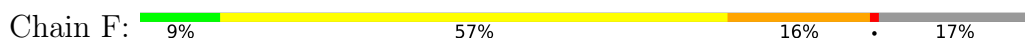
● Molecule 4: BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O



● Molecule 4: BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O



● Molecule 5: RNA polymerase principal sigma factor (RpoD); CHAIN F, P







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.09Å 235.09Å 250.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.00 46.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-3.00) 96.0 (46.80-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.289 0.221 , 0.274	Depositor DCC
$R_{free}$ test set	2351 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.8	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.499 for -h,-k,l 0.047 for h,-h-k,-l 0.047 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	56149	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: MPD, PO4, ZN, MG, NE6

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	0.43	0/1848	0.73	0/2512
1	B	0.39	0/1936	0.68	0/2633
1	K	0.43	0/1848	0.72	1/2512 (0.0%)
1	L	0.41	0/1936	0.70	0/2633
2	C	0.43	0/8997	0.73	8/12164 (0.1%)
2	M	0.43	0/8997	0.73	3/12164 (0.0%)
3	D	0.44	0/12073	0.77	11/16324 (0.1%)
3	N	0.46	2/12073 (0.0%)	0.76	9/16324 (0.1%)
4	E	0.40	0/783	0.69	0/1054
4	O	0.41	0/783	0.65	0/1054
5	F	0.40	0/2874	0.72	1/3866 (0.0%)
5	P	0.40	0/2874	0.69	1/3866 (0.0%)
All	All	0.43	2/57022 (0.0%)	0.74	34/77106 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	N	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	58	CYS	CB-SG	-5.87	1.72	1.81
3	N	60	CYS	CB-SG	-5.42	1.73	1.81

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	831	GLY	N-CA-C	-12.95	80.74	113.10
3	N	831	GLY	N-CA-C	-11.03	85.51	113.10
2	C	177	GLU	N-CA-C	-8.93	86.88	111.00
5	F	313	GLU	N-CA-C	8.15	133.01	111.00
2	M	58	ASP	N-CA-C	-8.08	89.18	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	N	1117	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	1816	0	1871	279	0
1	B	1902	0	1951	321	0
1	K	1816	0	1871	296	0
1	L	1902	0	1951	318	0
2	C	8829	0	8933	1694	0
2	M	8829	0	8933	1598	0
3	D	11864	0	12094	2489	0
3	N	11864	0	12094	2441	0
4	E	769	0	775	163	0
4	O	769	0	775	123	0
5	F	2829	0	2914	587	0
5	P	2829	0	2914	671	0
6	A	5	0	0	0	0
6	D	5	0	0	1	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	N	1	0	0	0	0
8	C	16	0	26	0	0
8	M	8	0	13	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	30	0	30	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	N	30	0	30	7	0
11	A	1	0	0	1	0
11	B	1	0	0	1	0
11	C	7	0	0	2	0
11	D	10	0	0	0	0
11	F	1	0	0	1	0
11	M	5	0	0	1	0
11	N	4	0	0	0	0
11	O	1	0	0	0	0
All	All	56149	0	57175	10419	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 92.

The worst 5 of 10419 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:283:ILE:HG22	2:M:284:ARG:H	1.03	1.17
3:D:416:ALA:HB2	3:D:432:TYR:HA	1.19	1.17
3:D:1489:GLN:HA	3:D:1492:LEU:HG	1.23	1.17
3:N:272:LEU:HD12	3:N:280:ALA:HB3	1.23	1.16
1:A:14:ARG:HB2	1:B:233:VAL:HA	1.27	1.16

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	229/315 (73%)	160 (70%)	54 (24%)	15 (7%)	<b>1</b> <b>6</b>
1	B	241/315 (76%)	159 (66%)	64 (27%)	18 (8%)	<b>1</b> <b>5</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	229/315 (73%)	168 (73%)	50 (22%)	11 (5%)	2	13
1	L	241/315 (76%)	171 (71%)	55 (23%)	15 (6%)	1	8
2	C	1117/1119 (100%)	774 (69%)	251 (22%)	92 (8%)	1	4
2	M	1117/1119 (100%)	767 (69%)	246 (22%)	104 (9%)	0	3
3	D	1502/1524 (99%)	931 (62%)	422 (28%)	149 (10%)	0	2
3	N	1502/1524 (99%)	907 (60%)	445 (30%)	150 (10%)	0	2
4	E	93/99 (94%)	54 (58%)	25 (27%)	14 (15%)	0	1
4	O	93/99 (94%)	56 (60%)	27 (29%)	10 (11%)	0	2
5	F	347/423 (82%)	167 (48%)	130 (38%)	50 (14%)	0	1
5	P	347/423 (82%)	171 (49%)	117 (34%)	59 (17%)	0	0
All	All	7058/7590 (93%)	4485 (64%)	1886 (27%)	687 (10%)	0	2

5 of 687 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	112	ARG
1	A	155	LYS
1	B	75	VAL
1	B	118	ALA

### 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%)	192 (95%)	10 (5%)	24	60
1	B	210/273 (77%)	193 (92%)	17 (8%)	11	40
1	K	202/273 (74%)	190 (94%)	12 (6%)	19	54
1	L	210/273 (77%)	196 (93%)	14 (7%)	16	49
2	C	941/941 (100%)	863 (92%)	78 (8%)	11	39
2	M	941/941 (100%)	859 (91%)	82 (9%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1264/1279 (99%)	1152 (91%)	112 (9%)	9	35
3	N	1264/1279 (99%)	1141 (90%)	123 (10%)	8	31
4	E	83/87 (95%)	76 (92%)	7 (8%)	11	38
4	O	83/87 (95%)	74 (89%)	9 (11%)	6	26
5	F	304/371 (82%)	274 (90%)	30 (10%)	8	30
5	P	304/371 (82%)	266 (88%)	38 (12%)	4	20
All	All	6008/6448 (93%)	5476 (91%)	532 (9%)	9	35

5 of 532 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	1299	PHE
3	N	1442	ASN
3	N	1285	GLU
5	P	355	GLU
3	D	1217	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	729	HIS
3	N	973	GLN
5	P	186	HIS
3	D	744	GLN
3	D	729	HIS

### 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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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
8	MPD	C	1120	-	7,7,7	2.22	1 (14%)	9,10,10	1.16	0
8	MPD	C	1121	-	7,7,7	2.24	1 (14%)	9,10,10	1.11	0
10	NE6	N	1528	-	29,30,30	3.64	7 (24%)	27,39,39	1.81	4 (14%)
8	MPD	M	1120	-	7,7,7	2.12	1 (14%)	9,10,10	1.09	0
6	PO4	D	1528	-	4,4,4	1.63	0	6,6,6	0.44	0
6	PO4	A	316	-	4,4,4	1.57	0	6,6,6	0.44	0
10	NE6	D	1529	-	29,30,30	3.60	7 (24%)	27,39,39	1.77	4 (14%)

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
8	MPD	C	1120	-	-	5/5/5/5	-
8	MPD	C	1121	-	-	0/5/5/5	-
10	NE6	N	1528	-	1/1/9/13	11/26/46/46	0/1/1/1
8	MPD	M	1120	-	-	2/5/5/5	-
10	NE6	D	1529	-	1/1/9/13	9/26/46/46	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	1528	NE6	C11-C12	-14.72	1.35	1.49
10	D	1529	NE6	C11-C12	-14.09	1.35	1.49
10	D	1529	NE6	O4-C4	10.74	1.38	1.22
10	N	1528	NE6	O4-C4	10.57	1.38	1.22
8	C	1121	MPD	O2-C2	-5.47	1.30	1.44



The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	1528	NE6	O14-C13-N12	4.67	114.87	108.77
10	D	1529	NE6	O14-C13-N12	4.36	114.46	108.77
10	D	1529	NE6	O1-C2-O2	4.30	121.05	116.94
10	N	1528	NE6	O1-C2-O2	4.18	120.94	116.94
10	D	1529	NE6	O4-C4-C5	-3.84	114.87	121.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	D	1529	NE6	C3
10	N	1528	NE6	C3

5 of 27 torsion outliers are listed below:

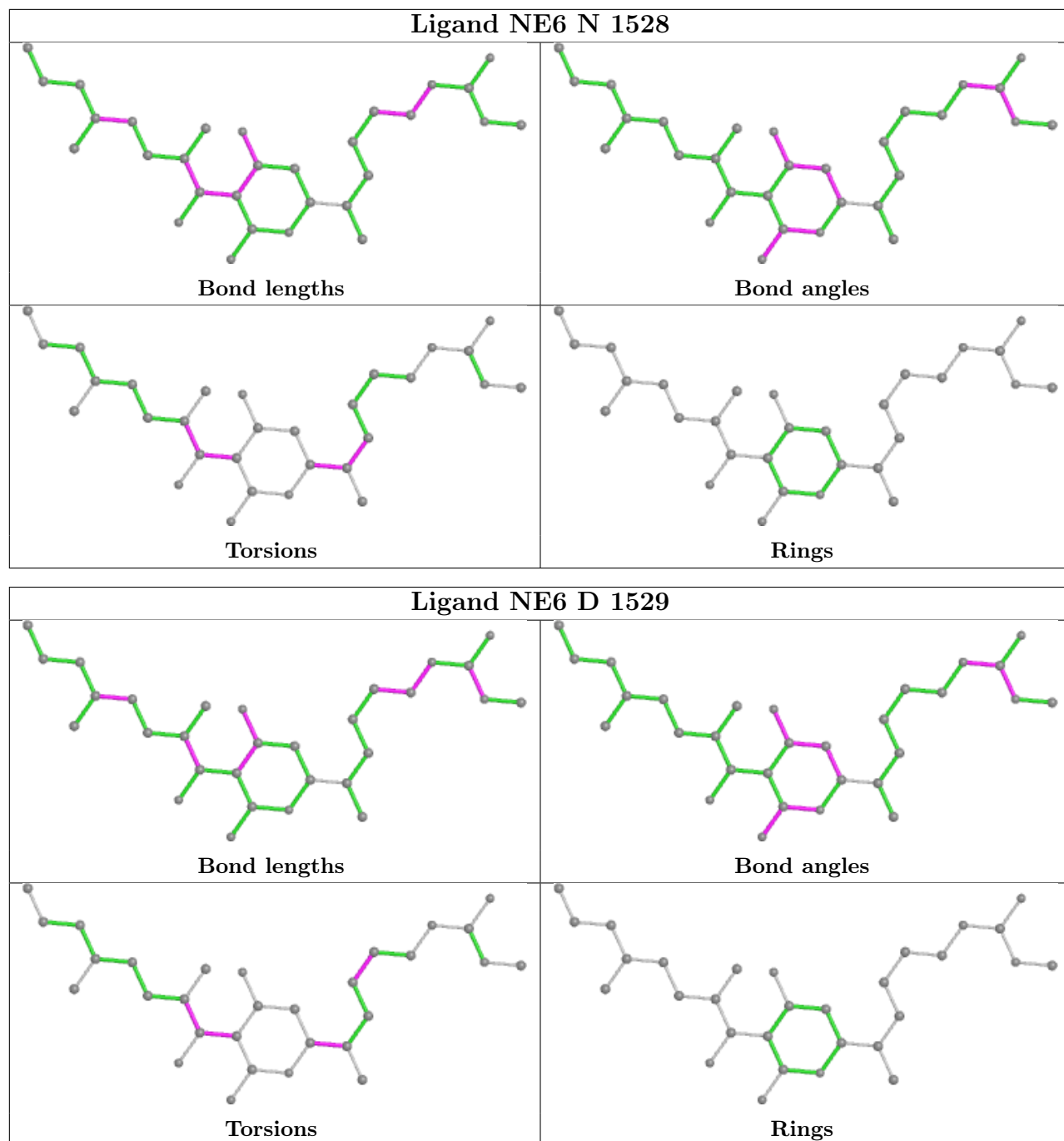
Mol	Chain	Res	Type	Atoms
8	C	1120	MPD	C1-C2-C3-C4
8	C	1120	MPD	O2-C2-C3-C4
10	D	1529	NE6	O15-C15-C3-C2
10	D	1529	NE6	O1-C6-C7-C8
10	D	1529	NE6	O1-C6-C7-C9

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	1528	NE6	7	0
6	D	1528	PO4	1	0
10	D	1529	NE6	8	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, 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	231/315 (73%)	-0.66	0 100 100	43, 72, 100, 115	0
1	B	243/315 (77%)	-0.82	0 100 100	51, 93, 113, 117	0
1	K	231/315 (73%)	-0.68	0 100 100	45, 73, 105, 117	0
1	L	243/315 (77%)	-0.81	0 100 100	56, 89, 112, 117	0
2	C	1119/1119 (100%)	-0.73	0 100 100	36, 77, 115, 117	0
2	M	1119/1119 (100%)	-0.72	0 100 100	31, 79, 115, 117	0
3	D	1504/1524 (98%)	-0.70	1 (0%) 95 89	35, 78, 117, 117	0
3	N	1504/1524 (98%)	-0.68	3 (0%) 95 87	34, 75, 113, 117	0
4	E	95/99 (95%)	-0.81	0 100 100	51, 88, 113, 117	0
4	O	95/99 (95%)	-0.78	0 100 100	52, 85, 109, 116	0
5	F	349/423 (82%)	-0.85	0 100 100	52, 84, 110, 117	0
5	P	349/423 (82%)	-0.81	0 100 100	51, 85, 110, 117	0
All	All	7082/7590 (93%)	-0.72	4 (0%) 95 89	31, 79, 115, 117	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	243	ALA	4.1
3	N	242	LEU	3.2
3	N	328	GLY	3.0
3	D	329	GLU	2.1

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

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

### 6.3 Carbohydrates [i](#)

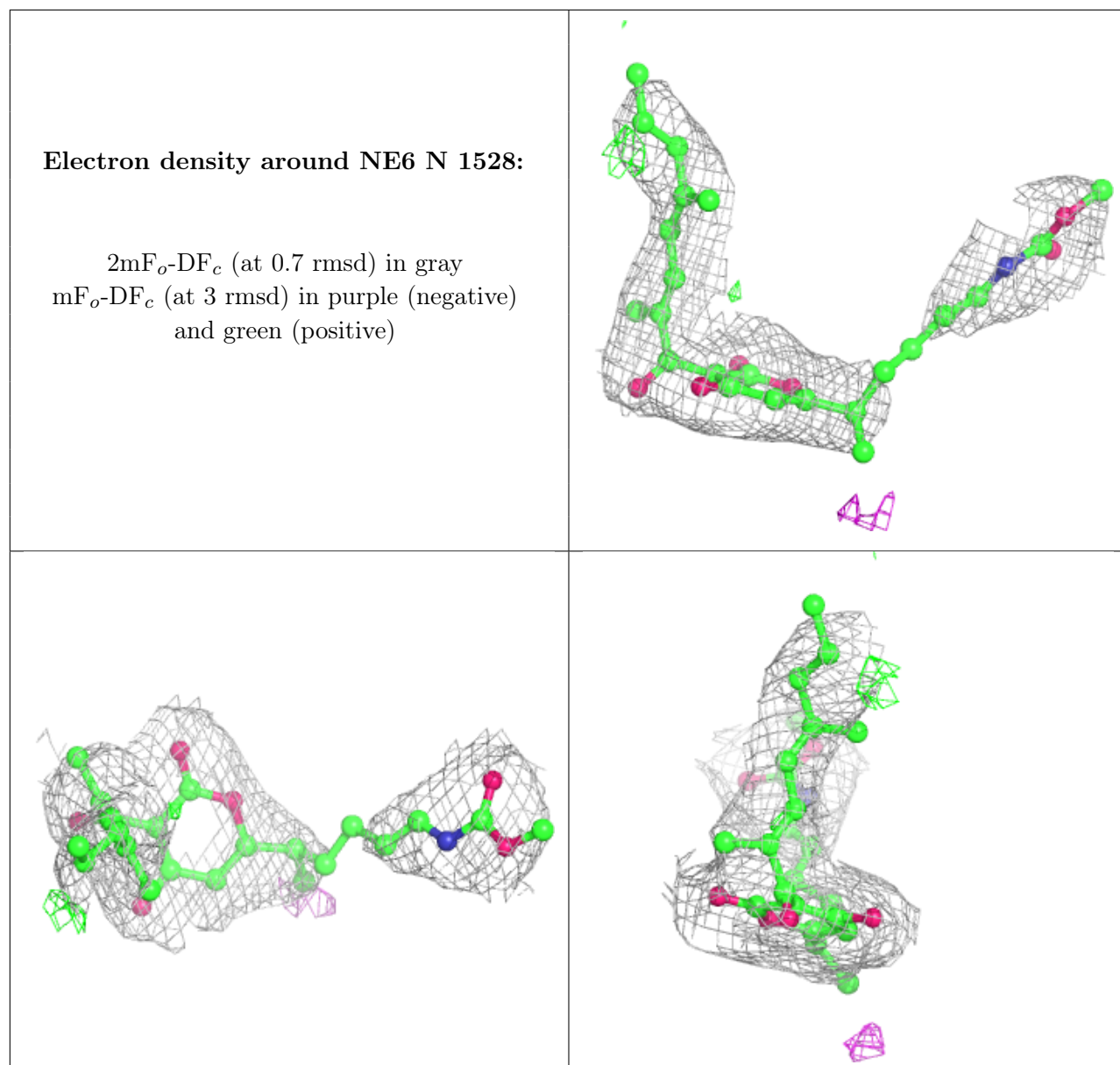
There are no monosaccharides in this entry.

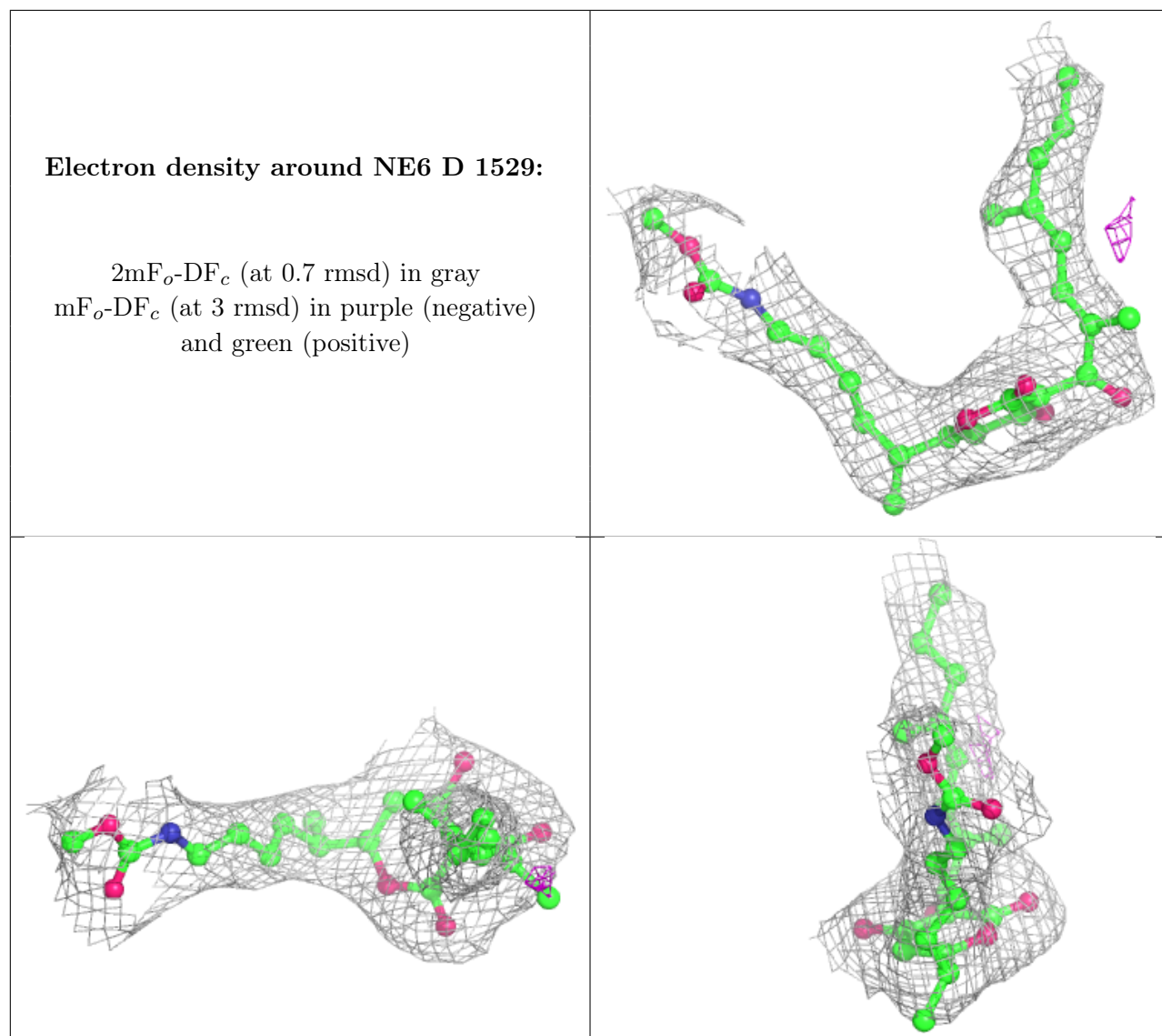
### 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
8	MPD	M	1120	8/8	0.92	0.17	71,79,84,85	0
10	NE6	N	1528	30/30	0.94	0.29	72,84,90,91	0
7	MG	D	1527	1/1	0.96	0.07	79,79,79,79	0
8	MPD	C	1121	8/8	0.96	0.15	70,72,73,73	0
6	PO4	A	316	5/5	0.96	0.18	71,73,77,77	0
9	ZN	D	1525	1/1	0.96	0.17	91,91,91,91	0
10	NE6	D	1529	30/30	0.96	0.22	52,70,81,85	0
6	PO4	D	1528	5/5	0.96	0.14	86,86,86,89	0
8	MPD	C	1120	8/8	0.97	0.17	51,56,57,57	0
7	MG	B	701	1/1	0.97	0.20	55,55,55,55	0
7	MG	N	1527	1/1	0.97	0.04	56,56,56,56	0
9	ZN	N	1525	1/1	0.99	0.19	50,50,50,50	0
9	ZN	D	1526	1/1	1.00	0.18	77,77,77,77	0
9	ZN	N	1526	1/1	1.00	0.18	55,55,55,55	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.





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

There are no such residues in this entry.