



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:08 PM UTC

PDB ID : 4XLS / pdb_00004xls
Title : Crystal structure of T. aquaticus transcription initiation complex with CarD containing upstream fork promoter.
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-13
Resolution : 4.01 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:

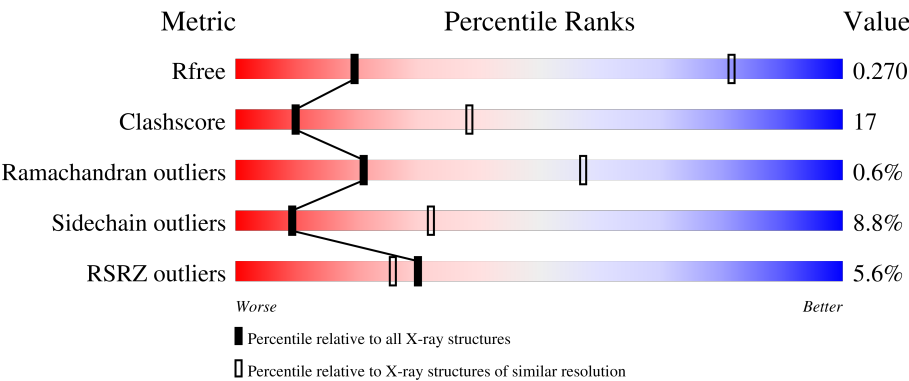
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.01 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	1095 (4.24-3.80)
Clashscore	190562	1142 (4.24-3.80)
Ramachandran outliers	187476	1074 (4.24-3.80)
Sidechain outliers	187428	1065 (4.24-3.80)
RSRZ outliers	180081	1095 (4.24-3.80)

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	314	4% 40% 29% • 28%
1	B	314	4% 43% 27% • 28%
1	G	314	9% 40% 29% • 28%
1	H	314	4% 38% 32% • 28%
2	C	1119	6% 55% 39% 5% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	M	164	
6	N	164	
7	O	30	
7	R	30	
8	P	24	
8	S	24	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 58966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a protein called CarD-like transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	162	Total	C	N	O	S	0	0	0
			1274	807	234	231	2			
6	N	162	Total	C	N	O	S	0	0	0
			1274	807	234	231	2			

- Molecule 7 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			
7	R	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			

- Molecule 8 is a DNA chain called DNA (5'-D(P*GP*CP*AP*CP*AP*AP*TP*TP*TP*AP*AP*CP*AP*CP*TP*TP*TP*TP*GP*TP*CP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	24	Total	C	N	O	P	0	0	0
			489	235	86	144	24			
8	S	24	Total	C	N	O	P	0	0	0
			489	235	86	144	24			

- 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	J	2	Total	Zn	0	0
			2	2		

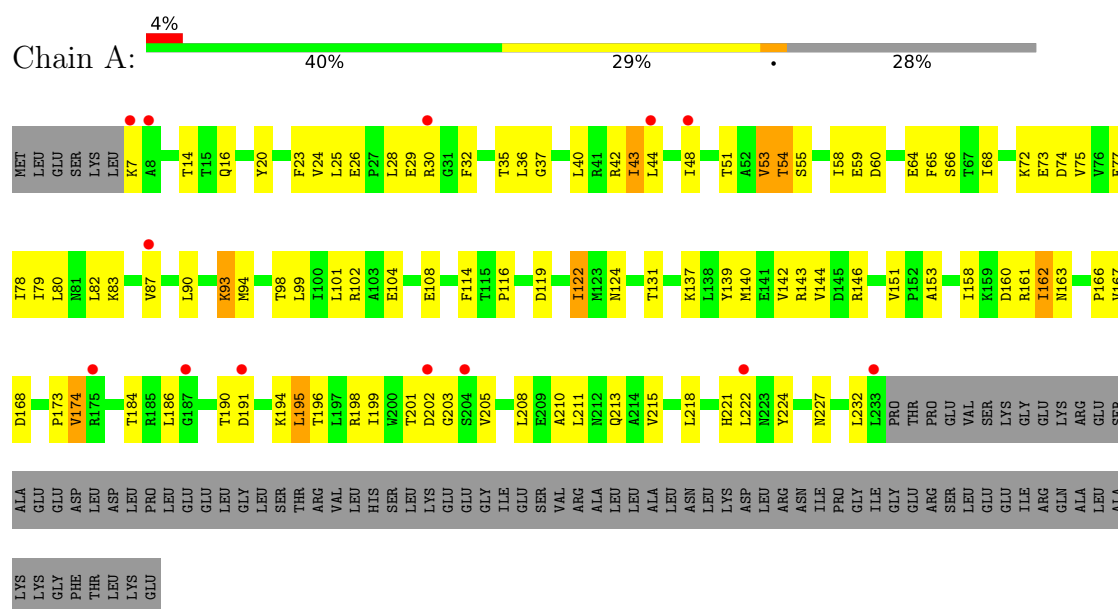
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total 1	Mg 1	0	0
10	J	1	Total 1	Mg 1	0	0

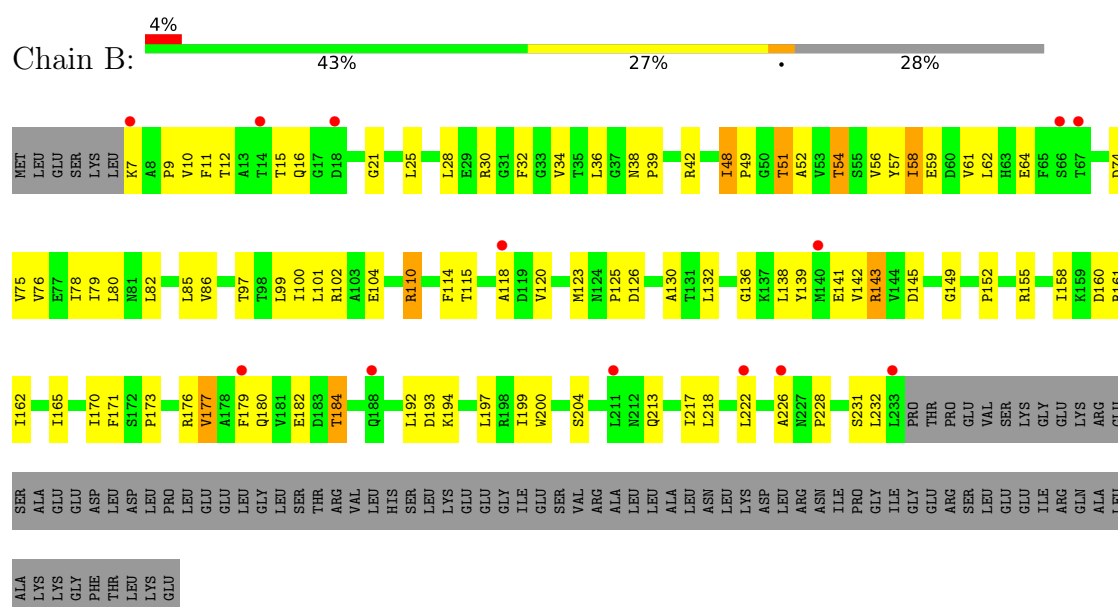
3 Residue-property plots [i](#)

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



• Molecule 1: DNA-directed RNA polymerase subunit alpha



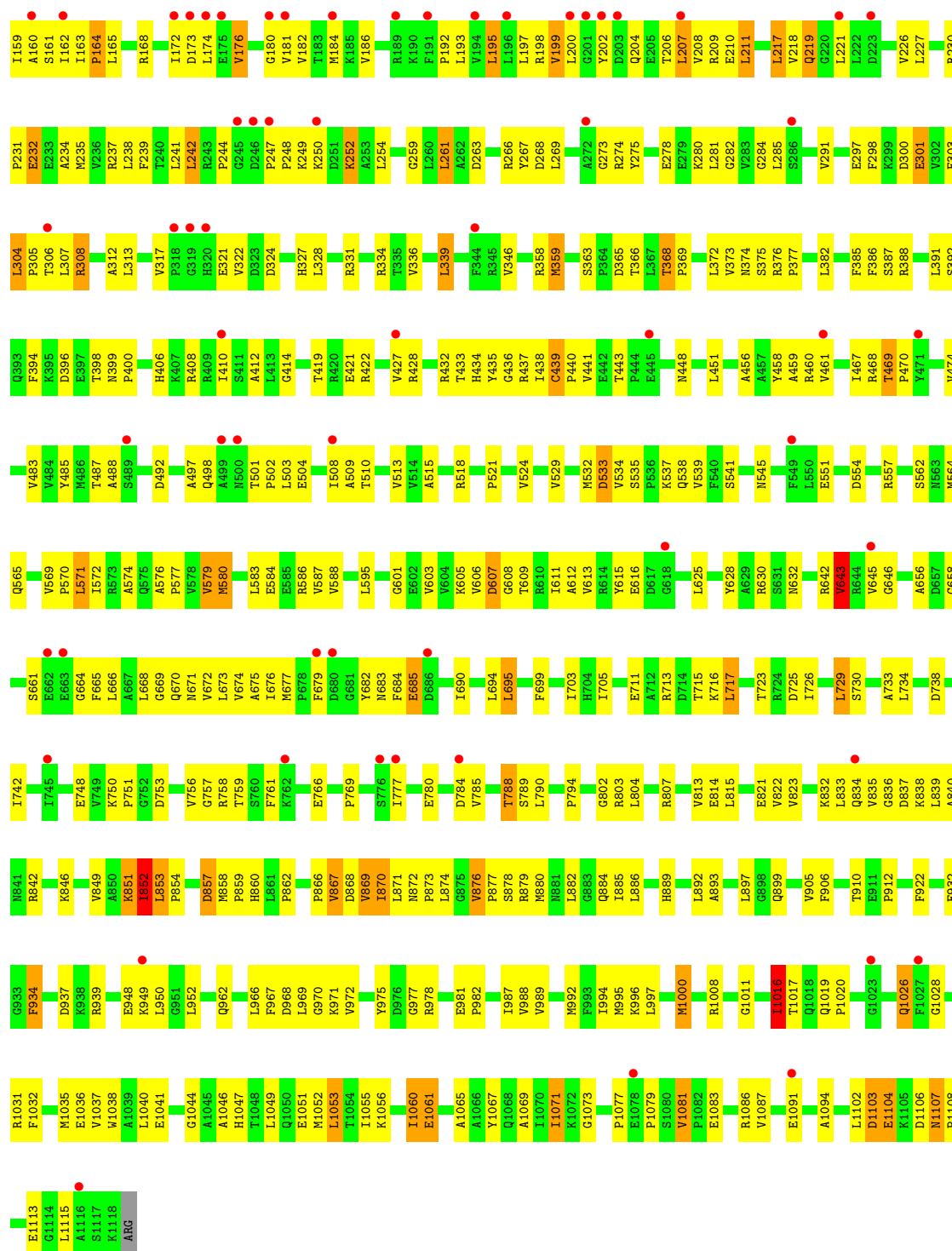
[illegible]

Chain H:

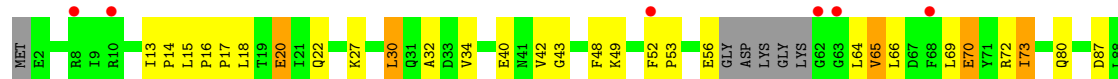
Residue Type	Count
Other	28
Non-polar	32
Polar	38
Other (Small)	4

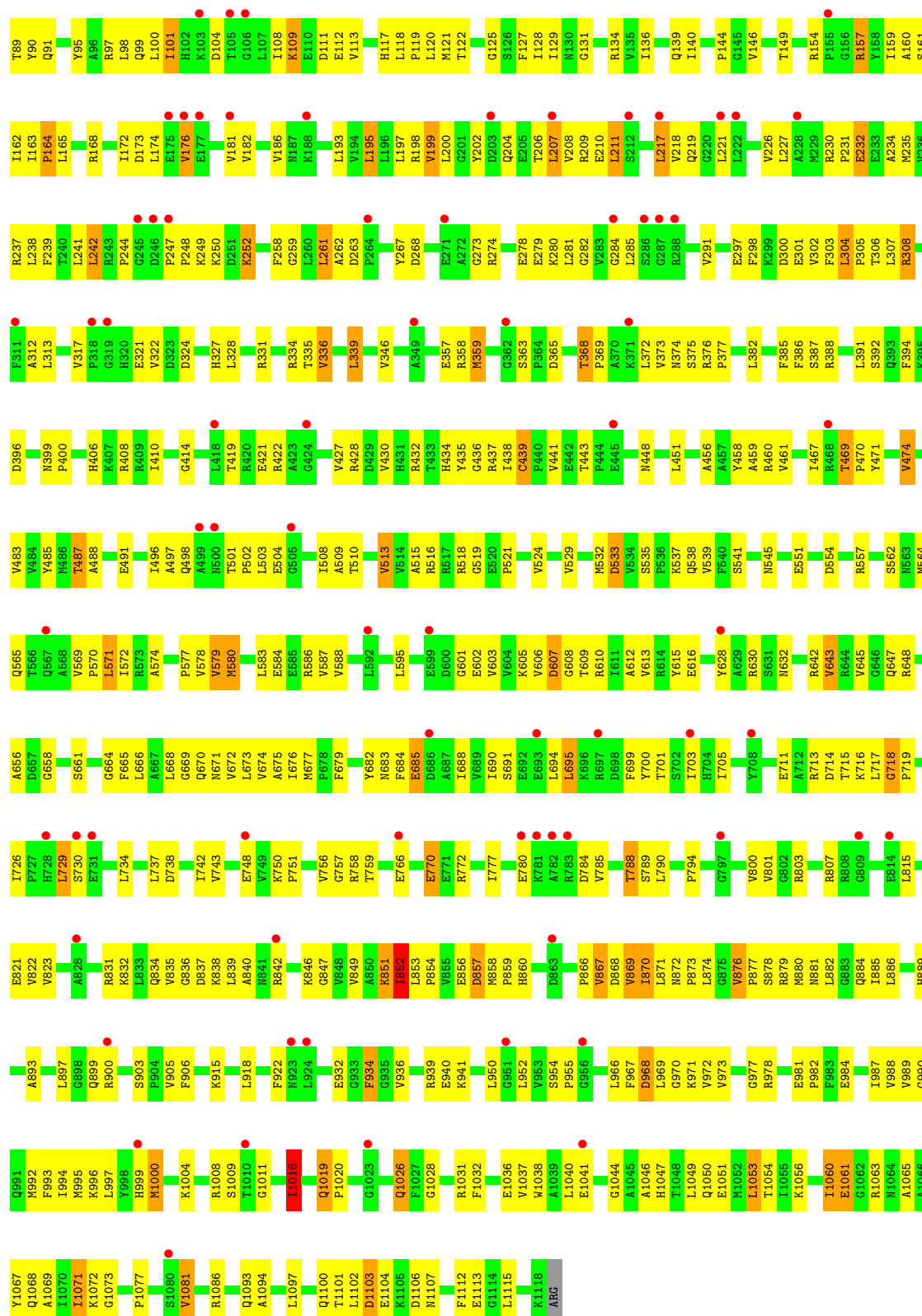
Chain C:

Amino Acid	Count	Category
K86	1	Other
D87	1	Other
L88	1	Other
T89	1	Other
Y90	1	Other
Q91	1	Other
A92	1	Other
P93	1	Other
L94	1	Other
Y95	1	Other
A96	1	Other
R97	1	Other
L98	1	Other
Q99	1	Other
L100	1	Other
I101	1	Other
D104	1	Other
I108	1	Other
K109	1	Other
E110	1	Other
D111	1	Other
E112	1	Other
V113	1	Other
F114	1	Other
L115	1	Other
G116	1	Other
H117	1	Other
L118	1	Other
P119	1	Other
L120	1	Other
M121	1	Other
G125	1	Other
S126	1	Other
F127	1	Other
I128	1	Other
I129	1	Other
N130	1	Other
G131	1	Other
R134	1	Other
V135	1	Other
I136	1	Other
Q139	1	Other
I140	1	Other
H141	1	Other
P144	1	Other
G145	1	Other
V146	1	Other
T149	1	Other
R154	1	Other
R157	1	Other
L158	1	Other
MET	1	Other
E2	1	Other
R10	1	Other
E11	1	Other
V12	1	Other
I13	1	Other
P14	1	Other
L15	1	Other
P16	1	Other
P17	1	Other
L18	1	Other
T19	1	Other
E20	1	Other
I21	1	Other
Q22	1	Other
K27	1	Other
L30	1	Other
Q31	1	Other
A32	1	Other
F36	1	Other
V42	1	Other
Q43	1	Other
A46	1	Other
A47	1	Other
F48	1	Other
K49	1	Other
E50	1	Other
T51	1	Other
F52	1	Other
E56	1	Other
GLY	1	Other
ASP	1	Other
LYS	1	Other
GLY	1	Other
LYS	1	Other
G62	1	Other
G63	1	Other
L64	1	Other
V65	1	Other
L66	1	Other
L69	1	Other
E70	1	Other
Y71	1	Other
R72	1	Other
I73	1	Other
G74	1	Other
G75	1	Other
Q80	1	Other
R84	1	Other
R95	1	Other



• Molecule 2: DNA-directed RNA polymerase subunit beta

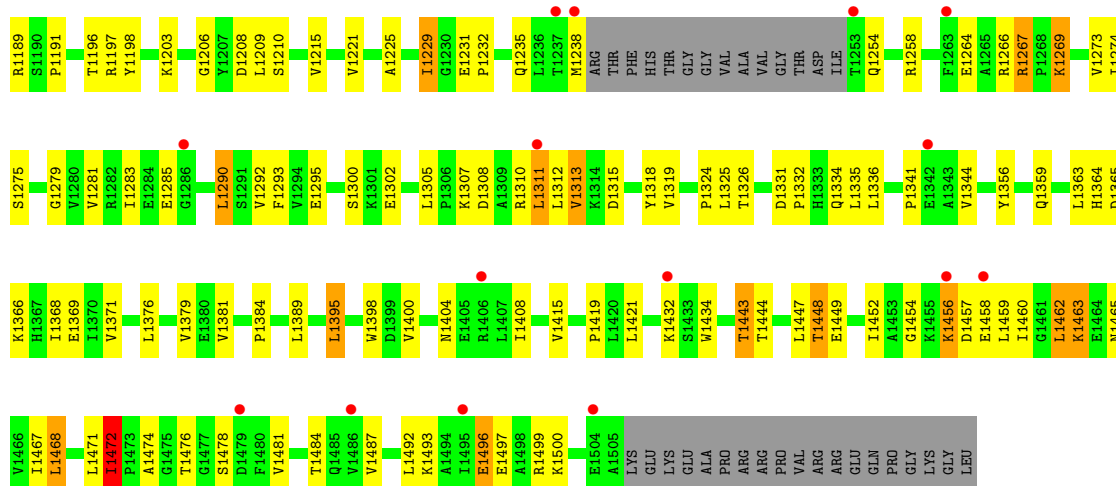




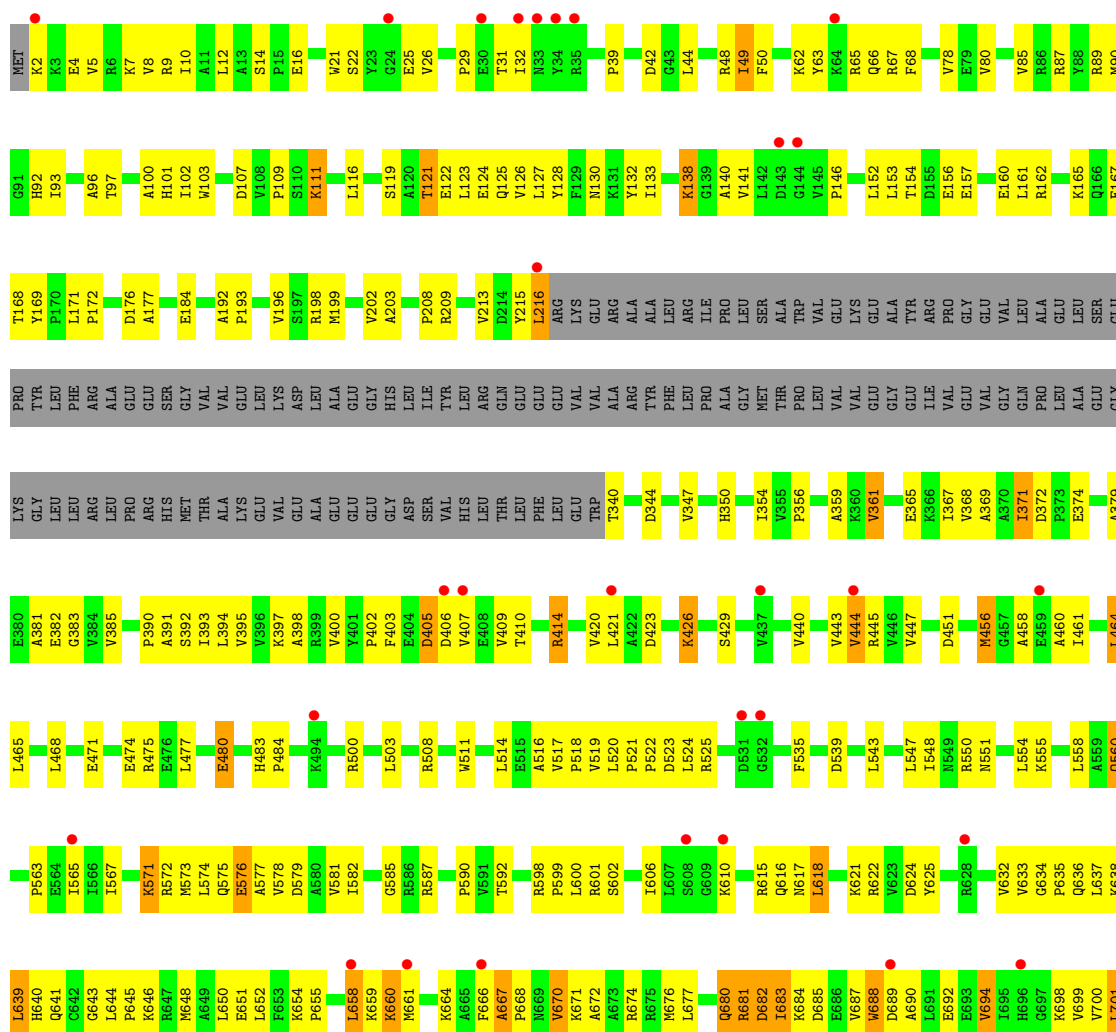
• Molecule 3: DNA-directed RNA polymerase subunit beta'

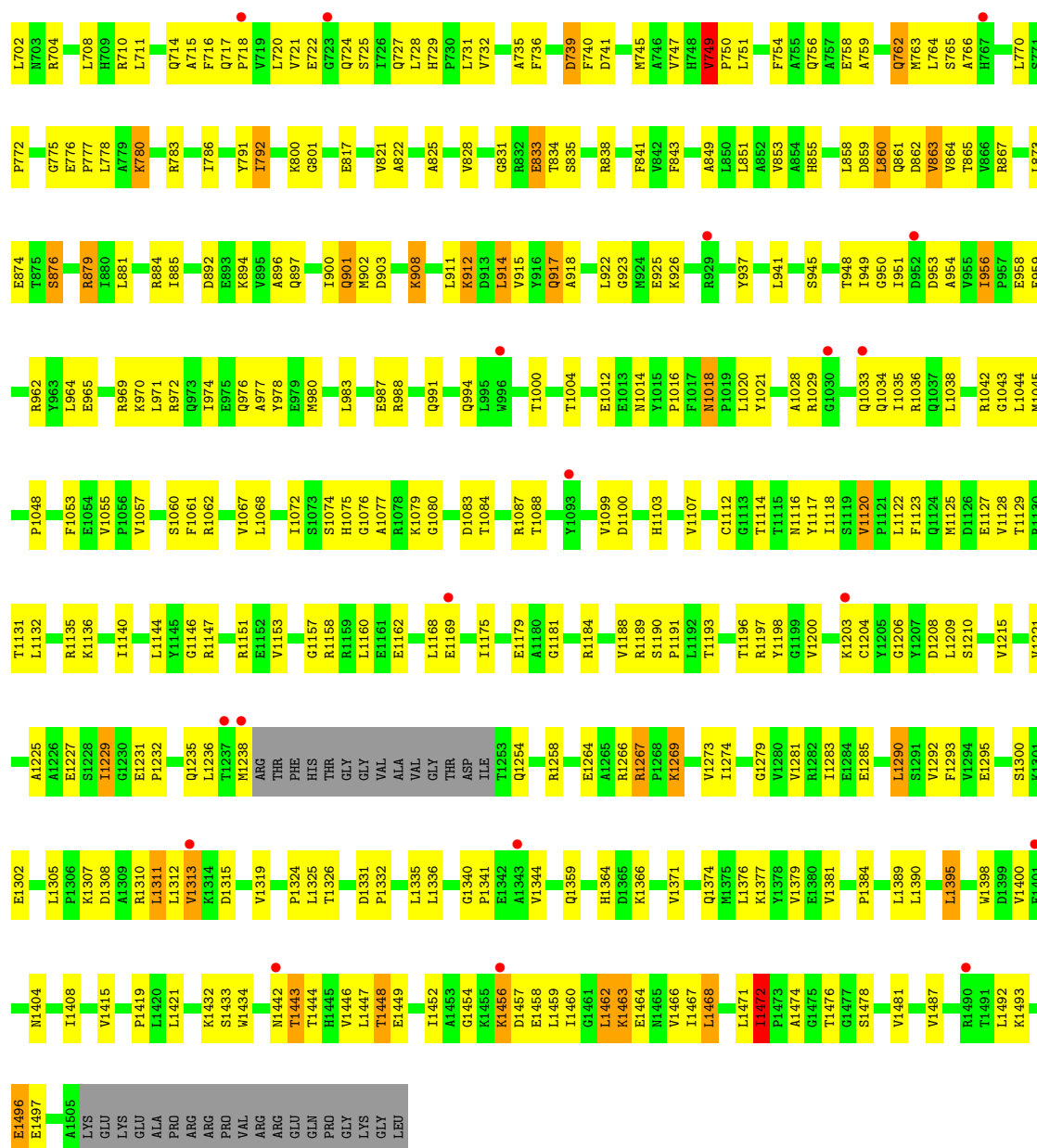


V1099	H1103	C1112	Y1117	I1118	S1119	P1120	P1121	L1122	F1123	G1124	M1125	E1127	T1128	T1129	R1130	R1135	K1136	I1140	E1141	G1142	G1143	G1144	R1147	R1151	E1152	E1153	E1154	R1158	L1159	L1160	E1162	L1168	E1169	D1170	V1171	I1175	E1179	A1180	G1181	R1184	V1188																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
K1009	M1014	Y1015	P1016	P1019	L1020	M1023	A1028	R1029	G1030	Q1033	L1034	T1035	R1036	Q1037	G1039	G1040	A854	M1041	R1042	G1043	L1044	M1045	P1048	F1053	E1054	V1055	P1056	S1059	F1060	R1061	R1062	V1067	L1068	I1072	S1073	S1074	H1075	G1076	A1077	R1078	G1080	D1083	Y1093																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
E817	V821	A822	A825	Q831	R832	E833	T834	S835	R838	F841	F842	F843	A849	L850	L851	R853	A854	H855	L858	D859	L860	Q861	D862	R863	L864	L873	S876	R879	L880	R881	R884	I885	D892	E893	K894	V895	A896	Q897	I900	Q901	R902	D903	E907	K908																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L911	K912	D913	L914	V915	Y916	Q917	A918	A919	L922	G923	K926	Y936	L941	S945	G946	I947	T948	G950	I951	D952	L953	A954	V955	I956	P957	E958	E959	L964	K970	L971	I974	Q976	A977	D978	E979	K980	L981	R982	L983	E987	R988	Q989	I990	V993																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
Q724	S725	I726	Q727	L728	H729	P730	L731	V732	A735	F736	D739	F740	M745	V746	V747	V748	P750	L751	F754	A755	Q756	E757	D758	L759	F763	M764	S765	A766	L770	S771	P772	G775	E776	L777	A778	K779	R780	R783	I786	Y787	I792	T793	K800	G801																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
K659	K660	M661	E662	E663	K664	A665	F666	A667	V670	K671	A672	A673	R674	M675	L676	L677	F678	R679	Q680	R681	D682	L683	K684	A685	H686	E687	D688	E689	A690	L691	E692	K693	V694	R695	L696	M697	L698	P699	V700	L701	L702	R703	R704	T707	L708	H709	R710	L711	Q714	A715	F716	Q717	F718	V719	L720	V721	E722	G723																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
L477	E480	H483	P484	S485	A486	R500	L503	R508	W511	M512	L513	L514	V517	P518	V519	L520	P521	P522	D523	L524	R525	D539	L543	L547	S548	N549	R550	N551	L554	K555	L558	A559	Q560	L565	L566	L567	M568	A649	L650	E651	L652	F653	K654	P655	E656	V657	L658																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
V400	Y401	P402	D405	D406	V407	V409	T410	T411	G412	D413	P417	G418	D419	V420	L421	D423	K426	V427	K428	S429	E430	L431	Y432	G433	R434	V435	E436	G437	A359	R441	H442	V443	V444	R445	V446	V447	D451	W456	E459	A460	I461	L464	L465	L468	E471	V472	R473	R474	E475	D476																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
T318	V322	E323	D405	D406	V407	S330	L333	T334	L335	F336	L337	E338	W339	E341	P342	Y345	K346	V347	A348	P349	H350	M351	N352	V353	I354	V355	P356	G357	A359	E365	K366	L367	V368	A369	A370	D372	V377	I378	A379	V385	H386	L387	P390	L394	V395	R396	K397	E475	D476																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
E167	T168	L171	P172	V179	K180	D181	E184	K187	L191	A192	P193	V196	S197	H198	M199	A203	S199	A200	T121	E122	L123	E207	P208	Q209	L210	V211	R212	V213	D214	N215	L216	R217	K218	E219	R220	L223	R224	T225	P226	A229	W230	V231	E232	G307	K308	E234	D235	E156	E157	E160	P314	R315	E240	H316	V241	L242																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
A243	E244	L245	S246	F251	R252	A253	E254	E260	L261	L264	A265	E266	G267	H268	L269	I270	Y271	L272	R273	Q274	E275	E276	E277	V278	V279	R281	L284	P285	A286	G287	M288	V293	E299	Q302	P303	L304	A305	E306	G307	K308	E309	L310	L311	R312	L313	P314	R315	E316	K317	L318	V241	L242																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
R86	R87	Y88	R89	G91	H92	R93	A96	T97	A100	H101	I102	W103	F104	P109	S110	H268	K111	S119	A120	T121	E122	L123	E207	P208	Q209	L210	V211	R212	V213	D214	N215	L216	R217	K218	E219	R220	L223	R224	T225	P226	A229	W230	V231	E232	G307	K308	E234	D235	E156	E157	E160	P314	R315	E240	H316	V241	L242																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
K2	K3	E4	V5	R6	K7	R9	R10	A11	L12	A13	S14	P15	E16	S22	E25	V26	P29	E36	T31	I32	N33	Y34	P39	D42	G43	L44	F45	D46	E47	R48	I49	F50	Y56	K62	Y63	K64	R65	Q66	R67	F68	R75	V78	E79	V80	T81	L82	K165	V166																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
MET																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										</

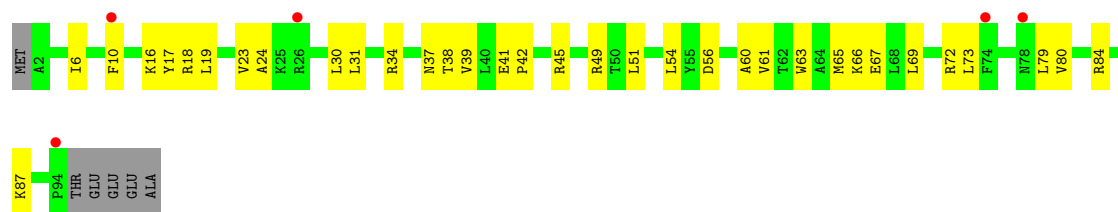


• Molecule 3: DNA-directed RNA polymerase subunit beta'



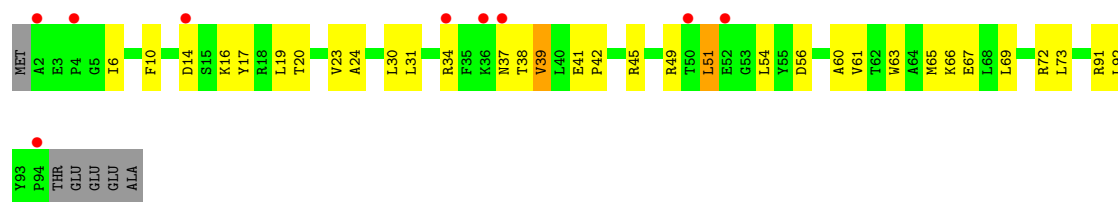


• Molecule 4: DNA-directed RNA polymerase subunit omega

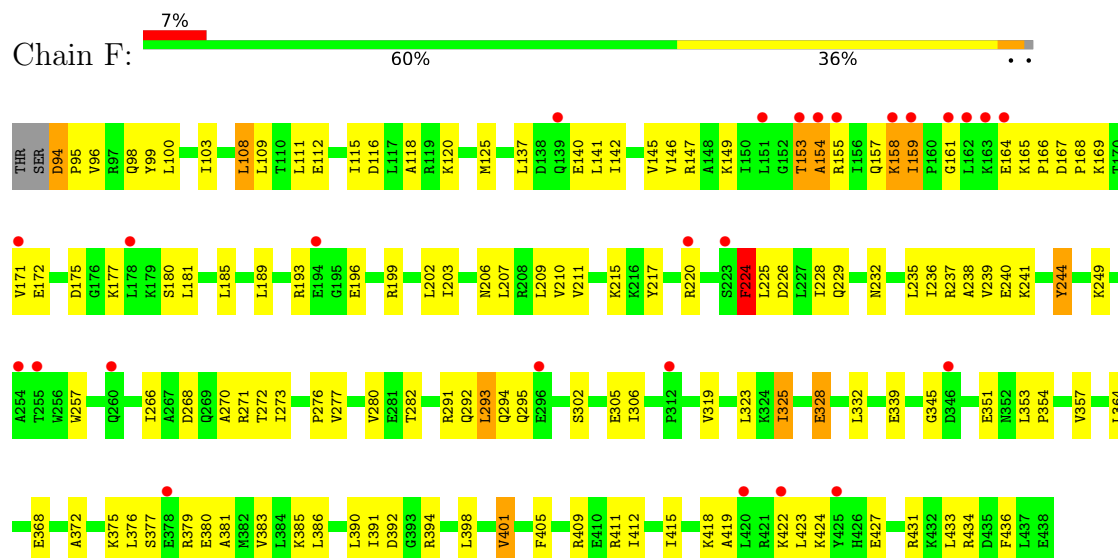


• Molecule 4: DNA-directed RNA polymerase subunit omega

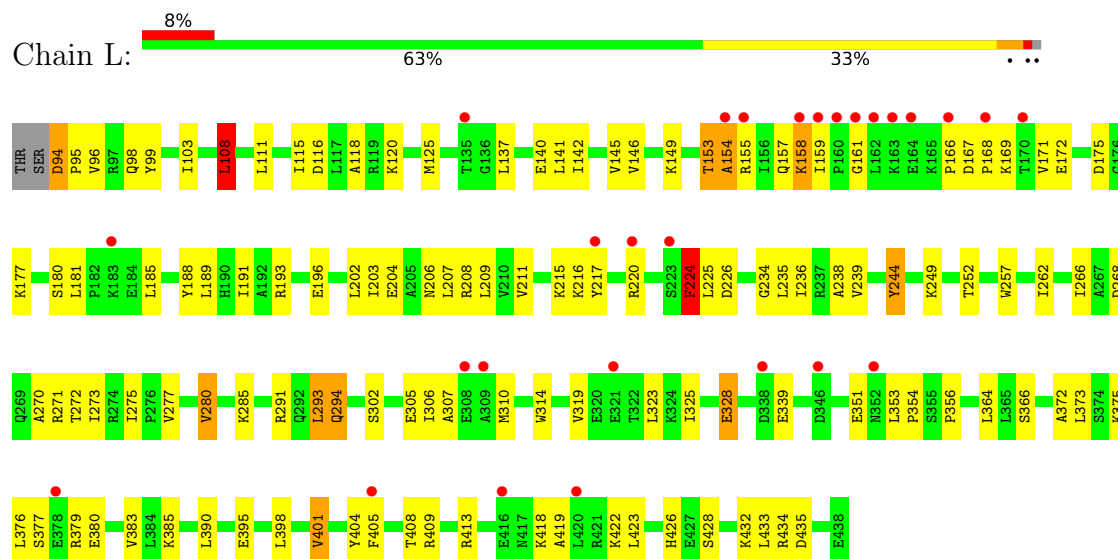




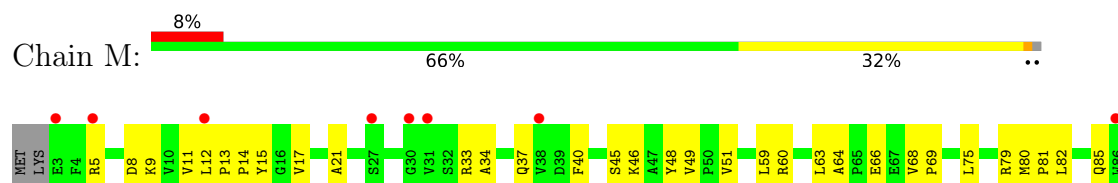
• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 5: RNA polymerase sigma factor SigA

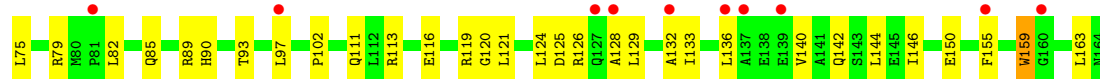
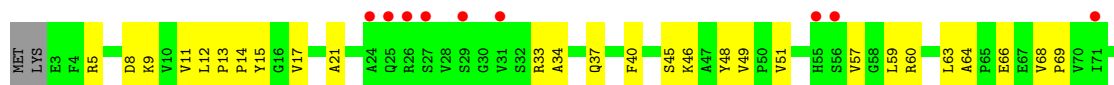


• Molecule 6: CarD-like transcriptional regulator





- Molecule 6: CarD-like transcriptional regulator



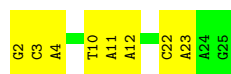
- Molecule 7: DNA (30-MER)



- Molecule 7: DNA (30-MER)



- Molecule 8: DNA (5'-D(P*GP*CP*AP*CP*AP*AP*TP*TP*TP*AP*AP*CP*AP*CP*TP*T
P*TP*TP*GP*TP*CP*AP*AP*G)-3')



- Molecule 8: DNA (5'-D(P*GP*CP*AP*CP*AP*AP*TP*TP*TP*AP*AP*CP*AP*CP*TP*T
P*TP*TP*GP*TP*CP*AP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	293.15Å 293.15Å 539.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 4.01 49.79 – 4.01	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.79-4.01) 75.7 (49.79-4.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.79 (at 4.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1839)	Depositor
R, R_{free}	0.232 , 0.272 0.234 , 0.270	Depositor DCC
R_{free} test set	7463 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	146.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 243.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	58966	wwPDB-VP
Average B, all atoms (Å ²)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.37	0/1804	0.88	2/2455 (0.1%)
1	B	0.39	0/1804	0.87	3/2455 (0.1%)
1	G	0.39	0/1804	0.87	6/2455 (0.2%)
1	H	0.41	0/1804	0.87	5/2455 (0.2%)
2	C	0.36	0/8905	0.88	16/12040 (0.1%)
2	I	0.37	0/8905	0.88	16/12040 (0.1%)
3	D	0.36	1/11963 (0.0%)	0.86	18/16165 (0.1%)
3	J	0.37	1/10959 (0.0%)	0.86	13/14802 (0.1%)
4	E	0.31	0/783	0.82	0/1054
4	K	0.32	0/783	0.82	0/1054
5	F	0.34	0/2829	0.85	6/3804 (0.2%)
5	L	0.36	0/2829	0.86	4/3804 (0.1%)
6	M	0.34	0/1302	0.89	3/1765 (0.2%)
6	N	0.35	0/1302	0.84	2/1765 (0.1%)
7	O	0.12	0/687	0.56	0/1059
7	R	0.13	0/687	0.59	0/1059
8	P	0.13	0/547	0.66	0/841
8	S	0.14	0/547	0.66	1/841 (0.1%)
All	All	0.36	2/60244 (0.0%)	0.85	95/81913 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	670	VAL	C-O	6.50	1.31	1.24
3	D	670	VAL	C-O	5.96	1.30	1.24

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	414	GLY	CA-C-N	7.59	129.32	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	414	GLY	C-N-CA	7.59	129.32	119.84
5	L	277	VAL	N-CA-C	7.54	117.66	110.42
3	J	1472	ILE	CA-C-N	7.16	126.83	119.82
3	J	1472	ILE	C-N-CA	7.16	126.83	119.82

There are no chirality outliers.

There are no planarity outliers.

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	1770	0	1799	76	0
1	B	1770	0	1799	61	0
1	G	1770	0	1799	79	0
1	H	1770	0	1799	75	0
2	C	8739	0	8841	373	0
2	I	8739	0	8841	374	0
3	D	11761	0	11976	464	0
3	J	10779	0	10993	410	0
4	E	768	0	784	27	0
4	K	768	0	784	27	0
5	F	2787	0	2866	87	0
5	L	2787	0	2866	80	0
6	M	1274	0	1288	34	0
6	N	1274	0	1288	39	0
7	O	613	0	343	14	0
7	R	613	0	343	9	0
8	P	489	0	273	7	0
8	S	489	0	273	5	0
9	D	2	0	0	0	0
9	J	2	0	0	0	0
10	D	1	0	0	0	0
10	J	1	0	0	0	0
All	All	58966	0	58955	2059	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 17.

The worst 5 of 2059 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)
5:F:149:LYS:HB3	5:F:193:ARG:HH12	1.35	0.91
2:I:204:GLN:HB2	2:I:227:LEU:HD21	1.54	0.90
2:C:502:PRO:HG3	2:C:510:THR:HG22	1.56	0.88
5:L:149:LYS:HB3	5:L:193:ARG:HH12	1.37	0.88
2:C:199:VAL:HA	2:C:231:PRO:HB3	1.55	0.88

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	225/314 (72%)	198 (88%)	26 (12%)	1 (0%)	30	65
1	B	225/314 (72%)	199 (88%)	25 (11%)	1 (0%)	30	65
1	G	225/314 (72%)	200 (89%)	24 (11%)	1 (0%)	30	65
1	H	225/314 (72%)	199 (88%)	25 (11%)	1 (0%)	30	65
2	C	1108/1119 (99%)	980 (88%)	119 (11%)	9 (1%)	16	51
2	I	1108/1119 (99%)	977 (88%)	123 (11%)	8 (1%)	18	54
3	D	1486/1524 (98%)	1333 (90%)	143 (10%)	10 (1%)	18	54
3	J	1361/1524 (89%)	1227 (90%)	126 (9%)	8 (1%)	21	57
4	E	91/99 (92%)	79 (87%)	12 (13%)	0	100	100
4	K	91/99 (92%)	80 (88%)	11 (12%)	0	100	100
5	F	343/347 (99%)	309 (90%)	32 (9%)	2 (1%)	21	57
5	L	343/347 (99%)	309 (90%)	31 (9%)	3 (1%)	14	48
6	M	160/164 (98%)	142 (89%)	18 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	N	160/164 (98%)	141 (88%)	19 (12%)	0	100	100
All	All	7151/7762 (92%)	6373 (89%)	734 (10%)	44 (1%)	21	57

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	683	ILE
3	D	1128	VAL
1	G	53	VAL
3	J	681	ARG

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	194/270 (72%)	180 (93%)	14 (7%)	13	37
1	B	194/270 (72%)	175 (90%)	19 (10%)	7	27
1	G	194/270 (72%)	178 (92%)	16 (8%)	10	34
1	H	194/270 (72%)	175 (90%)	19 (10%)	7	27
2	C	931/936 (100%)	849 (91%)	82 (9%)	9	32
2	I	931/936 (100%)	847 (91%)	84 (9%)	9	31
3	D	1252/1281 (98%)	1124 (90%)	128 (10%)	7	25
3	J	1150/1281 (90%)	1041 (90%)	109 (10%)	8	28
4	E	83/88 (94%)	80 (96%)	3 (4%)	31	53
4	K	83/88 (94%)	78 (94%)	5 (6%)	17	42
5	F	296/299 (99%)	273 (92%)	23 (8%)	11	35
5	L	296/299 (99%)	272 (92%)	24 (8%)	11	34
6	M	131/133 (98%)	128 (98%)	3 (2%)	44	64
6	N	131/133 (98%)	128 (98%)	3 (2%)	44	64
All	All	6060/6554 (92%)	5528 (91%)	532 (9%)	9	32

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

Mol	Chain	Res	Type
3	J	976	GLN
3	J	1285	GLU
3	J	971	LEU
5	L	339	GLU
3	D	863	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	37	ASN
5	L	263	ASN
4	E	28	GLN
3	D	1334	GLN
5	L	294	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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	227/314 (72%)	0.48	13 (5%) 29 26	120, 182, 228, 247	0
1	B	227/314 (72%)	0.44	13 (5%) 29 26	83, 155, 210, 239	0
1	G	227/314 (72%)	0.70	27 (11%) 9 12	127, 193, 236, 261	0
1	H	227/314 (72%)	0.47	14 (6%) 26 24	93, 165, 210, 245	0
2	C	1112/1119 (99%)	0.47	67 (6%) 27 25	70, 174, 245, 303	0
2	I	1112/1119 (99%)	0.49	78 (7%) 22 21	82, 182, 250, 314	0
3	D	1490/1524 (97%)	0.34	50 (3%) 48 35	66, 147, 206, 277	0
3	J	1367/1524 (89%)	0.35	48 (3%) 47 35	70, 153, 211, 274	0
4	E	93/99 (93%)	0.60	5 (5%) 31 27	93, 158, 217, 254	0
4	K	93/99 (93%)	0.67	9 (9%) 13 15	106, 166, 222, 247	0
5	F	345/347 (99%)	0.58	26 (7%) 20 20	108, 178, 259, 323	0
5	L	345/347 (99%)	0.60	27 (7%) 19 19	119, 184, 260, 323	0
6	M	162/164 (98%)	0.68	13 (8%) 18 19	154, 223, 269, 295	0
6	N	162/164 (98%)	0.77	19 (11%) 9 12	161, 228, 271, 302	0
7	O	30/30 (100%)	0.14	0 100 100	139, 200, 269, 277	0
7	R	30/30 (100%)	0.15	0 100 100	156, 209, 257, 267	0
8	P	24/24 (100%)	0.23	0 100 100	162, 229, 257, 280	0
8	S	24/24 (100%)	0.28	0 100 100	173, 222, 252, 265	0
All	All	7297/7870 (92%)	0.45	409 (5%) 30 26	66, 168, 242, 323	0

The worst 5 of 409 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	161	GLY	6.4
2	C	207	LEU	6.0
5	F	159	ILE	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	L	159	ILE	5.5
2	I	221	LEU	5.5

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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MG	J	2003	1/1	0.65	0.13	219,219,219,219	0
10	MG	D	2003	1/1	0.85	0.10	198,198,198,198	0
9	ZN	J	2002	1/1	0.99	0.04	242,242,242,242	0
9	ZN	D	2002	1/1	0.99	0.03	203,203,203,203	0
9	ZN	J	2001	1/1	0.99	0.05	200,200,200,200	0
9	ZN	D	2001	1/1	1.00	0.02	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.