



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 07:58 PM UTC

PDB ID : 4G7O / pdb_00004g7o
Title : Crystal structure of Thermus thermophilus transcription initiation complex containing 2 nt of RNA
Authors : Zhang, Y.; Ebright, R.H.
Deposited on : 2012-07-20
Resolution : 2.99 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

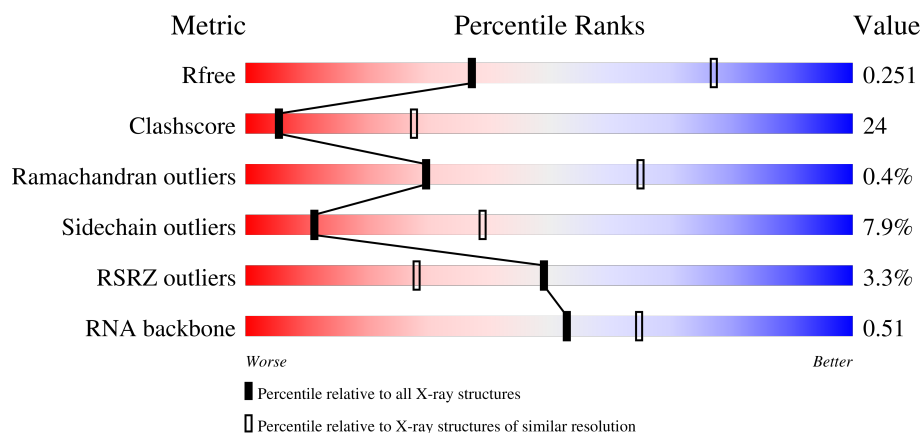
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	315	42%27%•28%
1	B	315	2% 39%26%5%30%
1	K	315	46%24%•28%
1	L	315	2% 42%25%•29%

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Mol	Chain	Length	Quality of chain
2	C	1119	
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	G	21	
6	Q	21	
7	H	27	
7	R	27	
8	I	2	
8	S	2	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 57231 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	L	225	Total	C	N	O	S	0	0	0
			1773	1133	308	330	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1482	Total	C	N	O	S	0	0	0
			11704	7421	2059	2189	35			
3	N	1489	Total	C	N	O	S	0	0	0
			11746	7446	2066	2198	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	P	347	Total	C	N	O	S	0	0	0
			2814	1774	510	526	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1
P	-19	MET	-	expression tag	UNP Q5SKW1
P	-18	GLY	-	expression tag	UNP Q5SKW1
P	-17	SER	-	expression tag	UNP Q5SKW1
P	-16	SER	-	expression tag	UNP Q5SKW1
P	-15	HIS	-	expression tag	UNP Q5SKW1
P	-14	HIS	-	expression tag	UNP Q5SKW1
P	-13	HIS	-	expression tag	UNP Q5SKW1
P	-12	HIS	-	expression tag	UNP Q5SKW1
P	-11	HIS	-	expression tag	UNP Q5SKW1
P	-10	HIS	-	expression tag	UNP Q5SKW1
P	-9	SER	-	expression tag	UNP Q5SKW1
P	-8	SER	-	expression tag	UNP Q5SKW1
P	-7	GLY	-	expression tag	UNP Q5SKW1
P	-6	LEU	-	expression tag	UNP Q5SKW1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	expression tag	UNP Q5SKW1
P	-4	PRO	-	expression tag	UNP Q5SKW1
P	-3	ARG	-	expression tag	UNP Q5SKW1
P	-2	GLY	-	expression tag	UNP Q5SKW1
P	-1	SER	-	expression tag	UNP Q5SKW1
P	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			
6	Q	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			

- Molecule 7 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*C P*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			
7	R	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a RNA chain called 5'-R(*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			
8	S	2	Total	C	N	O	P	0	0	0
			42	20	10	11	1			

- 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	N	2	Total	Zn	0	0
			2	2		

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

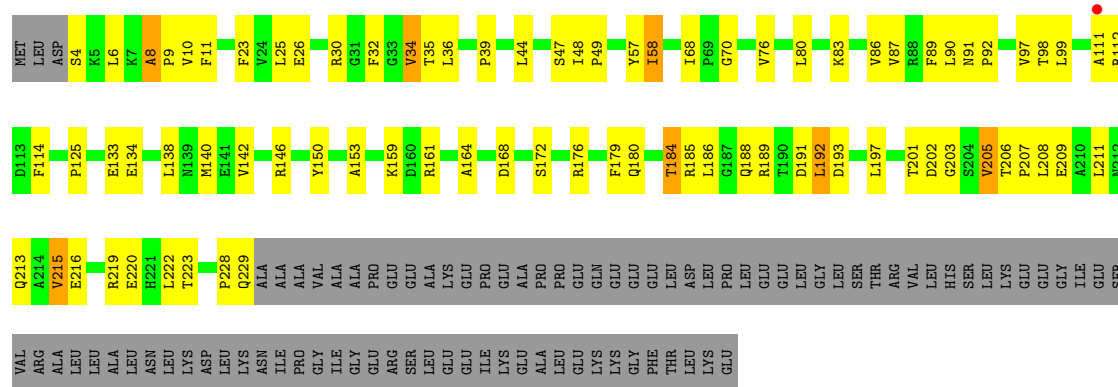
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	2	Total Mg 2 2	0	0
10	K	1	Total Mg 1 1	0	0
10	N	2	Total Mg 2 2	0	0

- Molecule 11 is water.

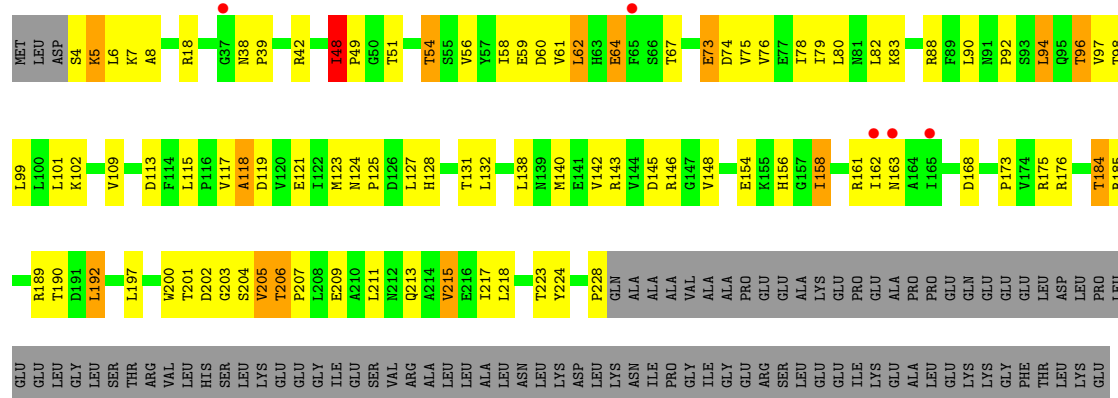
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	14	Total O 14 14	0	0
11	B	3	Total O 3 3	0	0
11	C	53	Total O 53 53	0	0
11	D	58	Total O 58 58	0	0
11	E	8	Total O 8 8	0	0
11	F	10	Total O 10 10	0	0
11	G	5	Total O 5 5	0	0
11	H	2	Total O 2 2	0	0
11	K	4	Total O 4 4	0	0
11	L	3	Total O 3 3	0	0
11	M	33	Total O 33 33	0	0
11	N	52	Total O 52 52	0	0
11	O	5	Total O 5 5	0	0
11	P	16	Total O 16 16	0	0
11	Q	2	Total O 2 2	0	0
11	R	3	Total O 3 3	0	0
11	S	1	Total O 1 1	0	0

- Molecule 1: DNA-directed RNA polymerase subunit alpha

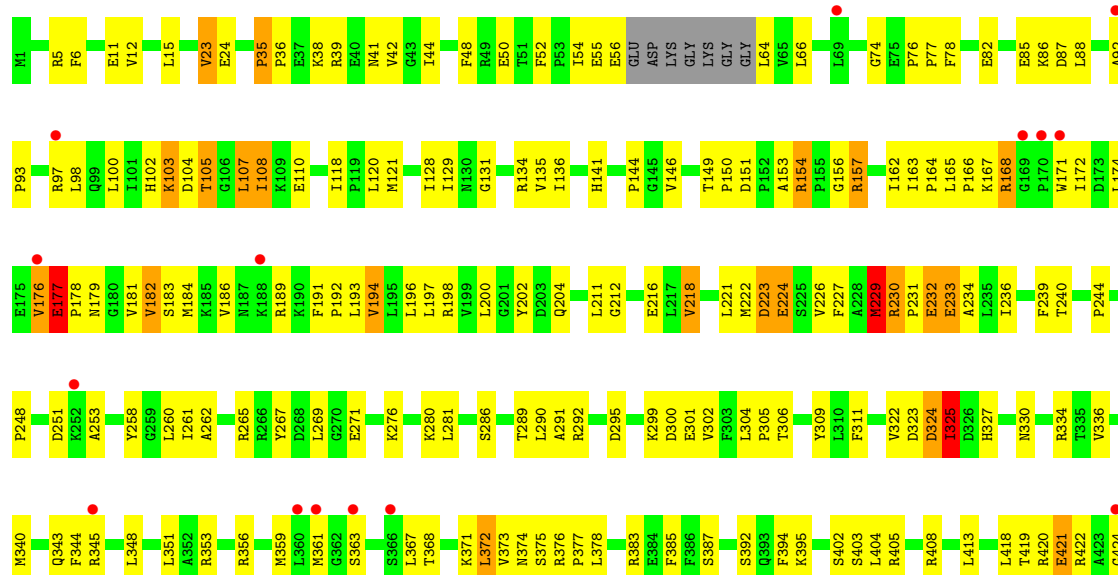


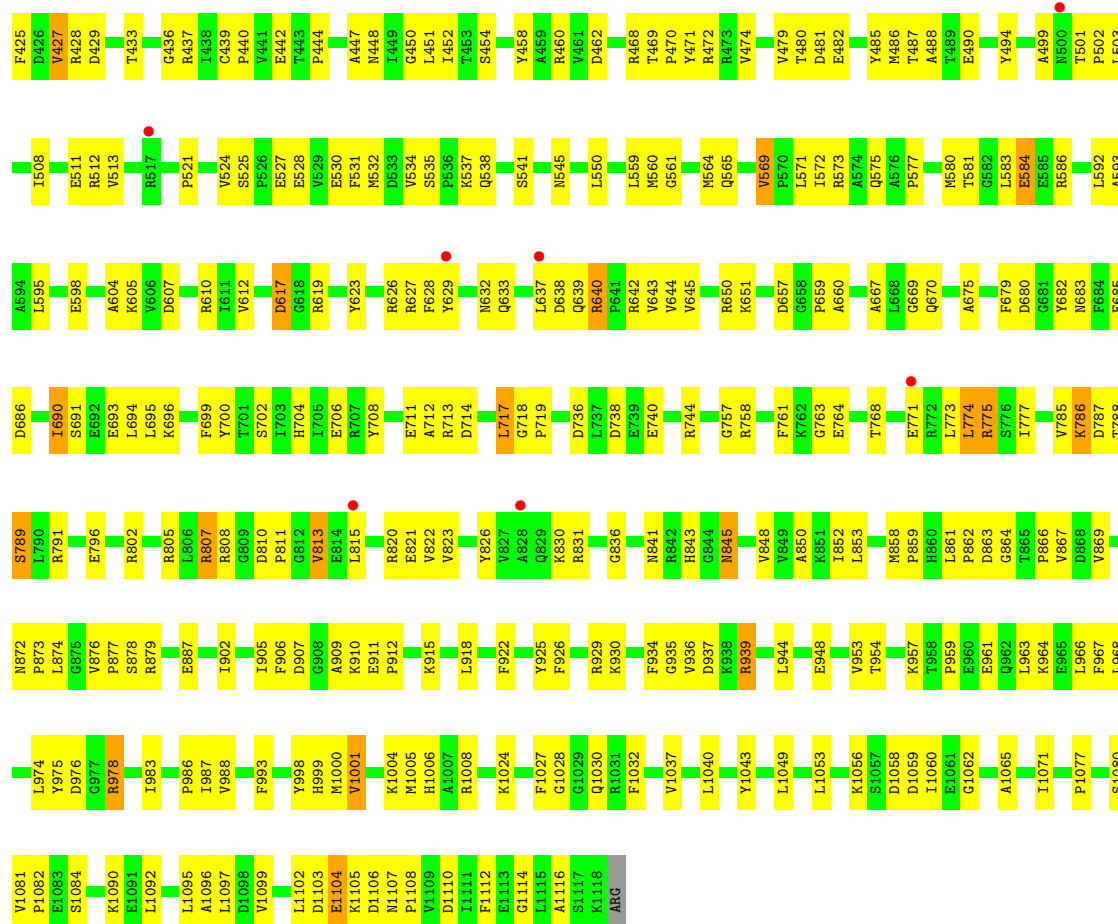


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

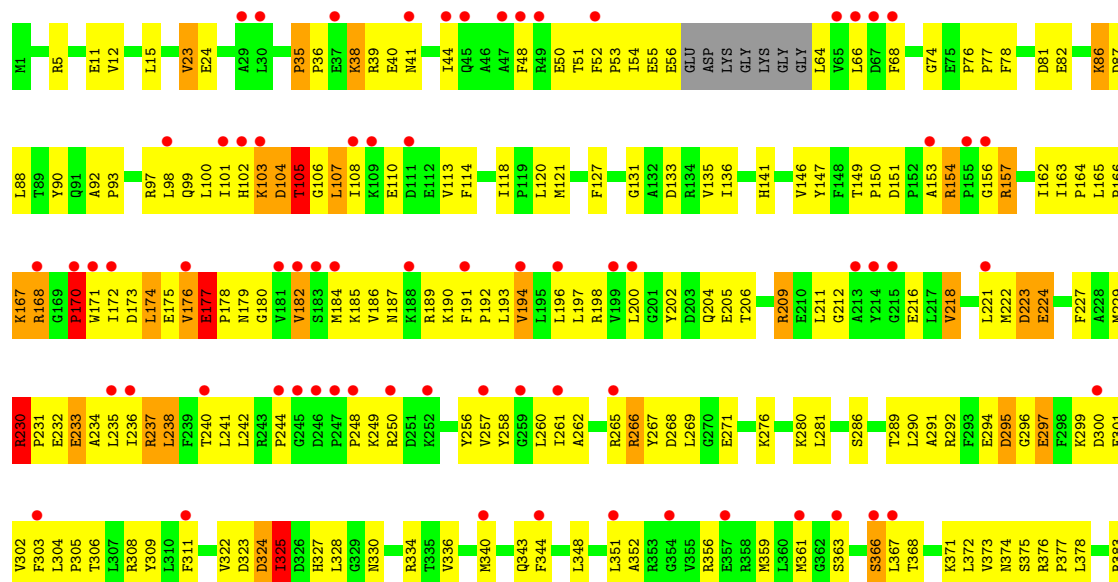


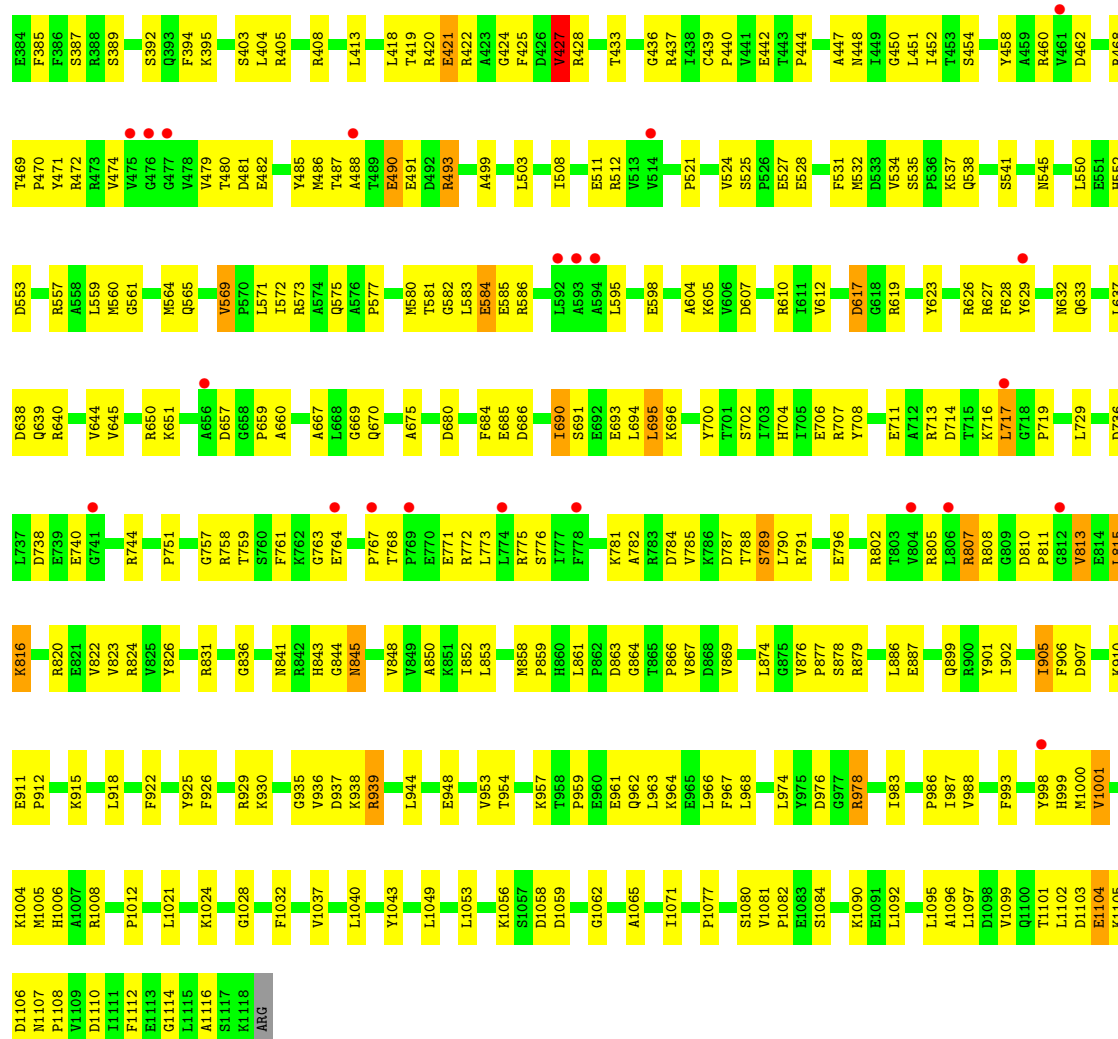


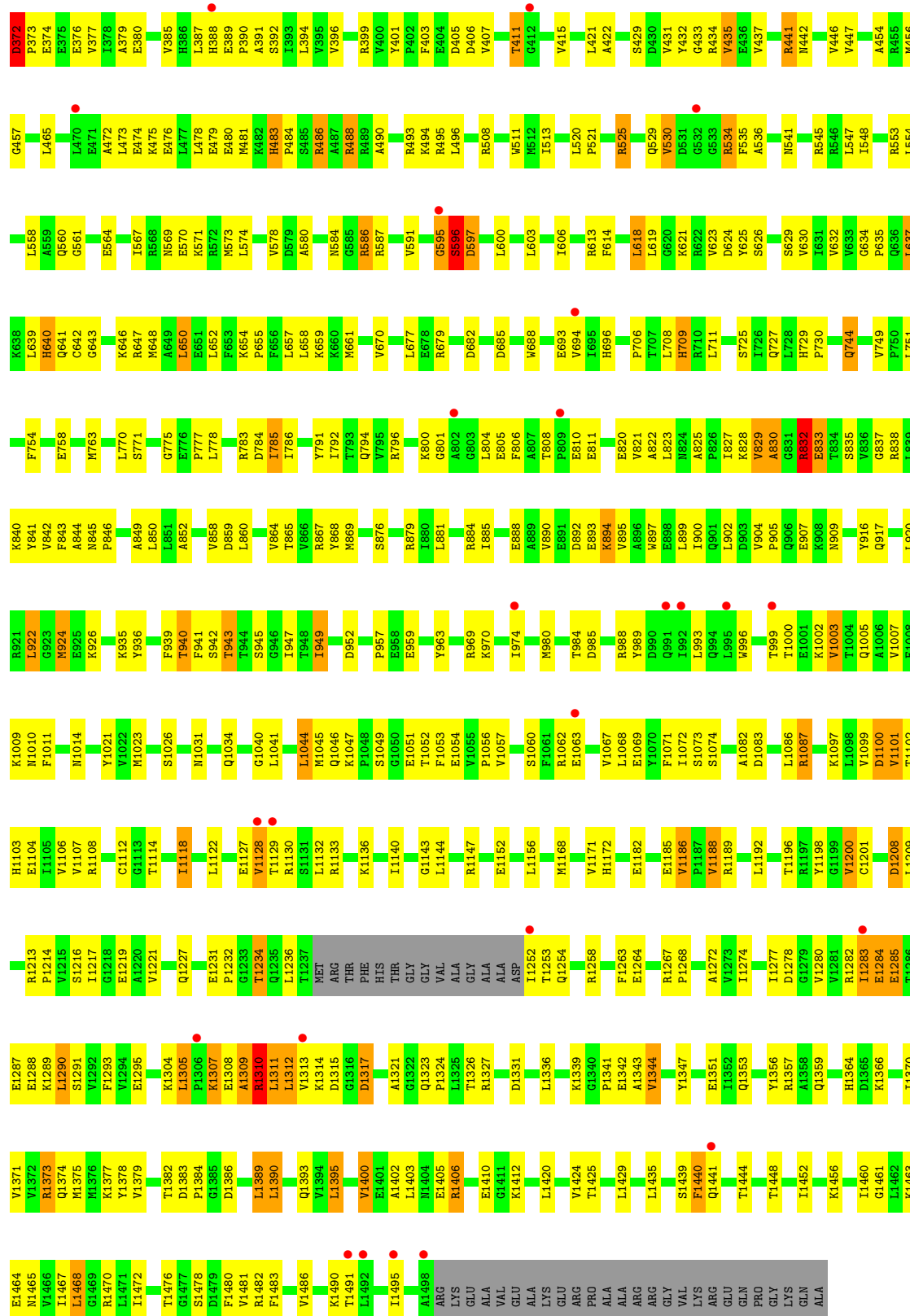
• Molecule 2: DNA-directed RNA polymerase subunit beta



Chain M:



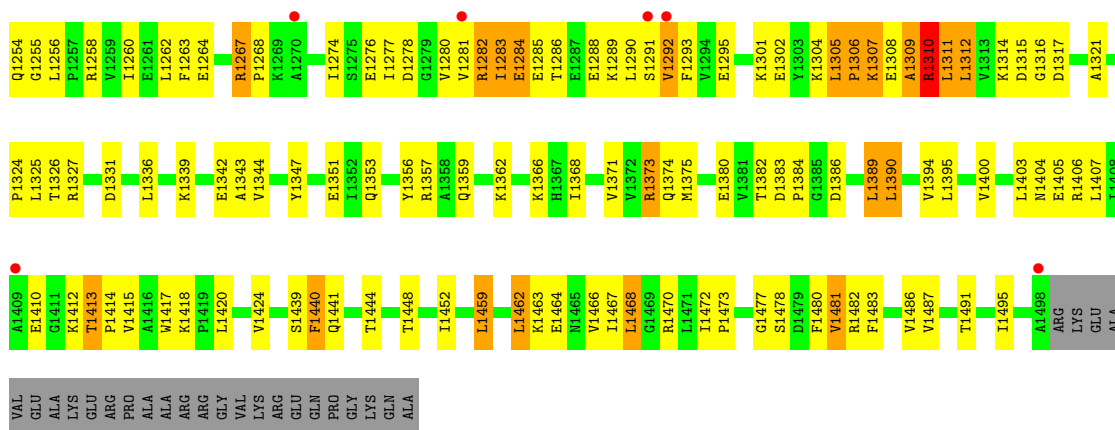




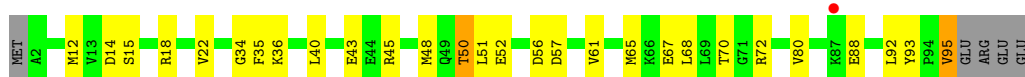
• Molecule 3: DNA-directed RNA polymerase subunit beta'



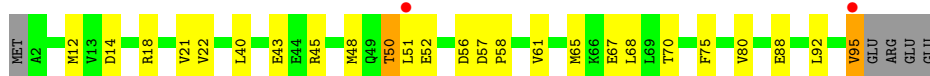
I1140	K1047	M869	L787	K671	G595	R495	A422	E338	E255	L171	R86	MET
G1143	P1048	S876	Y791	R675	S596	L496	S429	W339	E256	D181	R87	LYS
R1147	S1049	E958	Y792	R676	E497	V498	D430	V347	V259	E184	R88	K3
L1156	E1051	R879	L793	L677	P599	R598	Y431	Q348	E260	K187	R89	E4
R1159	T1052	I880	Q794	R678	L600	W511	Y432	Q349	L264	T97	R90	V5
V1171	F1053	L881	R795	R679	R601	M512	G433	P349	E265	P96	R91	R6
I1175	E1054	R884	R796	Q680	S602	I513	R434	H550	E266	K187	R92	K7
E1182	P1055	I885	R800	R681	L603	E525	V435	M351	E267	L191	S14	
V1188	P1056	E888	G801	D682	Q606	P526	E436	V353	F269	W103	P15	
R1189	V1057	E889	L804	D685	R613	R525	D438	V355	L270	K106	K17	
C1194	F1061	V890	E805	W688	F614	P527	V437	P356	V271	D107	I18	
Y1198	R1062	E891	F06	E693	L618	M527	R441	A359	L272	V108	R19	
G1199	V1067	D892	T808	V694	L619	V530	R445	V368	E275	W109	S20	
V1200	E1069	K894	P809	R706	G620	R534	V446	V377	E276	K111	E30	
C1204	Y1070	W897	E810	T707	R622	R535	V447	I371	E277	T114	I32	
D1208	F1071	E898	E820	L708	V623	A536	Y450	P373	V279	L115	N33	
R1213	I1072	L899	V821	H709	B624	F548	D451	P208	E280	L116	R35	
P1214	S1073	I900	R710	R710	V625	I541	I452	T281	T281	T121	T36	
V1215	S1074	Q901	A822	L711	S626	R545	D453	E376	Y282	E124	L37	
E1219	A1082	L902	L823	W719	V630	R546	A454	I378	E283	L217	K38	
Q1227	D1083	V904	A825	L720	V631	R547	R455	A379	L284	L127	P39	
E1231	L1086	P905	P826	W721	V632	I548	M456	E380	E285	K131	L44	
P1232	L1087	Q906	K827	S725	V633	R553	G457	V385	G287	I132	F45	
T1234	R1087	K908	V829	L726	G634	L558	A460	H886	M288	I133	D46	
M1238	Y1093	N909	A830	Q727	L637	A562	Q463	L387	V298	V134	E47	
ARG	K1097	Y916	G831	L728	R636	P563	L464	H888	E299	L135	R48	
THR	L1098	Q917	R832	H729	L639	E570	L465	E389	K300	D136	D47	
HIS	V1099	F1008	E833	P730	H640	E564	L466	P390	G301	K138	R48	
THR	D1100	K1009	T834	L731	G641	I565	L468	A391	Q302	G139	I53	
GLY	V1101	N1010	S835	Q744	G643	I566	L468	S392	P303	A140	K54	
V1246	T1102	L922	G837	R749	R646	I567	A472	L394	E306	I141	D55	
A1247	P1107	K926	R838	P750	R647	N569	L473	V395	A307	L142	Y56	
G1248	R1108	L931	L839	L751	M648	E570	K475	V396	L310	N143	R65	
A1249	F1123	K935	L840	P754	L650	K571	L477	R399	L311	V230	Q66	
A1250	Q1124	Y936	L842	R754	E551	E572	L478	V400	R312	G144	R67	
D1251	P1125	F939	N845	W763	P653	M573	L479	Y401	M313	P146	F68	
T1253	D1126	T940	P846	F754	R654	L574	E479	P402	P314	V147	E69	
	E1127	F941	P846	P754	R655	V578	M481	E404	Q316	K149	G70	
	V1128	F942	V842	R754	P655	D579	K482	D405	V317	R150	V72	
	T1129	S942	L850	S774	L657	A580	H483	D406	E323	L152	C73	
	R1130	S942	V858	G774	L658	N584	P484	V407	E326	L242	E74	
	S1131	T944	D859	G775	R659	G585	S485	S410	E326	A243	R75	
	L1132	S945	L860	E776	R659	R586	R486	T411	E244	D155	C76	
	R1133	G946	L860	P777	R660	R587	A487	G412	L245	D155	G77	
	E1134	I947	V864	L778	N661	R587	R488	D413	V332	R159	V78	
	R1135	T948	T865	R783	E662	R587	R488	D413	V332	F160	F79	
	K1136	I949	R866	D784	E663	V591	K491	R414	L333	L161	V80	
	R1137	M1045	R867	I785	N669	T592	A492	V415	T334	R162	I84	
		D952	Y868	I786	V670	P594	K494		L337	P170	R85	



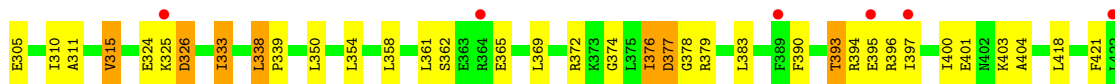
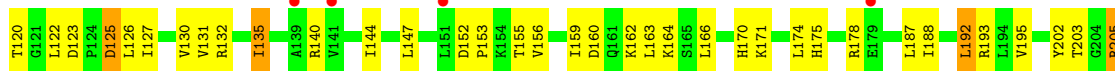
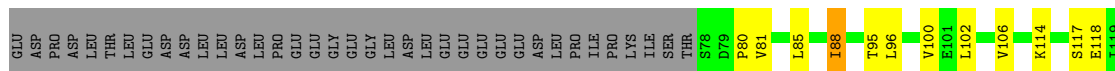
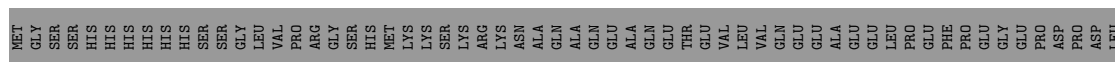
- Molecule 4: DNA-directed RNA polymerase subunit omega



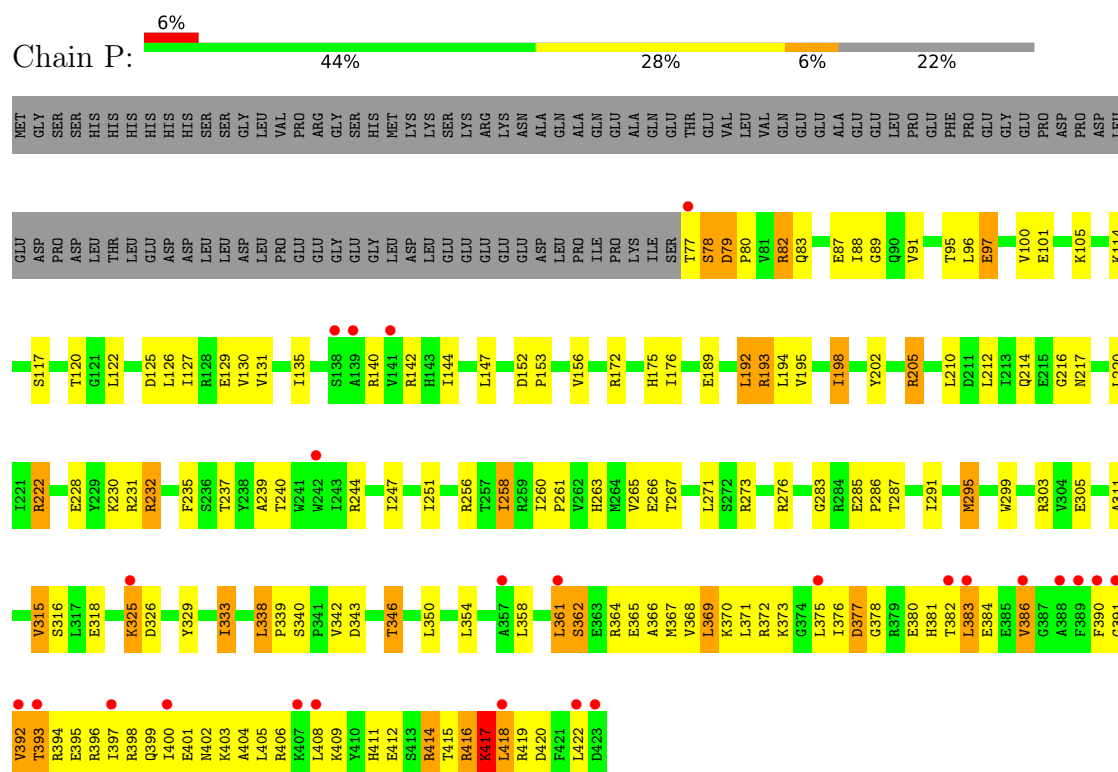
- Molecule 4: DNA-directed RNA polymerase subunit omega



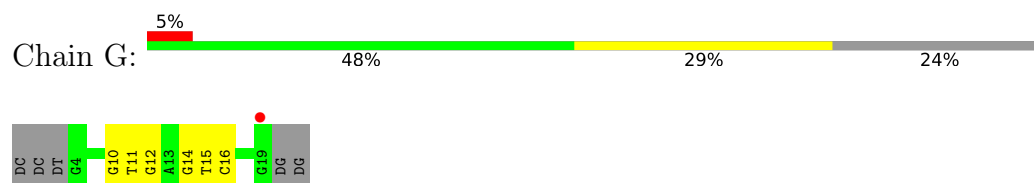
- Molecule 5: RNA polymerase sigma factor



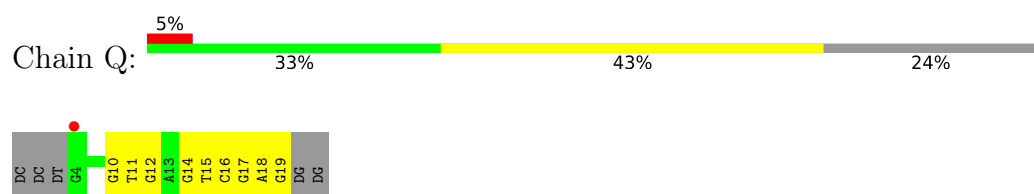
• Molecule 5: RNA polymerase sigma factor



• Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'



• Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'



• Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

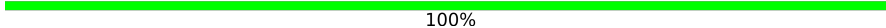


- Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain R:  59% 30% 11%

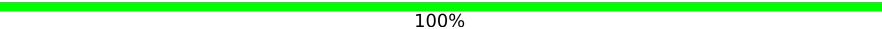


- Molecule 8: 5'-R(*GP*A)-3'

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: 5'-R(*GP*A)-3'

Chain S:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	185.48Å 103.88Å 297.34Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	46.61 – 2.99 46.61 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.61-2.99) 95.5 (46.61-2.99)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.205 , 0.247 0.209 , 0.251	Depositor DCC
R_{free} test set	1946 reflections (0.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	57231	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0787e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.39	1/1814 (0.1%)	0.90	6/2466 (0.2%)
1	B	0.35	0/1782	0.88	4/2424 (0.2%)
1	K	0.34	0/1814	0.88	6/2466 (0.2%)
1	L	0.34	0/1805	0.90	7/2454 (0.3%)
2	C	0.40	0/8937	0.82	12/12087 (0.1%)
2	M	0.41	1/8937 (0.0%)	0.85	18/12087 (0.1%)
3	D	0.41	1/11910 (0.0%)	0.82	22/16105 (0.1%)
3	N	0.40	2/11952 (0.0%)	0.83	20/16162 (0.1%)
4	E	0.33	0/775	0.78	0/1045
4	O	0.31	0/775	0.77	0/1045
5	F	0.36	0/2852	0.81	7/3837 (0.2%)
5	P	0.35	0/2859	0.80	6/3847 (0.2%)
6	G	0.21	0/368	0.64	0/567
6	Q	0.17	0/368	0.59	0/567
7	H	0.18	0/556	0.71	0/858
7	R	0.18	0/556	0.68	0/858
8	I	0.16	0/47	0.29	0/72
8	S	0.16	0/47	0.25	0/72
All	All	0.39	5/58154 (0.0%)	0.83	108/79019 (0.1%)

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
2	M	0	1
5	P	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	599	PRO	C-N	9.84	1.46	1.33
3	D	105	VAL	C-N	7.81	1.45	1.33
1	A	62	LEU	C-N	6.48	1.41	1.33
2	M	366	SER	C-N	6.20	1.41	1.33
3	N	744	GLN	C-N	5.37	1.41	1.33

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	421	GLU	N-CA-C	-8.64	101.34	112.23
2	M	421	GLU	N-CA-C	-8.64	101.35	112.23
2	M	105	THR	N-CA-C	-8.06	103.04	113.12
2	M	296	GLY	N-CA-C	7.79	122.74	112.77
5	P	326	ASP	N-CA-C	7.67	121.89	112.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	104	ASP	Peptide
5	P	82	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	86	0
1	B	1750	0	1797	97	0
1	K	1782	0	1834	61	0
1	L	1773	0	1826	79	0
2	C	8770	0	8872	451	0
2	M	8770	0	8871	531	2
3	D	11704	0	11934	563	1
3	N	11746	0	11974	697	0
4	E	761	0	778	29	0
4	O	761	0	778	27	0
5	F	2807	0	2882	112	0
5	P	2814	0	2888	177	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	328	0	181	4	0
6	Q	328	0	181	6	0
7	H	495	0	272	8	0
7	R	495	0	272	14	0
8	I	42	0	23	0	0
8	S	42	0	23	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	2	0	0	0	0
10	K	1	0	0	0	0
10	N	2	0	0	0	0
11	A	14	0	0	0	0
11	B	3	0	0	0	0
11	C	53	0	0	0	0
11	D	58	0	0	0	0
11	E	8	0	0	0	0
11	F	10	0	0	0	0
11	G	5	0	0	0	0
11	H	2	0	0	0	0
11	K	4	0	0	0	0
11	L	3	0	0	0	0
11	M	33	0	0	1	0
11	N	52	0	0	1	0
11	O	5	0	0	0	0
11	P	16	0	0	0	0
11	Q	2	0	0	0	0
11	R	3	0	0	0	0
11	S	1	0	0	0	0
All	All	57231	0	57220	2720	2

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 2720 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157:ARG:NH1	2:M:176:VAL:HG11	1.23	1.47
2:C:64:LEU:N	2:C:103:LYS:NZ	1.61	1.47
2:M:229:MET:HE3	2:M:233:GLU:C	1.41	1.45
2:M:64:LEU:N	2:M:103:LYS:NZ	1.64	1.45
2:M:107:LEU:HD12	2:M:108:ILE:N	1.11	1.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1314:LYS:NZ	2:M:784:ASP:OD2[1_445]	1.83	0.37
2:M:40:GLU:OE1	5:P:364:ARG:NH1[1_545]	2.03	0.17

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	224/315 (71%)	218 (97%)	5 (2%)	1 (0%)	30	65
1	B	220/315 (70%)	212 (96%)	6 (3%)	2 (1%)	14	48
1	K	224/315 (71%)	218 (97%)	6 (3%)	0	100	100
1	L	223/315 (71%)	213 (96%)	8 (4%)	2 (1%)	14	48
2	C	1107/1119 (99%)	1066 (96%)	37 (3%)	4 (0%)	30	65
2	M	1107/1119 (99%)	1063 (96%)	39 (4%)	5 (0%)	24	60
3	D	1478/1524 (97%)	1423 (96%)	53 (4%)	2 (0%)	48	80
3	N	1485/1524 (97%)	1423 (96%)	57 (4%)	5 (0%)	36	70
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
4	O	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
5	F	344/443 (78%)	335 (97%)	9 (3%)	0	100	100
5	P	345/443 (78%)	329 (95%)	12 (4%)	4 (1%)	10	40
All	All	6941/7630 (91%)	6677 (96%)	239 (3%)	25 (0%)	30	65

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	325	ILE
2	M	325	ILE
5	P	78	SER

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Mol	Chain	Res	Type
5	P	417	LYS
3	D	1310	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	199/273 (73%)	185 (93%)	14 (7%)	14	44
1	B	195/273 (71%)	178 (91%)	17 (9%)	9	35
1	K	199/273 (73%)	184 (92%)	15 (8%)	12	41
1	L	198/273 (72%)	182 (92%)	16 (8%)	11	38
2	C	936/941 (100%)	873 (93%)	63 (7%)	15	46
2	M	936/941 (100%)	864 (92%)	72 (8%)	12	40
3	D	1250/1279 (98%)	1137 (91%)	113 (9%)	9	34
3	N	1253/1279 (98%)	1150 (92%)	103 (8%)	10	37
4	E	83/88 (94%)	80 (96%)	3 (4%)	31	65
4	O	83/88 (94%)	80 (96%)	3 (4%)	31	65
5	F	301/388 (78%)	281 (93%)	20 (7%)	15	46
5	P	302/388 (78%)	273 (90%)	29 (10%)	8	31
All	All	5935/6484 (92%)	5467 (92%)	468 (8%)	11	39

5 of 468 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	34	VAL
5	P	193	ARG
2	M	223	ASP
4	O	95	VAL
3	N	1044	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	744	GLN
5	P	263	HIS
3	N	1103	HIS
3	N	1227	GLN
5	F	263	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0
8	S	1/2 (50%)	0	0
All	All	2/4 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 9 ligands modelled in this entry, 9 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	226/315 (71%)	0.02	0 100 100	47, 67, 98, 118	0
1	B	222/315 (70%)	0.25	7 (3%) 50 29	50, 79, 119, 142	0
1	K	226/315 (71%)	0.14	1 (0%) 88 76	49, 73, 103, 122	0
1	L	225/315 (71%)	0.36	5 (2%) 62 39	51, 81, 126, 148	0
2	C	1111/1119 (99%)	0.07	22 (1%) 65 41	34, 62, 122, 168	0
2	M	1111/1119 (99%)	0.46	91 (8%) 17 9	38, 76, 142, 179	0
3	D	1482/1524 (97%)	0.11	40 (2%) 56 33	32, 66, 130, 178	1 (0%)
3	N	1489/1524 (97%)	0.15	30 (2%) 65 41	34, 69, 129, 201	1 (0%)
4	E	94/99 (94%)	0.21	1 (1%) 78 57	44, 66, 113, 121	0
4	O	94/99 (94%)	0.04	2 (2%) 63 40	49, 72, 116, 130	0
5	F	346/443 (78%)	0.20	10 (2%) 53 31	42, 70, 124, 147	0
5	P	347/443 (78%)	0.55	25 (7%) 21 11	46, 83, 156, 214	0
6	G	16/21 (76%)	-0.05	1 (6%) 26 13	42, 78, 172, 179	0
6	Q	16/21 (76%)	-0.02	1 (6%) 26 13	53, 80, 182, 183	0
7	H	24/27 (88%)	0.22	0 100 100	67, 95, 146, 201	0
7	R	24/27 (88%)	0.24	0 100 100	65, 106, 160, 210	0
8	I	2/2 (100%)	-0.82	0 100 100	50, 50, 50, 55	0
8	S	2/2 (100%)	-0.43	0 100 100	62, 62, 62, 63	0
All	All	7057/7730 (91%)	0.20	236 (3%) 49 28	32, 71, 132, 214	2 (0%)

The worst 5 of 236 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	P	391	GLY	5.1
2	M	191	PHE	5.0
3	N	1249	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	M	196	LEU	4.7
5	P	375	LEU	4.5

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	K	1001	1/1	0.76	0.35	69,69,69,69	0
10	MG	N	2004	1/1	0.79	0.31	65,65,65,65	0
10	MG	D	2004	1/1	0.84	0.29	63,63,63,63	0
10	MG	N	2003	1/1	0.93	0.08	46,46,46,46	0
10	MG	D	2003	1/1	0.93	0.08	40,40,40,40	0
9	ZN	N	2002	1/1	0.99	0.03	107,107,107,107	0
9	ZN	D	2001	1/1	0.99	0.01	62,62,62,62	0
9	ZN	D	2002	1/1	0.99	0.02	83,83,83,83	0
9	ZN	N	2001	1/1	1.00	0.05	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.