



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 11, 2024 – 09:02 PM EDT

PDB ID : 6N61
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

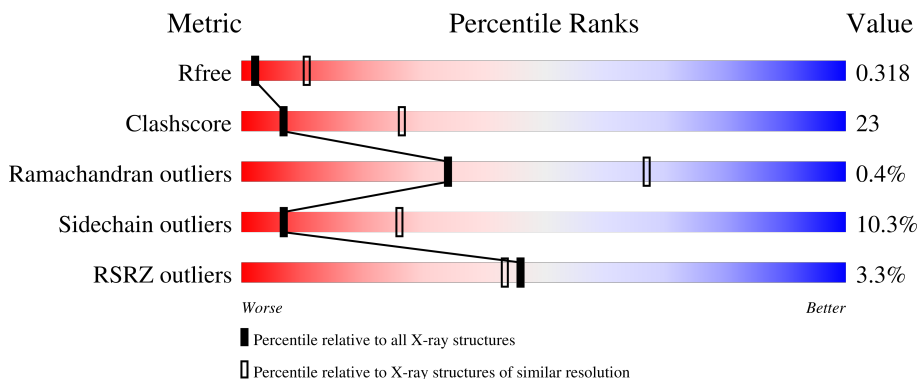
1 Overall quality at a glance

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}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (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	
1	B	239	
2	C	1342	
3	D	1409	
4	E	90	

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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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
4	E	79	627	382	118	126	1	0	0	0

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

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

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
			Total	C	N	O	P			
6	N	29	595	284	106	176	29	0	0	0

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

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

- Molecule 8 is a protein called Capistrain.

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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

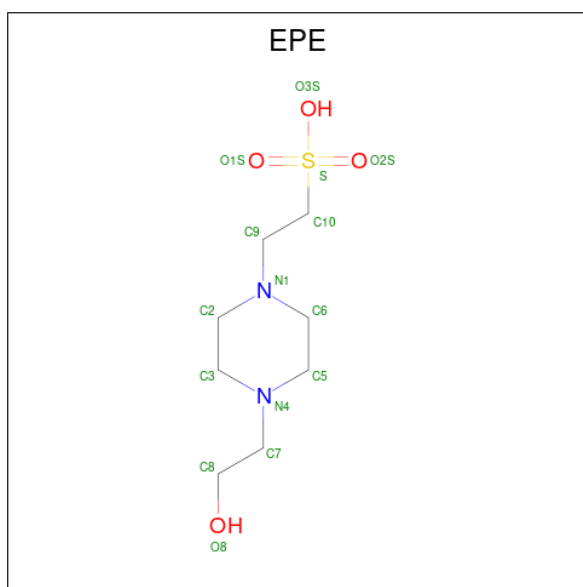
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 12 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

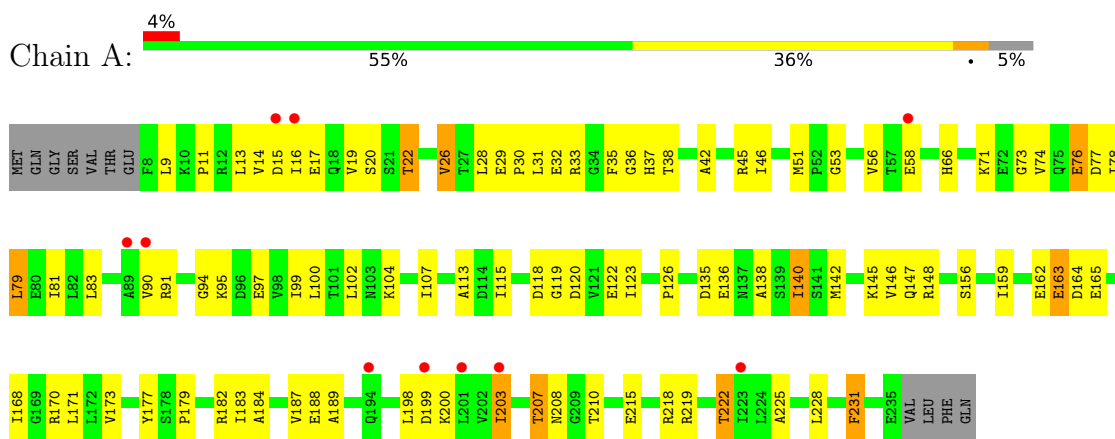
- Molecule 13 is water.

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

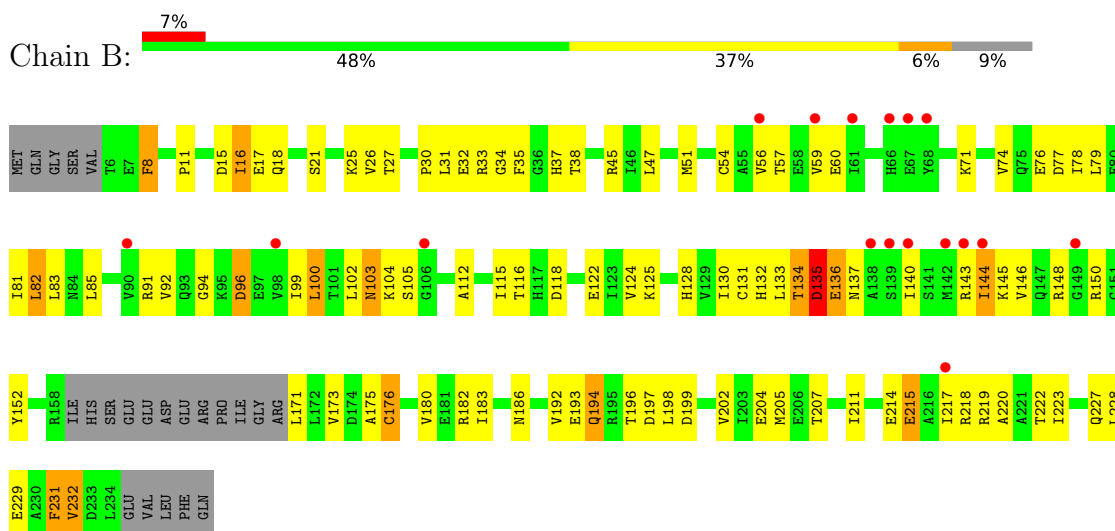
3 Residue-property plots

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

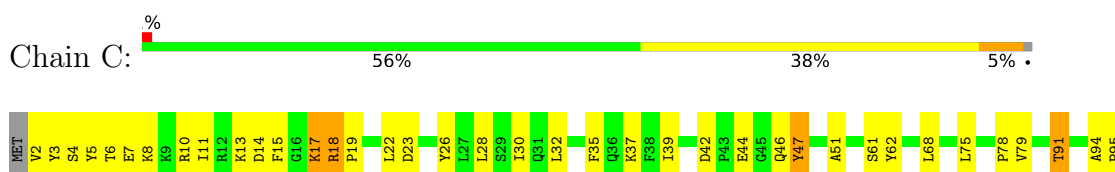
- Molecule 1: DNA-directed RNA polymerase subunit alpha

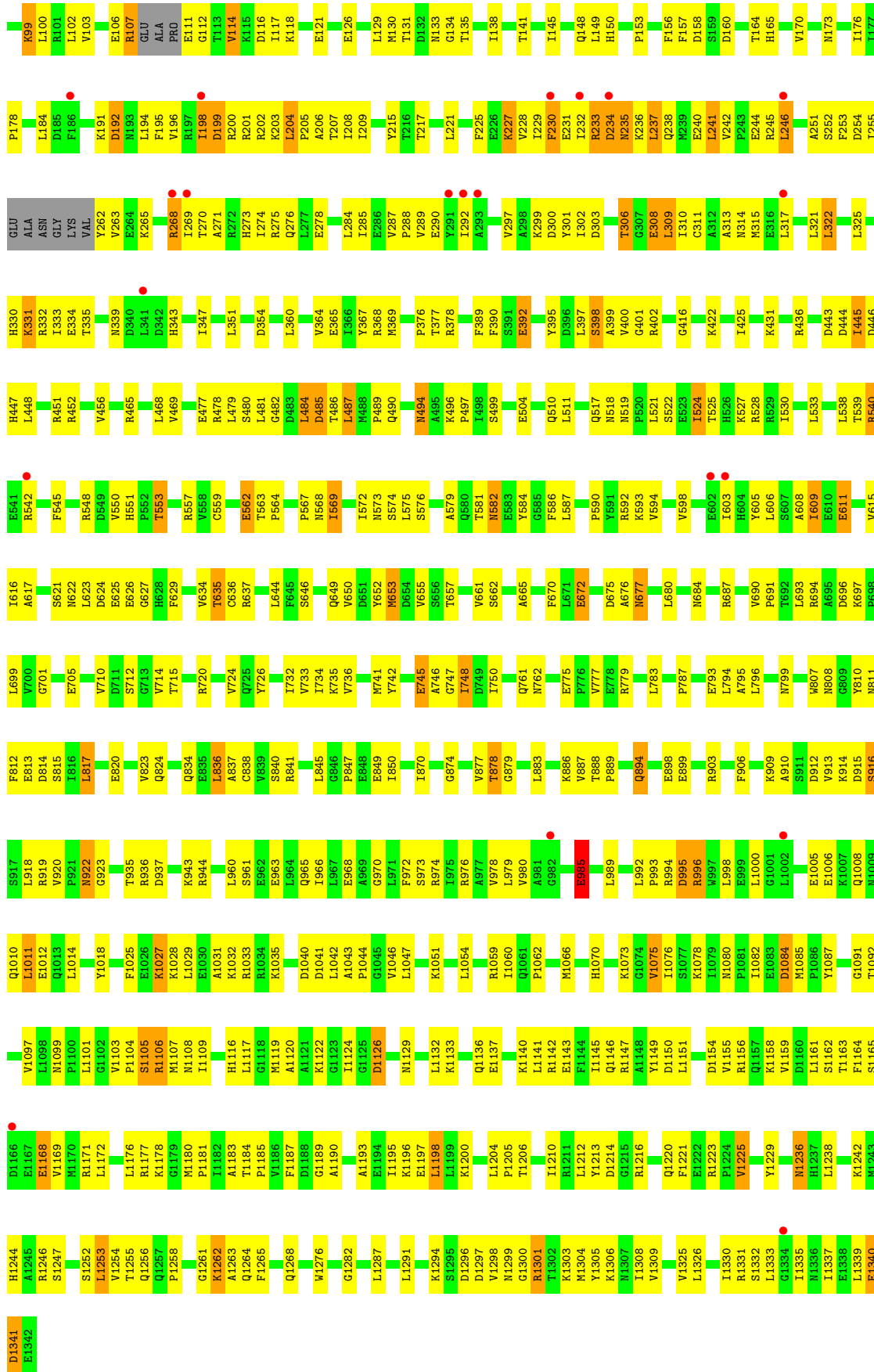


- Molecule 1: DNA-directed RNA polymerase subunit alpha

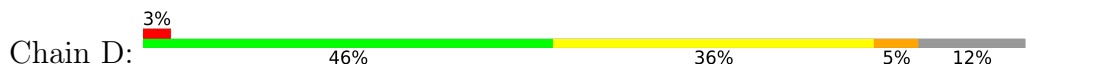


- Molecule 2: DNA-directed RNA polymerase subunit beta

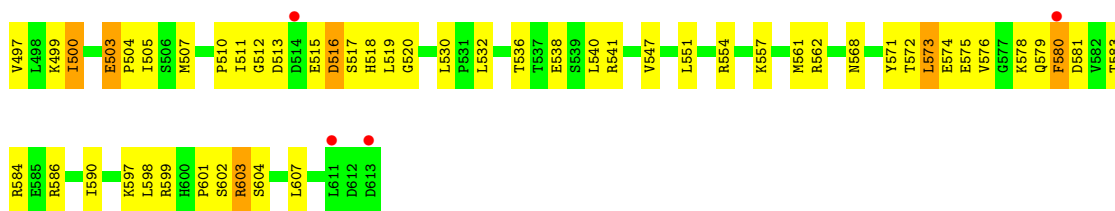




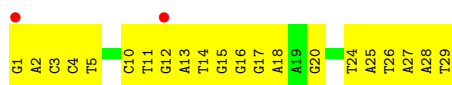
• Molecule 3: DNA-directed RNA polymerase subunit beta'



VAL	C85	Q157	K325	M400	A494	W580	T674	E756	V839	A919	E1009	ALA
LYS	E86	Q158	S326	V401	M495	K585	R678	I757	L840	Q1010	GLY	GLY
ASP	R87	T161	L327	E405	E497	R680	R679	P758	G841	P758	GLY	GLY
LEU	C88	T162	A328	E406	E498	S589	K681	Y759	R842	G924	LYS	LYS
LEU	G89	Q164	D329	I408	I499	S590	K682	N762	V843	E925	ASP	ASP
PHE	V90	Q165	M330	V408	I500	I591	V682	N763	E846	P926	LEU	LEU
LEU	R93	D167	K332	I411	P501	V592	V683	R763	D847	F935	ARG	ARG
LEU	Q94	G173	K333	V415	L510	M593	S694	R764	V848	F936	PRO	PRO
ALA	R95	D174	K334	V416	A600	Q594	R686	N768	L849	H936	ALA	ALA
GLN	K96	R175	R337	I417	S603	Q595	W686	V769	L850	I937	LEU	LEU
THR	V97	E176	F338	R417	Q504	A596	A689	L770	K850	G938	LYS	LYS
LYS	R98	F176	R339	E418	L596	L597	A690	O771	P851	P851	ILE	ILE
THR	R99	D177	R340	E418	V606	G597	V683	O772	G852	O771	VAL	VAL
GLU	E100	A178	Q340	R425	V607	K598	S694	Y772	T853	Y772	ASP	ASP
GLU	F17	E183	N341	A426	L511	K599	R697	F773	A854	F773	THR	THR
F17	M102	E183	N342	P427	L512	A600	M697	I774	A855	I774	GLN	GLN
LEU	M103	Q186	L342	A427	M513	A601	M697	S775	R857	R775	ASN	ASN
LEU	H104	A187	L343	H430	T514	S602	N700	H776	V858	I776	VAL	VAL
VAL	I105	A188	R345	H431	R515	K603	L701	H777	P859	H777	VAL	VAL
LEU	L107	L189	R346	R431	D516	M604	Q702	R780	R860	R860	LEU	LEU
LEU	L108	K190	V347	L432	A520	K615	E704	K781	S861	S948	THR	THR
THR	N29	K191	D348	L433	A521	P616	E705	G782	T862	S949	GLU	GLU
THR	S109	L194	L265	E438	E523	P620	V706	D785	L864	L864	SER	SER
THR	P110	L194	L266	E439	G524	F620	I707	T786	H865	H865	GLY	GLY
GLU	M101	E195	L267	I442	M525	I624	M708	A787	W868	W868	PHE	PHE
GLU	R101	Q196	L268	E443	M625	I625	R709	L788	C869	C869	VAL	VAL
GLU	M102	Q196	Y269	E444	M626	L641	D710	A788	R869	R869	VAL	VAL
LEU	G103	C198	R270	Q448	T528	I642	G711	K789	L872	L872	ARG	ARG
LEU	H113	C198	R271	Q449	G529	M644	G712	T797	L873	L873	GLN	GLN
LEU	I114	E199	V272	Q450	L449	V645	Q712	R798	M875	M875	THR	THR
LEU	W115	L201	I273	H451	P630	V646	E713	R798	S876	S876	THR	THR
LEU	K118	S119	R274	H452	K631	S638	I717	V801	D877	D877	GLU	GLU
LEU	S119	L202	M874	L453	E532	I641	R718	D802	D878	D878	GLY	GLY
LEU	S119	R202	N875	V453	E533	M644	S721	V803	R883	R883	GLY	GLY
LEU	P121	E203	R275	V454	S543	V645	M725	L804	S884	S884	GLN	GLN
LEU	S122	E204	R278	V455	L644	V646	R731	A804	V885	V885	LEU	LEU
LEU	R123	E204	L279	A459	L645	P647	R732	Q805	V886	V886	GLN	GLN
LEU	I124	L205	L382	F461	H645	E648	M735	D812	S887	S887	GLY	GLY
LEU	G125	N209	L382	D462	V648	K649	A736	D813	C888	C888	THR	THR
LEU	L126	S210	D289	E375	V548	K650	I737	C814	D889	D889	THR	THR
LEU	L127	E211	D289	E376	V549	K650	R738	G815	T890	T890	GLY	GLY
LEU	L128	T121	I290	L376	L646	V648	Q739	D816	V894	V894	VAL	VAL
LEU	D129	K213	I291	F377	E648	V649	L740	D817	C988	C988	THR	THR
LEU	M130	R214	V292	F377	E649	V649	L740	C815	Y899	Y899	THR	THR
LEU	M130	K215	R293	K378	A559	V650	L741	G816	G900	G900	SER	SER
LEU	L131	K215	N294	P379	A560	V651	M743	T816	R901	R901	GLY	GLY
LEU	L132	K216	M294	F380	N560	V652	R744	H617	D902	D902	ASP	ASP
LEU	L133	L217	E295	F380	N561	V653	R745	R617	L904	L904	VAL	VAL
LEU	R133	L217	K296	Y382	V564	V654	G746	R618	A904	A904	LEU	LEU
LEU	D134	L217	E296	L474	V565	V655	L747	E619	R905	R905	LEU	LEU
LEU	L135	L224	K297	L474	V566	V656	L748	G619	G906	G906	ASP	ASP
LEU	E136	R220	M298	Q477	A569	V657	M749	D622	G906	G906	VAL	VAL
LEU	E137	R221	R298	Q478	A569	V658	R749	T623	A913	A913	THR	THR
LEU	V138	L223	E386	L478	N560	V659	K749	P624	E914	E914	LEU	LEU
LEU	V138	L223	E386	E479	V563	V660	R750	V625	Y915	Y915	LEU	LEU
LEU	V145	L224	L387	A482	V564	V661	P750	R826	G906	G906	ASP	ASP
LEU	V145	L224	L388	L483	V565	V662	P751	R827	A914	A914	THR	THR
LEU	I147	G231	R389	A483	V566	V663	P752	R828	E915	E915	THR	THR
LEU	G231	G231	G389	L483	V567	V664	P753	R829	L1003	L1003	GLN	GLN
LEU	G231	G231	G389	L484	V568	V665	P754	R830	A1004	A1004	GLU	GLU
LEU	G231	G231	G389	L485	V569	V666	P755	R831	K1005	K1005	THR	THR
LEU	G231	G231	G389	L486	V570	V667	P756	R832				
LEU	G231	G231	G389	L487	V571	V668	P757	R833				
LEU	G231	G231	G389	L488	V572	V669	P758	R834				
LEU	G231	G231	G389	L489	V573	V670	P759	R835				
LEU	G231	G231	G389	L490	V574	V671	P760	R836				
LEU	G231	G231	G389	L491	V575	V672	P761	R837				
LEU	G231	G231	G389	L492	V576	V673	P762	R838				
LEU	G231	G231	G389	L493	V577	V674	P763	R839				
LEU	G231	G231	G389	L494	V578	V675	P764	R840				
LEU	G231	G231	G389	L495	V579	V676	P765	R841				
LEU	G231	G231	G389	L496	V580	V677	P766	R842				
LEU	G231	G231	G389	L497	V581	V678	P767	R843				
LEU	G231	G231	G389	L498	V582	V679	P768	R844				
LEU	G231	G231	G389	L499	V583	V680	P769	R845				
LEU	G231	G231	G389	L500	V584	V681	P770	R846				
LEU	G231	G231	G389	L501	V585	V682	P771	R847				
LEU	G231	G231	G389	L502	V586	V683	P772	R848				
LEU	G231	G231	G389	L503	V587	V684	P773	R849				
LEU	G231	G231	G389	L504	V588	V685	P774	R850				
LEU	G231	G231	G389	L505	V589	V686	P775	R851				
LEU	G231	G231	G389	L506	V590	V687	P776	R852				
LEU	G231	G231	G389	L507	V591	V688	P777	R853				
LEU	G231	G231	G389	L508	V592	V689	P778	R854				
LEU	G231	G231	G389	L509	V593	V690	P779	R855				
LEU	G231	G231	G389	L510	V594	V691	P780	R856				
LEU	G231	G231	G389	L511	V595	V692	P781	R857				
LEU	G231	G231	G389	L512	V596	V693	P782	R858				
LEU	G231	G231	G389	L513	V597	V694	P783	R859				
LEU	G231	G231	G389	L514	V598	V695	P784	R860				
LEU	G231	G231	G389	L515	V599	V696	P785	R861				
LEU	G231	G231	G389	L516	V600	V697	P786	R862				
LEU	G231	G231	G389	L517	V601	V698	P787	R863				
LEU	G231	G231	G389	L518	V602	V699	P788	R864				
LEU	G231	G231	G389	L519	V603	V700	P789	R865				
LEU	G231	G231	G389	L520	V604	V701	P790	R866				
LEU	G231	G231	G389	L521	V605	V702	P791	R867				
LEU	G231	G231	G389	L522	V606	V703	P792	R868				
LEU	G231	G231	G389	L523	V607	V704	P793	R869				
LEU	G231	G231	G389	L524	V608	V705	P794	R870				
LEU	G231	G231	G389	L525	V609	V706	P795	R871				
LEU	G231	G231	G389	L526	V610	V707	P796	R872				
LEU	G231	G231	G389	L527	V611	V708	P797	R873				
LEU	G231	G231	G389	L528	V612	V709	P798	R874				
LEU	G231	G231	G389	L529	V613	V710	P799	R875				
LEU	G231	G231	G389	L530	V614	V711	P800	R876				
LEU	G231	G231	G389	L531	V615	V712	P801	R877				
LEU	G231	G231	G389	L532	V616	V713	P802	R878				
LEU	G231	G231	G389	L533	V617	V714	P803	R879				
LEU	G231	G231	G389	L534	V618	V715	P804	R880				
LEU	G231	G231	G389	L535	V619	V716	P805	R881				
LEU	G231	G231	G389	L536	V620	V717	P806	R882				
LEU	G231	G231	G389	L537	V621	V718	P807	R883				
LEU	G231	G231	G389	L538	V622	V719	P808	R884				
LEU	G231	G231	G389	L539	V623	V720	P809	R885				
LEU	G231	G231	G389	L540	V624	V721	P810	R886				
LEU	G231	G231	G389	L541	V625	V722	P811	R887				
LEU	G231	G231	G389	L542	V626	V723	P812	R888				
LEU	G231	G231	G389	L543	V627	V724	P813	R889				
LEU	G231	G231	G389	L544	V628	V725	P814	R890				
LEU	G231	G231	G389	L545	V629	V726	P815	R891				
LEU	G231	G231	G389	L546	V630	V727	P816	R892				
LEU	G231	G231	G389	L547	V631	V728	P817	R893				
LEU	G231	G231	G389	L548	V632	V729	P818	R894				
LEU	G231											



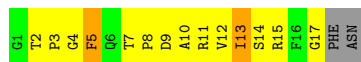
- Molecule 6: non-template strand DNA



- 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 49.44 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.45-3.25) 99.0 (49.44-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.273 , 0.316 0.277 , 0.318	Depositor DCC
R_{free} test set	1980 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å ²)	99.1	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, ZN, EDO, 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	0.24	0/1729	0.46	0/2349
1	B	0.24	0/1677	0.47	0/2274
2	C	0.25	0/10654	0.43	0/14375
3	D	0.25	0/9794	0.44	0/13212
4	E	0.22	0/629	0.39	0/847
5	F	0.24	0/3239	0.40	0/4352
6	N	0.55	1/666 (0.2%)	0.90	0/1026
7	T	0.57	1/552 (0.2%)	0.84	0/849
8	I	0.30	0/129	0.55	0/173
All	All	0.26	2/29069 (0.0%)	0.46	0/39457

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	DA	C1'-N9	-5.97	1.38	1.47
6	N	12	DG	C1'-N9	-5.60	1.39	1.47

There are no bond angle outliers.

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	86	0
2	C	10489	0	10490	455	0
3	D	9649	0	9859	531	0
4	E	627	0	634	31	0
5	F	3197	0	3251	148	0
6	N	595	0	329	36	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	1306	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 23.

The worst 5 of 1306 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 [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	226/239 (95%)	206 (91%)	19 (8%)	1 (0%)	34	67
1	B	213/239 (89%)	196 (92%)	14 (7%)	3 (1%)	11	40
2	C	1326/1342 (99%)	1245 (94%)	75 (6%)	6 (0%)	29	62
3	D	1231/1409 (87%)	1145 (93%)	83 (7%)	3 (0%)	47	77
4	E	77/90 (86%)	73 (95%)	3 (4%)	1 (1%)	12	41
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%)	34	67

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 [i](#)

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%)	166 (92%)	15 (8%)	11	36
1	B	181/206 (88%)	163 (90%)	18 (10%)	8	28
2	C	1144/1157 (99%)	1033 (90%)	111 (10%)	8	29
3	D	1035/1170 (88%)	921 (89%)	114 (11%)	6	24
4	E	67/74 (90%)	64 (96%)	3 (4%)	27	58
5	F	350/540 (65%)	308 (88%)	42 (12%)	5	20
8	I	13/15 (87%)	11 (85%)	2 (15%)	2	12
All	All	2971/3368 (88%)	2666 (90%)	305 (10%)	7	26

5 of 305 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	890	THR
5	F	487	MET
3	D	1024	THR
4	E	36	ASP
5	F	581	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	164	GLN
5	F	589	GLN
3	D	594	GLN
5	F	518	HIS
5	F	131	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 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
12	EPE	D	1504	-	15,15,15	0.90	1 (6%)	18,20,20	2.09	6 (33%)
9	EDO	C	1401	-	3,3,3	0.44	0	2,2,2	0.58	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
12	EPE	D	1504	-	-	3/9/19/19	0/1/1/1
9	EDO	C	1401	-	-	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	3.09	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	4.36	122.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	1504	EPE	O2S-S-C10	3.98	111.71	106.92
12	D	1504	EPE	C5-N4-C3	3.13	115.88	108.83
12	D	1504	EPE	C7-N4-C3	2.85	118.52	111.23
12	D	1504	EPE	O3S-S-C10	2.64	110.04	105.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	1504	EPE	7	0
9	C	1401	EDO	1	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 [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	228/239 (95%)	0.22	10 (4%) 34 32	73, 115, 173, 204	0
1	B	217/239 (90%)	0.39	17 (7%) 13 12	74, 133, 174, 188	0
2	C	1332/1342 (99%)	-0.04	20 (1%) 73 71	36, 92, 163, 211	0
3	D	1239/1409 (87%)	0.12	42 (3%) 45 42	45, 104, 181, 218	0
4	E	79/90 (87%)	-0.04	1 (1%) 77 75	71, 95, 155, 183	0
5	F	395/613 (64%)	0.28	26 (6%) 18 17	68, 140, 182, 213	0
6	N	29/29 (100%)	-0.13	2 (6%) 16 16	124, 171, 253, 256	0
7	T	24/24 (100%)	-0.22	0 100 100	114, 179, 256, 268	0
8	I	17/19 (89%)	0.12	0 100 100	97, 108, 127, 131	0
All	All	3560/4004 (88%)	0.09	118 (3%) 46 43	36, 107, 178, 268	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	6.9
3	D	972	LYS	6.1
3	D	973	LEU	6.0
2	C	230	PHE	5.9
5	F	352	GLY	5.8

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, 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
12	EPE	D	1504	15/15	0.70	0.33	114,143,172,178	0
9	EDO	C	1401	4/4	0.83	0.20	98,117,137,139	0
11	ZN	D	1503	1/1	0.90	0.24	108,108,108,108	0
11	ZN	D	1502	1/1	0.95	0.14	126,126,126,126	0
10	MG	D	1501	1/1	0.99	0.31	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.