



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:09 AM UTC

PDB ID : 6UU0 / pdb_00006uu0
Title : E. coli sigma-S transcription initiation complex with a 3-nt RNA and a mismatching GTP ("Fresh" crystal soaked with GTP for 1 hour)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 3.90 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

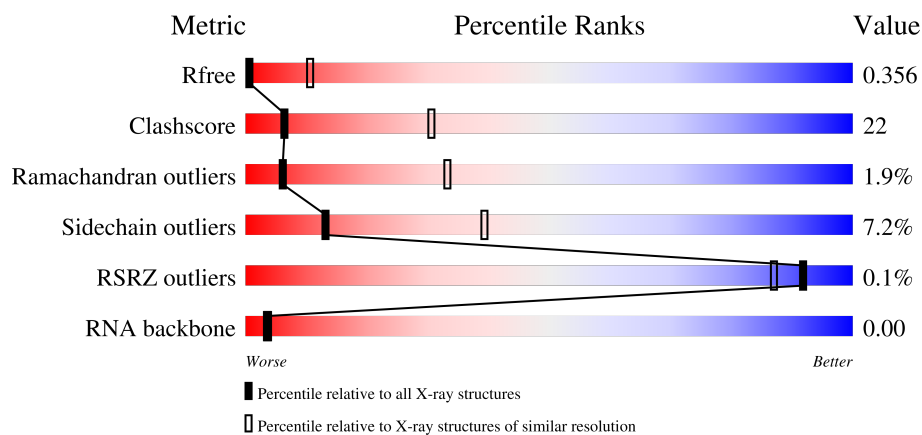
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

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	AAA	242	 60% 31% 5%
1	BBB	242	 61% 30% 6%
2	CCC	1342	 61% 34%
3	DDD	1407	 56% 36%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	EEE	90	
5	FFF	336	
6	111	50	
7	222	50	
8	333	3	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28977 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	AAA	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	BBB	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP A0A377D9Q8
AAA	-5	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-4	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-3	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-2	HIS	-	expression tag	UNP A0A377D9Q8
AAA	-1	HIS	-	expression tag	UNP A0A377D9Q8
AAA	0	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-6	ALA	-	expression tag	UNP A0A377D9Q8
BBB	-5	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-4	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-3	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-2	HIS	-	expression tag	UNP A0A377D9Q8
BBB	-1	HIS	-	expression tag	UNP A0A377D9Q8
BBB	0	HIS	-	expression tag	UNP A0A377D9Q8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1350	Total	C	N	O	S	0	0	0
			10478	6578	1867	1984	49			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	FFF	277	Total	C	N	O	S	0	0	0
			2253	1411	415	423	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP P13445
FFF	33	GLU	GLN	conflict	UNP P13445
FFF	329	LEU	-	expression tag	UNP P13445
FFF	330	GLU	-	expression tag	UNP P13445
FFF	331	HIS	-	expression tag	UNP P13445
FFF	332	HIS	-	expression tag	UNP P13445
FFF	333	HIS	-	expression tag	UNP P13445
FFF	334	HIS	-	expression tag	UNP P13445
FFF	335	HIS	-	expression tag	UNP P13445
FFF	336	HIS	-	expression tag	UNP P13445

- Molecule 6 is a DNA chain called Synthetic DNA 50-MER (promoter non-template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	32	Total	C	N	O	P	0	0	0
			660	313	122	193	32			

- Molecule 7 is a DNA chain called Synthetic DNA 50-MER (promoter template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	35	Total	C	N	O	P	0	0	0
			716	342	132	208	34			

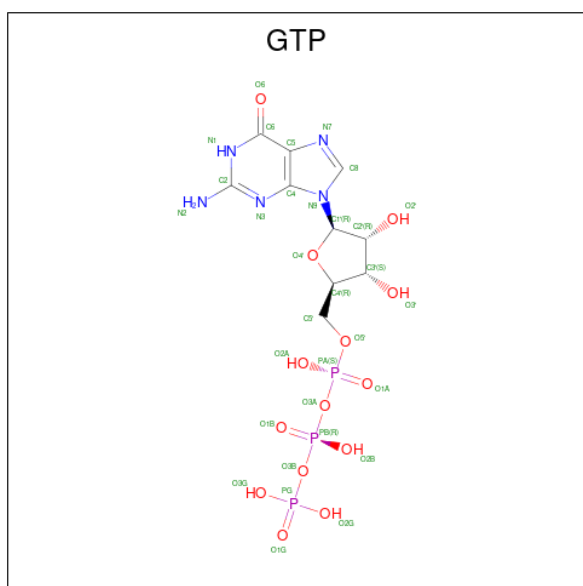
- Molecule 8 is a RNA chain called RNA 3-mer (de novo synthesized).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	333	3	Total	C	N	O	P	0	0	0
			77	30	15	27	5			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	CCC	1	Total	Mg	0	0
			1	1		
9	333	1	Total	Mg	0	0
			1	1		

- Molecule 10 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	CCC	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

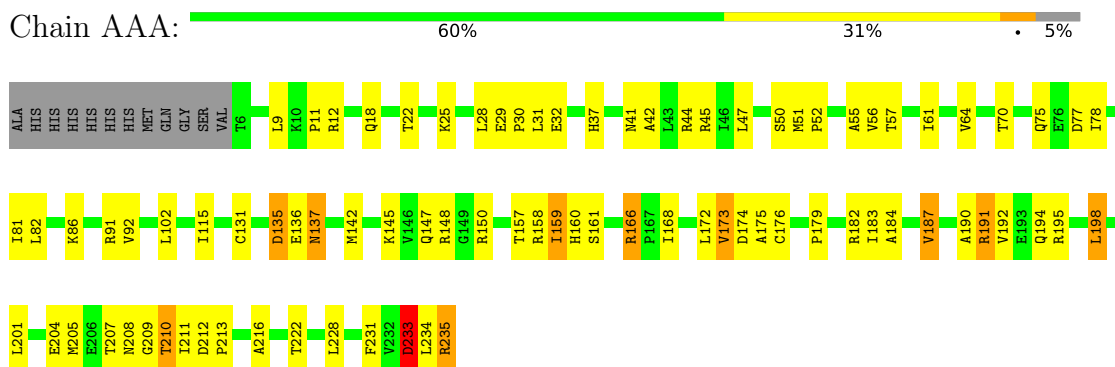
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

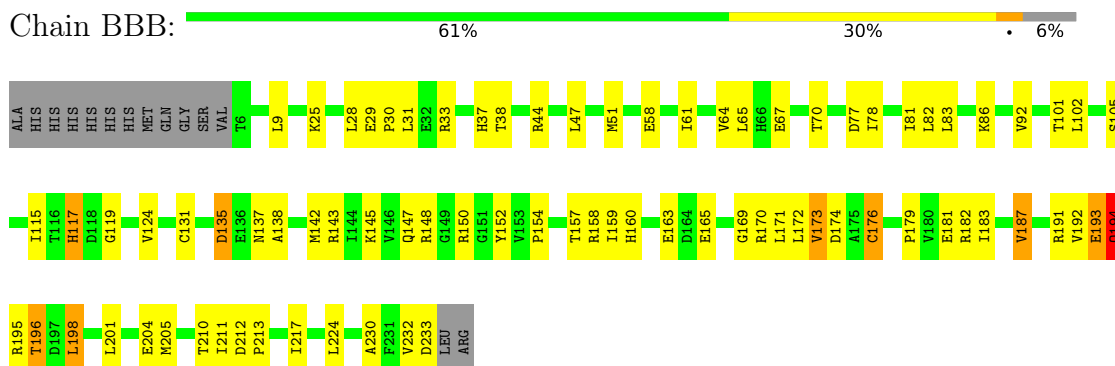
3 Residue-property plots [i](#)

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

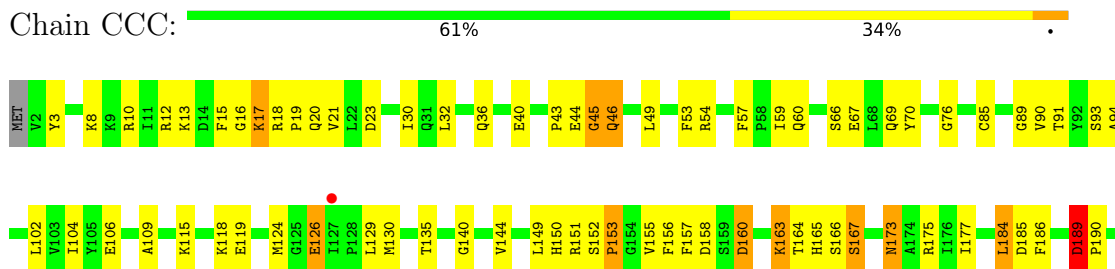
- Molecule 1: DNA-directed RNA polymerase subunit alpha

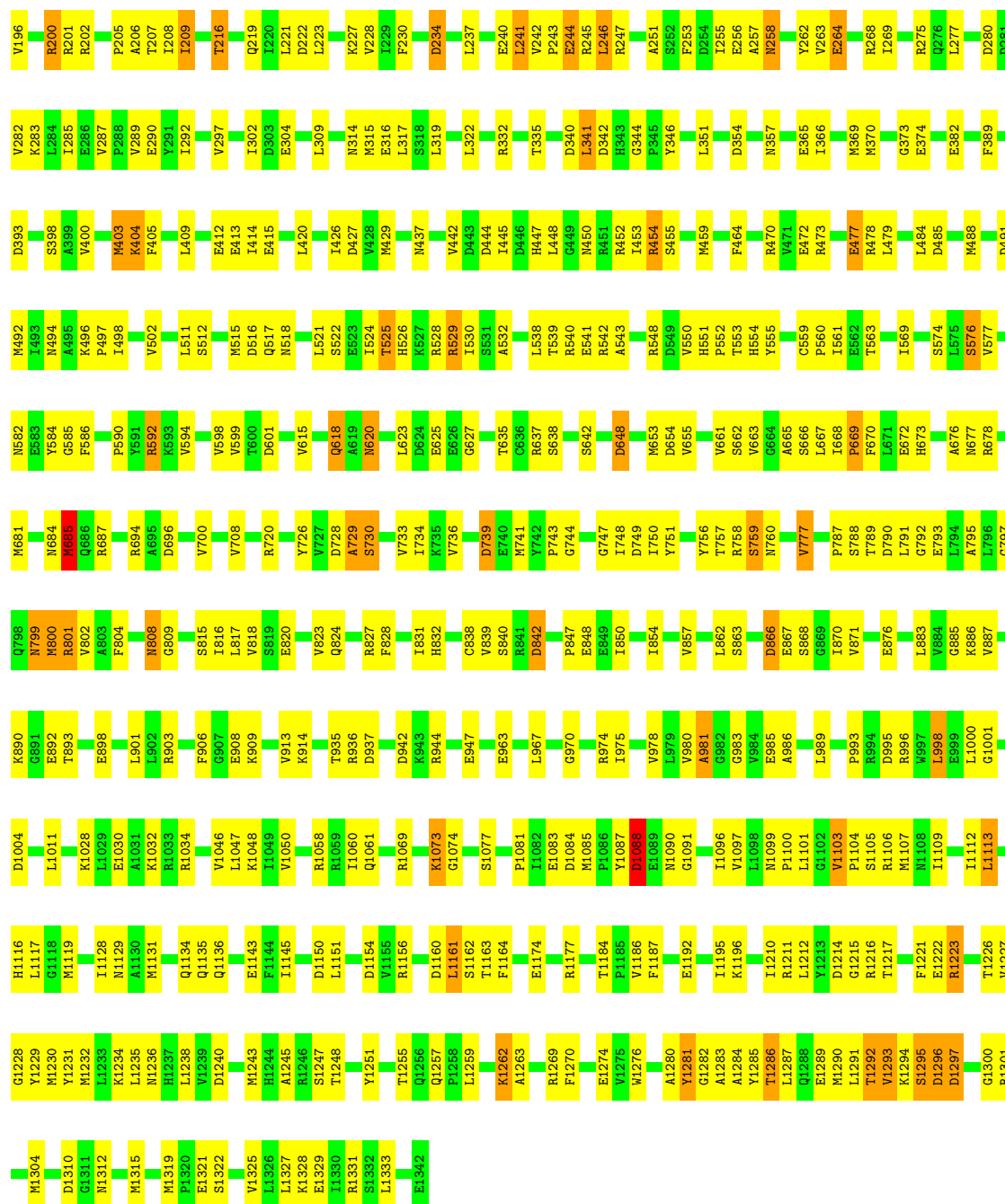


- Molecule 1: DNA-directed RNA polymerase subunit alpha



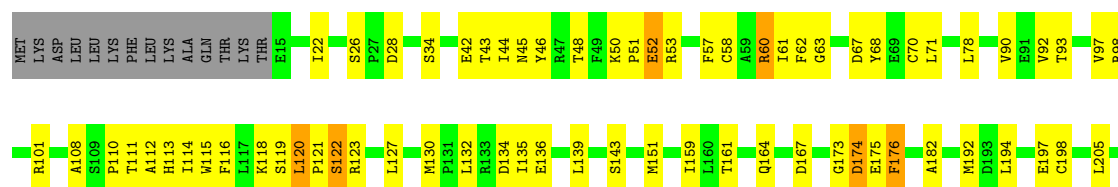
- Molecule 2: DNA-directed RNA polymerase subunit beta





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

Chain DDD: 56% 36%



ASN	T1310	E1200	D1087	V997	H897	H821	T787	G589	G597	N519	R426	R339	N209
ALA	K1311	R1206	V1088	V997	C898	M822	P788	S670	K598	A520	A426	Q340	S210
GLY	A1312	G1207	L1089	G1000	R901	M823	T789	V673	K599	E523	T428	N341	N310
LEU	S1313	D1208	L1090	G1000	R901	P824	T790	V673	A600	E523	L429	L342	R214
GLY	T1316	V1209	P1091	L1003	K911	V825	A761	R678	G524	G524	H430	G344	R220
SER	F1319	I1210	F1091	V1011	I915	G829	N762	Y679	M525	M525	H430	K345	L223
ASP	S1324	L1223	F1100	V1011	I915	D830	F763	R680	V526	V526	H430	R346	L224
ASN	S1324	R1224	G1103	A1018	I923	H831	R764	K681	L527	L527	H430	D348	L224
GLU	T1329	G1225	G1103	N1019	G924	K832	L767	W686	T528	T528	H430	P234	P234
ALA	V1226	V1226	I1106	V1020	E925	L835	V769	W686	G529	G529	H430	M237	M237
LEU	H1227	H1227	D1021	P1022	P926	R836	L770	R692	P530	P530	H430	P234	P234
ASP	T1230	T1230	E1110	P1022	S927	W839	Q771	M697	K531	K531	H430	S353	S353
ASN	Q1238	Q1238	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	T356	T356
GLU	R1242	R1242	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	P359	P359
ALA	L1243	L1243	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	Y360	Y360
LEU	G1245	G1245	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	L361	L361
GLY	V1246	V1246	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	R362	R362
ASP	N1249	N1249	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	Q365	Q365
ASN	D1250	D1250	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	G367	G367
GLU	V1255	V1255	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	K370	K370
ALA	I1256	I1256	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	M372	M372
LEU	V1257	V1257	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	E375	E375
GLY	R1258	R1258	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	L376	L376
ASP	G1259	G1259	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	F377	F377
ASN	M1260	M1260	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	K378	K378
GLU	L1261	L1261	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	P379	P379
LEU	K1262	K1262	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	F380	F380
ALA	V1263	V1263	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	I381	I381
LEU	G1270	G1270	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	Y382	Y382
ALA	L1275	L1275	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	G383	G383
LEU	E1276	E1276	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	K384	K384
GLY	Y1282	Y1282	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	L385	L385
ASP	S1283	S1283	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	E386	E386
LEU	K1286	K1286	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	L387	L387
GLY	R1290	R1290	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	R388	R388
ASN	L1291	L1291	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	I392	I392
GLY	L1292	L1292	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	T392	T392
ASP	G1296	G1296	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	T393	T393
LEU	K1297	K1297	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	I394	I394
ALA	V1298	V1298	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	K395	K395
GLY	S1303	S1303	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	K398	K398
LEU	L1307	L1307	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	K399	K399
GLY	G1308	G1308	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	I411	I411
LEU	I1309	I1309	D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	E414	E414
ALA			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	V415	V415
GLY			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	T514	T514
LEU			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	R515	R515
ALA			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	D516	D516
GLY			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	C517	C517
LEU			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	L423	L423
ALA			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	V421	V421
GLY			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	L422	L422
LEU			D1111	H1023	T928	R842	F773	Q702	E533	E533	H430	N424	N424

• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain EEE:  58% 28% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.80Å 156.16Å 233.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.90 49.20 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.20-3.90) 98.2 (49.20-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.314 , 0.368 0.307 , 0.356	Depositor DCC
R_{free} test set	2123 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	168.6	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 227.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28977	wwPDB-VP
Average B, all atoms (Å ²)	287.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: GTP, MG, ZN

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	AAA	0.95	0/1809	1.23	0/2450
1	BBB	0.96	0/1789	1.23	3/2425 (0.1%)
2	CCC	0.92	0/10745	1.31	22/14499 (0.2%)
3	DDD	0.94	0/10636	1.29	9/14362 (0.1%)
4	EEE	0.88	0/629	1.39	0/847
5	FFF	0.97	0/2282	1.35	2/3076 (0.1%)
6	111	0.33	0/739	0.60	0/1137
7	222	0.34	0/803	0.59	1/1238 (0.1%)
8	333	0.45	0/50	0.95	0/76
All	All	0.91	0/29482	1.27	37/40110 (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	CCC	0	1

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	563	THR	CB-CA-C	9.02	122.90	109.63
2	CCC	1084	ASP	CA-CB-CG	7.57	120.17	112.60
2	CCC	454	ARG	CB-CA-C	-6.76	99.60	111.22
2	CCC	153	PRO	N-CD-CG	-6.65	93.23	103.20
3	DDD	460	ASP	CA-CB-CG	6.51	119.11	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	CCC	1282	GLY	Peptide

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	AAA	1787	0	1813	76	0
1	BBB	1767	0	1789	84	0
2	CCC	10576	0	10591	470	0
3	DDD	10478	0	10691	581	2
4	EEE	627	0	634	22	0
5	FFF	2253	0	2298	120	1
6	111	660	0	362	57	1
7	222	716	0	396	58	1
8	333	77	0	32	7	0
9	333	1	0	0	0	0
9	CCC	1	0	0	0	0
10	CCC	32	0	12	7	0
11	DDD	2	0	0	1	0
All	All	28977	0	28618	1260	3

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 22.

The worst 5 of 1260 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)
3:DDD:525:MET:O	3:DDD:548:VAL:HG22	1.37	1.23
3:DDD:572:THR:HG21	3:DDD:589:TYR:OH	1.35	1.22
3:DDD:525:MET:N	3:DDD:548:VAL:HG23	1.58	1.18
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:NH1	1.60	1.17
2:CCC:1106:ARG:NH1	10:CCC:1402:GTP:O1G	1.79	1.16

All (3) 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:DDD:1174:ARG:NH2	7:222:32:DA:OP1[3_644]	1.88	0.32
3:DDD:210:SER:OG	6:111:28:DA:OP2[3_644]	1.89	0.31
5:FFF:67:TYR:O	5:FFF:299:ARG:NH2[3_644]	2.06	0.14

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	AAA	228/242 (94%)	211 (92%)	11 (5%)	6 (3%)	4	28
1	BBB	226/242 (93%)	207 (92%)	14 (6%)	5 (2%)	5	31
2	CCC	1339/1342 (100%)	1244 (93%)	68 (5%)	27 (2%)	6	32
3	DDD	1346/1407 (96%)	1231 (92%)	90 (7%)	25 (2%)	6	33
4	EEE	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
5	FFF	275/336 (82%)	251 (91%)	20 (7%)	4 (2%)	8	37
All	All	3491/3659 (95%)	3217 (92%)	207 (6%)	67 (2%)	6	33

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	117	HIS
1	BBB	193	GLU
1	BBB	194	GLN
2	CCC	46	GLN
2	CCC	247	ARG

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	AAA	198/208 (95%)	178 (90%)	20 (10%)	7	27
1	BBB	196/208 (94%)	182 (93%)	14 (7%)	13	40
2	CCC	1156/1157 (100%)	1067 (92%)	89 (8%)	12	37
3	DDD	1127/1168 (96%)	1051 (93%)	76 (7%)	15	41
4	EEE	67/74 (90%)	64 (96%)	3 (4%)	24	49
5	FFF	240/292 (82%)	226 (94%)	14 (6%)	18	44
All	All	2984/3107 (96%)	2768 (93%)	216 (7%)	13	39

5 of 216 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	CCC	1248	THR
3	DDD	443	GLU
4	EEE	8	ASP
2	CCC	1292	THR
3	DDD	132	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	333	1/3 (33%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	333	16	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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
10	GTP	CCC	1402	9	33,34,34	1.19	3 (9%)	50,54,54	1.79	13 (26%)

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
10	GTP	CCC	1402	9	-	3/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	CCC	1402	GTP	PB-O3B	3.30	1.63	1.59
10	CCC	1402	GTP	C4-N9	-2.82	1.30	1.38
10	CCC	1402	GTP	C5-C4	2.71	1.46	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	CCC	1402	GTP	C6-C5-N7	4.59	138.64	130.29
10	CCC	1402	GTP	C2-N3-C4	4.08	119.32	112.30
10	CCC	1402	GTP	C8-N9-C4	3.34	112.30	106.03
10	CCC	1402	GTP	C5-C4-N3	-3.28	123.16	128.39
10	CCC	1402	GTP	C6-C5-C4	-3.19	114.04	118.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

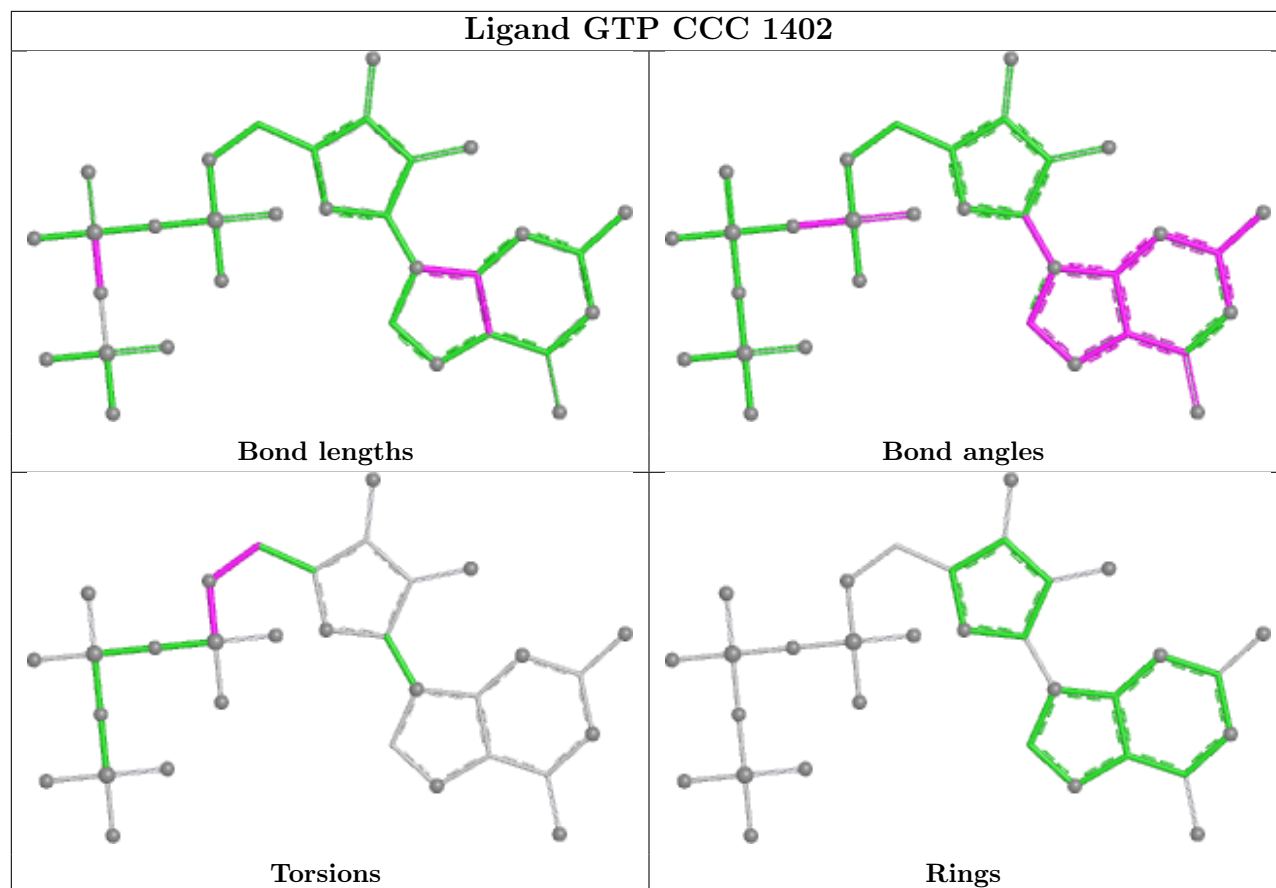
Mol	Chain	Res	Type	Atoms
10	CCC	1402	GTP	C5'-O5'-PA-O3A
10	CCC	1402	GTP	C5'-O5'-PA-O2A
10	CCC	1402	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	CCC	1402	GTP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	AAA	230/242 (95%)	-0.96	0 100 100	226, 314, 364, 413	0
1	BBB	228/242 (94%)	-0.85	0 100 100	225, 304, 376, 418	0
2	CCC	1341/1342 (99%)	-0.96	1 (0%) 92 87	142, 264, 377, 490	0
3	DDD	1350/1407 (95%)	-0.94	2 (0%) 92 87	159, 274, 397, 472	0
4	EEE	79/90 (87%)	-1.05	0 100 100	206, 300, 449, 524	0
5	FFF	277/336 (82%)	-0.94	0 100 100	207, 306, 397, 435	0
6	111	32/50 (64%)	-0.88	0 100 100	241, 310, 392, 431	0
7	222	35/50 (70%)	-0.75	0 100 100	224, 303, 435, 475	0
8	333	2/3 (66%)	-1.49	0 100 100	261, 261, 261, 291	0
All	All	3574/3762 (95%)	-0.94	3 (0%) 92 87	142, 283, 392, 524	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	1332	LEU	2.3
2	CCC	127	ILE	2.2
3	DDD	1145	PHE	2.1

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](#)

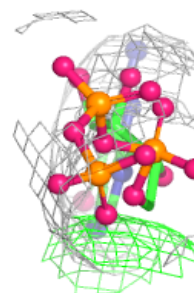
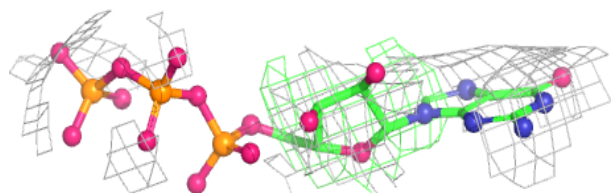
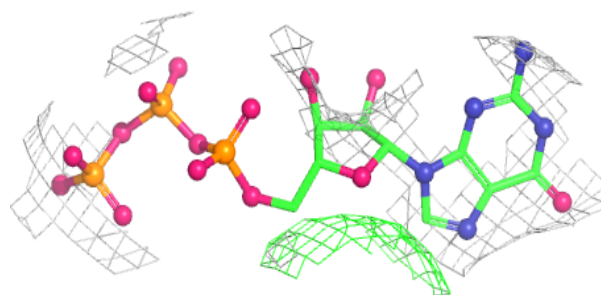
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	GTP	CCC	1402	32/32	0.79	0.07	180,256,340,342	0
9	MG	CCC	1401	1/1	0.97	0.03	309,309,309,309	0
9	MG	333	101	1/1	0.99	0.01	154,154,154,154	0
11	ZN	DDD	1501	1/1	0.99	0.05	436,436,436,436	0
11	ZN	DDD	1502	1/1	0.99	0.02	351,351,351,351	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP CCC 1402:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.