



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:27 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

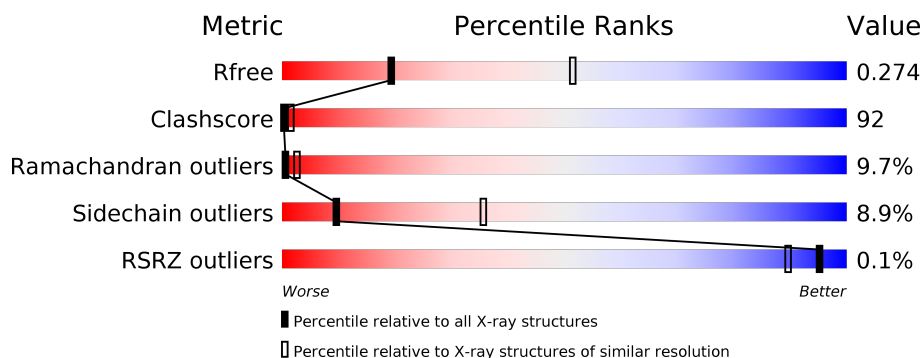
1 Overall quality at a glance ⓘ

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	<div> <div>15%</div> <div>51%</div> <div>6%</div> <div>27%</div> </div>
1	B	315	<div> <div>16%</div> <div>52%</div> <div>9%</div> <div>23%</div> </div>
1	K	315	<div> <div>17%</div> <div>50%</div> <div>6%</div> <div>27%</div> </div>
1	L	315	<div> <div>15%</div> <div>55%</div> <div>7%</div> <div>23%</div> </div>
2	C	1119	<div> <div>18%</div> <div>70%</div> <div>12%</div> <div>•</div> </div>
2	M	1119	<div> <div>17%</div> <div>69%</div> <div>13%</div> <div>•</div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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			

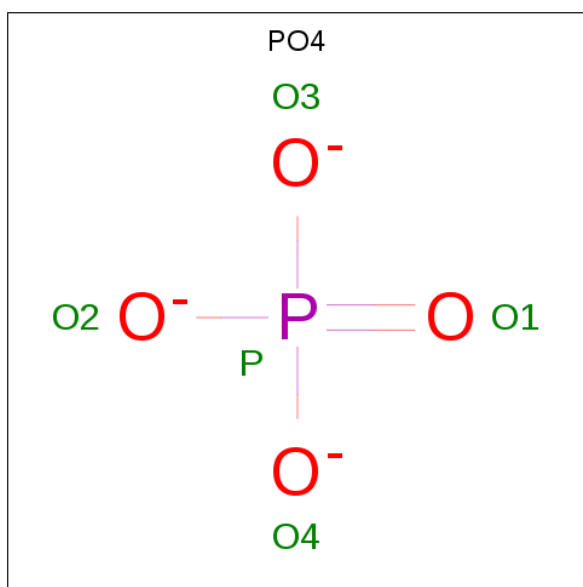
There are 6 discrepancies between the modelled and reference sequences:

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 (three-letter code: PO4) (formula: O₄P).

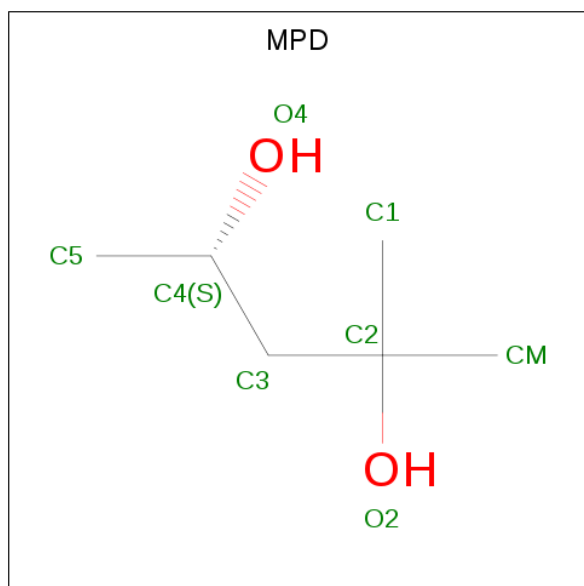


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (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: C₆H₁₄O₂).

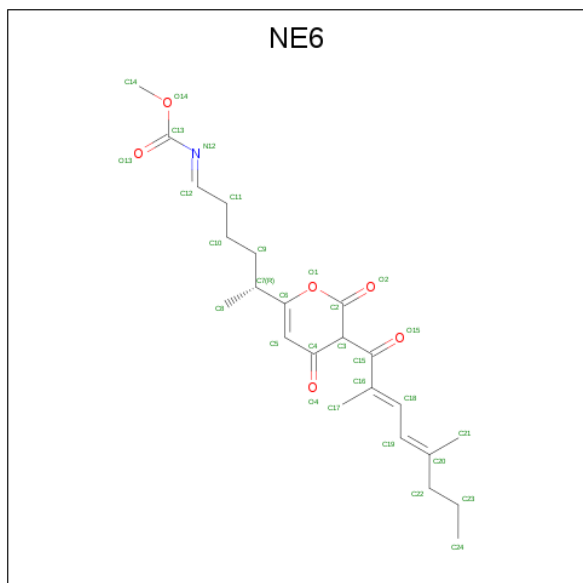


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			8	6	2		
8	C	1	Total	C	O	0	0
			8	6	2		
8	M	1	Total	C	O	0	0
			8	6	2		

- Molecule 9 is ZINC ION (three-letter code: 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-dihydro-3,4-dihydro-2H-pyran-6-yl}hexylidene]carbamate (three-letter code: NE6) (formula: C₂₃H₃₁NO₆).



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

- Molecule 11 is water.

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

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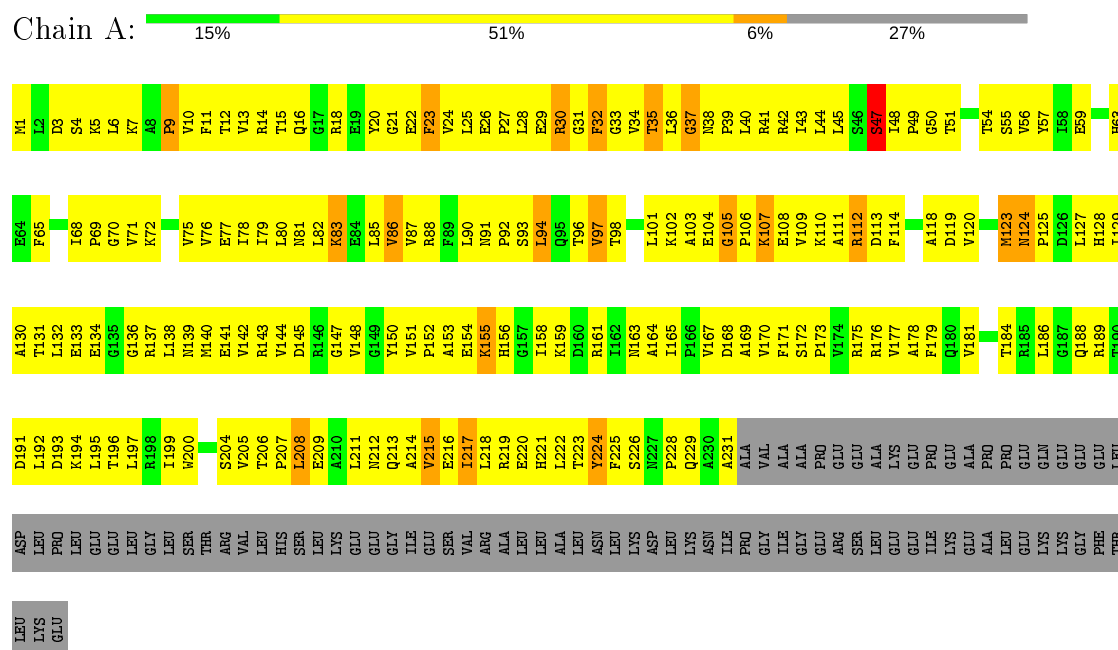
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	5	Total 5	O 5	0	0
11	N	4	Total 4	O 4	0	0
11	O	1	Total 1	O 1	0	0

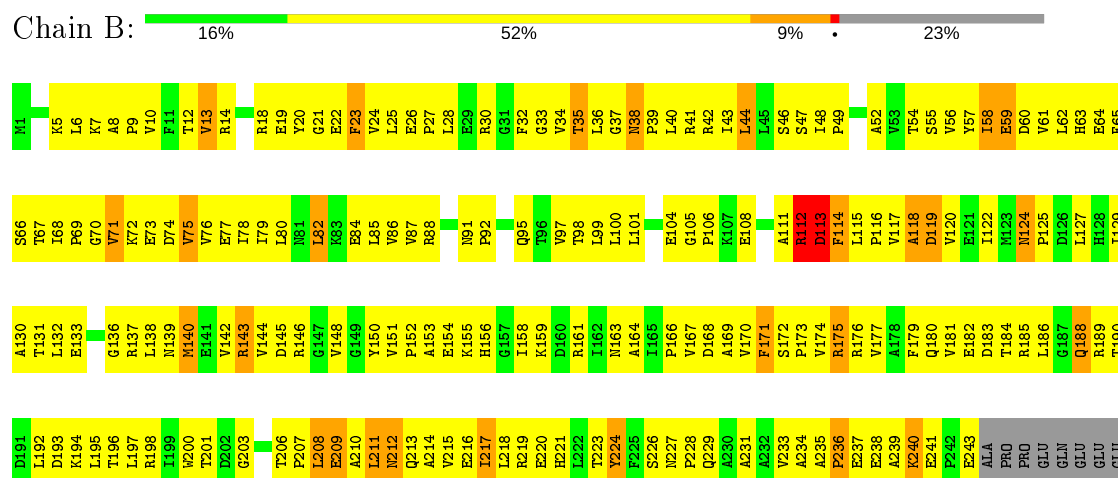
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

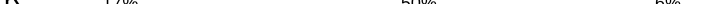


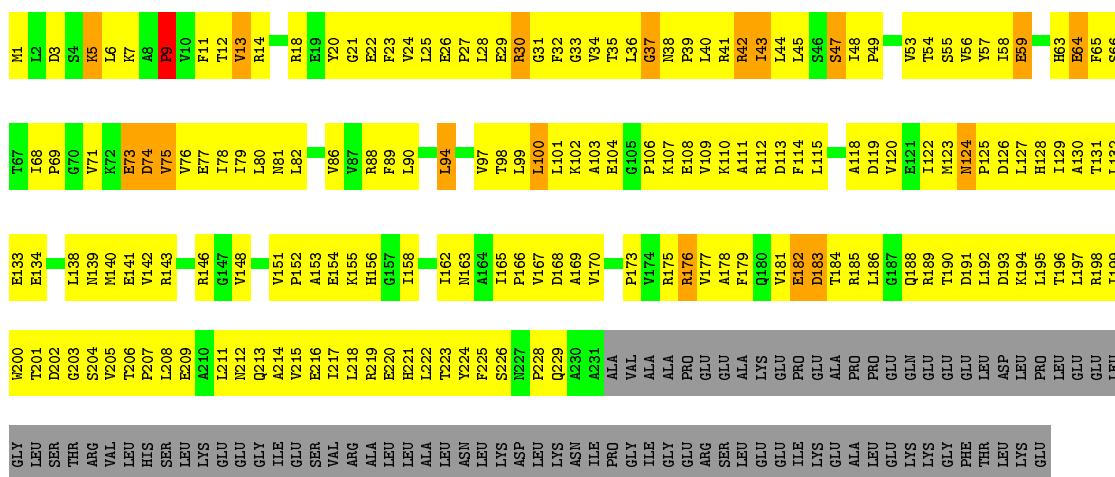
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L



THR	LEU	ASP	PRO	GLU	GLU	GLY	LEU	SER	THR	ARG	VAL	HIS	SER	LEU	LYS	GLU	GLU	GLY	ILE	GLU	SER	GLU	VAL	ARG	ALA	LEU	LEU	ALA	LEU	ASN	LEU	LYS	ASP	LEU	LYS	ASN	ILE	PRO	GLY	ILE	GLY	ARG	SER	LEU	GLU	GLU	ILE	LYS	GLU	ALA	LEU	LYS	GLY	PRO
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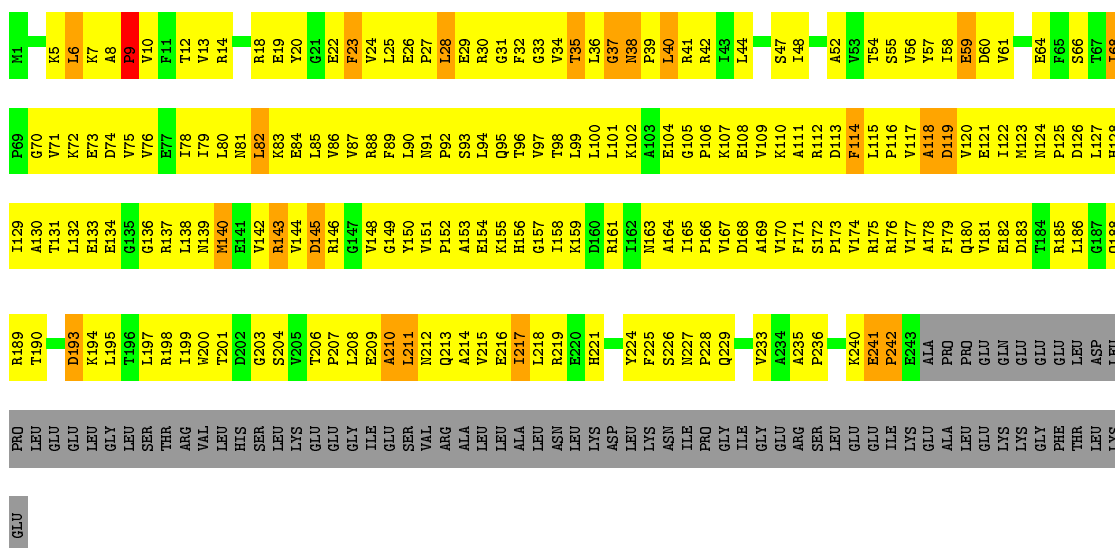
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

Chain K:  17% 50% 6% 27%

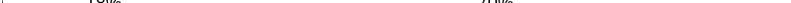


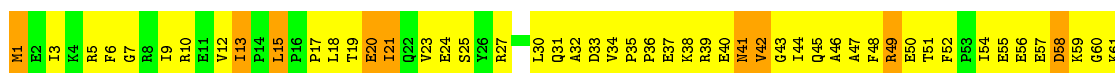
- Molecule 1: DNA-directed RNA polymerase subunit alpha; CHAIN A, B, K, L

Chain L: 15% 55% 7% 23%

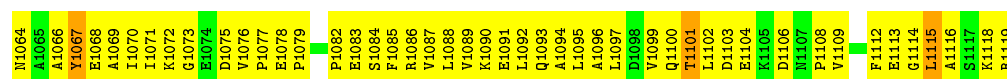


- Molecule 2: BACTERIAL RNA POLYMERASE BETA SUBUNIT; CHAIN C, M

Chain C:  18% 70% 12%

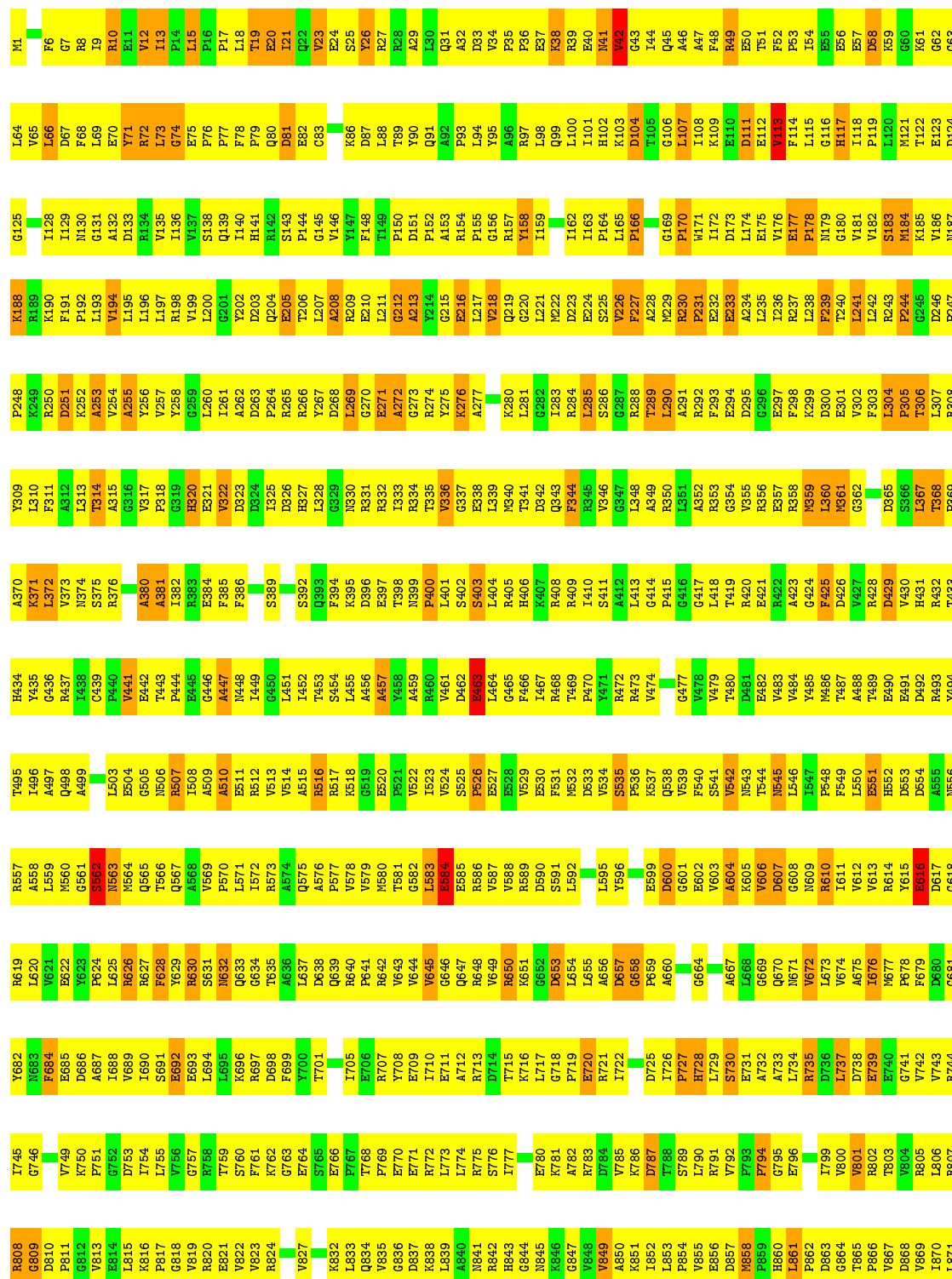


K938	K939	K940	K941	K942	K943	K944	K945	K946	K947	K948	K949	K950	K951	K952	K953	K954	K955	K956	K957	K958	K959	K960	K961	K962	K963	K964	K965	K966	K967	K968	K969	K970	K971	K972	K973	K974	K975	K976	K977	K978	K979	K980	K981	K982	K983	K984	K985	K986	K987	K988	K989	K990	K991	K992	K993	K994	K995	K996	K997	K998	K999	M1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
V1001	E1002	D1003	K1004	M1005	H1006	L1007	L1008	R1009	L1010	L1011	P1012	L1013	S1014	L1015	L1016	L1017	L1018	L1019	L1020	L1021	L1022	L1023	L1024	L1025	L1026	L1027	L1028	L1029	L1030	L1031	L1032	L1033	L1034	L1035	L1036	L1037	L1038	L1039	L1040	L1041	L1042	L1043	L1044	L1045	L1046	L1047	L1048	L1049	L1050	L1051	L1052	L1053	L1054	L1055	L1056	L1057	L1058	L1059	L1060	L1061	L1062	L1063																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
Y876	P877	S878	R879	K880	K881	L882	G883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	M1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
P811	G812	E813	E814	L815	K816	P817	G818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	M1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
W43	A747	E748	K749	K750	K751	P752	G753	G754	L755	L756	G757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	M1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
P880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	M1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L62	G63	L64	V65	L66	D67	F68	L69	E70	Y71	L72	L73	G74	E75	P76	P77	F78	F79	R80	E81	E82	R83	R84	D87	Y90	Q91	A92	P93	L94	Y95	A96	R97	L98	L99	I100	I101	I102	D104	K103	G106	L107	L108	K109	E110	D111	E112	V113	F114	L115	G116	H117	I118	P119	S120	M121	K122	L123	P124	F127	K128	K129	P130	G131	A132	D133	R134	V135	L136	V137	S138	Q139	P140	H141	R142	E205	S143	P144	G145	F148	T149	D151	P152	A153	R154	P155	G156	R157	A158	I159	I162	I163	P164	L165	P166	K167	L205	R168	G169	P170	L171	I172	D173	E174	E175	I236	R237	E177	L238	F239	T240	F302	L241	F303	L242	L243	P305	R243	T306	L307	G245	K308	D246	P247	Y309	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L311	A312	T314	A315	G316	P317	P318	E321	V322	R323	E324	I325	R326	I327	R328	S329	L330	L331	R332	R333	R334	T335	G336	G337	R338	L339	P340	L401	E278	L403	R405	F406	K407	G347	L265	R266	S267	G268	T269	L290	A291	R292	F293	E294	L295	G296	E297	D300	E301	V302	L304	L305	L306	L307	L308	L309	L310	L3



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

Chain M: 17% 69% 13%



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

Chain D: 15% 69% 14% ...

R615	K494	R434	I371	K308	E247	EL83	Tl21	G61
K555	R495	V435	D372	G309	P248	EL84	E122	R62
K556	L496	E436	P373	G310	Y249	V185	L123	V63
L557	E497	V437	E374	L311	L250	K186	E124	K64
L558	V498	D438	E375	R312	P251	K187	Q125	R65
A559	V499	L439	E376	M313	K252	G188	V126	Q66
K601	R500	V440	V377	P314	K253	Q189	L127	R67
K621	A501	R441	I378	R315	E254	EL90	K128	K78
A562	F502	M442	A379	Q316	K255	L191	F129	R69
P563	F503	M443	E380	V317	E256	A192	S130	I110
D624	D504	V444		Q318	G257	P193	K131	A111
Y625	S505	R445	V384	R318	V258	G194	V132	K71
P665	G506	V446	V385	A319	V259	V195	I133	V72
G627	N507	V447	H386					C73
R628	R508	E448	L387	E323	L261	R198	V134	E74
S629	P509	S449	H388	E323	K262	L135	L135	R75
P630	E510	Y450	H389	A324	K263	D199	D136	C76
E570	E510	E451	E390	E325	E263	D200	P137	G77
K571	M511	D451	P390	E326	L264		K138	K17
R572	M512	L452	A391	E327	E265	A203		V78
M573	E513	D453	S392	G328	E266	G139	R19	E79
K574	L514	E454	L393	E329	G267	I141	A140	R81
Q636	E515	R455	L394	T330	A268	R206	L142	K32
K637	A516	M456	V395	V331	P269	N143	N143	V23
A577	V517	G457	V396	V332	L270	P208	G144	G24
K639	P518	R458	K397	L333	V271	R209	V145	R85
D579	V519	E459	A398	T334	L272	R210	P146	V26
A580	L520	A460	R399	L335	R273	V211	V147	R87
L581	P521	I461	V400	F336	K274	R212	E148	Y88
G642	P522	Q462	Y401	L337		K149		R29
G643	D523	Q463	P402	E338	E277	V213	R150	E30
L644	L524	L464	F403	T339	P278	E214	Q151	T31
P645	R525	L465	E404	V340	V279	V215	L152	I32
K646	P526	K466	D405	E341	A280	R217	L153	N33
R647	M527	D467	D406	P342	T281	K218	T154	Y34
M648	V528	L468	V407	K343	Y282	E219	D155	R35
A649	Q529	D469	E408	D44	F283	R220	E156	R36
L650	V530	L470	V409	Y345	L284	A221	E157	L37
E651	D531	E471	S410	R346	P285	G222	R158	P38
L652	G532	A472	T411	V347	V286	L223	R159	A99
F653	G533	L473	G412	Q348	G287	R224	E160	A100
K654	R534	E474	D413	P349	K288	L225	L161	R41
P655	F535	K475	R414	H550	T289	P226	R182	H101
A656	A536	E476	V415	R351	P290			D42
L657	T537	L477	A416	N352	L291	L227	Y183	G43
R598	A538	R478	P417	V353	V292		G164	L44
K659	S538	L479	G418	V354	V293	V231	K165	F45
K660	D539	E479		V355	H294	E232	Q166	D46
M661	L540	E480	L421	V355	G295	R233	E167	E47
E662	M541	M481		E357	E296	V230	T168	R48
S602	D542	K482	A422	E357	G295	E234	Y169	P109
L603	L543	H483	D423	G358	V298	A236	P170	F50
T604	Y544	P484	G424	A359	L297	Y236	L171	S110
D605	R545	S485	G425	R360	E299	K237	P172	K111
I606	R546	R486	K426	K360	K300	P238	G113	P52</



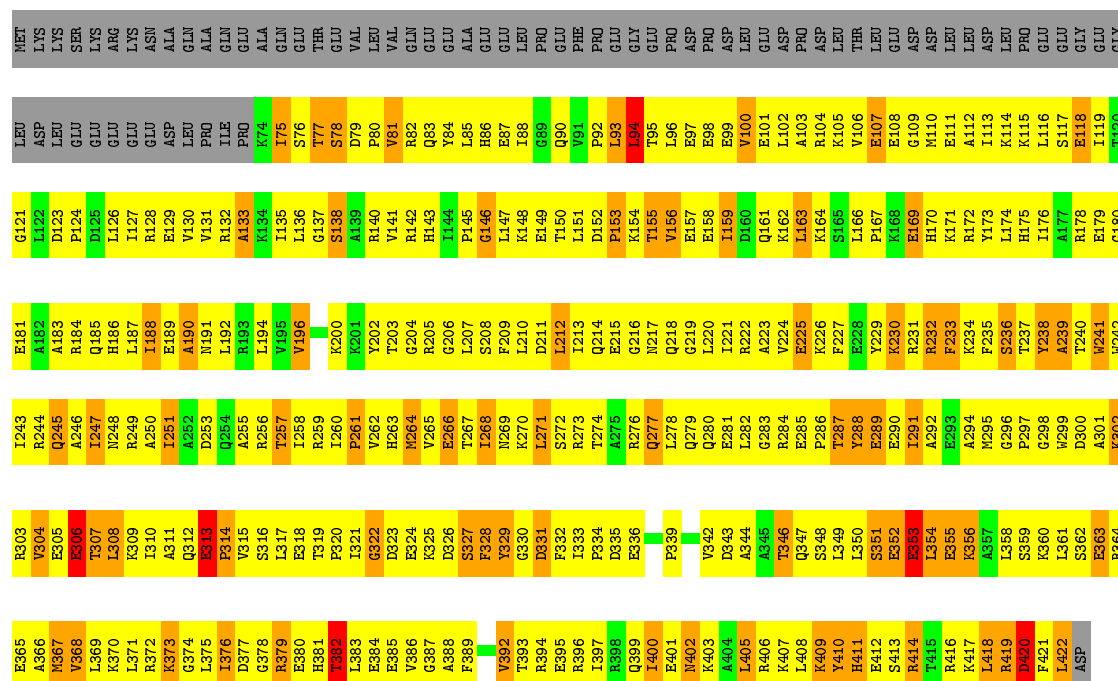
T997	L930	Y868	T808	A746	L677	Q616	K555	R495	V435	A370	G309	P248	V186	K64
E996	L931	K871	P809	V747	E678	M617	K556	L496	E436	L371	L310	Y249	K187	R65
T999	D932	K872	E811	V748	R679	L618	L557	E497	V437	B372	L311	L250	G188	Q66
T1000	A933	R873	E812	V749	Q680	L619	L558	V498	D438	P373	R312	F251	P189	E69
E1001	L934	L873	A813	P750	Q681		A559	R500	V439	E374	R313	R252	E190	F129
K1002	K935	E874	L813	P751			Q560	R501	V440	E375	R314	R253	E191	G70
T1003	Y936	T875	A814		I683	R622	G561	A501	R441	E376	R315	E254	K131	K71
T1004	Y937	S876	A815	F754	K684	V623	A562	F502	M442	R377	Q316	E255	Y132	W72
Q1005	G938	R877	R816	A755	D685	D624	P663	L503	V443	L378	V317	E256	Y195	C73
A1006	P939	G878	R817	A756	E686	Y625	E564	D504	V444	A379	R318	G257	V196	E74
V1007	T940	R879	R818	A757	S626	S627	I565	S505	R445	E380	R319	V258	S197	R75
F1008	F941	I880	G819	E758	R628	R629	I566	G506	V446	A381	A320	V259	R198	C76
K1009	S942	L881	E820	A759	L691	S629	I567	N507	V447		Q321	E260	P137	G77
H1010	T943	F882	V821	R760	E692	V630	R568	R508	E448		V322	L261	L199	G77
F1011	T944	A883	A822	I761	E693	I631	I569	P509	S449	V385	E329	L262	D200	V78
N1012	S945	L884	L823	Q762	V694	V632	E570	E510	Y450	L387	E323	R263	G201	E79
E1013	E946	I885	N824	N763	I695	V633	K571	N511	D451	L388	A324	E264	V202	V80
H1014	I947	V886	A825	L764	G634	G635	R572	N512	I452	R389	E325	L264	A203	T81
Y1015	T948	A887	R826	S765	G697	P635	R573	L513	D453	E389	E326	E265	L204	T82
P1016	I949	E888	I827	A766	K698	Q636	L574	L514	A454	P390	E327	E266	Y205	S83
F1017	G950	A889	K828	H767	V699	L637	Q575	E515	A455	A391	G326	G267	R206	I84
N1018	I951	V890	V829	A768	V700	K638	E576	A516	N456	S392	E329	A268	P208	V85
P1019	D952	E891	A830	L769	L701	L639	A577	V517	Q457	L394	V330	F269	P146	R86
L1020	D953	D892	G831	L770	L702	H640	N578	P518	A458	V395	V332	L270	R209	R87
A954	Y1021	E893	R832	S771	N703	O641	D579	V519	E459	V396	L333	L272	R210	Y88
V1022	V955	K894	E833	P772	R704	C642	A580	L520	A460	K397	T334	R273	R212	R89
M1023	I956	A895	T834	A773	H709	G643	L581	P521	I461	A398	L335	R274	E213	M90
A1024	S957	A896	S835	S774	R710	P645	L582	P522	Q462	K399	E336	E275	V214	G91
E958	E958	V897	V836	Q775	R711	K646	N584	D523	Q463	V400	L337	D276	E215	R92
S1026	E959	E998	G837		L711	G646	N584	L524	L464	Y401	E338	E277	V216	I93
G1027	K960	L899	R838	A778	G712	R647	G585	R525	L465	P402	V339	P278	K217	E94
A1028	K961	I900	L839	L778	I713	M648	R586	P526	K466	P403	T340	V279	K218	L95
R1029	Q962	Q901	R840	K780	Q714	A649	R587	N527	E467	E404	E341	A280	E219	A86
G1030	Y963	L902	D964	P781	A715	L650	P590	V528	L468	P405	P342	T281	R220	T97
M1031	L964	L903	Y841	S782	F716	L651	V591	L530	L469	D406	E343	Y282	A221	P88
P1032	E965	V904	F943	R783	Q717	L652	T592	D531	L470	V407		F283	G222	A99
E966	E966	P905	A844	D784	F653	K654	T593	D532	E471	E408	R346	L284	L223	A100
A967	A967	Q906	N845	I785	K654	P655	N593	G533	A472	V409	V347	P285	E224	H01
D968	D968	E907	P846	I786	F656	P656	G595	R534	E474	S410	Q348	R286	L225	I102
R1036	R969	K908	D847	L787	Q724	L657	S596	F535	K475	Q412	P349	G287	P226	M03
Q1037	K970	N909	E848	G788	S725	L658	D597	A536	E476	D413	R350	M288	L227	F104
L1038	L971	S910	A949	L789	I726	K659	R598	T537	L477	R414	K351	T289	A228	V105
C1039	L972	L911	L850	Y790	Q727	K660	P599	S538	L478	V415	V353	P290	A229	K106
G1040	Q973	K912	L851	Y791	L728	M661	P599	D539	E479	V416	V354	L281	W230	D107
L1041	I974		A852	I792	H729	M662	L800	S539	E480	A416	V355	V282		V108
G1043		V915	V853	F793	F730	E662	R601	L540	E481	P417	V356	V293	K233	P109
	L983	Y916	A854	Q794	L731	E663	S602	N541	D481	Q418	P356	H294	E234	S110
	T984	Q117	R855	V795	V732	K664	L603	D542	K482	D419	E357	G295	A235	I112
	D985	A918	G856	R796	Q733	G665	T604	L543	H483	V420	G358	E296	Y236	G113
K1047	R986	F919	I857	K797	E734	I666	D605	V544	P484	L421	A359	L297	K237	T114
P1048	E987	L820	V858	E798	A735	A667	I806	R545	S488	A422	K360	V298	P238	L115
S1049	R988	R821	D859	K799	F736	P668	L607	R546	R486	D423	V361	E299	G239	D176
G1050	Y989	L922	L860	N737	M669	V670	S608	L547	A487		E362	K300	E240	L116
E1051	D990	G923	Q861	A738	R738	V670	G609	L548	R488	K428	A363	Q301	I241	D117
T1052	Q991	N924	D862	A802	D739	K671	K610	N549	R489	S429	G364	Q302	L242	L118
F1053		E925	V863	G803	F740	A672	Q611	R550	A490	D430	D365	A243	K180	S119
	L993	K926	V864	L804	A673	A673	G612	N551	K491	V431	K366	E244	E244	T121
P1056	V1056	T927	T865	E805	D743	R674	R613	N552	A492	Y432	I367	L245	P246	E122
V1057	F066	Q744	V866	F806	Q744	R675	F614	R553	R493	G433	V368	A307	P368	E183
R1058		V996	R867	A807	M745	M676	R615	L554	K494	R434	A369	K308	E247	E124



V368	L308	Q245	A182	G121	LEU	MET
L369	R309	A246	A183	L122	ASP	LYS
K370	L310	A247	R184	D123	LEU	LYS
L371	A311	M248	Q185	P124	GLU	LYS
K372	R312		H186	D125	GLU	SER
K373	E313	T251	L187	L126	GLU	ARG
G374	G314		T188	I127	GLU	LYS
L375	P315	A255	E189	R128	GLU	ASN
L376	S316	R256	A190	E129	ASP	ALA
D377	L317	T257	M191	V130	LEU	ALA
G378	E318	L258	L192	V131	PRO	ALA
R379	T319	E259	R193	A132	ILE	GLN
E380	P320	T260	L194	R133	PRO	GLU
H381	L321	P261	V195	K134	K74	ALA
T382	G322	T262	V196	I135	I75	GLN
L383	D323	D263	S197	L136	S76	GLU
E384	E324	M264	L198	G137	T77	THR
E385	K325	V265		S138	S78	GLU
V386	D326	E266	T203	A139	D79	VAL
G387	S327	T267	G204	R140	PRO	LEU
A388	F328	T268	R205	V141	V81	VAL
	Y329	M269	G206	R142	R82	GLN
V392	G330	K270	L207	H143	Q83	GLU
T393	B331	L271	S208	I144	Y84	GLU
F394	F332	S272	P209	P145	L85	ALA
E395	I333	R273	L210	G146	H86	GLU
R396	K334	T274	D211	L147	E87	GLU
I397	D335	A275	L212	K148	I88	LEU
R398	E336	R276	T213	E149	G89	PRO
Q399	H337	Q277	Q214	T150	Q90	GLU
L400	L338	L278	E215	L151	V91	PHI
E401	P339	Q279	G216	D152	P92	PRO
K402	S340	Q280	N217	P153	L93	GLU
K403	P341	E281	Q218	K154	L94	GLY
A404	V342	L282	G219	T155	T95	GLU
L405	D343	G283	L220	V156	L96	PRO
R406	A344	R284	T221	E157	E97	ASP
K407	A345	E285	R222	E158	E98	PRO
L408	T346	T286	A223	I159	E99	ASP
K409	Q347	T287	V224	D160	V100	LEU
Y410	S348	T288	E225	Q161	E101	GLU
H411	L349	E289	K226	K162	L102	ASP
A412	L350	E290	F227	L163	A103	PRO
S413	S351	T291	E228	K164	R104	ASP
R414	E352	A292	Y229	S165	K105	LEU
T415	E353	E293	K230	L166	V106	THR
R416	L354	A294	R231	P167	E107	LEU
K417	E355	M295	R232	K168	E108	GLU
L418	L356	G296	F233	E169	G109	ASP
R419	A357	T297	K234	H170	M110	ASP
D420	L358	F238	F235	K171	E111	LEU
F421	S359	W299	S236	R172	A112	LEU
L422	K360	D300	T237	Y173	I113	ASP
	L361	A301	Y238	L174	K114	LEU
	S362	R302	A239	H175	K115	PRO
	E363	R303	T240	I176	L116	GLU
	R364	V304	W241	A177	S117	GLY
	E365	E305	W242	R178	E118	GLY
	A366	E306	T243	I119	T120	GLY
	W367	T207		F181		

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

Chain P: 9% 55% 18% • 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	235.09 Å 235.09 Å 250.88 Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.01 Å)	Xtriage
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 ²)	83.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 46.6	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	0.95	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	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

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%)	1 6
1	B	241/315 (76%)	159 (66%)	64 (27%)	18 (8%)	1 5

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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 ⓘ

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
5	F	335	ASP
2	M	184	MET
4	O	86	GLN
5	F	398	ARG
1	L	68	ILE

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

Mol	Chain	Res	Type
3	D	1489	GLN
1	K	81	ASN
5	P	170	HIS
4	E	86	GLN
5	F	263	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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	1121	-	7,7,7	2.24	1 (14%)	9,10,10	1.11	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
8	MPD	C	1120	-	7,7,7	2.22	1 (14%)	9,10,10	1.16	0
10	NE6	N	1528	-	29,30,30	3.64	7 (24%)	27,39,39	1.81	4 (14%)
10	NE6	D	1529	-	29,30,30	3.60	7 (24%)	27,39,39	1.77	4 (14%)
8	MPD	M	1120	-	7,7,7	2.12	1 (14%)	9,10,10	1.09	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	C	1121	-	-	0/5/5/5	-
10	NE6	N	1528	-	1/1/9/13	11/26/46/46	0/1/1/1
10	NE6	D	1529	-	1/1/9/13	9/26/46/46	0/1/1/1
8	MPD	C	1120	-	-	5/5/5/5	-
8	MPD	M	1120	-	-	2/5/5/5	-

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	N	1528	NE6	C3
10	D	1529	NE6	C3

5 of 27 torsion outliers are listed below:

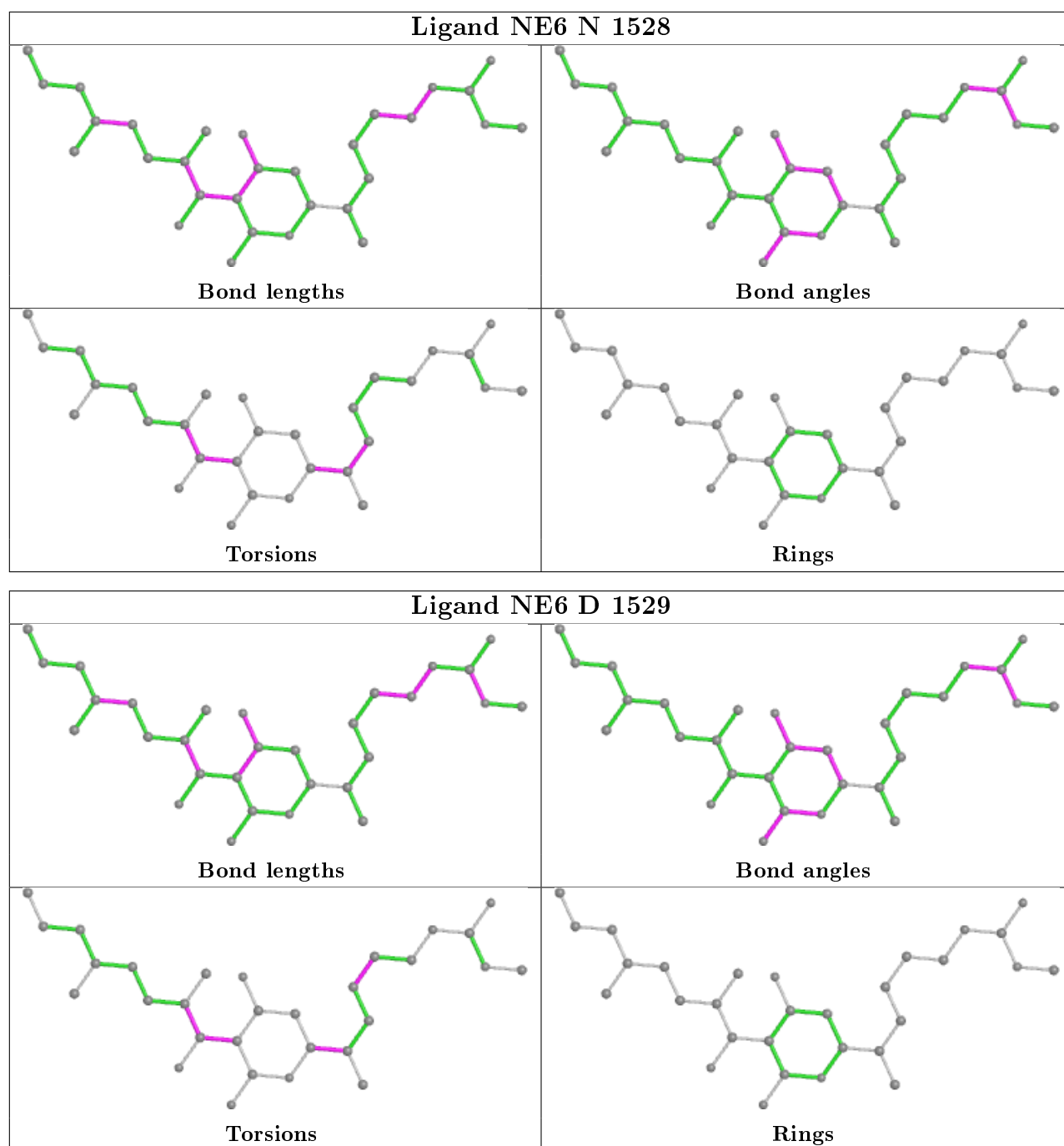
Mol	Chain	Res	Type	Atoms
8	C	1120	MPD	C1-C2-C3-C4
8	C	1120	MPD	O2-C2-C3-C4
10	N	1528	NE6	O1-C6-C7-C8
10	N	1528	NE6	O1-C6-C7-C9
10	N	1528	NE6	C8-C7-C9-C10

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1528	PO4	1	0
10	N	1528	NE6	7	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, 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%)	-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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

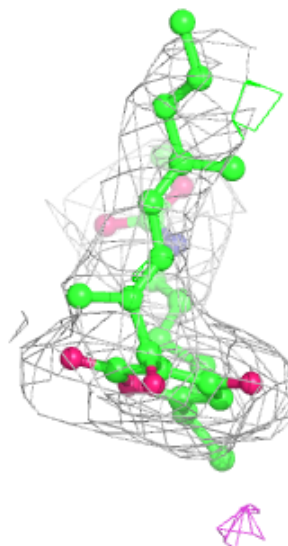
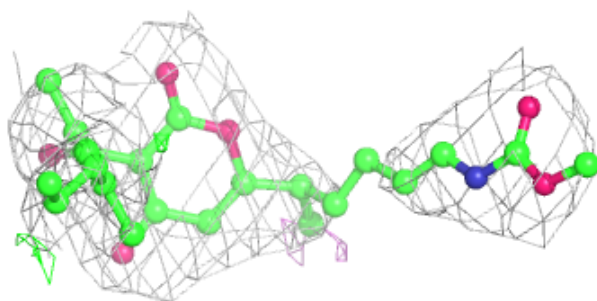
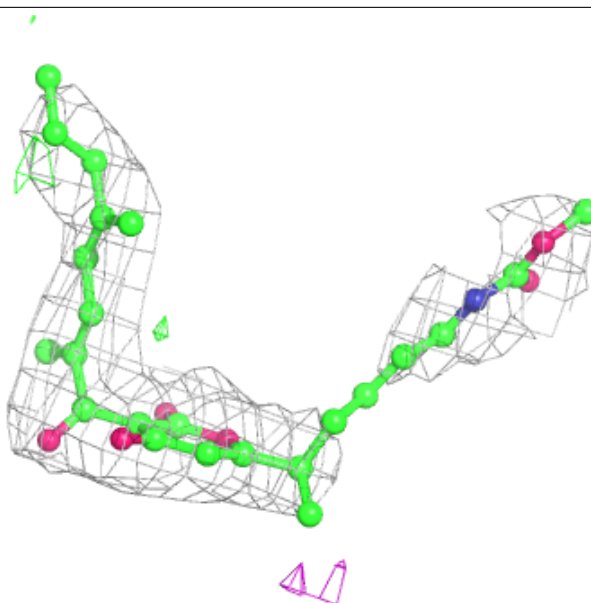
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

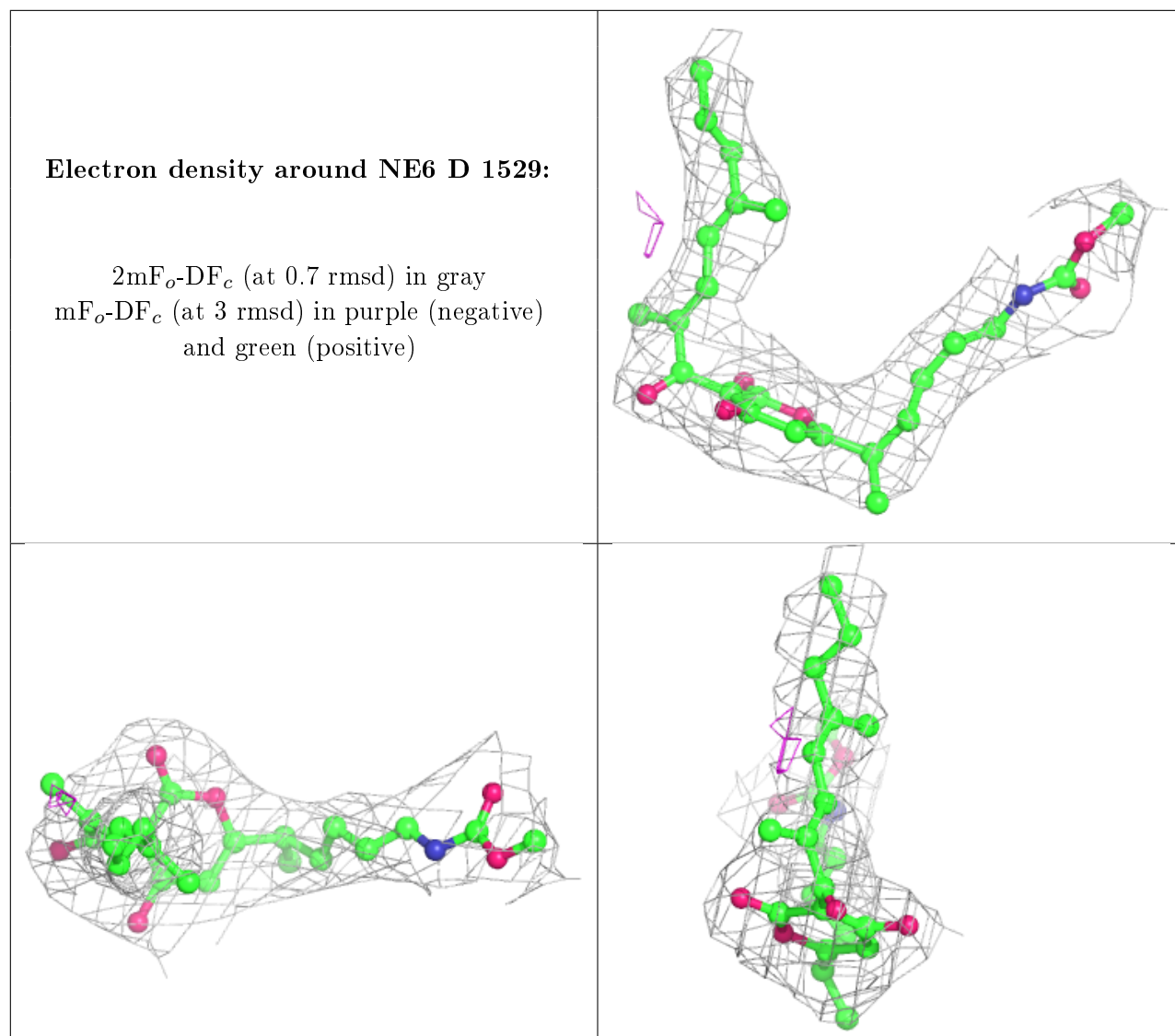
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MPD	M	1120	8/8	0.92	0.17	71,79,84,85	0
10	NE6	N	1528	30/30	0.94	0.29	72,84,90,91	0
7	MG	D	1527	1/1	0.96	0.07	79,79,79,79	0
6	PO4	A	316	5/5	0.96	0.18	71,73,77,77	0
9	ZN	D	1525	1/1	0.96	0.17	91,91,91,91	0
8	MPD	C	1121	8/8	0.96	0.15	70,72,73,73	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
7	MG	N	1527	1/1	0.97	0.04	56,56,56,56	0
7	MG	B	701	1/1	0.97	0.20	55,55,55,55	0
8	MPD	C	1120	8/8	0.97	0.17	51,56,57,57	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.

Electron density around NE6 N 1528:

$2mF_o-DF_c$ (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.