



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 11:19 PM UTC

PDB ID : 9N5D / pdb_00009n5d
Title : RNA polymerase II elongation complex with 8-oxoG at +1 site, CMP added
Authors : Oh, J.; Wang, D.
Deposited on : 2025-02-04
Resolution : 3.35 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

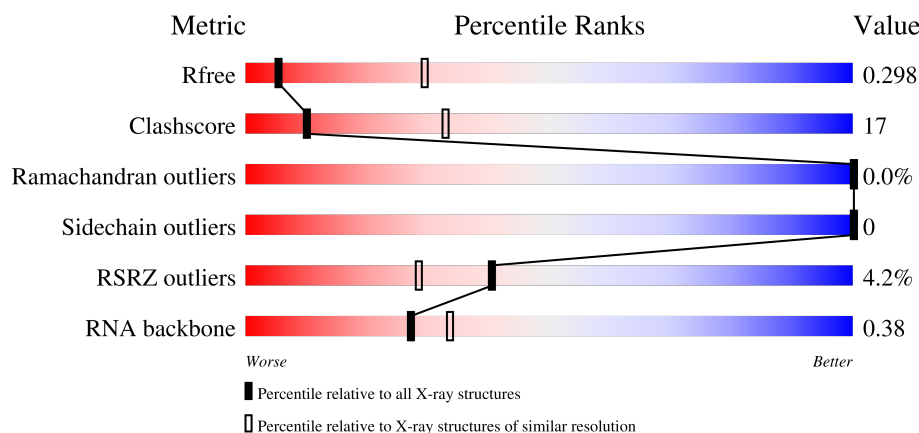
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)
RNA backbone	3983	1110 (3.72-3.00)

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	R	10	10% 90% 10%
2	T	29	31% 59% 10%
3	N	18	11% 72% 17%
4	A	1733	4% 49% 31% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29066 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			219	97	43	69	10			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			521	250	80	165	26			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	15	Total	C	N	O	P	0	0	0
			317	148	71	83	15			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1385	Total	C	N	O	S	0	0	0
			10831	6833	1895	2043	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1121	Total	C	N	O	S	0	0	0
			8849	5601	1550	1645	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	213	Total	C	N	O	S	0	0	0
			1728	1099	301	317	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1064	670	179	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			946	582	170	184	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

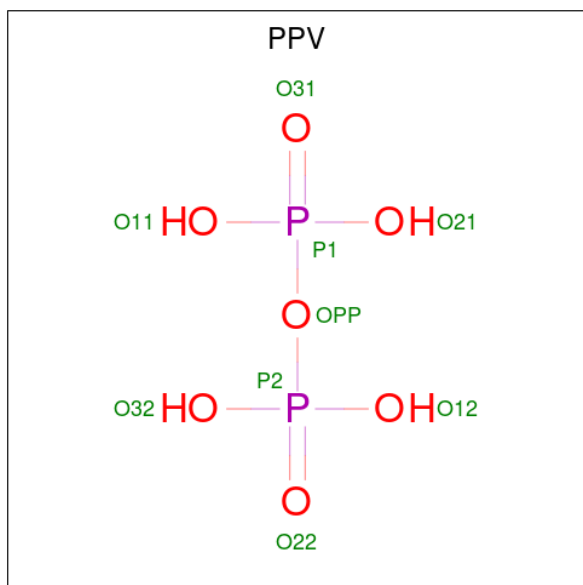
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is PYROPHOSPHATE (CCD ID: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).

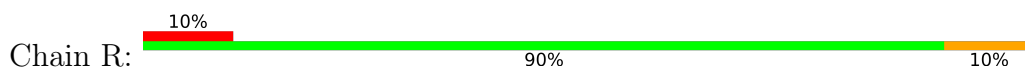


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	A	1	Total 9	O 7	P 2	0	0

3 Residue-property plots

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

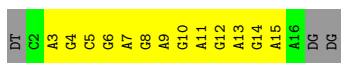
- Molecule 1: RNA



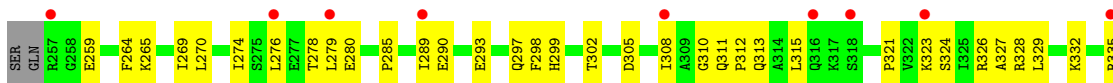
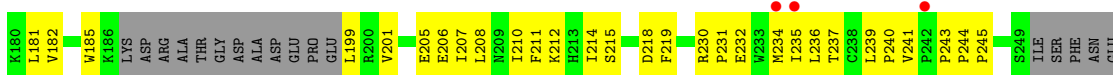
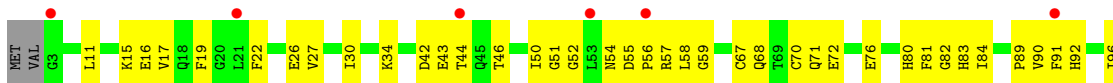
- Molecule 2: Template strand DNA



- Molecule 3: Non-template strand DNA

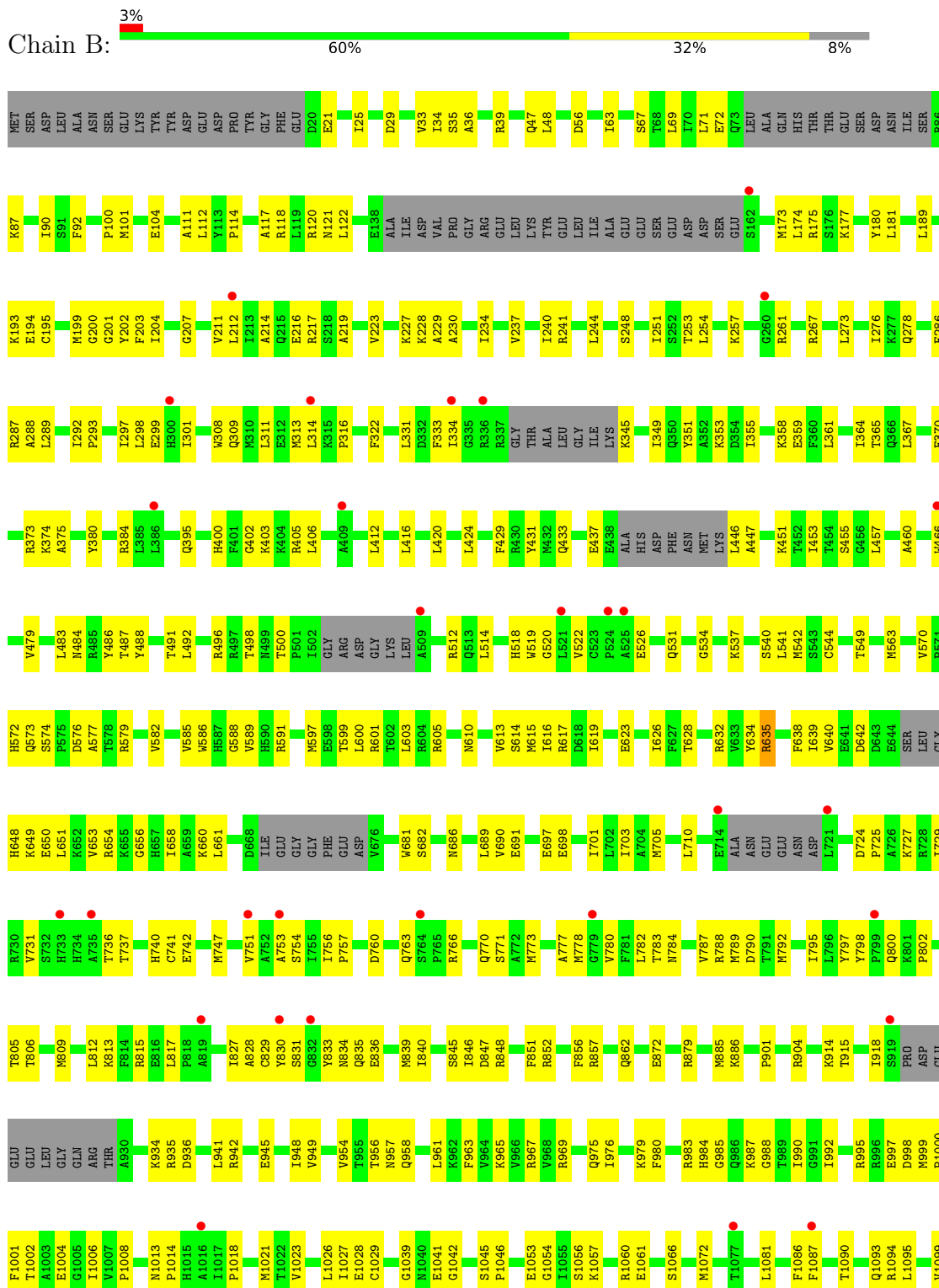


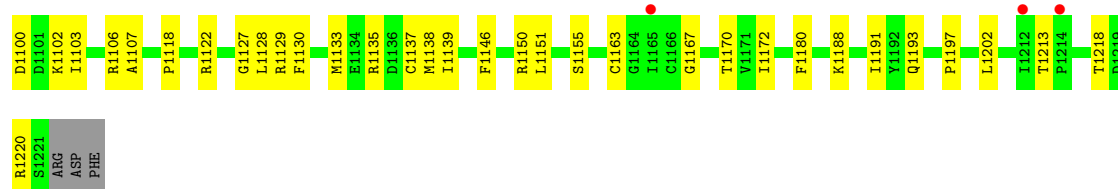
- Molecule 4: DNA-directed RNA polymerase II subunit RPB1



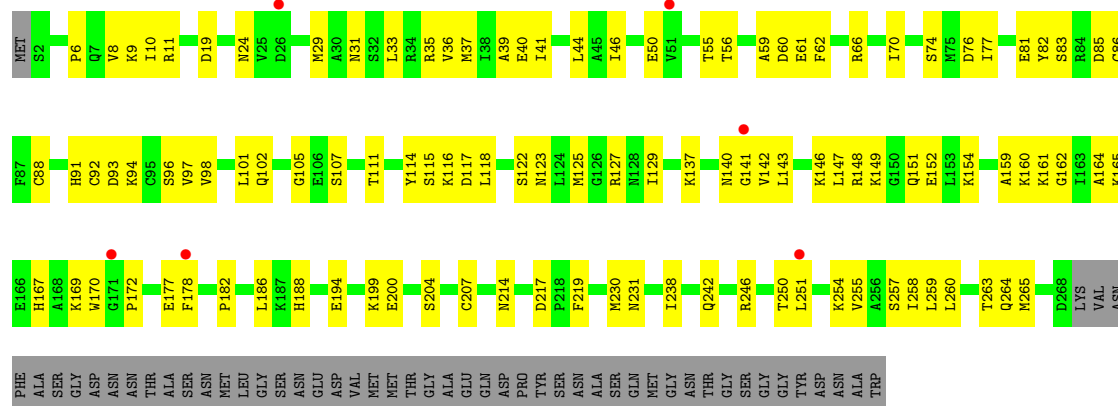
TYR	GLY	GLN	M1364	M1267	L1192	K1112	P910	G820	T709	I607	P514	R434	I336
SER	GLU	LYS	I1365	L1268	L1193	T1113	L914	R821	L710	I607	N517	R337	R337
PRO	ALA	ILE	R1366	I1271	P1114	S1115	E914	E822	R711	Q611	N518	G338	G338
THR	THR	THR	L1195	L1196	L1116	S1116	S915	G823	L722	Q612	P519	N339	N339
PRO	PRO	ILE	L1197	L1198	T1117	G916	G916	L824	L732	I613	C520	L340	L340
SER	PHE	GLU	D1198	R1199	V1118	V1119	S917	R825	L732	I613	Q525	R344	R344
TYR	GLY	ASP	V1276	V1276	T1119	T1119	E918	D826	L732	I613	Q525	R344	R344
PRO	ALA	GLN	V1374	V1374	L1120	L1120	I919	R827	N736	V617	Q525	F347	F347
THR	TYR	ASP	I1279	I1279	A1125	A1125	L923	R828	N736	E618	L528	R350	R350
PRO	GLY	GLN	E1280	E1280	L1207	L1207	L923	R829	K737	K619	C529	T351	T351
SER	GLU	GLY	R1281	R1281	T1208	T1208	K924	K830	K738	K620	L450	V352	V352
PRO	ALA	GLY	V1282	V1282	M1209	M1209	L925	T831	D739	S624	L531	I353	I353
SER	PRO	VAL	V1283	V1283	Q1130	Q1130	Q826	R840	N741	I630	R532	S354	S354
TYR	THR	THR	M1284	M1284	A1131	A1131	V927	R841	K744	I630	K533	S454	S454
SER	PRO	THR	V1384	V1384	L1132	L1132	L936	K843	Q745	R635	L534	M455	M455
PRO	SER	PRO	T1385	T1385	L1133	L1133	Y933	R844	Q745	R635	L534	M456	M456
PRO	PRO	THR	R1386	R1386	L1134	L1134	Y933	L845	Q745	R635	L534	M456	M456
THR	GLY	THR	H1387	H1387	I1138	I1138	L936	E846	Q745	R635	L534	M456	M456
SER	PHE	ASN	T1295	T1295	I1138	I1138	L936	E847	Q745	R635	L534	M456	M456
PRO	GLY	GLU	K1217	K1217	T1141	T1141	D939	R848	Q745	R635	L534	M456	M456
SER	VAL	GLY	Q1218	Q1218	T1141	T1141	R849	R849	Q745	R635	L534	M456	M456
TYR	SER	LEU	F1220	F1220	K1144	K1144	V850	V850	Q745	R635	L534	M456	M456
PRO	PRO	VAL	L1224	L1224	I1148	I1148	K941	K941	Q745	R635	L534	M456	M456
THR	GLY	ASN	F1225	F1225	L1148	L1148	L943	L943	Q745	R635	L534	M456	M456
SER	PHE	ALA	V1226	V1226	A1149	A1149	E944	E944	Q745	R635	L534	M456	M456
PRO	SER	ASP	I1227	I1227	S1150	S1150	R945	R945	Q745	R635	L534	M456	M456
TYR	THR	ASP	D1309	D1309	E1151	E1151	E945	E945	Q745	R635	L534	M456	M456
SER	THR	ASP	A1412	A1412	E1152	E1152	A952	A952	Q745	R635	L534	M456	M456
PRO	PRO	LYS	L1313	L1313	Y1153	Y1153	N953	N953	Q745	R635	L534	M456	M456
THR	THR	ASP	S1314	S1314	Y1154	Y1154	L956	L956	Q745	R635	L534	M456	M456
PRO	TYR	GLU	E1417	E1417	D1155	D1155	L956	L956	Q745	R635	L534	M456	M456
PRO	SER	LEU	D1418	D1418	P1156	P1156	L956	L956	Q745	R635	L534	M456	M456
TYR	THR	PHE	C1421	C1421	D1157	D1157	L956	L956	Q745	R635	L534	M456	M456
PRO	PRO	PRO	M1427	M1427	S1160	S1160	L956	L956	Q745	R635	L534	M456	M456
THR	ALA	LEU	V1428	V1428	T1161	T1161	L956	L956	Q745	R635	L534	M456	M456
SER	TYR	VAL	I1429	I1429	V1162	V1162	L956	L956	Q745	R635	L534	M456	M456
PRO	ASP	ASP	L1430	L1430	E1165	E1165	L956	L956	Q745	R635	L534	M456	M456
SER	PRO	SER	G1431	G1431	D1166	D1166	L956	L956	Q745	R635	L534	M456	M456
TYR	THR	GLY	Q1432	Q1432	E1167	E1167	L956	L956	Q745	R635	L534	M456	M456
SER	SER	SER	M1433	M1433	E1168	E1168	L956	L956	Q745	R635	L534	M456	M456
PRO	PRO	ASN	I1436	I1436	I1169	I1169	L956	L956	Q745	R635	L534	M456	M456
THR	THR	ALA	F1441	F1441	I1170	I1170	L956	L956	Q745	R635	L534	M456	M456
SER	PRO	ALA	G1445	G1445	L1176	L1176	L956	L956	Q745	R635	L534	M456	M456
TYR	SER	GLY	GLU	GLU	LEU	LEU	L956	L956	Q745	R635	L534	M456	M456
PRO	PRO	PHE	GLU	GLU	ASP	ASP	L956	L956	Q745	R635	L534	M456	M456
THR	SER	THR	SER	SER	GLU	GLU	L956	L956	Q745	R635	L534	M456	M456
SER	PRO	THR	SER	SER	GLU	GLU	L956	L956	Q745	R635	L534	M456	M456
TYR	TYR	ALA	R1343	R1343	ALA	ALA	L956	L956	Q745	R635	L534	M456	M456
PRO	THR	THR	R1345	R1345	GLU	GLU	L956	L956	Q745	R635	L534	M456	M456
SER	TYR	ALA	VAL	VAL	GLU	GLU	L956	L956	Q745	R635	L534	M456	M456
PRO	PRO	TYR	LYS	LYS	D1257	D1257	L956	L956	Q745	R635	L534	M456	M456
SER	SER	GLY	TYR	TYR	K1262	K1262	L956	L956	Q745	R635	L534	M456	M456
TYR	THR	GLY	TYR	TYR	E1264	E1264	L956	L956	Q745	R635	L534	M456	M456
PRO	SER	ALA	MET	MET	I1355	I1355	L956	L956	Q745	R635	L534	M456	M456
PRO	PRO	ASP	PRO	PRO	I1356	I1356	L956	L956	Q745	R635	L534	M456	M456
THR	SER	THR	GLU	GLU	GLU	GLU	L956	L956	Q745	R635	L534	M456	M456

- Molecule 5: DNA-directed RNA polymerase II subunit RPB2

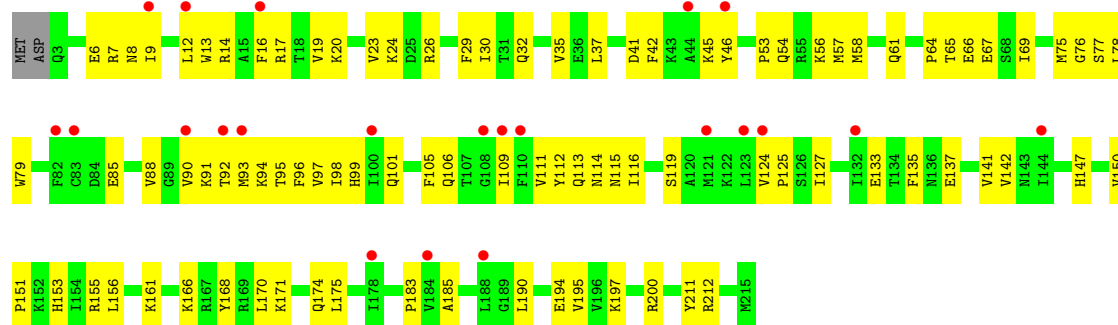




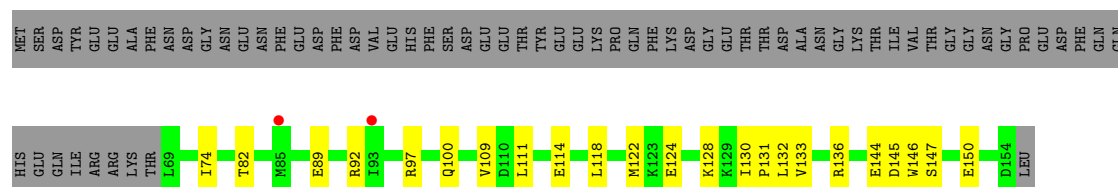
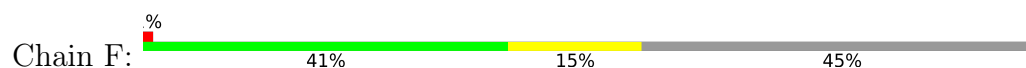
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



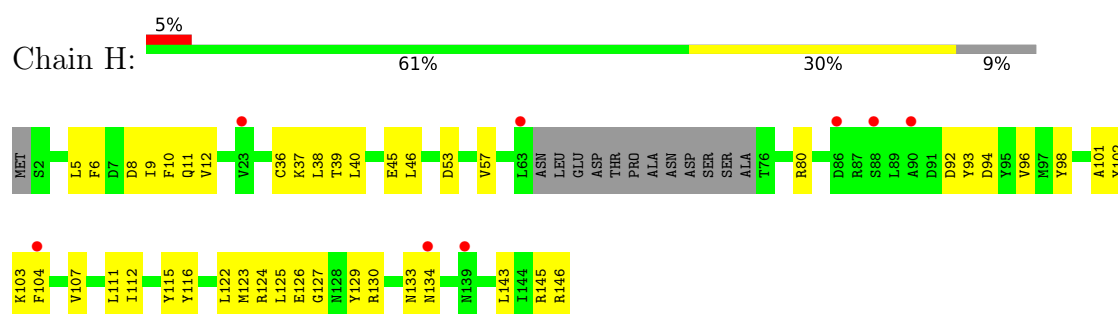
• Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



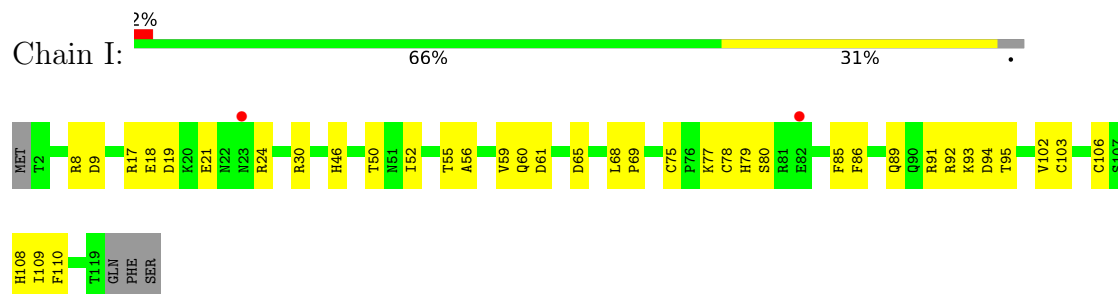
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



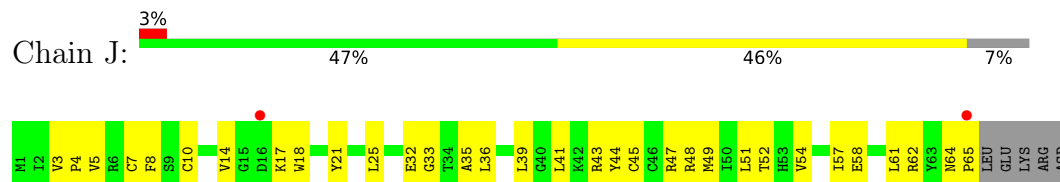
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



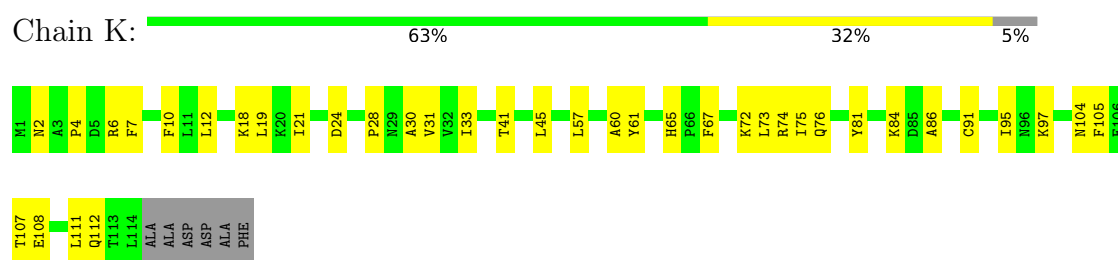
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



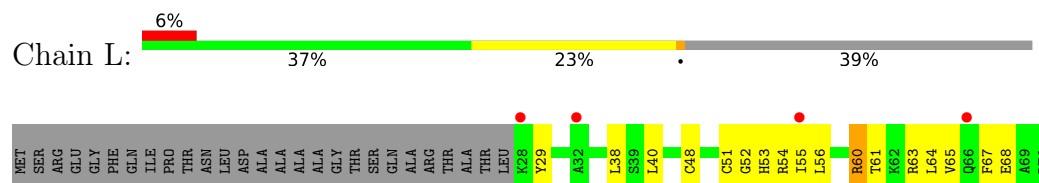
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.90Å 222.27Å 193.15Å 90.00° 100.27° 90.00°	Depositor
Resolution (Å)	49.31 – 3.35 49.31 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.31-3.35) 98.8 (49.31-3.35)	Depositor EDS
R_{merge}	0.51	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.265 , 0.300 0.264 , 0.298	Depositor DCC
R_{free} test set	2000 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 75.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29066	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 8OG, PPV

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	R	0.14	0/245	0.32	0/379
2	T	0.23	0/551	0.49	0/843
3	N	0.21	0/359	0.39	0/553
4	A	0.15	0/11023	0.39	0/14912
5	B	0.14	0/9020	0.35	0/12172
6	C	0.14	0/2139	0.34	0/2899
7	E	0.15	0/1764	0.39	0/2376
8	F	0.13	0/696	0.36	0/943
9	H	0.14	0/1082	0.42	0/1466
10	I	0.16	0/964	0.40	0/1301
11	J	0.17	0/541	0.40	0/727
12	K	0.14	0/937	0.36	0/1265
13	L	0.16	0/339	0.41	0/450
All	All	0.15	0/29660	0.38	0/40286

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
4	A	0	1
5	B	0	2
13	L	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	311	GLN	Peptide
5	B	267	ARG	Sidechain
5	B	635	ARG	Sidechain
13	L	60	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	R	219	0	110	1	0
2	T	521	0	297	19	0
3	N	317	0	166	14	0
4	A	10831	0	10873	419	1
5	B	8849	0	8808	311	0
6	C	2101	0	2058	85	0
7	E	1728	0	1744	79	0
8	F	684	0	692	18	0
9	H	1064	0	1029	40	0
10	I	946	0	888	36	1
11	J	532	0	544	38	0
12	K	919	0	929	35	0
13	L	337	0	354	15	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	A	9	0	0	0	0
All	All	29066	0	28492	991	1

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 17.

The worst 5 of 991 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:E:96:PHE:HA	7:E:99:HIS:HD2	1.26	1.00
6:C:66:ARG:NH2	11:J:3:VAL:O	2.03	0.91
7:E:96:PHE:HA	7:E:99:HIS:CD2	2.08	0.88
4:A:567:LYS:HB2	9:H:96:VAL:HB	1.56	0.88
11:J:36:LEU:HD13	11:J:47:ARG:HD3	1.55	0.86

All (1) 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)
4:A:917:SER:OG	10:I:21:GLU:OE1[4_546]	2.18	0.02

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	1371/1733 (79%)	1334 (97%)	36 (3%)	1 (0%)	48	76
5	B	1101/1224 (90%)	1078 (98%)	23 (2%)	0	100	100
6	C	265/318 (83%)	260 (98%)	5 (2%)	0	100	100
7	E	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
10	I	116/122 (95%)	112 (97%)	4 (3%)	0	100	100
11	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
12	K	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
13	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	3493/4173 (84%)	3407 (98%)	85 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	958	VAL

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	1194/1520 (79%)	1194 (100%)	0	100	100
5	B	955/1061 (90%)	955 (100%)	0	100	100
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	192/197 (98%)	192 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	116/128 (91%)	116 (100%)	0	100	100
10	I	109/116 (94%)	109 (100%)	0	100	100
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3070/3657 (84%)	3070 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	1093	GLN
5	B	1141	HIS
7	E	153	HIS
4	A	881	GLN
4	A	877	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
2	8OG	T	19	1,2	22,25,26	4.09	18 (81%)	26,37,40	1.68	7 (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
2	8OG	T	19	1,2	-	3/7/21/22	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	8OG	C8-N7	7.45	1.52	1.38
2	T	19	8OG	C8-N9	6.09	1.51	1.40
2	T	19	8OG	C2-N3	6.01	1.47	1.33
2	T	19	8OG	C4-N3	5.81	1.47	1.34
2	T	19	8OG	C2-N2	4.96	1.45	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	8OG	C2-N3-C4	4.50	120.05	112.30
2	T	19	8OG	O6-C6-C5	-3.11	119.77	127.26
2	T	19	8OG	C2-N1-C6	-2.71	120.19	125.11
2	T	19	8OG	C5-C6-N1	2.68	119.49	112.13
2	T	19	8OG	C5-N7-C8	-2.50	106.02	109.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	8OG	O4'-C4'-C5'-O5'
2	T	19	8OG	C3'-C4'-C5'-O5'
2	T	19	8OG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
16	PPV	A	1804	-	6,8,8	0.79	0	12,13,13	0.80	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
16	PPV	A	1804	-	-	1/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

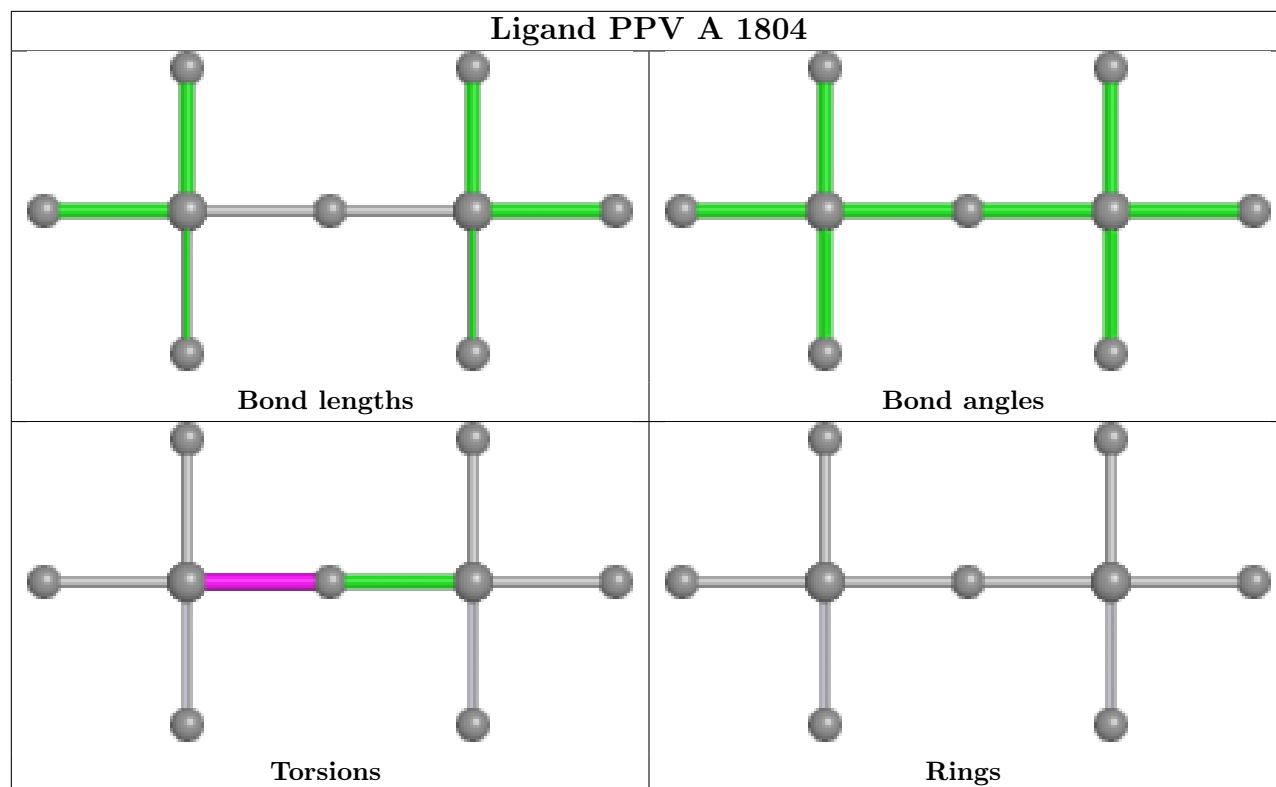
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	1804	PPV	P1-OPP-P2-O32

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](#)

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	R	10/10 (100%)	0.18	1 (10%) 12 12	81, 94, 140, 153	0
2	T	25/29 (86%)	0.37	0 100 100	76, 155, 214, 221	0
3	N	15/18 (83%)	0.15	0 100 100	150, 173, 221, 227	0
4	A	1385/1733 (79%)	0.56	72 (5%) 33 23	45, 87, 157, 209	0
5	B	1121/1224 (91%)	0.45	33 (2%) 53 39	48, 84, 142, 186	0
6	C	267/318 (83%)	0.31	6 (2%) 62 46	53, 86, 119, 147	0
7	E	213/215 (99%)	0.76	22 (10%) 12 11	61, 119, 178, 195	0
8	F	86/155 (55%)	0.27	2 (2%) 61 45	68, 93, 127, 156	0
9	H	133/146 (91%)	0.56	8 (6%) 27 20	83, 107, 147, 177	0
10	I	118/122 (96%)	0.42	2 (1%) 69 53	68, 100, 123, 135	0
11	J	65/70 (92%)	0.33	2 (3%) 51 38	59, 81, 108, 128	0
12	K	114/120 (95%)	0.32	0 100 100	52, 85, 111, 130	0
13	L	43/70 (61%)	0.81	4 (9%) 14 13	68, 120, 165, 186	0
All	All	3595/4230 (84%)	0.50	152 (4%) 40 28	45, 89, 156, 227	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	83	CYS	4.8
7	E	121	MET	4.7
4	A	1332	PHE	4.7
7	E	110	PHE	4.4
7	E	93	MET	4.4

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	8OG	T	19	23/24	0.71	0.12	86,107,128,146	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

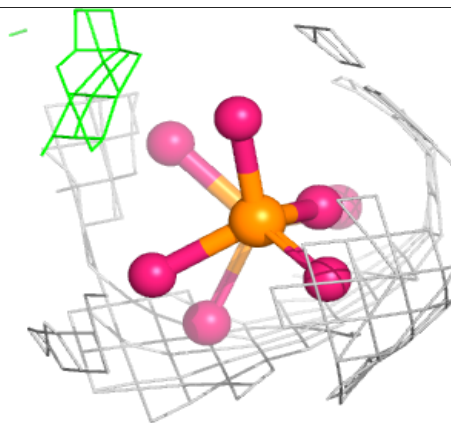
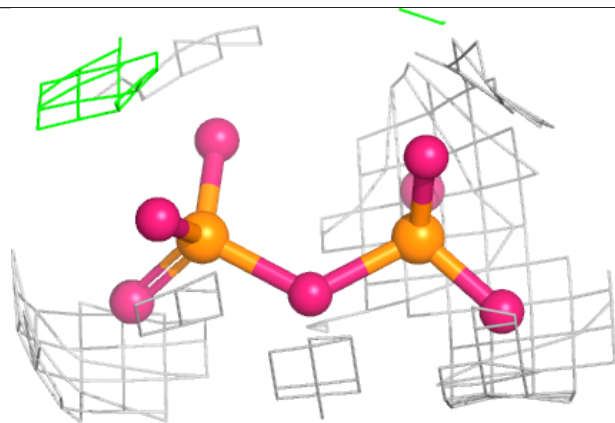
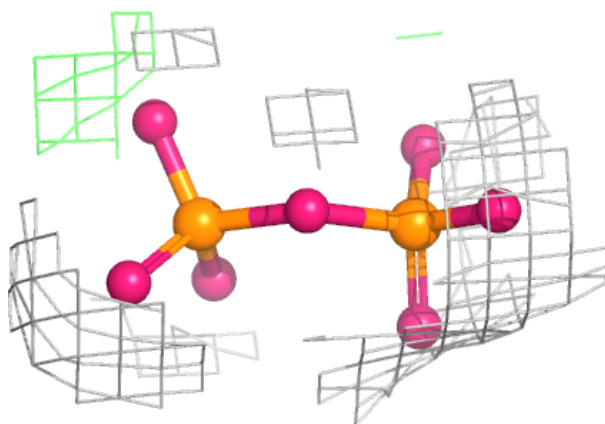
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	PPV	A	1804	9/9	0.42	0.12	134,142,165,171	0
14	ZN	L	101	1/1	0.75	0.14	174,174,174,174	0
15	MG	A	1803	1/1	0.83	0.08	88,88,88,88	0
14	ZN	I	202	1/1	0.86	0.10	157,157,157,157	0
14	ZN	B	1301	1/1	0.95	0.06	163,163,163,163	0
14	ZN	J	101	1/1	0.96	0.11	88,88,88,88	0
14	ZN	A	1801	1/1	0.96	0.05	233,233,233,233	0
14	ZN	I	201	1/1	0.97	0.04	89,89,89,89	0
14	ZN	A	1802	1/1	0.97	0.04	161,161,161,161	0
14	ZN	C	401	1/1	1.00	0.09	100,100,100,100	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 PPV A 1804:

$2mF_o-DF_c$ (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.