



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 09:48 AM UTC

PDB ID : 6N61 / pdb_00006n61
Title : Escherichia coli RNA polymerase sigma70-holoenzyme bound to upstream fork promoter DNA and Capistruin
Authors : Braffman, N.; Hauver, J.; Campbell, E.A.; Darst, S.A.
Deposited on : 2018-11-24
Resolution : 3.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

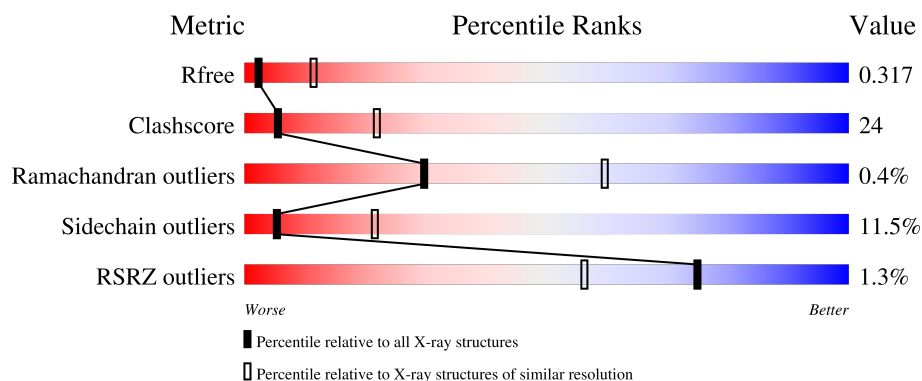
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	239	3% 54% 36% 5% 5%
1	B	239	4% 48% 35% 8% 9%
2	C	1342	% 54% 40% 6% •
3	D	1409	% 46% 36% 6% 12%
4	E	90	% 48% 38% • 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	613	
6	N	29	
7	T	24	
8	I	19	

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
12	EPE	D	1504	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28613 atoms, of which 23 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	228	Total	C	N	O	S	0	0	0
			1709	1067	300	336	6			
1	B	217	Total	C	N	O	S	0	0	0
			1658	1035	290	327	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP P0A7Z4
A	236	VAL	-	expression tag	UNP P0A7Z4
A	237	LEU	-	expression tag	UNP P0A7Z4
A	238	PHE	-	expression tag	UNP P0A7Z4
A	239	GLN	-	expression tag	UNP P0A7Z4
B	235	GLU	-	expression tag	UNP P0A7Z4
B	236	VAL	-	expression tag	UNP P0A7Z4
B	237	LEU	-	expression tag	UNP P0A7Z4
B	238	PHE	-	expression tag	UNP P0A7Z4
B	239	GLN	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1332	Total	C	N	O	S	0	0	0
			10489	6581	1829	2036	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1239	Total	C	N	O	S	0	0	0
			9649	6061	1733	1807	48			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	expression tag	UNP P0A8T7
D	1408	LEU	-	expression tag	UNP P0A8T7
D	1409	GLU	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	395	Total	C	N	O	S	0	0	0
			3197	1993	578	603	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	ASN	ASP	conflict	UNP Q0P6L9

- Molecule 6 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	N	29	Total	C	N	O	P	0	0	0
			595	284	106	176	29			

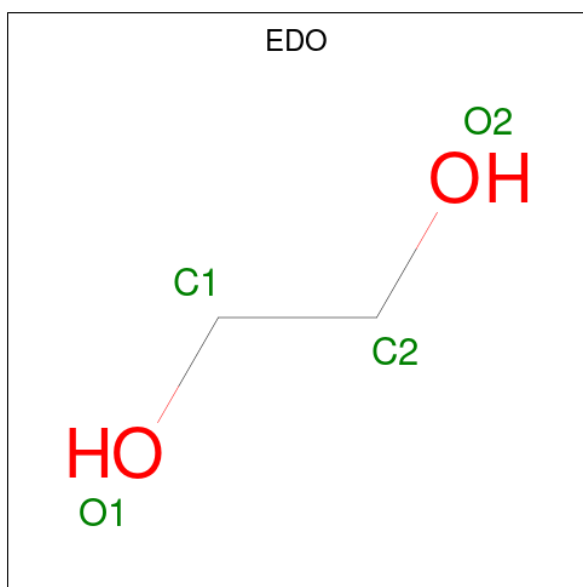
- Molecule 7 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	T	24	Total	C	N	O	P	0	0	0
			492	233	94	141	24			

- Molecule 8 is a protein called Capistrain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	17	Total	C	N	O	0	0	0
			126	80	24	22			

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	H	O	0	0
			10	2	6	2		

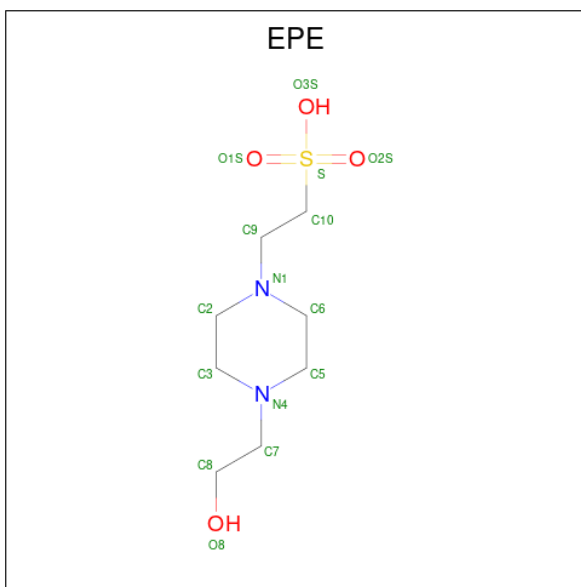
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

- Molecule 12 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	H	N	O	S	
			32	8	17	2	4	1	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	1	Total	O		
			1	1	0	0
13	B	2	Total	O		
			2	2	0	0
13	C	13	Total	O		
			13	13	0	0
13	D	3	Total	O		
			3	3	0	0
13	E	1	Total	O		
			1	1	0	0
13	F	5	Total	O		
			5	5	0	0
13	T	1	Total	O		
			1	1	0	0

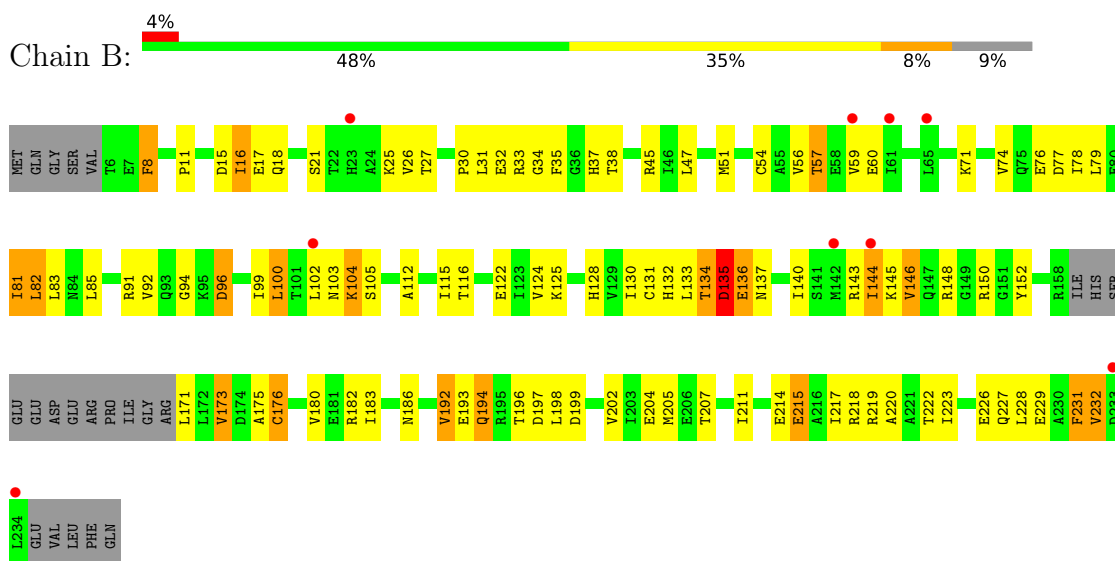
3 Residue-property plots

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

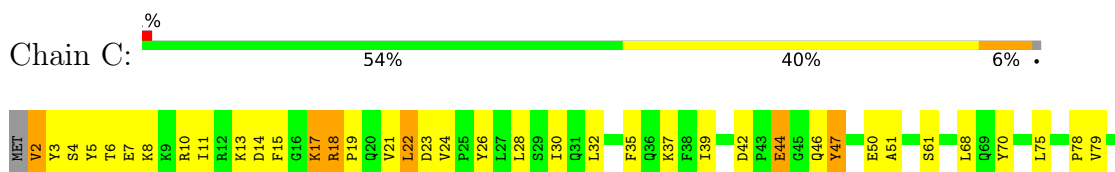
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta

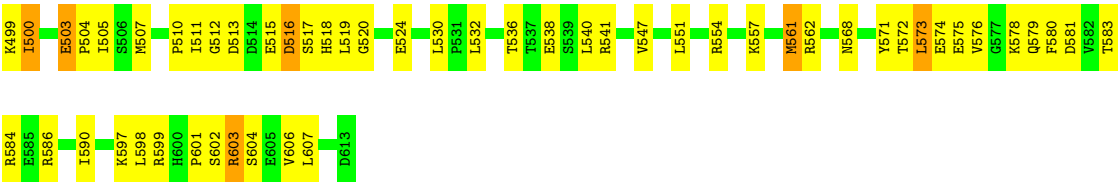


V1309	Q1220	D1150	I1076	L992	P787	I603	T525	K430	L321	A251	N173	T91
E1316	F1221	L1151	S1077	P993	E793	H604	H526	K431	L322	S252	N176	A94
P1317	R1223	D1154	K1078	R994	L794	Y605	K527	R436	L325	F253	I176	P95
V1325	P1224	V1155	N1080	E899	A795	S607	H529	D433	H330	I255	P177	K99
L1326	V1225	R1156	P1081	R903	L796	A608	I530	D443	K331	GLU	L178	L100
R1331	Q1157	K1157	T1082	F906	N799	E610	L533	D444	R332	ALA	L184	R101
S1332	V1227	L1160	E1083	G907	M800	E611	L538	D445	R333	ASN	D185	L102
L1333	G1228	D1161	M1085	E908	A796	E612	T539	D446	L334	GLY	F186	V103
G1334	Y1229	F1163	P1086	K909	L797	V615	H540	H447	T335	VAL	K191	E106
I1335	Y1087	T1087	Y1087	A910	G701	A617	H542	R451	R339	Y262	D192	R107
R1337	Q1008	Q1008	Q1008	V913	G701	S621	F545	R452	H343	V263	N193	GLU
E1338	N1009	N1009	N1009	K914	M704	N622	F545	V456	I347	E264	N195	PRO
L1339	D1010	D1010	D1010	F812	E705	L623	R548	R465	L351	R268	F196	E111
E1340	L1011	S916	E1012	E813	V710	D624	R549	R466	R352	I269	N197	G112
D1341	Q1013	S815	Q1013	S815	V711	E625	H550	L468	D354	T270	I198	T113
E1342	L1014	R816	L817	L817	S712	E626	H551	V469	R354	A271	D199	V114
	Y1018	P921	G713	G713	G713	H628	P552	E477	L360	H273	R200	A115
	F1026	N922	V714	V714	T715	G629	T553	R478	V364	I274	R201	D116
	E1026	G923	V823	V823	R720	T634	H557	R479	I366	O276	K203	K118
	K1027	T935	Q824	Q824	C636	T635	H558	S480	I367	L277	P205	E121
	K1028	R936	E825	E825	C636	L644	C559	S481	I368	E278	A206	E126
	M107	D937	D826	D826	G637	L645	H560	L482	I369	L284	I208	L129
	N108	P937	Q834	Q834	Q726	F645	H561	R483	I370	I285	I209	M130
	E1030	K943	R836	R836	V727	S646	P564	D485	P376	E287	Y215	T131
	A1031	R944	E836	E836	V727	S646	P564	R486	T377	V288	T216	D132
	K1032	L964	L836	L836	V727	S646	P564	L487	P378	V289	T217	N133
	R1033	L964	L836	L836	V727	S646	P564	L488	T379	E290	L221	G134
	R1034	L964	L836	L836	V727	S646	P564	L489	E379	Y291	F225	T135
	K1035	L964	L836	L836	V727	S646	P564	L490	E379	I292	F226	I138
	D1040	L964	L836	L836	V727	S646	P564	L491	E379	I292	F226	T141
	L1041	L964	L836	L836	V727	S646	P564	L492	E379	I292	F226	T141
	L1042	L964	L836	L836	V727	S646	P564	L493	E379	I292	F226	T141
	A1043	L964	L836	L836	V727	S646	P564	L494	E379	I292	F226	T141
	P1044	L964	L836	L836	V727	S646	P564	L495	E379	I292	F226	T141
	G1045	L964	L836	L836	V727	S646	P564	L496	E379	I292	F226	T141
	V1046	L964	L836	L836	V727	S646	P564	L497	E379	I292	F226	T141
	L1047	L964	L836	L836	V727	S646	P564	L498	E379	I292	F226	T141
	K1051	L964	L836	L836	V727	S646	P564	L499	E379	I292	F226	T141
	L1054	L964	L836	L836	V727	S646	P564	L500	E379	I292	F226	T141
	R1059	L964	L836	L836	V727	S646	P564	L501	E379	I292	F226	T141
	I1060	L964	L836	L836	V727	S646	P564	L502	E379	I292	F226	T141
	Q1061	L964	L836	L836	V727	S646	P564	L503	E379	I292	F226	T141
	P1062	L964	L836	L836	V727	S646	P564	L504	E379	I292	F226	T141
	M1066	L964	L836	L836	V727	S646	P564	L505	E379	I292	F226	T141
	H1070	L964	L836	L836	V727	S646	P564	L506	E379	I292	F226	T141
	K1073	L964	L836	L836	V727	S646	P564	L507	E379	I292	F226	T141
	V1075	L964	L836	L836	V727	S646	P564	L508	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L509	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L510	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L511	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L512	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L513	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L514	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L515	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L516	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L517	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L518	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L519	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L520	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L521	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L522	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L523	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L524	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L525	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L526	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L527	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L528	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L529	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L530	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L531	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L532	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L533	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L534	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L535	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L536	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L537	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L538	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L539	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L540	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L541	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L542	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L543	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L544	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L545	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L546	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L547	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L548	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L549	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L550	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L551	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L552	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L553	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L554	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L555	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L556	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L557	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L558	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L559	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L560	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L561	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L562	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L563	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L564	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L565	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L566	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L567	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L568	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L569	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L570	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L571	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L572	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L573	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L574	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L575	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L576	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L577	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L578	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L579	E379	I292	F226	T141
		L989	L836	L836	V727	S646	P564	L580	E379	I292	F226	T141

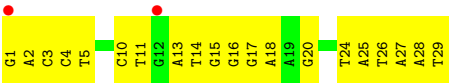
Chain D: % 46% 36% 6% 12%

Category	Item	Value	Color
VAL	VAL	154	Red
	LYS	86	Green
	ASP	87	Green
	LEU	131	Green
	LEU	158	Green
	LEU	90	Green
	LYS	59	Green
	PHE	92	Green
	LEU	93	Green
	LYS	94	Green
ALA	ALA	174	Green
	GLN	36	Green
	THR	97	Green
	LYS	98	Green
	THR	99	Green
	GLU	100	Green
	GLU	101	Green
	GLU	102	Green
	D18	103	Green
	A19	104	Green
L20	L20	105	Green
	E106	106	Green
	S26	107	Green
	S26	108	Green
	S109	109	Green
	P110	110	Green
	H113	111	Green
	I114	112	Green
	W115	113	Green
	E42	114	Green
N45	N45	115	Green
	Y46	116	Green
	P121	117	Green
	S122	118	Green
	R123	119	Green
	E52	120	Green
	R53	121	Green
	G125	122	Green
	L126	123	Green
	R293	124	Green
L56	L56	125	Green
	F57	126	Green
	C58	127	Green
	A59	128	Green
	D129	129	Green
	M130	130	Green
	P131	131	Green
	L132	132	Green
	R133	133	Green
	D134	134	Green
E69	E69	135	Green
	C70	136	Green
	L71	137	Green
	V138	138	Green
	L139	139	Green
	Y140	140	Green
	E235	141	Green
	W236	142	Green
	P323	143	Green
	L324	144	Green
L78	L78	145	Green
	H80	146	Green
	R81	147	Green
	K325	148	Green
	S326	149	Green
	L327	150	Green
	P243	151	Green
	Y244	152	Green
	L245	153	Green
	P246	154	Green
M330	M330	155	Green
	E405	156	Green
	V408	157	Green
	I411	158	Green
	V415	159	Green
	I416	160	Green
	R417	161	Green
	E418	162	Green
	R425	163	Green
	A426	164	Green
L342	L342	165	Green
	K345	166	Green
	R346	167	Green
	D347	168	Green
	D348	169	Green
	R352	170	Green
	E438	171	Green
	L441	172	Green
	I442	173	Green
	E443	174	Green
Y360	Y360	175	Green
	R270	176	Green
	R271	177	Green
	V272	178	Green
	I273	179	Green
	E199	180	Green
	L201	181	Green
	R202	182	Green
	R278	183	Green
	L279	184	Green
L205	L205	185	Green
	N209	186	Green
	S210	187	Green
	E211	188	Green
	R212	189	Green
	R123	190	Green
	I291	191	Green
	G125	192	Green
	R214	193	Green
	K213	194	Green
L230	L230	195	Green
	D289	196	Green
	L290	197	Green
	E375	198	Green
	V292	199	Green
	R293	200	Green
	N294	201	Green
	K216	202	Green
	L217	203	Green
	K296	204	Green
R297	205	Green	
L381	L381	206	Green
	Y382	207	Green
	G383	208	Green
	K384	209	Green
	L385	210	Green
	E386	211	Green
	L387	212	Green
	G388	213	Green
	L390	214	Green
	N320	215	Green
K321	K321	216	Green
	R322	217	Green
	P323	218	Green
	L324	219	Green
	K325	220	Green
	S326	221	Green
	L327	222	Green
	P243	223	Green
	Y244	224	Green
	L245	225	Green
M330			





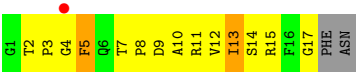
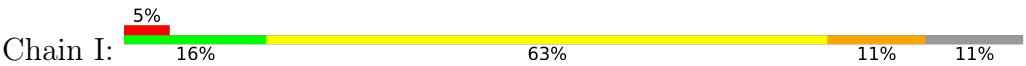
• Molecule 6: non-template strand DNA



• Molecule 7: template strand DNA



• Molecule 8: Capistruin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	172.89Å 172.89Å 385.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 3.25 49.45 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.45-3.25) 99.3 (49.45-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.273 , 0.316 0.276 , 0.317	Depositor DCC
R_{free} test set	1980 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28613	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: MG, EDO, ZN, EPE

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	0.13	0/1729	0.37	0/2349
1	B	0.11	0/1677	0.40	0/2274
2	C	0.13	0/10654	0.34	0/14375
3	D	0.13	0/9794	0.36	1/13212 (0.0%)
4	E	0.11	0/629	0.32	0/847
5	F	0.12	0/3239	0.33	0/4352
6	N	0.24	0/666	0.39	0/1026
7	T	0.26	0/552	0.41	1/849 (0.1%)
8	I	0.28	0/129	0.53	0/173
All	All	0.14	0/29069	0.36	2/39457 (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
1	B	0	2
2	C	0	4
3	D	0	2
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	D	1244	GLN	N-CA-C	8.11	123.21	113.16
7	T	11	DA	C4'-C3'-O3'	-5.64	101.54	110.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	135	ASP	Peptide
1	B	231	PHE	Peptide
2	C	198	ILE	Peptide
2	C	234	ASP	Peptide
2	C	985	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1709	0	1700	69	0
1	B	1658	0	1669	87	0
2	C	10489	0	10490	475	0
3	D	9649	0	9859	548	0
4	E	627	0	634	34	0
5	F	3197	0	3251	152	0
6	N	595	0	329	35	0
7	T	492	0	269	36	0
8	I	126	0	123	22	0
9	C	4	6	6	1	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
12	D	15	17	17	7	0
13	A	1	0	0	1	0
13	B	2	0	0	0	0
13	C	13	0	0	2	0
13	D	3	0	0	3	0
13	E	1	0	0	0	0
13	F	5	0	0	0	0
13	T	1	0	0	1	0
All	All	28590	23	28347	1348	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 24.

The worst 5 of 1348 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)
7:T:10:DC:H2''	7:T:11:DA:H5'	1.27	1.11
1:A:26:VAL:HG23	1:A:203:ILE:HG13	1.37	1.07
2:C:746:ALA:HB1	2:C:747:GLY:HA3	1.33	1.06
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.40	1.02
1:B:192:VAL:HG21	1:B:198:LEU:HD22	1.46	0.96

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	226/239 (95%)	206 (91%)	19 (8%)	1 (0%)	30	59
1	B	213/239 (89%)	196 (92%)	14 (7%)	3 (1%)	9	33
2	C	1326/1342 (99%)	1245 (94%)	75 (6%)	6 (0%)	24	55
3	D	1231/1409 (87%)	1145 (93%)	83 (7%)	3 (0%)	43	70
4	E	77/90 (86%)	73 (95%)	3 (4%)	1 (1%)	9	34
5	F	391/613 (64%)	378 (97%)	13 (3%)	0	100	100
8	I	15/19 (79%)	12 (80%)	3 (20%)	0	100	100
All	All	3479/3951 (88%)	3255 (94%)	210 (6%)	14 (0%)	30	59

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
2	C	199	ASP
2	C	200	ARG
3	D	1345	ARG
2	C	235	ASN

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	181/206 (88%)	162 (90%)	19 (10%)	6	24
1	B	181/206 (88%)	158 (87%)	23 (13%)	4	18
2	C	1144/1157 (99%)	1017 (89%)	127 (11%)	6	23
3	D	1035/1170 (88%)	908 (88%)	127 (12%)	4	19
4	E	67/74 (90%)	64 (96%)	3 (4%)	24	52
5	F	350/540 (65%)	309 (88%)	41 (12%)	5	21
8	I	13/15 (87%)	11 (85%)	2 (15%)	2	12
All	All	2971/3368 (88%)	2629 (88%)	342 (12%)	5	21

5 of 342 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	663	GLU
3	D	1243	LEU
3	D	685	ILE
3	D	876	SER
5	F	112	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1218	HIS
5	F	545	HIS
3	D	1235	ASN
5	F	271	ASN
2	C	762	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
9	EDO	C	1401	-	3,3,3	0.41	0	2,2,2	0.61	0
12	EPE	D	1504	-	15,15,15	0.89	1 (6%)	19,20,20	1.94	6 (31%)

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
9	EDO	C	1401	-	-	0/1/1/1	-
12	EPE	D	1504	-	-	3/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	1504	EPE	C10-S	3.07	1.81	1.77

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	1504	EPE	C7-N4-C5	4.18	122.38	111.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	1504	EPE	O2S-S-C10	3.30	111.71	106.73
12	D	1504	EPE	C5-N4-C3	3.27	115.88	108.84
12	D	1504	EPE	C7-N4-C3	2.73	118.52	111.24
12	D	1504	EPE	C6-N1-C2	2.49	114.21	108.84

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	1504	EPE	C9-C10-S-O3S
12	D	1504	EPE	C9-C10-S-O2S
12	D	1504	EPE	C8-C7-N4-C3

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1401	EDO	1	0
12	D	1504	EPE	7	0

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	228/239 (95%)	0.18	6 (2%) 57 38	73, 115, 173, 204	0
1	B	217/239 (90%)	0.37	9 (4%) 41 27	74, 133, 174, 188	0
2	C	1332/1342 (99%)	-0.13	10 (0%) 82 68	36, 92, 163, 211	0
3	D	1239/1409 (87%)	-0.02	11 (0%) 81 65	45, 104, 181, 218	0
4	E	79/90 (87%)	-0.19	1 (1%) 75 56	71, 95, 155, 183	0
5	F	395/613 (64%)	0.04	5 (1%) 75 56	68, 140, 182, 213	0
6	N	29/29 (100%)	0.13	2 (6%) 23 16	124, 171, 253, 256	0
7	T	24/24 (100%)	0.26	1 (4%) 40 26	114, 179, 256, 268	0
8	I	17/19 (89%)	0.25	1 (5%) 28 19	97, 108, 127, 131	0
All	All	3560/4004 (88%)	-0.02	46 (1%) 75 56	36, 107, 178, 268	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	134	ASP	4.6
1	B	142	MET	4.5
2	C	826	ASP	4.0
1	A	235	GLU	3.9
5	F	352	GLY	3.8

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

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

6.3 Carbohydrates ⓘ

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
12	EPE	D	1504	15/15	0.61	0.10	114,143,172,178	0
9	EDO	C	1401	4/4	0.62	0.12	98,117,137,139	0
11	ZN	D	1502	1/1	0.97	0.05	126,126,126,126	0
11	ZN	D	1503	1/1	0.98	0.07	108,108,108,108	0
10	MG	D	1501	1/1	0.99	0.08	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.