



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 10:15 PM EDT

PDB ID : 4XLS  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

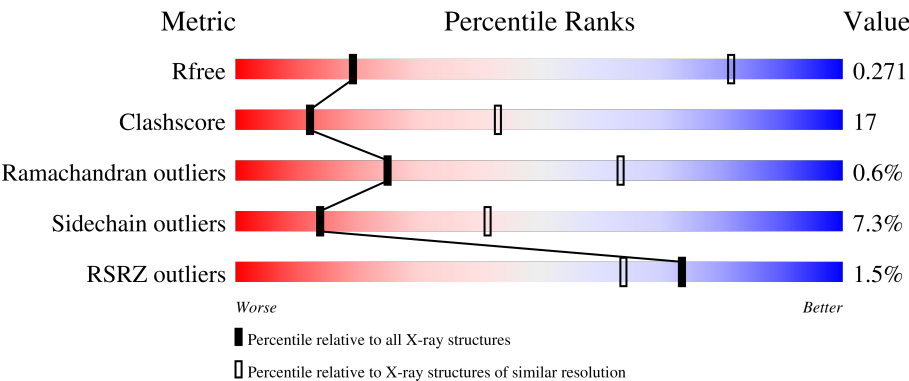
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

# 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 <sub>free</sub>	130704	1098 (4.34-3.70)
Clashscore	141614	1159 (4.34-3.70)
Ramachandran outliers	138981	1118 (4.34-3.70)
Sidechain outliers	138945	1108 (4.34-3.70)
RSRZ outliers	127900	1034 (4.38-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	314	<div><div></div><div>41%30%•28%</div></div>
1	B	314	<div><div></div><div>43%27%•28%</div></div>
1	G	314	<div><div>4%</div><div>42%29%•28%</div></div>
1	H	314	<div><div></div><div>38%32%•28%</div></div>
2	C	1119	<div><div>2%</div><div>58%38%••</div></div>

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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 (three-letter code: 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		

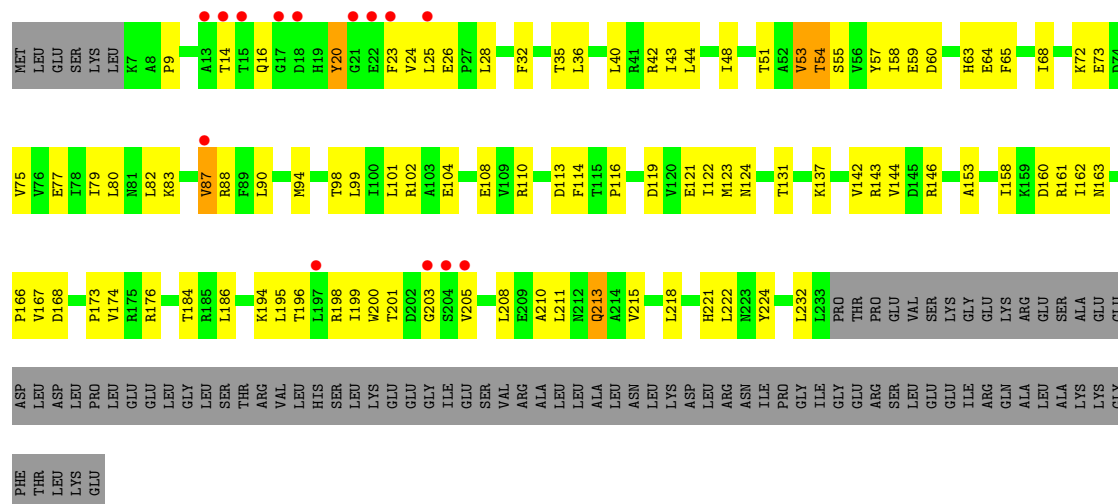
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



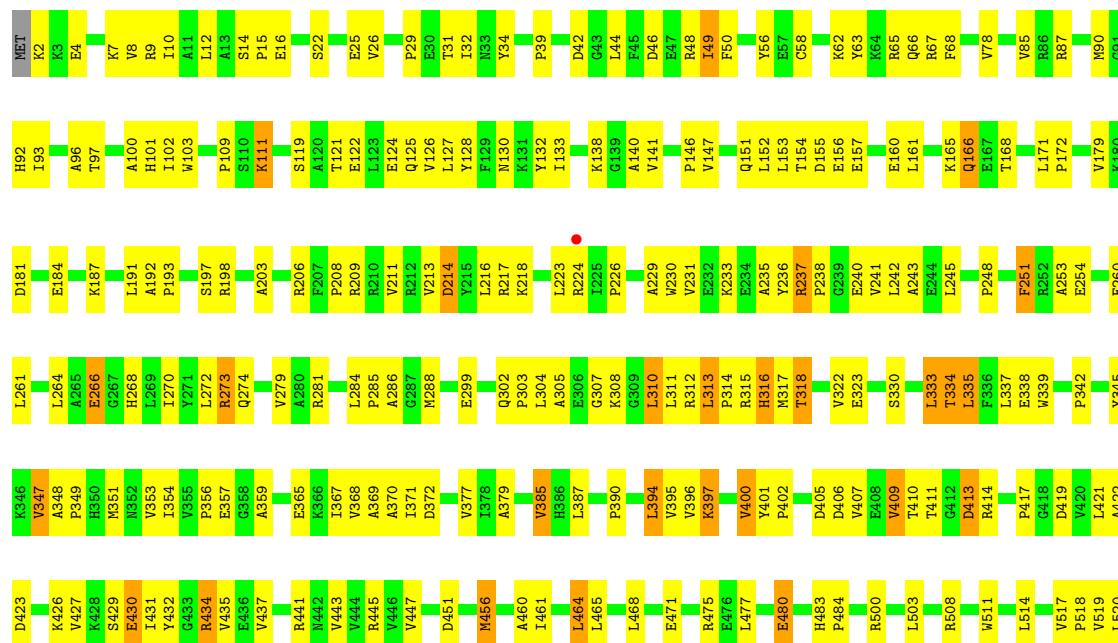
- Molecule 1: DNA-directed RNA polymerase subunit alpha

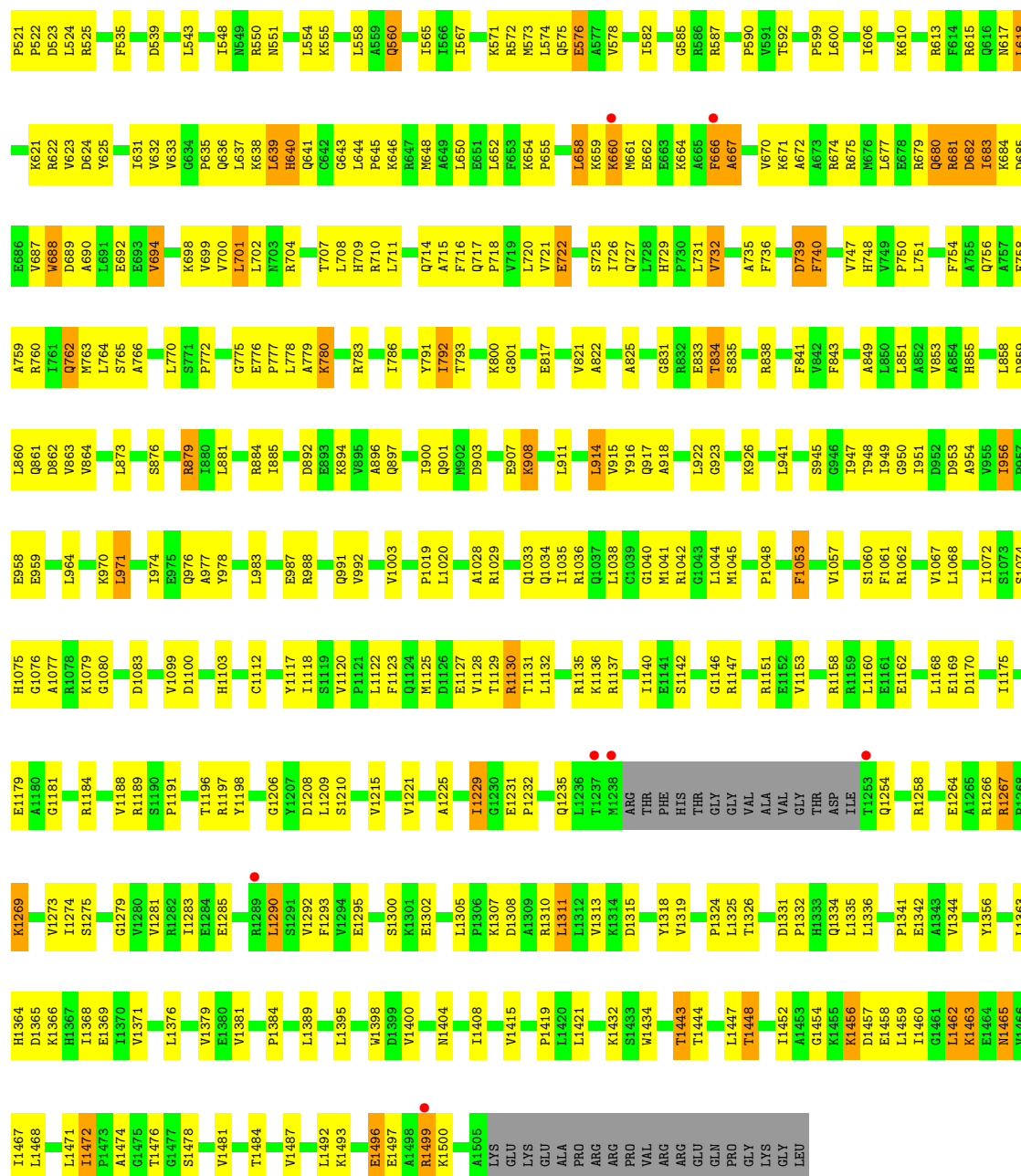




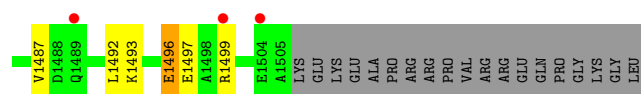






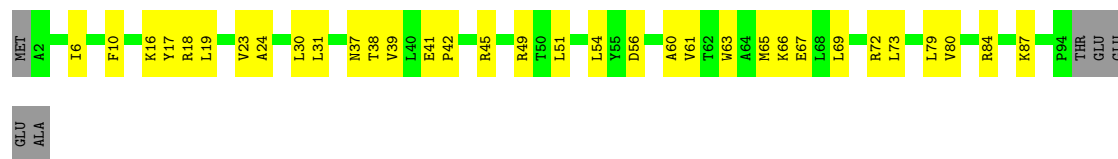


L1389	E1285	G1204	I1118	Y1021	A918	S835	D739	K659	P590	L503	V396	THR	VAL	E184
L1390	R1289	Y1205	S1119	A1028	L922	R838	D740	V670	Y591	R508	K397	ALA	VAL	A192
L1395	L1290	G1206	V1120	R1029	G923	R839	D741	A672	T592	L509	R399	GLY	GLU	P193
L1398	S1291	D1208	L1122	Q1033	M924	F841	V747	A673	P599	W511	Y400	VAL	LVS	R198
L1399	F1293	L1209	F1123	Q1034	E925	R842	H748	R674	L600	L514	Y401	ALA	LEU	R199
D1399	V1294	S1210	G1124	Q1035	K926	F843	V749	R675	R601	E515	P402	GLU	ALA	D200
V1400	E1295	V1215	M1125	I1036	Y937	A849	V751	L677	S602	E516	F403	GLY	ALA	G201
N1404	S1300	V1221	E1127	Q1037	L941	L850	L751	Q680	I606	P517	D405	GLY	GLY	V202
I1408	K1301	V1222	V1128	Q1038	L941	L851	F754	R681	K610	P518	D406	GLY	HIS	A203
V1415	E1302	A1225	R1130	M1041	S945	R853	F755	D682	V407	V519	V407	ASP	LEU	P208
P1419	L1305	A1226	T1131	R1042	T948	R855	Q756	I683	R615	P521	V409	SER	ILE	R209
L1420	P1306	L1228	L1132	G1043	I949	A854	A757	R684	Q616	P522	T410	VAL	TTR	
L1421	K1307	I1229	R1135	M1045	G950	R858	H758	D685	N617	D523		HIS	LEU	V213
K1432	D1308	L1230	R1136	P1048	I951	D859	A759	E686	L618	D524	R414	THR	GLN	D214
S1433	R1310	E1231	R1137	P1048	D952	L860	Q762	V687	K621	L524	L421	LEU	GLY	Y215
V1434	L1311	Q1235	I1140	F1053	D953	Q861	H763	D689	R622	F835	D422	PHE	GLY	L216
N1442	L1312	L1236	G1146	V1057	V955	D862	L764	A690	Y623	D539	A423	LEU	GLY	ARG
T1443	V1313	T1237	R1147	V1057	V956	H863	S765	E692	Y625	L543	K426	TRP	ALA	ARG
T1444	K1314	M1238	R1151	S1060	E957	V866	L770	E693	V632		S429	T340	ALA	ARG
H1445	D1315	THR	R1152	F1061	E958	R867	S771	V694	V633	I548	V443	D344	TYR	ALA
V1446	V1319	THR	V1153	R1062	E959	R873	P772	K698	P635	R549	V444	V347	PHE	LEU
L1447	P1324	H15	H157	V1067	R962	L873	G775	V699	G634	R550	R445		LEU	ARG
T1448	L1325	THR	G1157	L1068	Y963	E874	H776	W700	Q636	N551	V446	I354	ALA	PRO
I1452	T1326	GLY	R1158	I1072	E965	S876	L777	L702	L637	L554	V447	V355	GLY	LEU
G1453	D1331	VAL	R1159	S1073	R969	R879	A779	R703	L639	K555	D451	P356	MET	SER
A1454	P1332	ALA	L1160	H1074	K970	T880	K780	R704	H640	L558	M456	A359	THR	ALA
K1455	L1335	VAL	E1162	H1075	L971	L881	R783	L708	Q641	Q560	G457	K360	VAL	VAL
D1457	L1336	GLY	L1168	G1076	R972	R884	R786	R710	G643	P563	A458	V361	GLY	LVS
E1458	L1336	THR	E1169	A1077	Q973	T885	I786	L711	L644	E564	E459	E365	ALA	ALA
L1459	G1340	ASP	L1175	K1079	E975	D892	Y791	Q714	R647	I566	A460	K366	GLY	TYR
G1461	P1341	ILE	T1177	G1080	Q976	E893	L792	A715	M648	I567	I461	I367	ILE	ARG
L1462	A1343	Q1254	E1179	D1083	A977	K894	F716	F716	I566	L464	L465	A370	GLY	PRO
K1463	V1344	T1084	A1180	T1084	Y978	V895	K800	Q717	A649			D371	VAL	GLY
E1464	H1364	R1087	G1181	R1087	L983	A896	G801	P719	L650	K571	L468	E372	GLY	VAL
N1465	D1365	T1088	R1184	T1088	R988	Q897	A805	V719	L651	R572	E471	P373	LEU	LEU
V1466	K1366	V1099	V1188	V1099	Q981	I900	E817	L720	K654	M573	E474	E374	PRO	ALA
L1467	P1367	D1100	R1189	D1100	Q951	N902	V821	V721	P655	L574	R475	A379	ALA	LEU
L1468	V1371	H1103	S1190	H1103	Q954	D903	A822	E722	P655	Q575	E476	A381	SER	GLY
L1471	Q1374	V1192	P1191	V1192	Q954	D903	A822	V725	L658	E576	L477	E382	PRO	TYR
T1472	M1375	L1107	L1192	V1107	E1012	R908	A825	Q727	K659	V578	E480	V385	LEU	PHE
A1474	L1376	T1193	T1193	V1107	E1013	L911	A825	H729	M661	A580			LEU	LEU
G1475	V1378	R1196	R1196	G1112	Y1015	K912	V828	L730	E662	I582	H483	P390	ARG	ARG
T1476	V1379	T1197	R1197	G1113	Y1016	D913	V828	F730	E663		P484	A391	LEU	ALA
G1477	E1380	V1281	Y1198	T1114	F1017	L914	G831	L731	K664	G585		S392	PRO	GLY
S1478	V1381	G1199	N1018	T1115	F1017	V915	R832	V732	A685	R586		I393	ARG	GLY
V1481	P1384	V1200	P1019	T1116	P1019	Y916	E833	A735	A687	R587	R500	L394	HIS	SER
				Y1117	L1020	Q917	T834	F736	P668			V395	MET	GLY



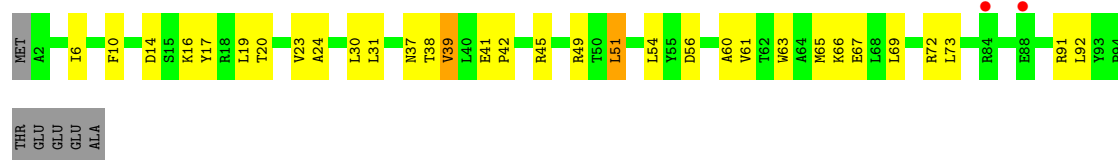
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 61% 33% 6%



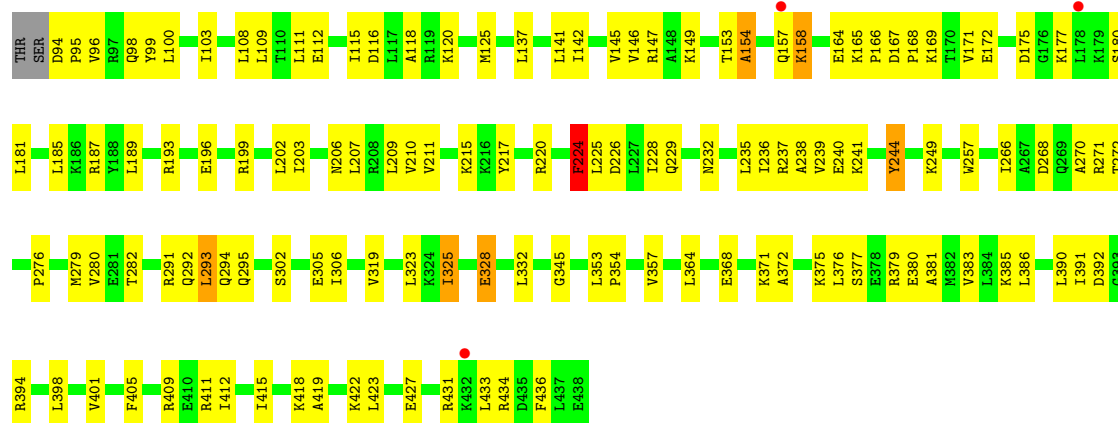
• Molecule 4: DNA-directed RNA polymerase subunit omega

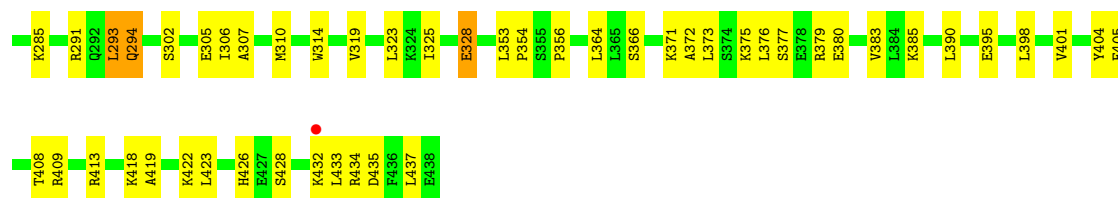
Chain K: 2% 62% 30% 6%



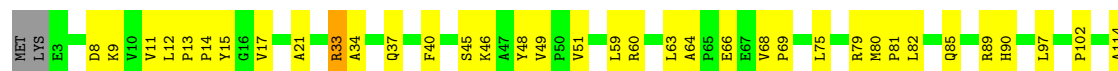
• Molecule 5: RNA polymerase sigma factor SigA

Chain F: 62% 35% 2%





- Molecule 6: CarD-like transcriptional regulator



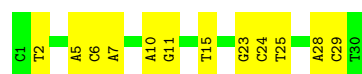
- Molecule 6: CarD-like transcriptional regulator



- Molecule 7: DNA (30-MER)

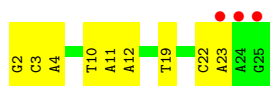


- Molecule 7: DNA (30-MER)



- 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')

Chain S:  75% 21% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	293.15Å 293.15Å 539.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 4.01 49.86 – 4.01	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.79-4.01) 75.7 (49.86-4.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.79 (at 4.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1839)	Depositor
R, $R_{free}$	0.232 , 0.272 0.232 , 0.271	Depositor DCC
$R_{free}$ test set	7463 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	146.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 190.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	58966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/1804	0.52	0/2455
1	B	0.27	0/1804	0.54	0/2455
1	G	0.27	0/1804	0.52	0/2455
1	H	0.28	0/1804	0.55	0/2455
2	C	0.26	0/8905	0.53	1/12040 (0.0%)
2	I	0.26	0/8905	0.53	1/12040 (0.0%)
3	D	0.27	0/11963	0.52	0/16165
3	J	0.27	0/10959	0.51	0/14802
4	E	0.25	0/783	0.52	0/1054
4	K	0.25	0/783	0.53	0/1054
5	F	0.27	0/2829	0.52	0/3804
5	L	0.27	0/2829	0.53	0/3804
6	M	0.26	0/1302	0.51	0/1765
6	N	0.26	0/1302	0.49	0/1765
7	O	0.46	0/687	1.08	0/1059
7	R	0.46	0/687	1.11	1/1059 (0.1%)
8	P	0.45	0/547	1.13	3/841 (0.4%)
8	S	0.48	0/547	1.18	2/841 (0.2%)
All	All	0.28	0/60244	0.56	8/81913 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	S	25	DG	P-O5'-C5'	-6.14	111.08	120.90
2	I	242	LEU	CA-CB-CG	5.95	128.99	115.30
2	C	242	LEU	CA-CB-CG	5.89	128.85	115.30
7	R	28	DA	O4'-C1'-N9	5.80	112.06	108.00
8	P	19	DT	C5-C4-O4	-5.26	121.22	124.90

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	75	0
1	B	1770	0	1799	61	0
1	G	1770	0	1799	78	0
1	H	1770	0	1799	74	0
2	C	8739	0	8841	357	0
2	I	8739	0	8841	363	0
3	D	11761	0	11976	449	0
3	J	10779	0	10993	397	0
4	E	768	0	784	27	0
4	K	768	0	784	27	0
5	F	2787	0	2866	86	0
5	L	2787	0	2866	79	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	2002	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 2002 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	34	71
1	B	225/314 (72%)	199 (88%)	25 (11%)	1 (0%)	34	71
1	G	225/314 (72%)	200 (89%)	24 (11%)	1 (0%)	34	71
1	H	225/314 (72%)	199 (88%)	25 (11%)	1 (0%)	34	71
2	C	1108/1119 (99%)	980 (88%)	119 (11%)	9 (1%)	19	58
2	I	1108/1119 (99%)	977 (88%)	123 (11%)	8 (1%)	22	61
3	D	1486/1524 (98%)	1333 (90%)	143 (10%)	10 (1%)	22	61
3	J	1361/1524 (89%)	1227 (90%)	126 (9%)	8 (1%)	25	63
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%)	25	63
5	L	343/347 (99%)	309 (90%)	31 (9%)	3 (1%)	17	55
6	M	160/164 (98%)	142 (89%)	18 (11%)	0	100	100
6	N	160/164 (98%)	141 (88%)	19 (12%)	0	100	100
All	All	7151/7762 (92%)	6373 (89%)	734 (10%)	44 (1%)	25	63

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%)	184 (95%)	10 (5%)	23	51
1	B	194/270 (72%)	176 (91%)	18 (9%)	9	32
1	G	194/270 (72%)	184 (95%)	10 (5%)	23	51
1	H	194/270 (72%)	176 (91%)	18 (9%)	9	32
2	C	931/936 (100%)	864 (93%)	67 (7%)	14	42
2	I	931/936 (100%)	863 (93%)	68 (7%)	14	41
3	D	1252/1281 (98%)	1139 (91%)	113 (9%)	9	34
3	J	1150/1281 (90%)	1062 (92%)	88 (8%)	13	40
4	E	83/88 (94%)	81 (98%)	2 (2%)	49	69
4	K	83/88 (94%)	79 (95%)	4 (5%)	25	53
5	F	296/299 (99%)	279 (94%)	17 (6%)	20	49
5	L	296/299 (99%)	275 (93%)	21 (7%)	14	42
6	M	131/133 (98%)	127 (97%)	4 (3%)	40	63
6	N	131/133 (98%)	127 (97%)	4 (3%)	40	63
All	All	6060/6554 (92%)	5616 (93%)	444 (7%)	14	41

5 of 444 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	87	VAL
6	N	159	TRP
2	I	427	VAL

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Mol	Chain	Res	Type
6	M	40	PHE
3	J	1371	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	213	GLN
2	I	899	GLN
5	L	263	ASN
1	H	38	ASN
2	I	538	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	227/314 (72%)	-0.15	0	100	100	120, 182, 228, 247	0
1	B	227/314 (72%)	-0.29	0	100	100	83, 155, 210, 239	0
1	G	227/314 (72%)	0.33	14 (6%)	20	17	127, 193, 236, 261	0
1	H	227/314 (72%)	-0.13	1 (0%)	92	87	93, 165, 210, 245	0
2	C	1112/1119 (99%)	-0.09	24 (2%)	62	52	70, 174, 245, 303	0
2	I	1112/1119 (99%)	-0.04	25 (2%)	62	52	82, 182, 250, 314	0
3	D	1490/1524 (97%)	-0.17	8 (0%)	91	85	66, 147, 206, 277	0
3	J	1367/1524 (89%)	-0.15	14 (1%)	82	74	70, 153, 211, 274	0
4	E	93/99 (93%)	-0.12	0	100	100	93, 158, 217, 254	0
4	K	93/99 (93%)	0.06	2 (2%)	62	52	106, 166, 222, 247	0
5	F	345/347 (99%)	-0.10	3 (0%)	84	77	108, 178, 259, 323	0
5	L	345/347 (99%)	-0.21	6 (1%)	70	60	119, 184, 260, 323	0
6	M	162/164 (98%)	0.16	3 (1%)	66	58	154, 223, 269, 295	0
6	N	162/164 (98%)	0.47	7 (4%)	35	29	161, 228, 271, 302	0
7	O	30/30 (100%)	0.15	3 (10%)	7	7	139, 200, 269, 277	0
7	R	30/30 (100%)	-0.35	0	100	100	156, 209, 257, 267	0
8	P	24/24 (100%)	0.23	3 (12%)	3	5	162, 229, 257, 280	0
8	S	24/24 (100%)	-0.47	0	100	100	173, 222, 252, 265	0
All	All	7297/7870 (92%)	-0.09	113 (1%)	73	64	66, 168, 242, 323	0

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	221	LEU	5.7
2	I	182	VAL	5.1
1	G	13	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
2	C	175	GLU	4.6
6	N	119	ARG	4.3

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	MG	J	2003	1/1	0.88	0.29	219,219,219,219	0
9	ZN	J	2001	1/1	0.93	0.20	200,200,200,200	0
9	ZN	D	2002	1/1	0.94	0.14	203,203,203,203	0
10	MG	D	2003	1/1	0.95	0.27	198,198,198,198	0
9	ZN	D	2001	1/1	0.97	0.13	96,96,96,96	0
9	ZN	J	2002	1/1	0.97	0.06	242,242,242,242	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.