



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:48 AM UTC

PDB ID : 1Y77 / pdb_00001y77
Title : Complete RNA Polymerase II elongation complex with substrate analogue GMPCPP
Authors : Kettenberger, H.; Armache, K.-J.; Cramer, P.
Deposited on : 2004-12-08
Resolution : 4.50 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

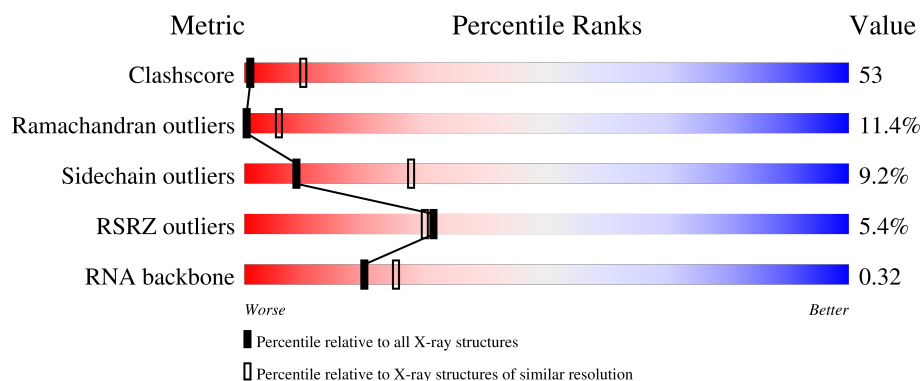
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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))
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)
RNA backbone	3983	1039 (5.90-3.10)

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	T	19	
2	N	7	
3	P	10	
4	A	1733	
5	B	1224	

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Mol	Chain	Length	Quality of chain
6	C	318	
7	D	221	
8	E	215	
9	F	155	
10	G	171	
11	H	146	
12	I	122	
13	J	70	
14	K	120	
15	L	70	

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
18	G2P	B	1308	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31835 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 DNA chain called 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*T*CP*GP*CP*CP*TP*GP*GP*TP*CP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	19	Total	C	N	O	P	21	0	0
			388	185	67	117	19			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	7	Total	C	N	O	P	20	0	0
			141	69	27	39	6			

- Molecule 3 is a RNA chain called 5'-R(*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1416	Total	C	N	O	S	0	0	0
			11140	7021	1946	2111	62			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1112	Total	C	N	O	S	0	0	0
			8836	5594	1548	1639	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 10 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 13 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 14 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

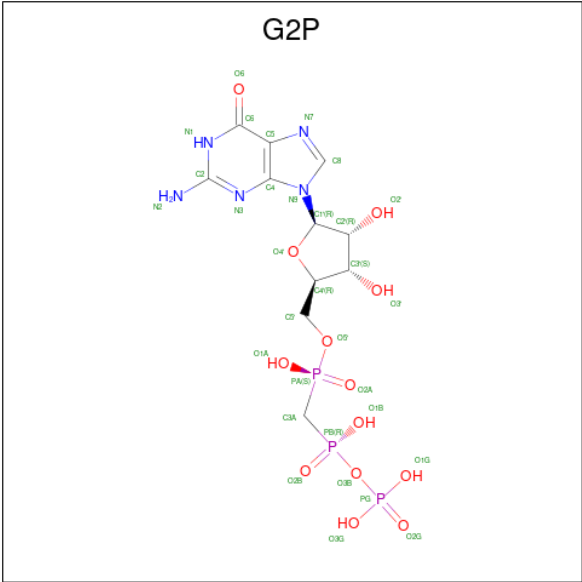
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Zn	0	0
			2	2		
16	B	1	Total	Zn	0	0
			1	1		
16	C	1	Total	Zn	0	0
			1	1		
16	I	2	Total	Zn	0	0
			2	2		
16	J	1	Total	Zn	0	0
			1	1		
16	L	1	Total	Zn	0	0
			1	1		

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

- Molecule 18 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).

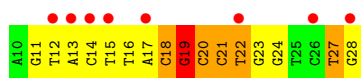
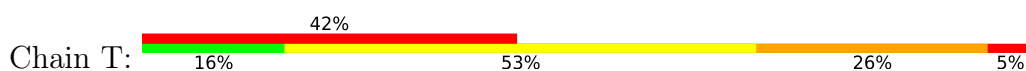


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total	C	N	O	P	32	0
			32	11	5	13	3		

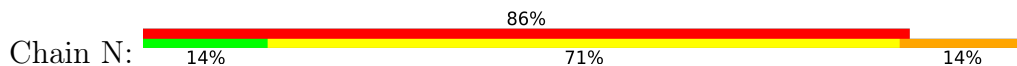
3 Residue-property plots

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.

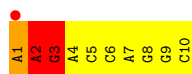
- Molecule 1: 5'-D(P*AP*GP*TP*AP*CP*TP*TP*AP*CP*T*CP*GP*CP*CP*TP*GP*GP*T P*CP*TP*G)-3'



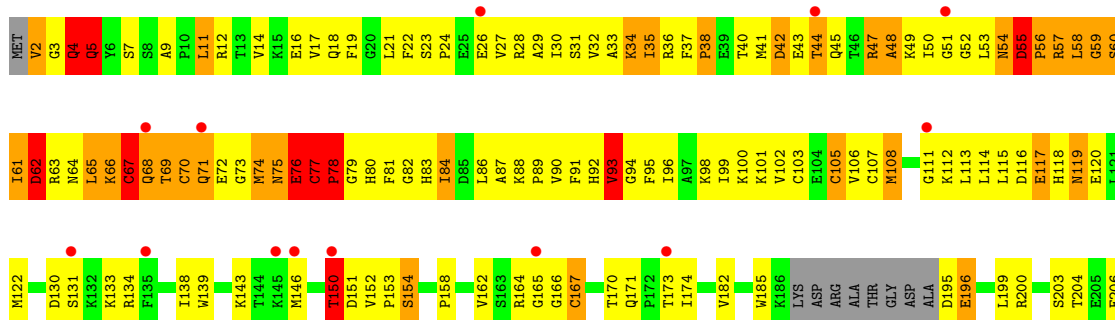
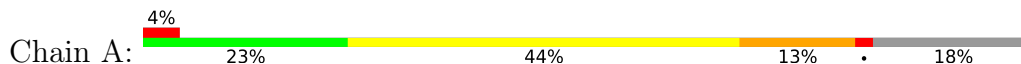
- Molecule 2: 5'-D(*AP*AP*GP*TP*AP*CP*T)-3'



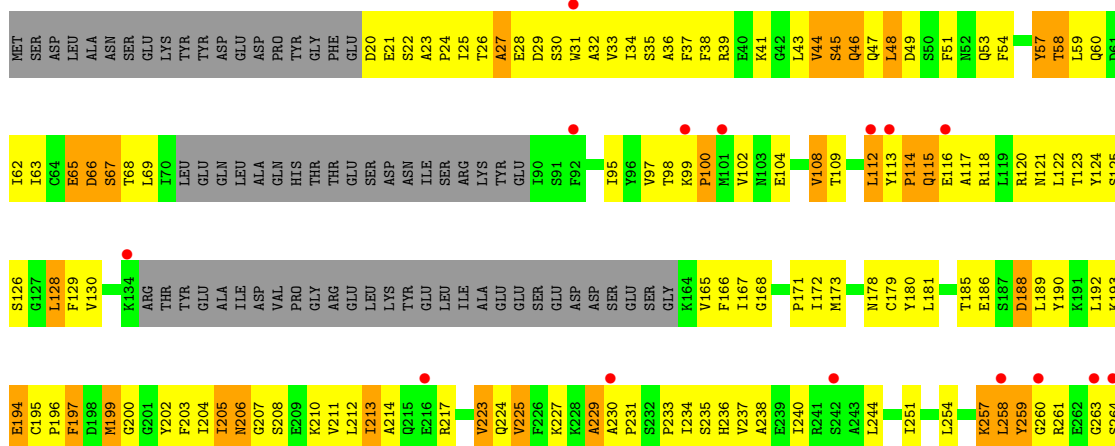
- Molecule 3: 5'-R(*AP*AP*GP*AP*CP*CP*AP*GP*GP*C)-3'

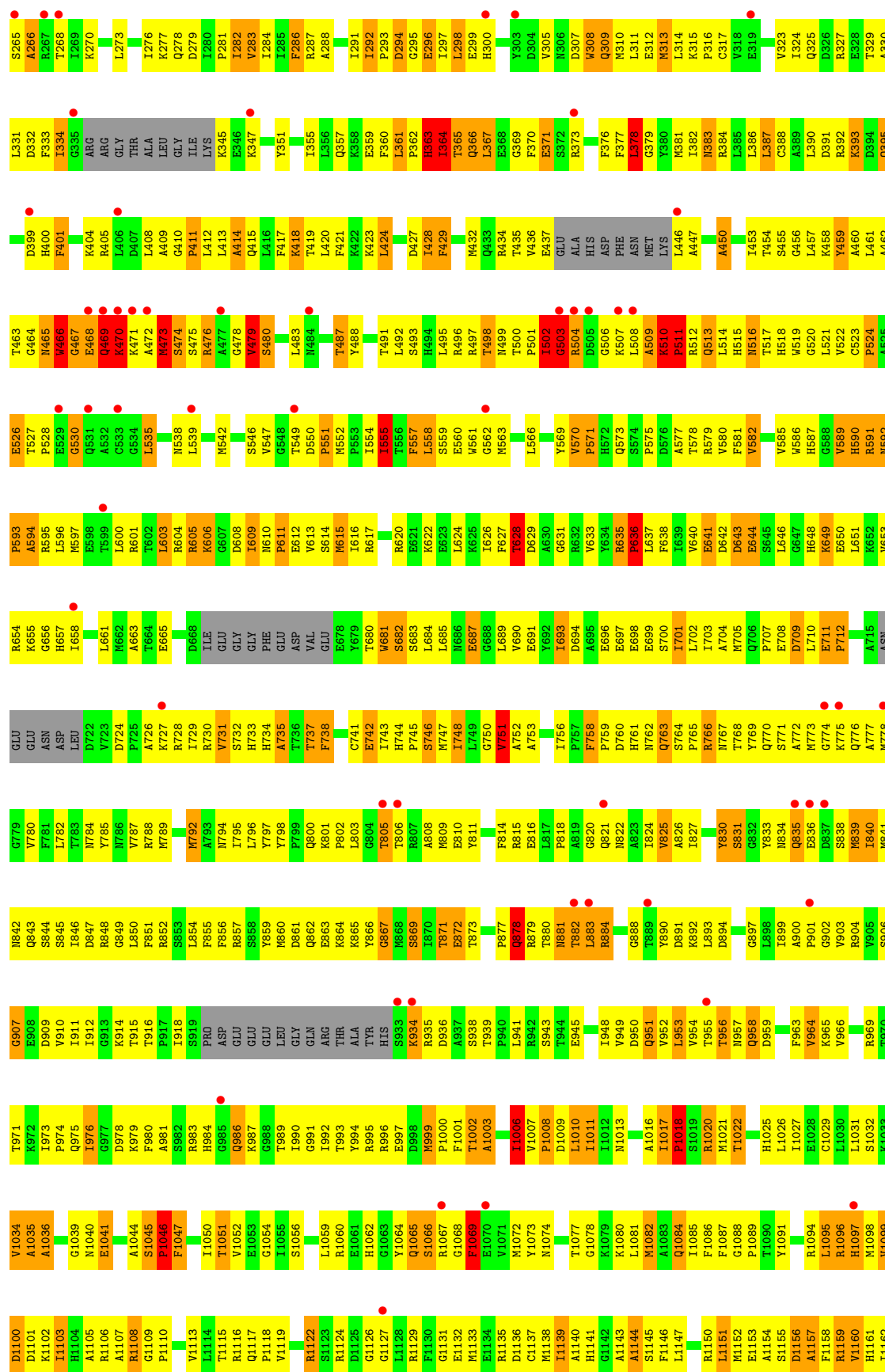


- Molecule 4: DNA-directed RNA polymerase II largest subunit



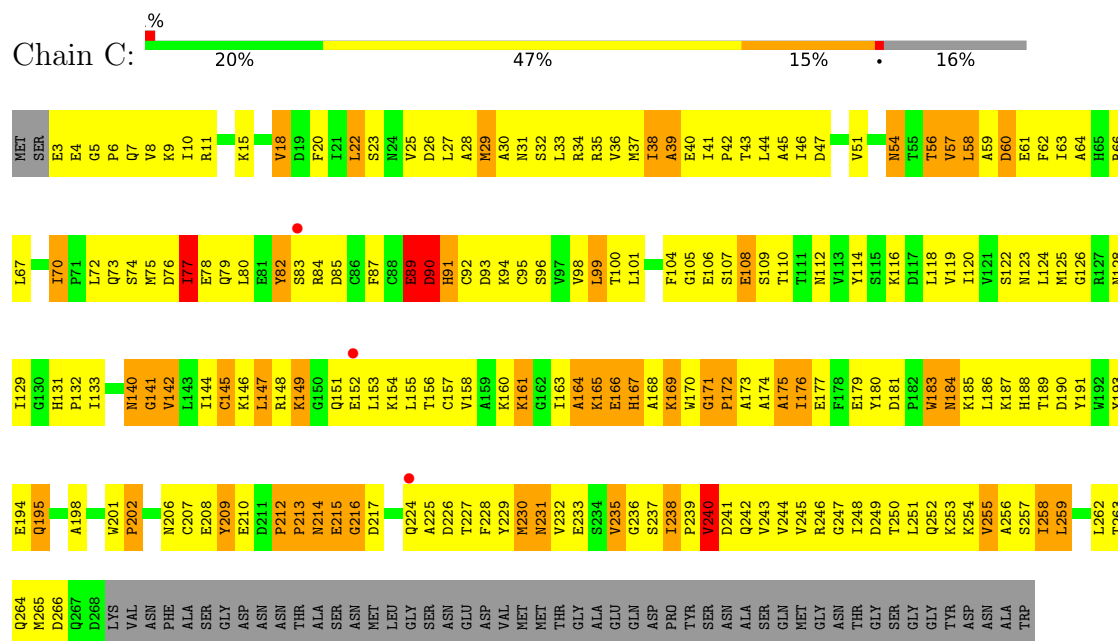




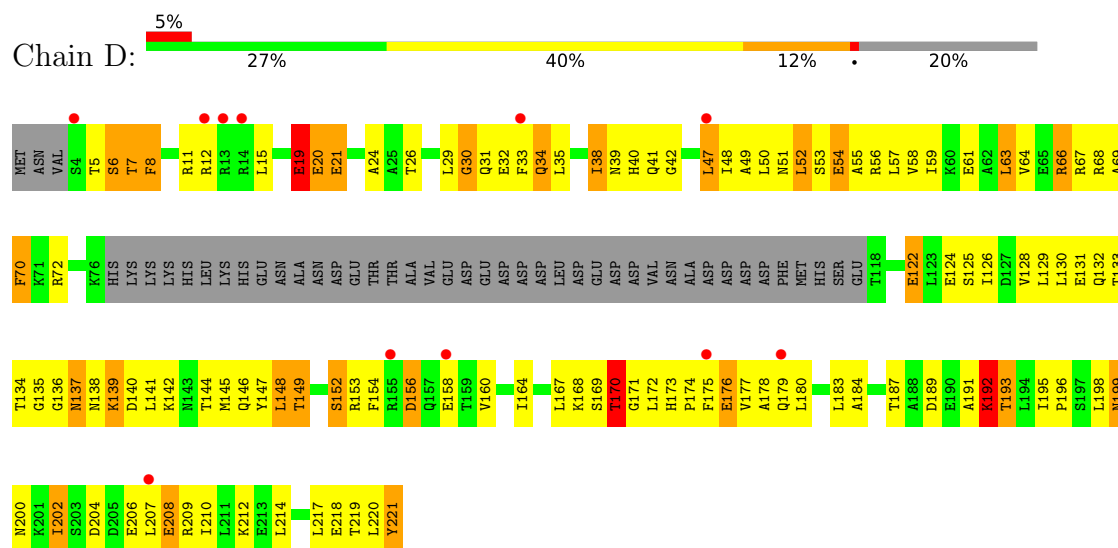




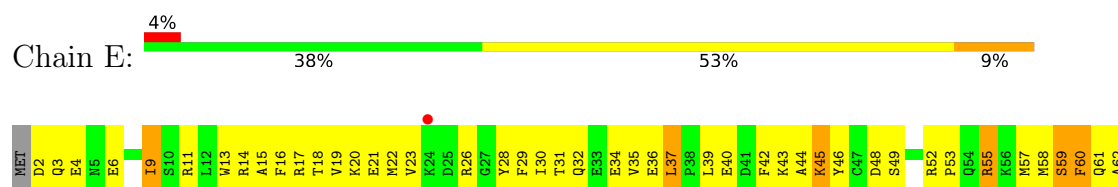
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide

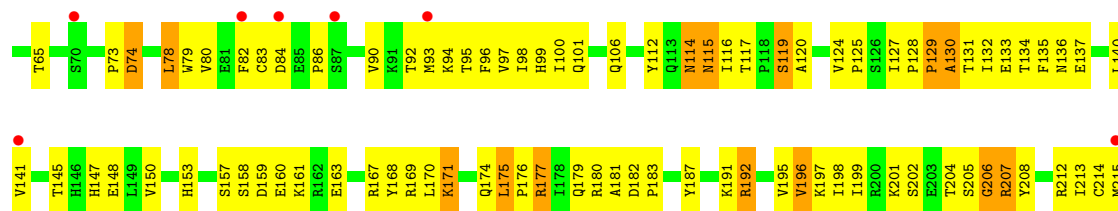


• Molecule 7: DNA-directed RNA polymerase II 32 kDa polypeptide

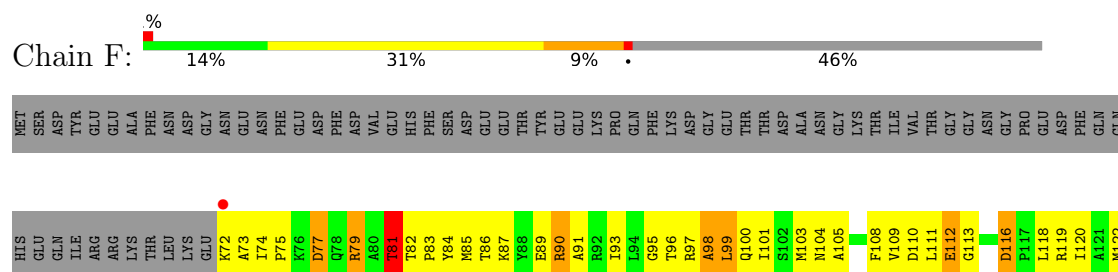


• Molecule 8: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

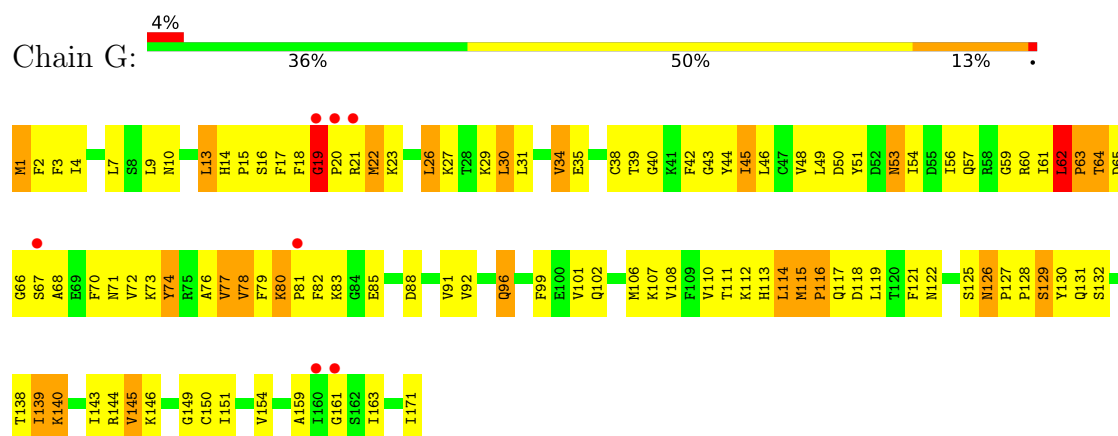




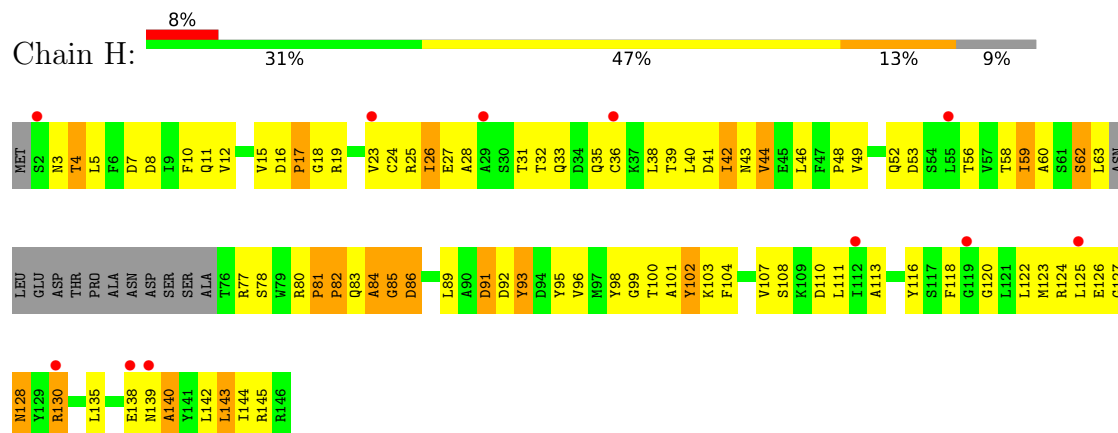
• Molecule 9: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



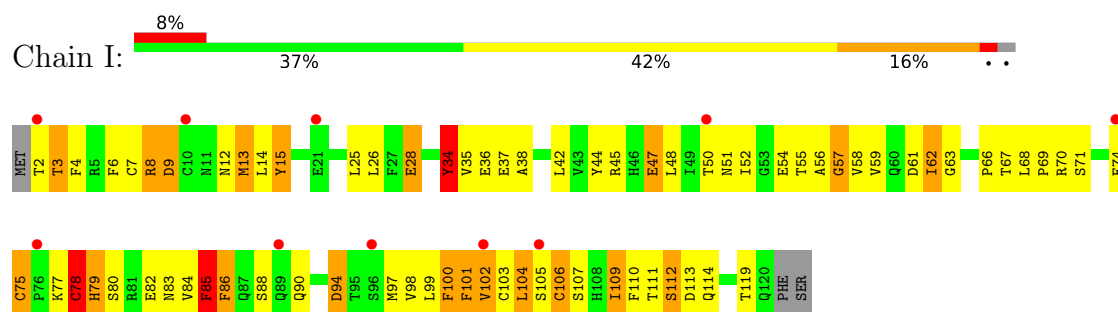
• Molecule 10: DNA-directed RNA polymerase II 19 kDa polypeptide



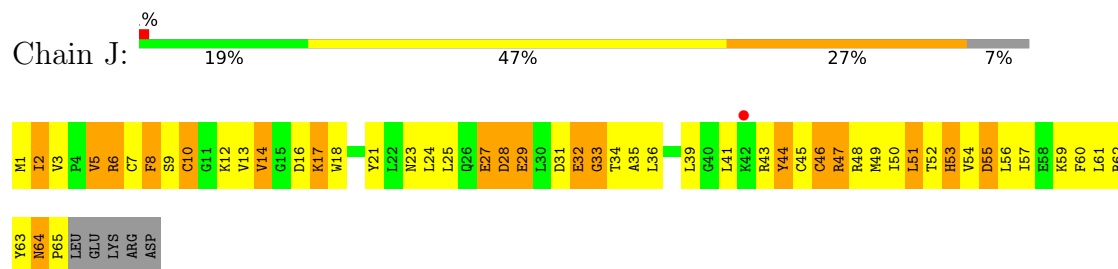
• Molecule 11: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



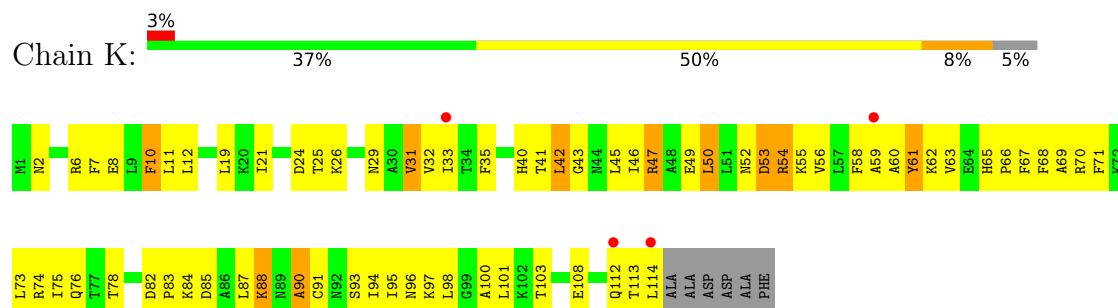
• Molecule 12: DNA-directed RNA polymerase II subunit 9



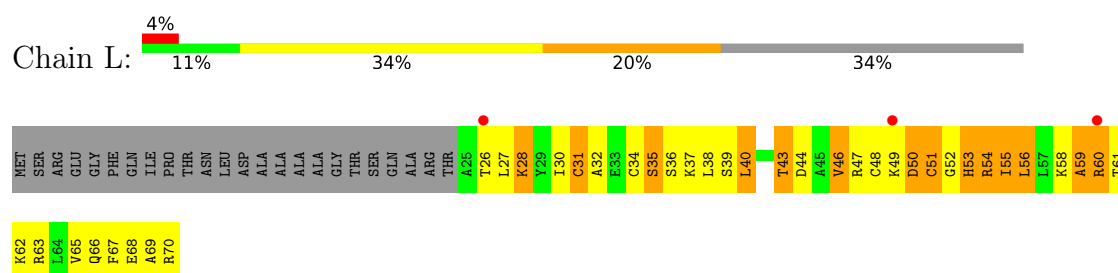
- Molecule 13: DNA-directed RNA polymerases I/II/III subunit 10



- Molecule 14: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 15: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	222.46Å 393.07Å 283.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.50 50.00 – 4.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.50) 78.5 (50.00-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 4.45Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.297 , (Not available) 0.270 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	137.1	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 83.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.030 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	31835	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: ZN, G2P, 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	T	0.66	0/433	1.24	5/666 (0.8%)
2	N	0.74	0/158	0.99	1/242 (0.4%)
3	P	0.84	0/240	1.76	7/373 (1.9%)
4	A	0.80	9/11339 (0.1%)	1.17	106/15334 (0.7%)
5	B	0.73	10/9008 (0.1%)	1.21	78/12146 (0.6%)
6	C	0.84	2/2133 (0.1%)	1.43	21/2891 (0.7%)
7	D	0.62	1/1365 (0.1%)	1.16	14/1837 (0.8%)
8	E	0.49	0/1788	0.99	10/2406 (0.4%)
9	F	0.67	0/691	1.22	10/933 (1.1%)
10	G	0.62	0/1368	1.13	15/1844 (0.8%)
11	H	0.46	0/1086	1.02	7/1470 (0.5%)
12	I	0.52	0/989	1.13	7/1331 (0.5%)
13	J	0.62	0/541	1.09	2/727 (0.3%)
14	K	0.56	0/937	1.02	3/1265 (0.2%)
15	L	0.56	0/365	1.01	1/485 (0.2%)
All	All	0.72	22/32441 (0.1%)	1.18	287/43950 (0.7%)

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	T	0	3
4	A	0	3
5	B	1	7
6	C	0	4
All	All	1	17

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	119	ASN	C-N	46.52	1.98	1.34
4	A	150	THR	C-N	-26.15	0.93	1.33
6	C	89	GLU	C-N	-23.16	1.00	1.33
5	B	363	HIS	C-N	-22.55	1.02	1.33
5	B	503	GLY	C-N	18.00	1.68	1.33

The worst 5 of 287 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	GLY	O-C-N	-29.99	83.71	122.70
6	C	89	GLU	O-C-N	-28.71	84.40	122.59
5	B	469	GLN	O-C-N	-27.77	84.36	122.97
6	C	89	GLU	CA-C-N	23.98	164.87	121.70
6	C	89	GLU	C-N-CA	23.98	164.87	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	364	ILE	CB

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	150	THR	Mainchain
4	A	77	CYS	Peptide
1	T	19	DG	Sidechain
1	T	20	DC	Sidechain
1	T	21	DC	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	T	388	0	216	52	0
2	N	141	0	81	8	0
3	P	214	0	111	19	0
4	A	11140	0	11218	1326	0
5	B	8836	0	8870	1061	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	2095	0	2049	260	0
7	D	1356	0	1319	127	0
8	E	1752	0	1776	159	0
9	F	679	0	701	86	0
10	G	1340	0	1357	159	0
11	H	1068	0	1040	107	0
12	I	971	0	928	105	0
13	J	532	0	542	101	0
14	K	919	0	929	90	0
15	L	363	0	387	46	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
18	B	32	0	12	0	0
All	All	31835	0	31536	3364	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 53.

The worst 5 of 3364 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:503:GLY:C	5:B:504:ARG:N	1.68	1.48
4:A:825:ILE:CG2	5:B:508:LEU:HD11	1.45	1.45
1:T:16:DT:C4'	4:A:1403:GLU:OE2	1.77	1.30
1:T:20:DC:H4'	4:A:447:GLN:NE2	1.44	1.29
4:A:56:PRO:O	4:A:57:ARG:HG3	1.28	1.28

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	
4	A	1406/1733 (81%)	962 (68%)	280 (20%)	164 (12%)	0	5
5	B	1096/1224 (90%)	740 (68%)	225 (20%)	131 (12%)	0	5
6	C	264/318 (83%)	158 (60%)	67 (25%)	39 (15%)	0	3
7	D	173/221 (78%)	121 (70%)	34 (20%)	18 (10%)	0	6
8	E	212/215 (99%)	149 (70%)	48 (23%)	15 (7%)	1	11
9	F	82/155 (53%)	64 (78%)	14 (17%)	4 (5%)	1	16
10	G	169/171 (99%)	131 (78%)	26 (15%)	12 (7%)	1	11
11	H	129/146 (88%)	84 (65%)	30 (23%)	15 (12%)	0	5
12	I	117/122 (96%)	81 (69%)	27 (23%)	9 (8%)	1	10
13	J	63/70 (90%)	37 (59%)	11 (18%)	15 (24%)	0	1
14	K	112/120 (93%)	89 (80%)	18 (16%)	5 (4%)	2	17
15	L	44/70 (63%)	18 (41%)	13 (30%)	13 (30%)	0	0
All	All	3867/4565 (85%)	2634 (68%)	793 (20%)	440 (11%)	0	6

5 of 440 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	4	GLN
4	A	5	GLN
4	A	48	ALA
4	A	54	ASN
4	A	55	ASP

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	
4	A	1239/1520 (82%)	1127 (91%)	112 (9%)	9	28
5	B	964/1061 (91%)	868 (90%)	96 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	234/274 (85%)	211 (90%)	23 (10%)	7	24
7	D	140/200 (70%)	119 (85%)	21 (15%)	3	14
8	E	196/197 (100%)	187 (95%)	9 (5%)	24	46
9	F	74/137 (54%)	65 (88%)	9 (12%)	5	18
10	G	152/152 (100%)	141 (93%)	11 (7%)	13	35
11	H	117/128 (91%)	109 (93%)	8 (7%)	14	37
12	I	113/116 (97%)	101 (89%)	12 (11%)	6	22
13	J	60/65 (92%)	54 (90%)	6 (10%)	7	24
14	K	99/102 (97%)	92 (93%)	7 (7%)	13	35
15	L	40/57 (70%)	38 (95%)	2 (5%)	22	43
All	All	3428/4009 (86%)	3112 (91%)	316 (9%)	8	27

5 of 316 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	D	32	GLU
11	H	102	TYR
7	D	126	ILE
8	E	215	MET
12	I	101	PHE

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

Mol	Chain	Res	Type
5	B	734	HIS
6	C	54	ASN
11	H	52	GLN
5	B	763	GLN
5	B	1062	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	P	9/10 (90%)	1 (11%)	1 (11%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	P	3	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	P	2	A

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 10 ligands modelled in this entry, 9 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	$\# Z > 2$
18	G2P	B	1308	-	30,34,34	2.53	9 (30%)	46,54,54	3.02	14 (30%)

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
18	G2P	B	1308	-	1/1/7/7	3/19/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	1308	G2P	C3'-C4'	-5.52	1.39	1.53
18	B	1308	G2P	C5'-C4'	5.45	1.67	1.51
18	B	1308	G2P	O2'-C2'	4.96	1.55	1.43
18	B	1308	G2P	C1'-N9	-4.81	1.33	1.47
18	B	1308	G2P	O4'-C4'	-4.25	1.35	1.45

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	1308	G2P	O4'-C4'-C5'	13.47	152.48	109.33
18	B	1308	G2P	C5'-C4'-C3'	-6.87	90.48	115.21
18	B	1308	G2P	O5'-C5'-C4'	6.85	132.31	108.99
18	B	1308	G2P	C2'-C1'-N9	-5.52	97.87	113.25
18	B	1308	G2P	O3'-C3'-C2'	-4.61	97.04	111.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	B	1308	G2P	C4'

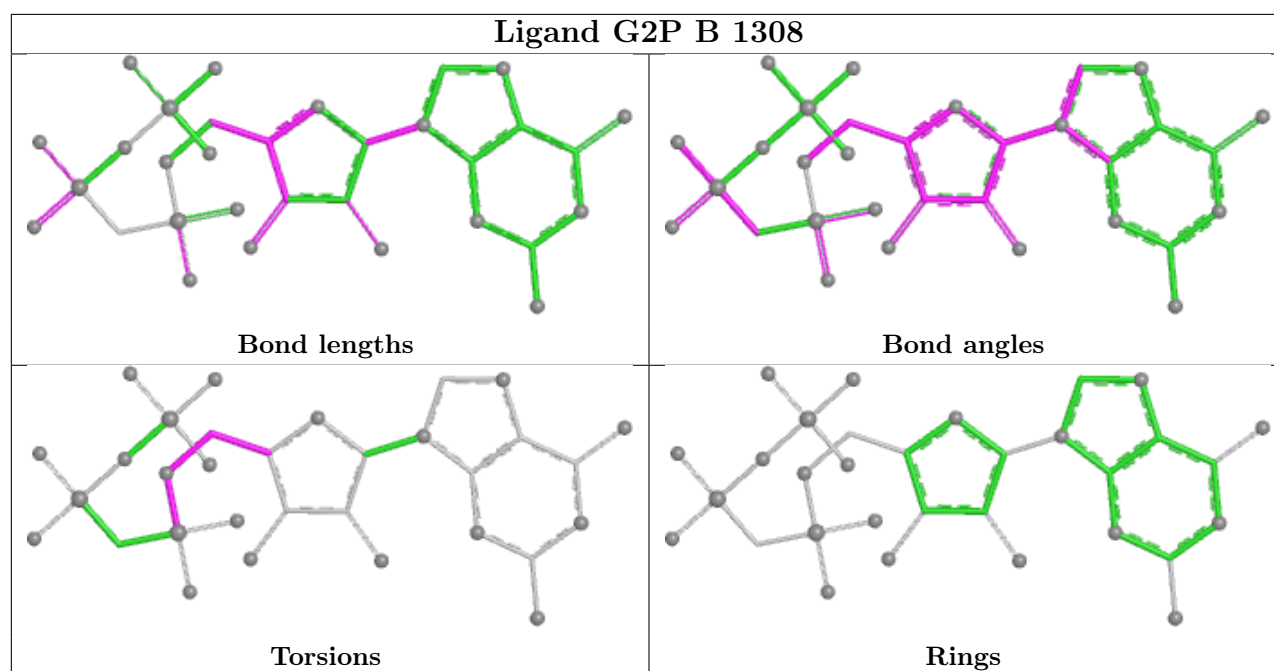
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	B	1308	G2P	C4'-C5'-O5'-PA
18	B	1308	G2P	O4'-C4'-C5'-O5'
18	B	1308	G2P	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	B	3
4	A	2
6	C	2

The worst 5 of 7 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	119:ASN	C	120:GLU	N	1.98
1	B	503:GLY	C	504:ARG	N	1.68
1	C	90:ASP	C	91:HIS	N	1.15
1	B	511:PRO	C	512:ARG	N	1.12
1	B	363:HIS	C	364:ILE	N	1.03

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	T	18/19 (94%)	1.97	8 (44%) 0 2	63, 85, 96, 104	0
2	N	6/7 (85%)	2.73	6 (100%) 0 0	51, 51, 51, 51	0
3	P	10/10 (100%)	1.09	1 (10%) 12 17	71, 75, 93, 93	0
4	A	1416/1733 (81%)	0.47	67 (4%) 36 33	45, 110, 184, 223	0
5	B	1112/1224 (90%)	0.60	71 (6%) 25 27	45, 119, 188, 216	0
6	C	266/318 (83%)	0.34	3 (1%) 78 63	60, 102, 161, 182	0
7	D	177/221 (80%)	0.67	11 (6%) 26 28	75, 131, 170, 187	0
8	E	214/215 (99%)	0.42	8 (3%) 45 37	79, 164, 209, 215	0
9	F	84/155 (54%)	0.18	1 (1%) 76 62	50, 81, 128, 147	0
10	G	171/171 (100%)	0.57	7 (4%) 41 36	79, 106, 137, 162	0
11	H	133/146 (91%)	0.72	11 (8%) 17 21	124, 161, 197, 206	0
12	I	119/122 (97%)	0.80	10 (8%) 17 21	97, 151, 181, 222	0
13	J	65/70 (92%)	0.32	1 (1%) 72 57	64, 102, 142, 149	0
14	K	114/120 (95%)	0.35	4 (3%) 47 38	65, 106, 136, 143	0
15	L	46/70 (65%)	1.03	3 (6%) 25 26	99, 158, 191, 199	0
All	All	3951/4601 (85%)	0.53	212 (5%) 31 30	45, 116, 188, 223	0

The worst 5 of 212 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1387	HIS	7.7
5	B	471	LYS	7.6
10	G	21	ARG	5.7
5	B	507	LYS	4.4
10	G	20	PRO	4.4

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](#)

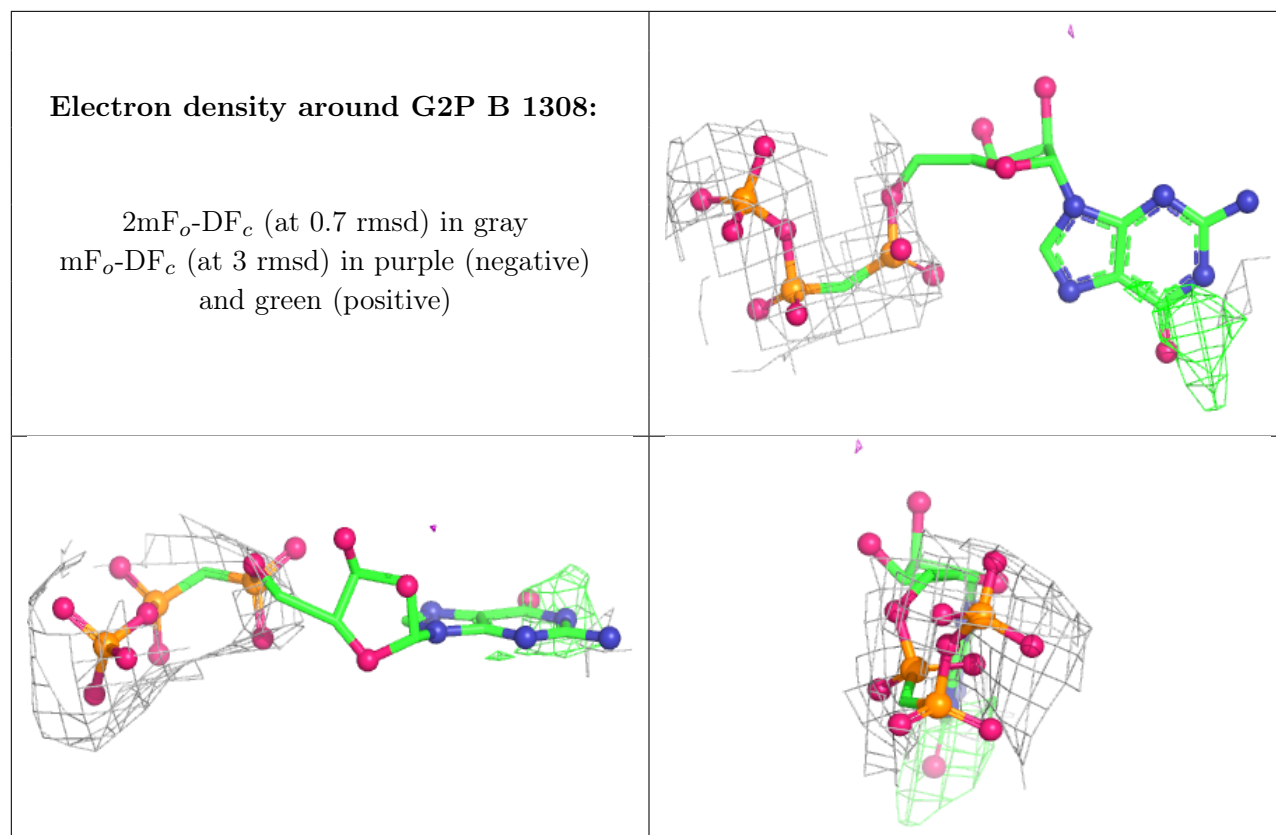
There are no oligosaccharides in this entry.

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
16	ZN	I	204	1/1	0.93	0.06	186,186,186,186	0
17	MG	A	1736	1/1	0.96	0.09	77,77,77,77	0
16	ZN	A	1734	1/1	0.97	0.06	112,112,112,112	0
16	ZN	B	1307	1/1	0.98	0.09	67,67,67,67	0
16	ZN	L	105	1/1	0.98	0.04	130,130,130,130	0
16	ZN	I	203	1/1	0.98	0.09	108,108,108,108	0
16	ZN	J	101	1/1	0.99	0.04	90,90,90,90	0
16	ZN	A	1735	1/1	0.99	0.03	68,68,68,68	0
16	ZN	C	319	1/1	0.99	0.06	63,63,63,63	0
18	G2P	B	1308	32/32	-	-	0,0,0,0	32

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.



6.5 Other polymers [i](#)

There are no such residues in this entry.