



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 3DXJ / pdb_00003dxj
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

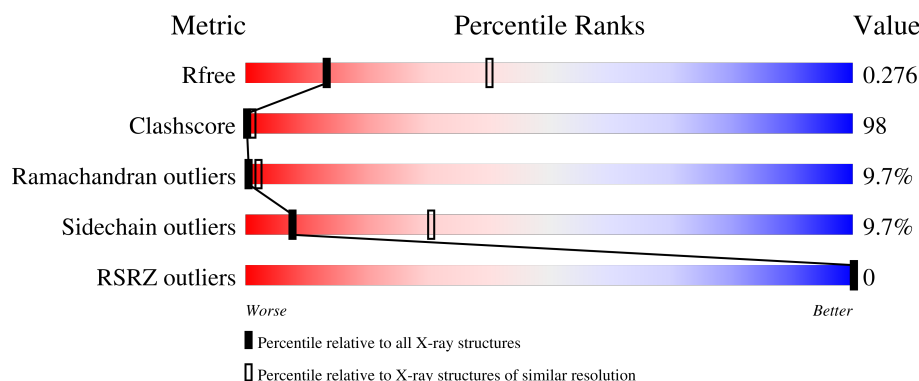
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 ≥ 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	14%	65%	19%	.
3	D	1524	12%	64%	20%	..
3	N	1524	13%	63%	21%	..
4	E	99	15%	61%	18%	. .
4	O	99	18%	61%	16%	. .
5	F	423	7%	55%	19%	. 17%
5	P	423	7%	52%	21%	. 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

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
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
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
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			

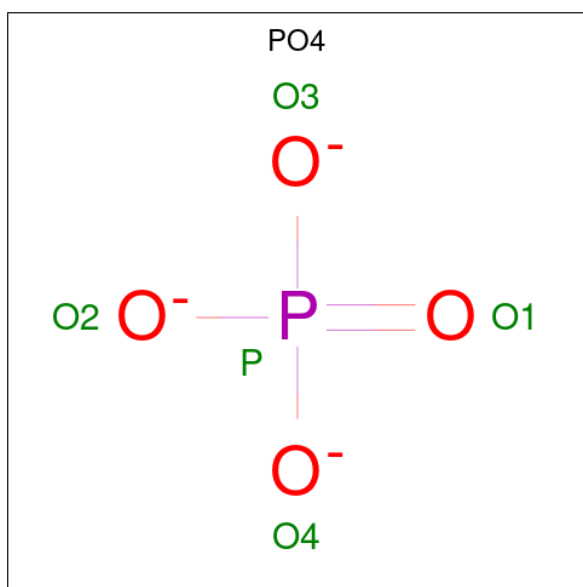
There are 6 discrepancies between the modelled and reference sequences:

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 (CCD ID: PO4) (formula: O₄P).

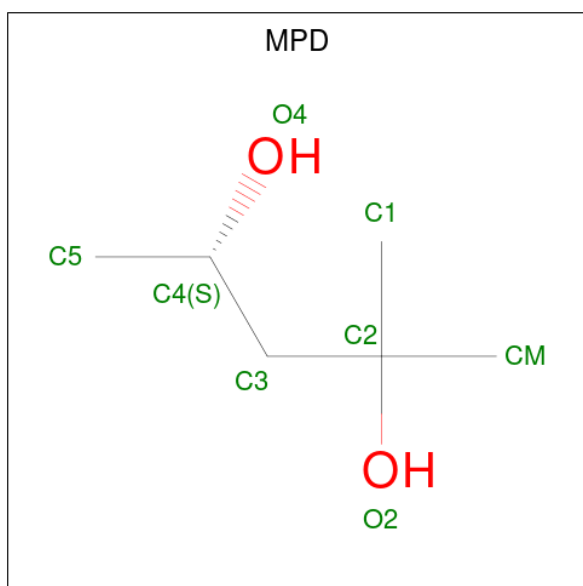


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: 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 (CCD ID: MPD) (formula: C₆H₁₄O₂).

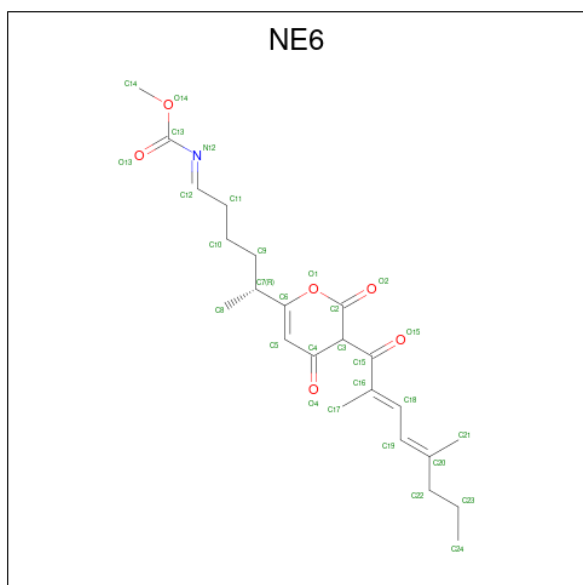


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			8	6	2		
8	C	1	Total	C	O	0	0
			8	6	2		
8	M	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is methyl [(1E,5R)-5-{(3S)-3-[(2E,4E)-2,5-dimethylocta-2,4-dienoyl]-2,4-dioxo-3,4-dihydro-2H-pyran-6-yl}hexylidene]carbamate (CCD ID: NE6) (formula: C₂₃H₃₁NO₆).



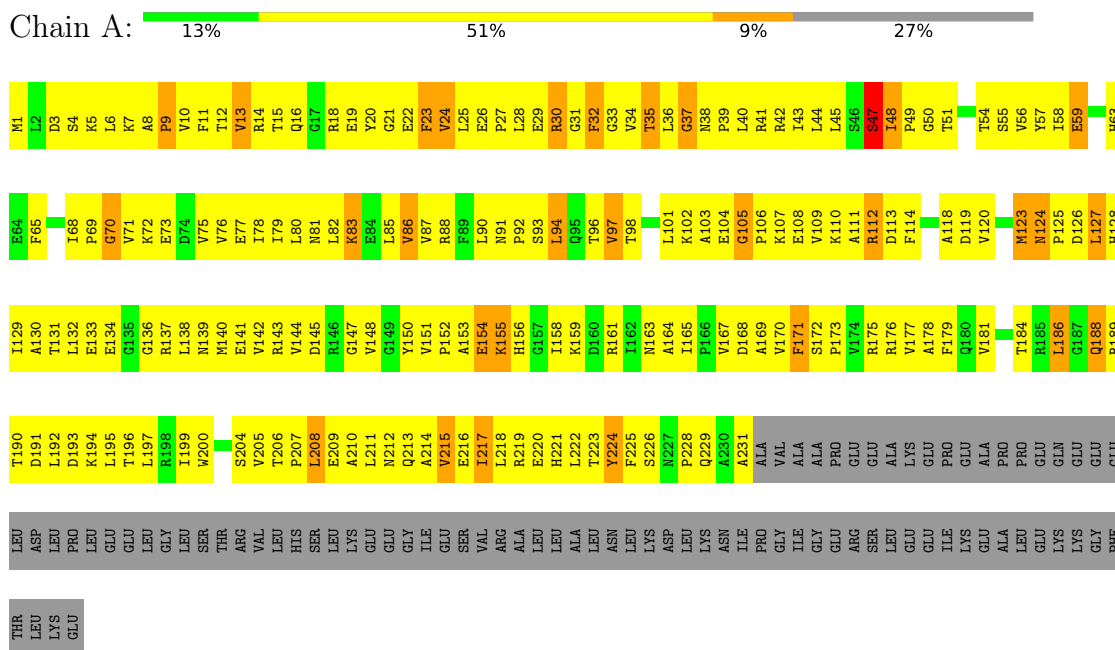
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	5	Total	O	0	0
			5	5		
11	N	4	Total	O	0	0
			4	4		
11	O	1	Total	O	0	0
			1	1		

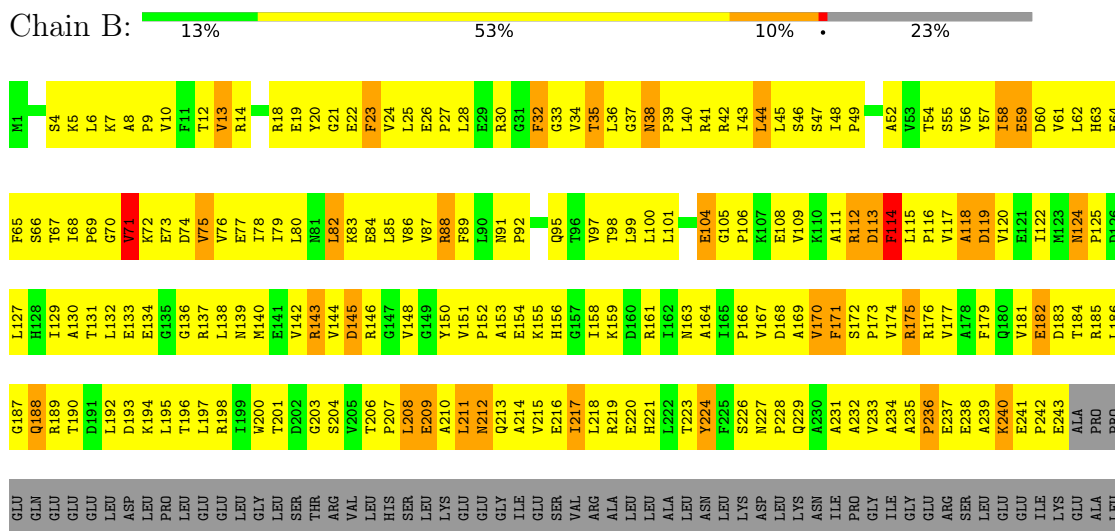
3 Residue-property plots

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



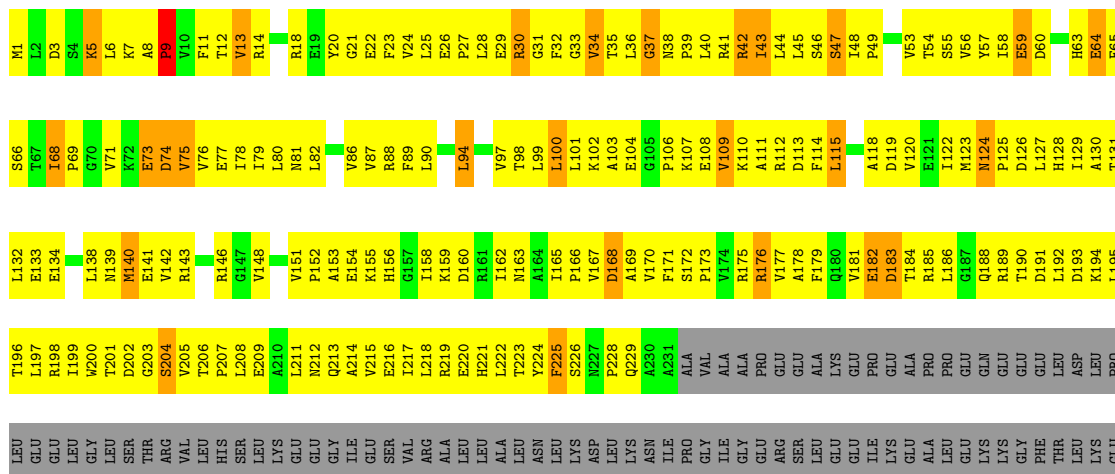
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L



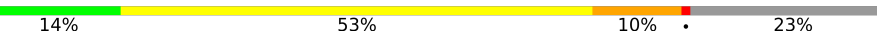
GLU
LYS
LYS
GLY
PHE
THR
LYS
GLU

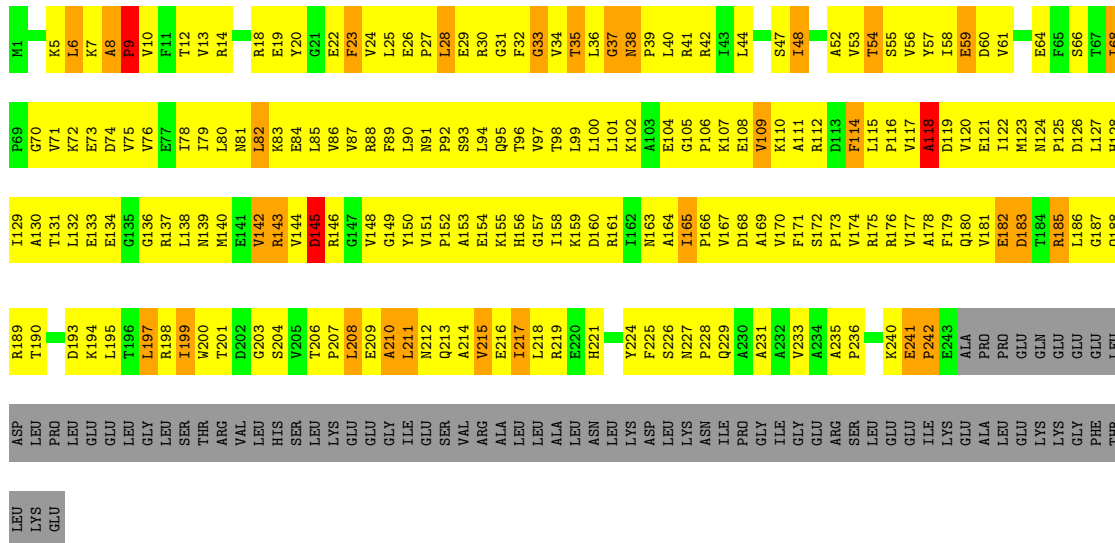
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

Chain K: 

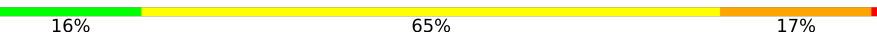


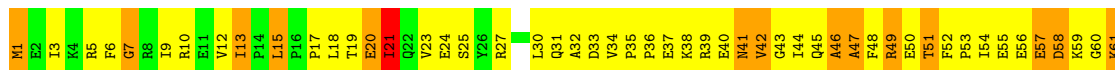
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

Chain L: 

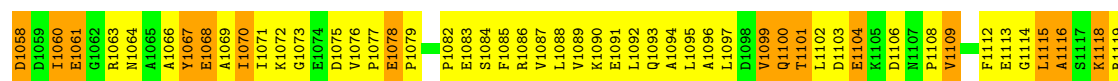


- Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M

Chain C: 

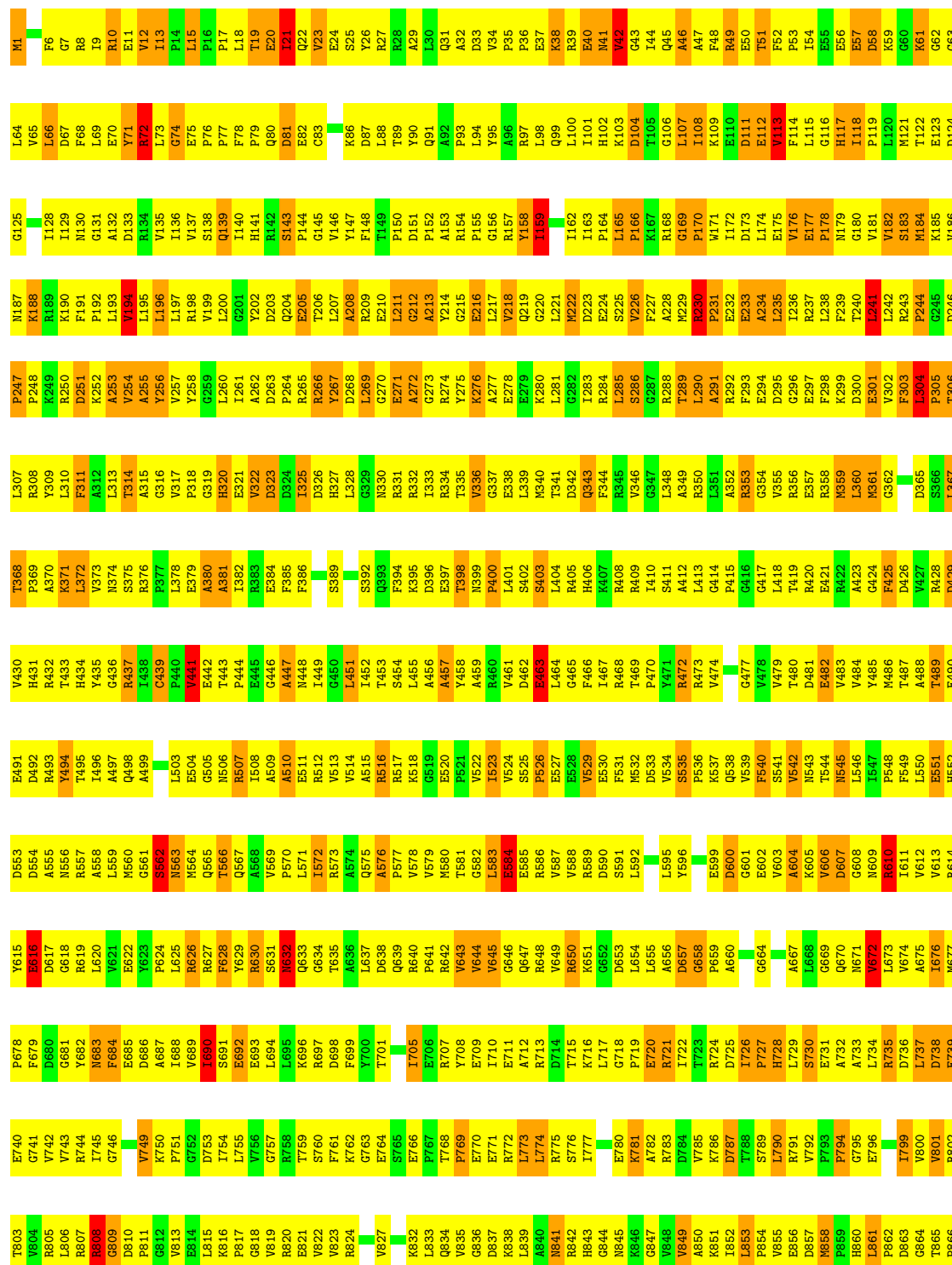


M995	K996	L997	Y998	H999	K1000	V1001	E1002	D1003	K1004	M1005	L1006	A1007	R1008	S1009	T1010	E1011	G1012	P1013	Y1014	L1015	I1016	T1017	P1018	Q1019	Q1020	L1021	Q1022	F1023	G1024	G1025	G1026	G1027	G1028	Q1029	L1030	F1031	F1032	G1033	G1034	M1035	E1036	L1037	M1038	L1039	E1040	L1041	A1042	Y1043	G1044	E1045	A1046	H1047	T1048	L1049	Q1050	E1051	M1052	L1053	T1054	L1055	K1056	S1057																																																																																																																																																																																							
E932	G933	F934	D935	K936	R937	E938	E939	E940	Y941	E942	Y943	L944	R945	R946	A947	E948	K949	L950	G951	L952	Y953	T954	P955	T956	P957	P958	P959	E960	E961	Q962	L963	K964	E965	L966	F967	L968	Q969	G970	K971	L972	Y973	Y974	Y975	D976	G977	R978	T979	Y980	E981	P982	L983	E984	G985	P986	Y987	Y988	Y989	G990	Q991	Y992	F993	L994																																																																																																																																																																																							
L871	H872	R873	L874	H875	H876	S877	S878	S879	H880	H881	L882	L883	R884	L885	L886	E887	T888	H889	L890	A891	A892	L893	L894	L895	L896	L897	G898	G899	E900	Q901	L902	S903	F904	L905	F906	D907	G908	A909	K910	E911	P912	E913	L914	K915	E916	E917	L918	L919	E920	E921	E922	E923	Y924	Y925	F926	G927	K928	R929	L930	Y931	L932	L933	L934	L935	L936	L937	L938	L939	L940																																																																																																																																																																																
R808	Q809	D810	P811	G812	G813	E814	L815	R816	P817	G818	H819	R820	E821	W822	G823	R824	W825	Y826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870																																																																																																																																																																																							
G741	W742	W743	A744	E745	W746	W747	W748	W749	W750	W751	W752	W753	W754	W755	W756	W757	W758	W759	W760	W761	W762	W763	W764	W765	W766	W767	W768	W769	W770	W771	W772	W773	W774	W775	W776	W777	W778	W779	W780	W781	W782	W783	W784	W785	W786	W787	W788	W789	W790	W791	W792	W793	W794	W795	W796	W797	W798	W799	W800	W801	W802	W803	W804	W805	W806	W807																																																																																																																																																																																			
P678	F679	D680	G681	Y682	H683	F684	E685	D686	A687	L688	W689	L690	S691	E692	E693	L694	L695	K696	R697	D698	F699	Y700	Y701	H702	W703	W704	W705	W706	W707	W708	W709	W710	W711	W712	W713	W714	W715	W716	W717	W718	W719	W720	W721	W722	W723	W724	W725	W726	W727	W728	W729	W730	W731	W732	W733	W734	W735	W736	W737	W738																																																																																																																																																																																									
E616	D617	G618	R619	E620	W621	W622	W623	W624	W625	W626	W627	W628	W629	W630	W631	W632	W633	W634	W635	W636	W637	W638	W639	W640	W641	W642	W643	W644	W645	W646	W647	W648	W649	W650	W651	W652	W653	W654	W655	W656	W657	W658	W659	W660	W661	W662	W663	W664	W665	W666	W667	W668	W669	W670	W671	W672	W673	W674	W675	W676	W677																																																																																																																																																																																								
A555	N556	R557	A558	Q559	N560	C561	S562	N563	N564	Q565	T566	W567	W568	P569	L570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	T581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	D600	G601	E602	G603	A604	K605	W606	D607	L608	E609	W610	W611	W612	W613	W614	W615																																																																																																																																																																																									
Y494	T495	L496	A497	Q498	A499	N500	T501	P502	E503	E504	Q505	N506	R507	L508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554																																																																																																																																																																																									
T433	H434	Y435	G436	R437	L438	C439	P440	E441	E442	T443	P444	E445	G446	A447	N448	L449	G450	L451	L452	L453	S454	L455	A456	A457	Y458	A459	R460	Y461	D462	S463	L464	A465	H466	L467	R468	E469	P470	M532	D533	Y534	S535	P536	Q537	G538	W539	F540	S541	Y542	N543	T544	N545	L546	M547	M548	W549	L550	E551	H552	D553	D554																																																																																																																																																																																									
V373	N374	R375	S376	P377	L378	E379	A380	A381	L382	R383	E384	F385	F386	S387	R388	S389	Q390	L391	S392	Q393	F394	K395	D396	E397	T398	N399	P400	G401	L402	S403	L404	H405	H406	R407	R408	R409	T410	S411	A412	L413	O414	P415	G416	C417	L418	T419	R420	E421	R422	A423	G424	D425	D426	W427	R428	L429	D430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474																																																																																																																																																
P247	P248	K249	R250	D251	P252	A253	V254	W255	W256	W257	G258	L259	T260	G261	Y262	P263	D264	Q265	Q266	E267	D268	L269	Q270	E271	A272	G273	R274	Y275	E276	A277	E278	E279	K280	L281	G282	I283	R284	L285	S286	R287	R288	L289	L290	A291	R292	P293	E294	D295	G296	E297	D300	E301	V302	F303	L304	P305	T306	K307	G308	R309																																																																																																																																																																																									
Y309	L310	F311	A312	L313	T314	A315	G316	P317	P318	E319	G320	D321	D322	D323	D324	D325	D326	D327	D328	D329	R330	R331	R332	R333	R334	T335	V336	G337	E338	L339	M340	T341	D342	Q343	F344	R345	V346	G347	L348	A349	R350	L351	A352	R353	G354	V355	R356	E357	R358	M359	S360	S361	S362	S363	S364	S365	S366	S367	S368	S369	S370	S371	S372	S373	S374	S375	S376	S377	S378	S379	S380	S381	S382	S383	S384	S385	S386	S387	S388	S389	S390	S391	S392	S393	S394	S395	S396	S397	S398	S399	S400	S401	S402	S403	S404	S405	S406	S407	S408	S409	S410	S411	S412	S413	S414	S415	S416	S417	S418	S419	S420	S421	S422	S423	S424	S425	S426	S427	S428	S429	S430	S431	S432	S433	S434	S435	S436	S437	S438	S439	S440	S441	S442	S443	S444	S445	S446	S447	S448	S449	S450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554
G62	G63	L64	V65	L66	D67	F68	L69	E70	Y71	W72	L73	G74	E75	P76	P77	F78	P79	Q80	D81	E82	G83	R84	D87	Y90	Q91	A92	P93	L94	Y95	A96	R97	L98	Q99	L100	L101	H102	K103	D104	T105	E106	G107	L108	K109	E110	D111	L112	E113	F114	L115	G116	H117	L118	P119	L120	M121	K122	E123																																																																																																																																																																																												
D124	F127	I128	L129	M130	G131	A132	D133	L134	V135	L136	W137	G138	Q139	I140	H141	R142	E143	P144	G145	F148	T149	P150	D151	P152	A153	P154	P155	G156	R157	Y158	I159	T162	D163	E164	L165	K167	R168	F227	A228	M229	P170	E171	I172	D173	L174	E175	W176	E177	P178	N179	G180	H181	V181	W182	S183	M184	K185	V186																																																																																																																																																																																											
N187	K188	R189	K190	F191	P192	L193	L194	L195	L196	L197	L198	V199	L200	G201	Y202	H203	Q204	E205	E206	L207	A208	R209	E210	L211	G212	A213	Y214	E215	E216	L217	Y218	Q219	G220	L221	M222	D223	E224	S225	F227	A228	M229	P170	E171	I172	D173	L174	E175	W176	E177	P178	N179	G180	H181	V181	W182	S183	M184	K185	V186																																																																																																																																																																																										



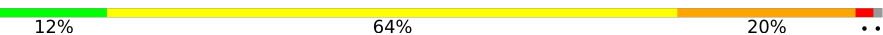
● Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M

Chain M: 14% 65% 19%



V687	G927	L1055	L1115
D688	K928	K1056	A1116
V689	K929	S1057	S1117
I870	K930	D1068	K1118
L871	G931	D1069	R1119
N872	E932	I1060	
P873	G933	E1061	
L874	F934	G1062	
G875		M1000	
V876		E1002	
P877	D937	R1063	
S878	K938	N1064	
R879	K939	A1004	
E940	R940	M1005	
M880	V941	Y1067	
N881	E942	E1068	
L882	E943	A1007	
G883	L944	R1008	
Q884	R945	S1009	
T885	R946	T1010	
L886	R947	G1012	
E887	A948	Y1013	
H888	K949	D1075	
L890	V953	V1076	
G891		P1077	
L892		E1078	
A893	K957	P1079	
G894	T958	S1080	
Y895	P959	V1081	
F896	E960	L1082	
L897	E961	E1083	
K898	E962	S1084	
Q899	K963	R1085	
R900	K964	F1086	
I902	E965	V1087	
S903	L966	L1088	
P904	Q969	V1089	
I905	G970	K1090	
D907	K971	G1029	
G908		Q1030	
A909	Y975	R1031	
K910	D976	F1032	
E911	G977	A1033	
P912	R978	E1034	
E913	T979	M1035	
I914	G980	A1096	
K915	E981	L1097	
E916	P982	D1098	
L917	I983	V1099	
L918	E984	M1038	
A919	G985	A1039	
Q920	P986	L1040	
A921	R987	E1041	
F922	V988	D1103	
E923	V989	E1104	
V924	G990	K1105	
F926	M992	D1106	
		N1107	
		T1048	
		P1108	
		V1109	
		Q1060	
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		L1111	
		M1052	
		E1113	
		L1053	
		Q1114	
		G1114	

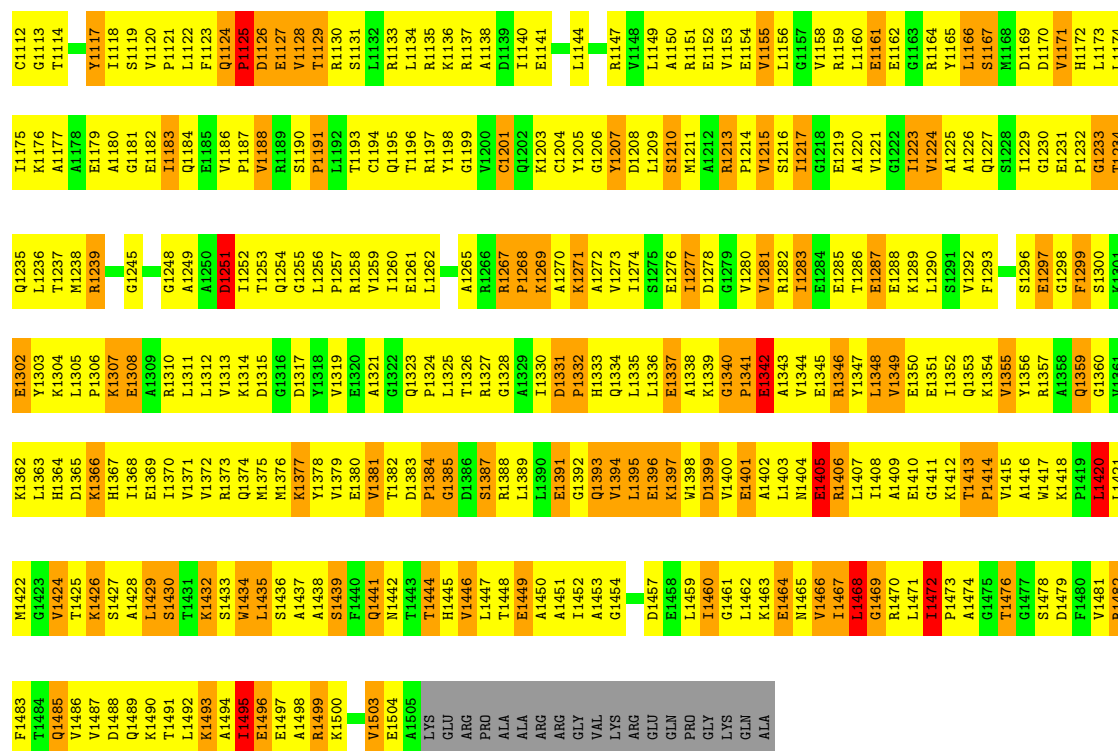
● Molecule 3: BACTERIAL RNA POLYMERASE BETA-PRIME SUBUNIT; CHAIN D, N

Chain D:  12% 64% 20% ..

Y67	K62	T121	G182	L245	E306	A369	Y432	A492	N552	R613
K63	E4	E122	E183	P246	A307	A370	G433	R493	R553	F614
K64	K3	L123	E184	E247	G308	A371	R434	R494	L554	R615
V5	K65	E124	V185	P248	G309	D372	R435	R495	K555	Q616
R6	R66	Q125	V186	Y249	L310	E374	E436	R496	L556	R617
K7	R67	V126	L187	L250	L311	P375	V437	E497	L557	L618
V8	E68	L127	G188	E253	R312	E376	D438	V498	L558	L619
R9	E69	Y128	Q189	R252	M313	V377	L439	V499	A559	G620
I10	E70	S130	L191	A253	P314	E378	V440	R500	Q560	K621
L12	A11	G70	K71	E254	R315	L378	R441	F501	A561	R622
V72	V72	S131	A192	E255	Q316	A379	M442	F502	G562	V623
C73	C73	Y132	G193	E256	V317	E380	V443	L503	P563	D624
S14	S14	L133	P194	C257	R318	E381	V444	L504	E564	Y625
R15	R15	V134	V195	V258	A319	V384	R445	S505	S565	S626
E16	E16	L135	V196	V259	V322	V385	V446	G506	S566	G627
K17	K17	D136	E197	E260	E323	H386	V447	N507	L567	R628
L18	L18	P137	R198	L261	E324	L387	E448	R508	R568	S629
R19	R19	K138	L199	K262	A324	H388	S449	P509	N569	V630
S20	S20	G139	D200	E263	E325	E389	Y450	E510	E570	I631
E21	E21	A140	A203	L264	E326	P390	D451	M511	K571	V632
V26	V26	L141	L204	L270	E327	A391	L452	P512	R572	G633
E27	E27	V147	L205	V271	E328	S392	D453	I513	M573	P634
K28	K28	E148	Y206	L272	E329	L394	R455	L514	L574	G635
P29	P29	K149	R207	R273	G267	L395	R456	E515	Q575	Q636
E30	E30	R150	F207	R274	A268	V331	M456	A516	E576	L637
T31	T31	Q151	V85	L275	E269	V332	G457	V517	K577	K638
L32	L32	L152	R86	L276	L270	V396	P402	P518	A578	L639
N33	N33	E153	R87	L277	L271	K397	L403	V519	D579	E640
Y34	Y34	T154	E94	L278	L272	A398	E404	L520	A580	Q641
R35	R35	D155	R89	R280	R273	L335	R465	L521	L581	G642
A96	A96	E156	N90	E281	R274	V400	K466	P522	L582	G643
L37	L37	E157	G91	L281	R275	Y401	E467	P523	G583	L644
K38	K38	Y158	H92	L282	E277	L402	L468	D524	L584	P645
P39	P39	R159	I93	L283	P278	F403	L469	E530	N591	E651
A99	A99	E160	I94	F284	V279	E404	L470	D531	T592	L652
A100	A100	G222	E94	P285	L284	D406	L471	D532	N593	F653
R41	R41	L161	L95	L286	E280	L407	A472	G533	P594	K654
D42	D42	R162	L96	G287	P342	D408	L473	G534	R595	G655
Q43	Q43	Y163	A96	E288	P343	E409	E474	R534	G596	P656
F104	F104	G164	F103	L289	P344	L413	K475	R535	S596	L657
V105	V105	K165	L104	L290	H350	R414	E476	A536	D597	P658
D46	D46	Q166	L105	L291	M351	V415	L477	T537	A598	K659
E47	E47	E167	K106	L292	N352	A416	L478	S538	P599	P660
R48	R48	T168	D107	V292	V353	P417	E479	D539	L600	M661
V108	V108	Y169	V108	V293	V354	G418	E480	L540	R601	E662
P109	P109	E170	P109	H294	V355		L481	N541	S602	G663
S110	S110	P170	S110	G295	P356	L421	K482	D542	L603	K664
K111	K111	L171	K111	E296	E357	A422	H483	R543	T604	G665
P52	P52	P172	L112	L297	G358	D423	L484	Y544	D605	I666
L53	L53	G113	G113	V298	V298	G424	P484	R545	I606	P667
K54	K54	T114	T114	E299	R360	G425	S485	R546	L607	A668
D55	D55	V175	L115	G300	V361	K426	R486	R547	P608	P669
V56	V56	A177	L116	K301	G301	V427	L487	L547	G609	V670
E57	E57	L176	D117	G302	D365	K428	R488	I548	K610	K671
C58	C58	V179	L118	P303	K366	S429	R489	N549	Q611	
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C60	C60	D181	A120	A305	V368	V431	K491	N551		

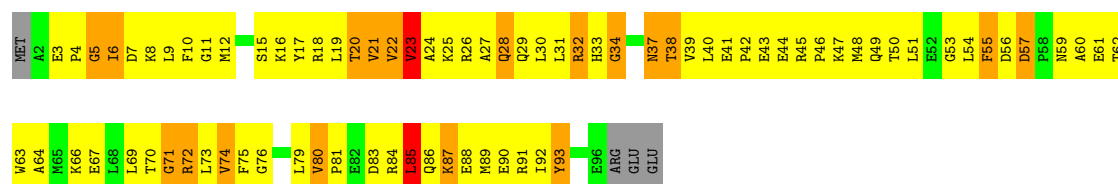
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L1367	L1368	L1369	L1370	L1371	L1372	L1373	L1374	L1375	L1376	L1377	L1378	L1379	L1380	L1381	L1382	L1383	L1384	L1385	L1386	L1387	L1388	L1389	L1390	L1391	L1392	L1393	L1394	L1395	L1396	L1397	L1398	L1399	L1400	L1401	L1402	L1403	L1404	L1405	L1406	L1407	L1408	L1409	L1410	L1411	L1412	L1413	L1414	L1415	L1416	L1417	L1418	L1419	L1420	L1421	L1422	L1423	L1424	L1425	L1426																																																																																																																																																																																																																																																					
L1427	L1428	L1429	L1430	L1431	L1432	L1433	L1434	L1435	L1436	L1437	L1438	L1439	L1440	L1441	L1442	L1443	L1444	L1445	L1446	L1447	L1448	L1449	L1450	L1451	L1452	L1453	L1454	L1455	L1456	L1457	L1458	L1459	L1460	L1461	L1462	L1463	L1464	L1465	L1466	L1467	L1468	L1469	L1470	L1471	L1472	L1473	L1474	L1475	L1476	L1477	L1478	L1479	L1480	L1481	L1482	L1483	L1484	L1485	L1486																																																																																																																																																																																																																																																					
L1487	L1488	L1489	L1490	L1491	L1492	L1493	L1494	L1495	L1496	L1497	L1498	L1499	L1500	L1501	L1502	L1503	L1504	L1505	L1506	L1507	L1508	L1509	L1510	L1511	L1512	L1513	L1514	L1515	L1516	L1517	L1518	L1519	L1520	L1521	L1522	L1523	L1524	L1525	L1526	L1527	L1528	L1529	L1530	L1531	L1532	L1533	L1534	L1535	L1536	L1537	L1538	L1539	L1540	L1541	L1542	L1543	L1544	L1545	L1546	L1547	L1548	L1549	L1550	L1551	L1552	L1553	L1554	L1555	L1556	L1557	L1558	L1559	L1560	L1561	L1562	L1563	L1564	L1565	L1566	L1567																																																																																																																																																																																																																																
L1568	L1569	L1570	L1571	L1572	L1573	L1574	L1575	L1576	L1577	L1578	L1579	L1580	L1581	L1582	L1583	L1584	L1585	L1586	L1587	L1588	L1589	L1590	L1591	L1592	L1593	L1594	L1595	L1596	L1597	L1598	L1599	L1600	L1601	L1602	L1603	L1604	L1605	L1606	L1607	L1608	L1609	L1610	L1611	L1612	L1613	L1614	L1615	L1616	L1617	L1618	L1619	L1620	L1621	L1622	L1623	L1624	L1625	L1626	L1627	L1628	L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647	L1648	L1649	L1650	L1651	L1652	L1653	L1654	L1655	L1656	L1657	L1658	L1659	L1660	L1661	L1662	L1663	L1664	L1665	L1666	L1667	L1668	L1669	L1670	L1671	L1672	L1673	L1674	L1675	L1676	L1677	L1678	L1679	L1680	L1681	L1682	L1683	L1684	L1685	L1686	L1687	L1688	L1689	L1690	L1691	L1692	L1693	L1694	L1695	L1696	L1697	L1698	L1699	L1700	L1701	L1702	L1703	L1704	L1705	L1706	L1707	L1708	L1709	L1710	L1711	L1712	L1713	L1714	L1715	L1716	L1717	L1718	L1719	L1720	L1721	L1722	L1723	L1724	L1725	L1726	L1727	L1728	L1729	L1730	L1731	L1732	L1733	L1734	L1735	L1736	L1737	L1738	L1739	L1740	L1741	L1742	L1743	L1744	L1745	L1746	L1747	L1748	L1749	L1750	L1751	L1752	L1753	L1754	L1755	L1756	L1757	L1758	L1759	L1760	L1761	L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780	L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799	L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818	L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837	L1838	L1839	L1840	L1841	L1842	L1843	L1844	L1845	L1846	L1847	L1848	L1849	L1850	L1851	L1852	L1853	L1854	L1855	L1856	L1857	L1858	L1859	L1860	L1861	L1862	L1863	L1864	L1865	L1866	L1867	L1868	L1869	L1870	L1871	L18





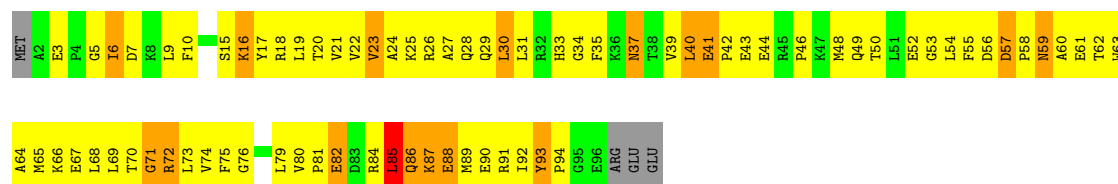
• Molecule 4: BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O

Chain E: 15% 61% 18%



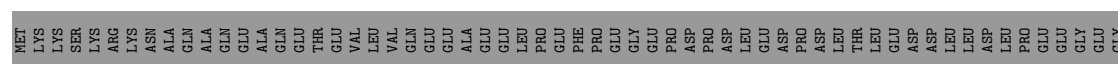
• Molecule 4: BACTERIAL RNA POLYMERASE OMEGA SUBUNIT; CHAIN E, O

Chain O: 18% 61% 16%



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

Chain F: 7% 55% 19% 17%



LEU	ASP	G121	A182	R244	E306	A366	G121	LEU	ASP	G121	A182	R244	E306	A366
LEU	LEU	L122	A183	Q245	T307	M367	L122	ASP	LEU	L122	A183	Q245	T307	M367
GLU	GLU	D123	R184	A246	L308	V368	D123	LEU	LEU	D123	R184	A246	L308	V368
P124	P124	P124	Q185	L247	L369	L369	P124	GLU	GLU	P124	Q185	L247	L369	L369
H186	H186	H186	H186	N248	K370	L371	H186	GLU	GLU	H186	H186	N248	K370	L371
L126	L126	L126	L187	R249	L371	L371	L126	GLU	GLU	L126	L187	R249	L371	L371
L127	L127	L127	L188	A250	Q312	R372	L127	GLU	GLU	L127	L188	A250	Q312	R372
R128	R128	R128	E189	L251	Q312	R372	R128	GLU	GLU	R128	E189	L251	Q312	R372
ASP	ASP	E129	E189	L251	Q312	R372	E129	GLU	GLU	E129	E189	L251	Q312	R372
LEU	LEU	V130	N191	A255	P314	G374	V130	LEU	LEU	V130	N191	A255	P314	G374
PRO	PRO	V131	L192	R256	S316	L376	V131	PRO	PRO	V131	L192	R256	S316	L376
ILE	ILE	R132	L193	R257	S316	D377	R132	ILE	ILE	R132	L193	R257	S316	D377
PRO	PRO	A133	L194	R258	S316	G378	A133	PRO	PRO	A133	L194	R258	S316	G378
K74	K74	K134	V195	R259	T319	R379	K74	K74	K74	K134	V195	R259	T319	R379
I75	I75	I135	V196	L260	P320	E380	I75	I75	I75	I135	V196	L260	P320	E380
S76	S76	L136	S197	P261	L321	H381	S76	S76	S76	L136	S197	P261	L321	H381
T77	T77	G137	I198	V262	G322	T382	T77	T77	T77	G137	I198	V262	G322	T382
S78	S78	S138	A199	M264	D323	L383	S78	S78	S78	S138	A199	M264	D323	L383
D79	D79	A139	T203	V265	G326	E386	D79	D79	D79	A139	T203	V265	G326	E386
P80	P80	R140	G204	E266	F332	V392	P80	P80	P80	R140	G204	E266	F332	V392
V81	V81	V141	G204	E266	F332	V392	V81	V81	V81	V141	G204	E266	F332	V392
R82	R82	R142	R205	T267	G327	G387	R82	R82	R82	R142	R205	T267	G327	G387
Q83	Q83	H143	G206	L268	F328	A388	Q83	Q83	Q83	H143	G206	L268	F328	A388
Y84	Y84	I144	L207	N269	Y329	F389	Y84	Y84	Y84	I144	L207	N269	Y329	F389
L85	L85	P145	S208	K270	G330	F390	L85	L85	L85	P145	S208	K270	G330	F390
H86	H86	G146	F209	L271	D331	G391	H86	H86	H86	G146	F209	L271	D331	G391
E87	E87	L147	L210	S272	F332	V392	E87	E87	E87	L147	L210	S272	F332	V392
I88	I88	K148	D211	R273	L333	T393	I88	I88	I88	K148	D211	R273	L333	T393
G89	G89	E149	L212	T274	P334	R394	G89	G89	G89	E149	L212	T274	P334	R394
Q90	Q90	T150	T213	A275	D335	E395	Q90	Q90	Q90	T150	T213	A275	D335	E395
V91	V91	L151	Q214	R276	E336	R396	V91	V91	V91	L151	Q214	R276	E336	R396
P92	P92	D152	E215	Q277	H337	I397	P92	P92	P92	D152	E215	Q277	H337	I397
L93	L93	P153	G216	L278	L338	R398	L93	L93	L93	P153	G216	L278	L338	R398
L94	L94	K154	N217	Q279	P339	Q399	L94	L94	L94	K154	N217	Q279	P339	Q399
T95	T95	T155	Q218	Q280	S340	I400	T95	T95	T95	T155	Q218	Q280	S340	I400
L96	L96	V156	G219	E281	E341	E401	L96	L96	L96	V156	G219	E281	E341	E401
E97	E97	E157	L220	L282	V342	R402	E97	E97	E97	E157	L220	L282	V342	R402
E98	E98	E158	I221	G283	D343	K403	E98	E98	E98	E158	I221	G283	D343	K403
E99	E99	I159	R222	R284	A344	A404	E99	E99	E99	I159	R222	R284	A344	A404
V100	V100	D160	A223	E285	L405	L405	V100	V100	V100	D160	A223	E285	L405	L405
E101	E101	K161	V224	P286	T346	R406	E101	E101	E101	K161	V224	P286	T346	R406
L102	L102	K162	E225	T287	K407	K407	L102	L102	L102	K162	E225	T287	K407	K407
A103	A103	L163	K226	Y288	S348	L408	A103	A103	A103	L163	K226	Y288	S348	L408
R104	R104	K164	F227	E289	L349	K409	R104	R104	R104	K164	F227	E289	L349	K409
K105	K105	S165	E228	E290	L350	Y410	K105	K105	K105	S165	E228	E290	L350	Y410
V106	V106	L166	Y229	T291	S351	R411	V106	V106	V106	L166	Y229	T291	S351	R411
E107	E107	P167	K230	A292	E352	E412	E107	E107	E107	P167	K230	A292	E352	E412
E108	E108	K168	R231	E293	E353	S413	E108	E108	E108	K168	R231	E293	E353	S413
G109	G109	E169	R232	A294	L354	R414	G109	G109	G109	E169	R232	A294	L354	R414
M110	M110	H170	F233	M295	E355	T415	M110	M110	M110	H170	F233	M295	E355	T415
E111	E111	K171	K234	G286	K356	R416	E111	E111	E111	K171	K234	G286	K356	R416
A112	A112	R172	F235	P297	A357	K417	A112	A112	A112	R172	F235	P297	A357	K417
I113	I113	Y173	L358	G298	L358	L418	I113	I113	I113	Y173	L358	G298	L358	L418
K114	K114	T237	Y299	R299	R419	R419	K114	K114	K114	T237	Y299	R299	R419	R419
K115	K115	H175	Y238	D300	K360	D420	K115	K115	K115	H175	Y238	D300	K360	D420
L116	L116	L176	A239	L301	L361	F421	L116	L116	L116	L176	A239	L301	L361	F421
S117	S117	A177	T240	K302	S362	L422	S117	S117	S117	A177	T240	K302	S362	L422
E118	E118	R178	W241	R303	E363	ASP	E118	E118	E118	R178	W241	R303	E363	ASP
I119	I119	W242	V304	R364	R364		I119	I119	I119	W242	V304	R364	R364	
T120	T120	E181	I243	E305	E365		T120	T120	T120	E181	I243	E305	E365	

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

Chain P: 7% 52% 21% 17%

A366	V304	R244	A182	G121	LEU	MET
M367	E305	Q245	A183	L122	ASP	LYS
V368	E306	A246	R184	D123	LEU	LYS
L369	T307	Q247	Q185	P124	GLU	SER
K370	L308	N248	H186	D125	GLU	LYS
L371	K309	R249	L187	L126	GLU	ARG
R372	L310	A250	L188	L127	GLU	LYS
K373	A311	T251	E189	R128	GLU	ASN
G374	K312	A252	A190	E129	ASP	ALA
L375	E313	D253	N191	V130	LEU	GLN
L376	P314	Q254	L192	V131	PRO	ALA
D377	V315	A255	L193	R132	ILE	GLN
G378	S316	R256	L194	A133	PRO	GLN
R379	L317	T257	V195	K134	K74	ALA
E380	E318	L258	V196	I135	I75	GLN
H381	T319	R259	G200	L136	S76	GLU
T382	P320	L260	K201	G137	T77	THR
L383	L321	P261	K201	S138	S78	GLU
E384	G322	V262	Y202	A139	D79	VAL
E385	D323	H263	T203	R140	P80	LEU
V386	E324	M264	G204	V141	V81	VAL
G387	K325	V265	R205	R142	R82	GLN
A388	D326	E266	G206	P145	O83	GLU
F389	S327	T267	L207	P145	Y84	GLU
F390	F328	L268	S208	G146	L85	ALA
G391	Y329	T269	F209	L147	H86	GLU
V392	G330	K270	L210	K148	E87	GLU
T393	D331	L271	D211	E149	I88	LEU
R394	F332	S272	L212	T150	G89	PRO
E395	I333	R273	T213	L151	Q90	GLU
R396	P334	T274	Q214	D152	V91	PHE
L397	D335	A275	E215	P153	P92	PRO
R398	E336	R276	G216	K154	L93	GLU
Q399		Q277	N217	T155	L94	GLY
A400	P339	L278	Q218	V156	T95	GLU
E401		Q279	G219	E157	L96	PRO
N402	V342	Q280	L220	E158	E97	ASP
K403	D343	E281	I221	L159	E98	PRO
A404	A344	L282	R222	D160	E99	ASP
L405	A345	G283	A223	Q161	V100	LEU
R406	T346	R284	V224	K162	E101	GLU
K407	Q347	E285	E225	L163	L102	ASP
L408	S348	P286	K226	K164	A103	PRO
K409	L349	T287	F227	S165	R104	ASP
Y410	L350	Y288	E228	L166	K105	LEU
H411	S351	E289	G229	P167	V106	THR
E412	E352	E290	K230	K168	E107	LEU
S413	E353	I291	R231	E168	E108	LEU
R414	L364	A292	R232	H170	G109	GLU
T415	E355	E293	K233	K171	M110	ASP
R416	K356	A294	F234	R172	E111	LEU
K417	G357	M295	F235	Y173	A112	LEU
L418	L358	G296	S236	L174	I113	ASP
R419	S359	P297	T237	H175	K114	LEU
F420	K360	G298	Y238	L116	K115	PRO
F421	L361	M299	A239	A177	L116	GLU
L422	S362	D300	T240	R178	S117	GLU
ASP	E363	A301	W241	E179	E118	GLY
	R364	K302	T242	G180	T119	GLY
	F365	E302	T243	F184	T120	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	235.09Å 235.09Å 250.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-3.00) 96.2 (50.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.289 0.221 , 0.276	Depositor DCC
R_{free} test set	2351 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	83.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l 0.047 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	56149	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, NE6, ZN, MPD

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	0.53	0/1848	1.08	9/2512 (0.4%)
1	B	0.46	0/1936	0.99	9/2633 (0.3%)
1	K	0.51	0/1848	1.08	13/2512 (0.5%)
1	L	0.48	0/1936	1.09	17/2633 (0.6%)
2	C	0.52	0/8997	1.15	88/12164 (0.7%)
2	M	0.51	0/8997	1.15	90/12164 (0.7%)
3	D	0.54	0/12073	1.17	135/16324 (0.8%)
3	N	0.55	1/12073 (0.0%)	1.15	127/16324 (0.8%)
4	E	0.43	0/783	1.05	6/1054 (0.6%)
4	O	0.45	0/783	0.98	2/1054 (0.2%)
5	F	0.46	0/2874	1.07	25/3866 (0.6%)
5	P	0.46	0/2874	1.04	19/3866 (0.5%)
All	All	0.52	1/57022 (0.0%)	1.13	540/77106 (0.7%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1268	PRO	C-O	5.79	1.30	1.23

The worst 5 of 540 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	177	GLU	CA-C-N	16.13	140.01	119.84
2	C	177	GLU	C-N-CA	16.13	140.01	119.84
3	D	131	LYS	N-CA-C	13.72	125.95	111.14
2	M	58	ASP	N-CA-C	-13.71	89.18	110.42
3	D	831	GLY	N-CA-C	-13.69	80.74	113.18

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	290	0
1	B	1902	0	1951	346	0
1	K	1816	0	1871	315	0
1	L	1902	0	1951	334	0
2	C	8829	0	8933	1779	0
2	M	8829	0	8933	1689	0
3	D	11864	0	12094	2646	0
3	N	11864	0	12094	2562	0
4	E	769	0	775	175	0
4	O	769	0	775	138	0
5	F	2829	0	2914	649	0
5	P	2829	0	2914	717	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	11069	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 98.

The worst 5 of 11069 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%)	1 5
1	B	241/315 (76%)	159 (66%)	64 (27%)	18 (8%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	229/315 (73%)	168 (73%)	50 (22%)	11 (5%)	2	11
1	L	241/315 (76%)	171 (71%)	55 (23%)	15 (6%)	1	6
2	C	1117/1119 (100%)	774 (69%)	251 (22%)	92 (8%)	0	3
2	M	1117/1119 (100%)	767 (69%)	246 (22%)	104 (9%)	0	2
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	0
4	O	93/99 (94%)	56 (60%)	27 (29%)	10 (11%)	0	1
5	F	347/423 (82%)	167 (48%)	130 (38%)	50 (14%)	0	0
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 ⓘ

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%)	190 (94%)	12 (6%)	18	50
1	B	210/273 (77%)	194 (92%)	16 (8%)	12	41
1	K	202/273 (74%)	188 (93%)	14 (7%)	14	45
1	L	210/273 (77%)	196 (93%)	14 (7%)	15	46
2	C	941/941 (100%)	853 (91%)	88 (9%)	8	32
2	M	941/941 (100%)	833 (88%)	108 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1264/1279 (99%)	1149 (91%)	115 (9%)	9	33
3	N	1264/1279 (99%)	1136 (90%)	128 (10%)	7	29
4	E	83/87 (95%)	76 (92%)	7 (8%)	10	37
4	O	83/87 (95%)	74 (89%)	9 (11%)	6	26
5	F	304/371 (82%)	276 (91%)	28 (9%)	8	33
5	P	304/371 (82%)	260 (86%)	44 (14%)	3	15
All	All	6008/6448 (93%)	5425 (90%)	583 (10%)	8	30

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	N	762	GLN
5	P	367	MET
3	N	851	LEU
3	N	745	MET
3	N	1441	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 160 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	881	ASN
3	N	1489	GLN
2	M	1030	GLN
3	N	703	ASN
5	P	214	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	M	1120	-	7,7,7	2.21	1 (14%)	9,10,10	1.08	0
8	MPD	C	1120	-	7,7,7	2.31	1 (14%)	9,10,10	1.14	0
6	PO4	A	316	-	4,4,4	1.62	0	6,6,6	0.48	0
10	NE6	D	1529	-	30,30,30	3.82	7 (23%)	28,39,39	1.91	7 (25%)
8	MPD	C	1121	-	7,7,7	2.33	1 (14%)	9,10,10	1.09	0
10	NE6	N	1528	-	30,30,30	3.85	7 (23%)	28,39,39	1.98	6 (21%)
6	PO4	D	1528	-	4,4,4	1.69	0	6,6,6	0.47	0

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	M	1120	-	-	1/5/5/5	-
8	MPD	C	1120	-	-	4/5/5/5	-
10	NE6	D	1529	-	1/1/9/13	11/26/46/46	0/1/1/1
8	MPD	C	1121	-	-	0/5/5/5	-
10	NE6	N	1528	-	1/1/9/13	12/26/46/46	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	-15.20	1.35	1.49
10	D	1529	NE6	C11-C12	-14.55	1.35	1.49
10	D	1529	NE6	O4-C4	11.49	1.38	1.22
10	N	1528	NE6	O4-C4	11.31	1.38	1.22
10	N	1528	NE6	C3-C4	-6.96	1.39	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	1528	NE6	O14-C13-N12	4.84	114.87	108.66
10	D	1529	NE6	O14-C13-N12	4.52	114.46	108.66
10	D	1529	NE6	O1-C2-O2	4.40	121.05	116.94
10	N	1528	NE6	O1-C2-O2	4.29	120.94	116.94
10	D	1529	NE6	O4-C4-C5	-3.97	114.87	121.46

All (2) chirality outliers are listed below:

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

5 of 28 torsion outliers are listed below:

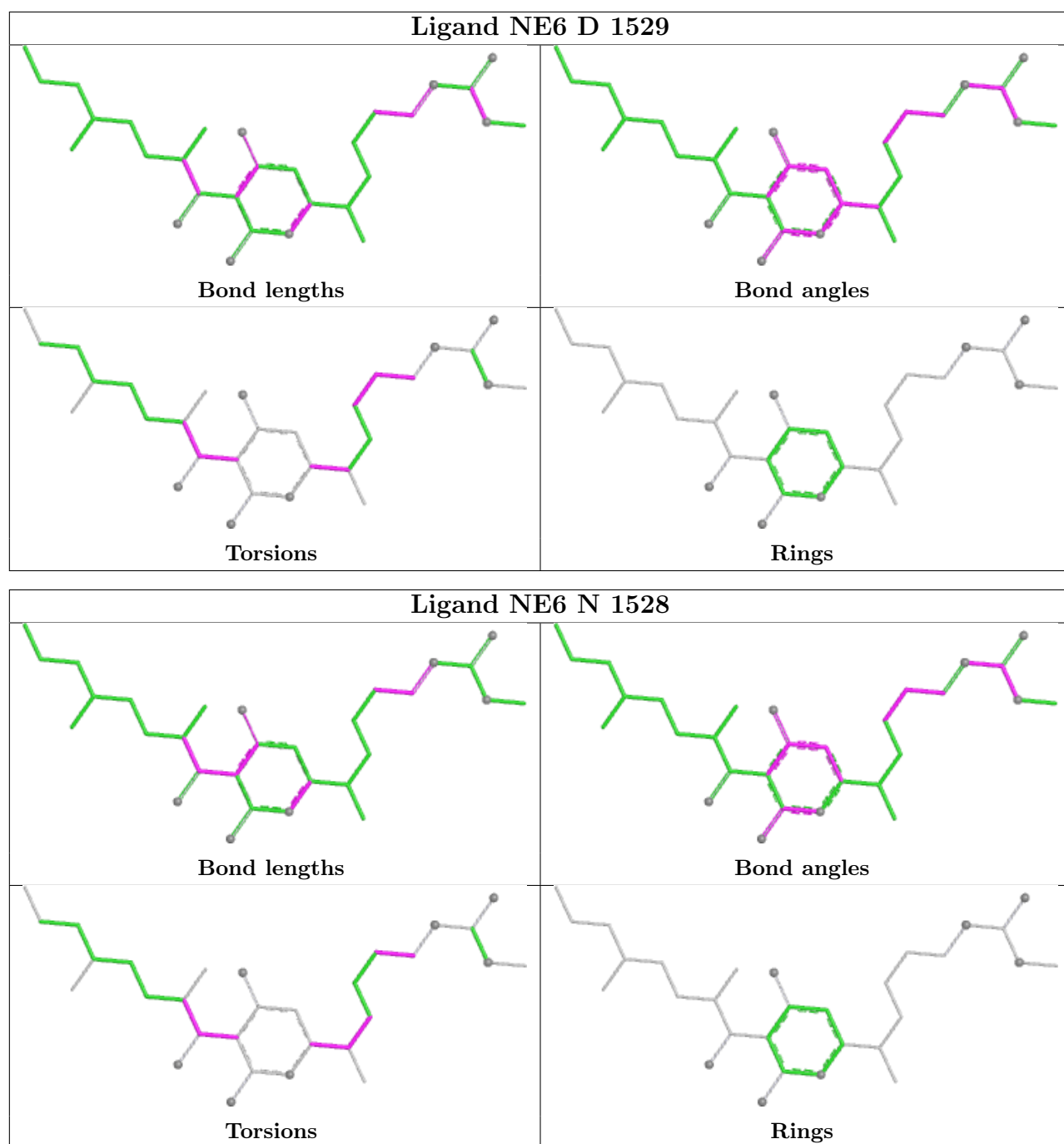
Mol	Chain	Res	Type	Atoms
8	C	1120	MPD	C1-C2-C3-C4
8	C	1120	MPD	O2-C2-C3-C4
10	D	1529	NE6	O15-C15-C3-C2
10	D	1529	NE6	O1-C6-C7-C8
10	D	1529	NE6	O1-C6-C7-C9

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1529	NE6	8	0
10	N	1528	NE6	7	0
6	D	1528	PO4	1	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	231/315 (73%)	-1.69	0 100 100	43, 72, 100, 115	0
1	B	243/315 (77%)	-1.65	0 100 100	51, 93, 113, 117	0
1	K	231/315 (73%)	-1.69	0 100 100	45, 73, 105, 117	0
1	L	243/315 (77%)	-1.64	0 100 100	56, 89, 112, 117	0
2	C	1119/1119 (100%)	-1.67	0 100 100	36, 77, 115, 117	0
2	M	1119/1119 (100%)	-1.68	0 100 100	31, 79, 115, 117	0
3	D	1504/1524 (98%)	-1.65	0 100 100	35, 78, 117, 117	0
3	N	1504/1524 (98%)	-1.64	0 100 100	34, 75, 113, 117	0
4	E	95/99 (95%)	-1.70	0 100 100	51, 88, 113, 117	0
4	O	95/99 (95%)	-1.65	0 100 100	52, 85, 109, 116	0
5	F	349/423 (82%)	-1.68	0 100 100	52, 84, 110, 117	0
5	P	349/423 (82%)	-1.67	0 100 100	51, 85, 110, 117	0
All	All	7082/7590 (93%)	-1.66	0 100 100	31, 79, 115, 117	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands

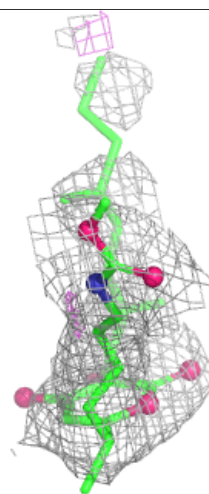
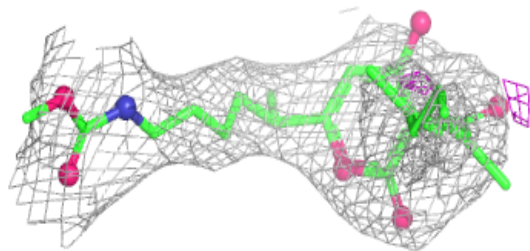
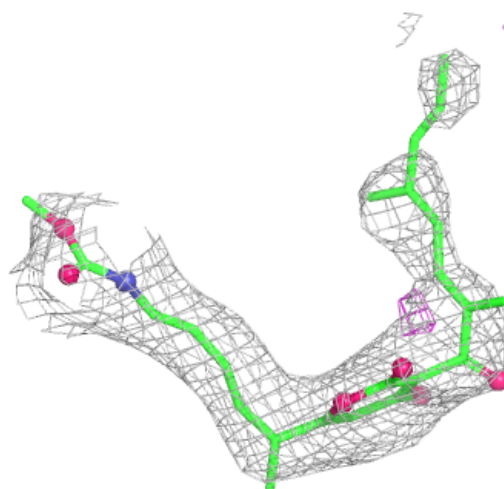
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

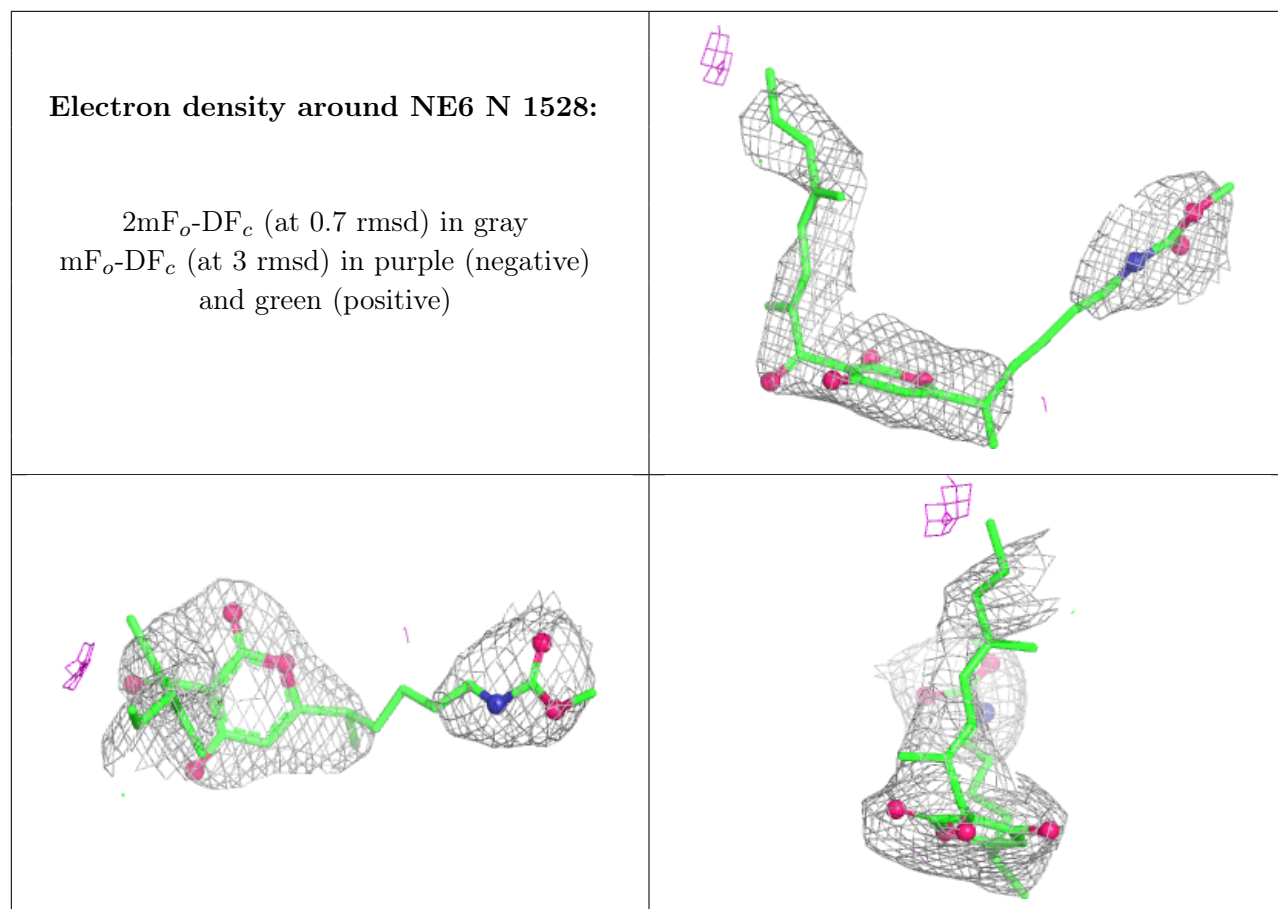
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MPD	M	1120	8/8	0.98	0.10	71,79,84,85	0
6	PO4	D	1528	5/5	0.99	0.03	86,86,86,89	0
8	MPD	C	1120	8/8	0.99	0.09	51,56,57,57	0
8	MPD	C	1121	8/8	0.99	0.06	70,72,73,73	0
6	PO4	A	316	5/5	0.99	0.06	71,73,77,77	0
7	MG	B	701	1/1	1.00	0.04	55,55,55,55	0
7	MG	D	1527	1/1	1.00	0.01	79,79,79,79	0
7	MG	N	1527	1/1	1.00	0.02	56,56,56,56	0
9	ZN	D	1525	1/1	1.00	0.02	91,91,91,91	0
9	ZN	D	1526	1/1	1.00	0.01	77,77,77,77	0
9	ZN	N	1525	1/1	1.00	0.01	50,50,50,50	0
9	ZN	N	1526	1/1	1.00	0.01	55,55,55,55	0
10	NE6	D	1529	30/30	1.00	0.04	52,70,81,85	0
10	NE6	N	1528	30/30	1.00	0.04	72,84,90,91	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 NE6 D 1529:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.