



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 31, 2021 – 01:17 PM EDT

PDB ID : 7KEF
Title : RNA polymerase II elongation complex with unnatural base dTPT3, rNaM in swing state
Authors : Oh, J.; Wang, D.
Deposited on : 2020-10-10
Resolution : 3.89 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

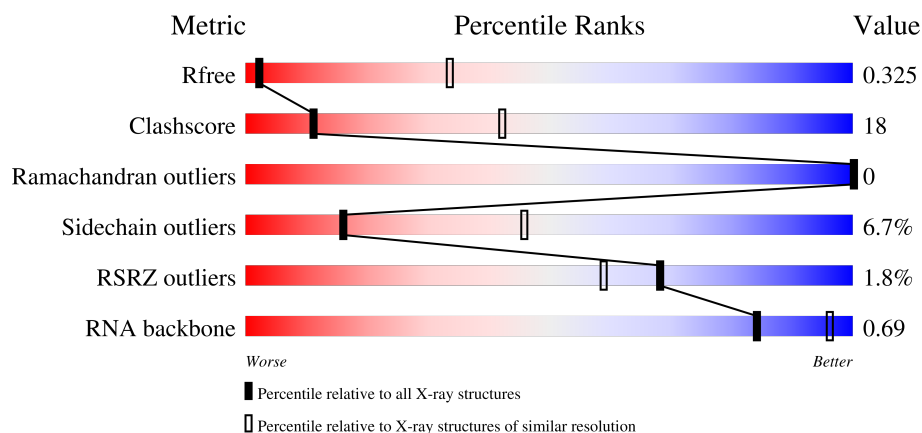
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






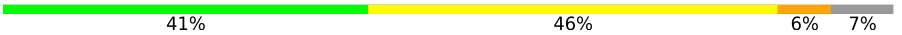

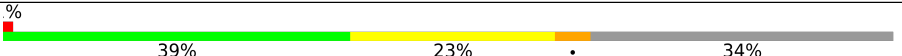
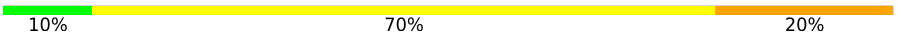
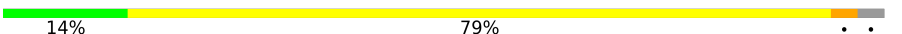

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

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	A	1733	<div> <div>5%</div> <div>48% 30% 20%</div> </div>
2	B	1224	<div> <div>2%</div> <div>51% 37% 10%</div> </div>
3	C	318	<div> <div>0%</div> <div>53% 30% 16%</div> </div>
4	E	215	<div> <div>5%</div> <div>67% 29%</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	10	
12	T	29	
13	N	16	

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29202 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1390	Total	C	N	O	S	0	0	0
			10920	6887	1913	2059	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2091	1315	348	415	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1748	1108	308	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			359	221	71	63	4			

- Molecule 11 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 12 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	28	Total	C	N	O	P	S	0	0
			566	273	100	164	27	2		

- Molecule 13 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	15	Total	C	N	O	P	0	0	0
			307	147	51	94	15			

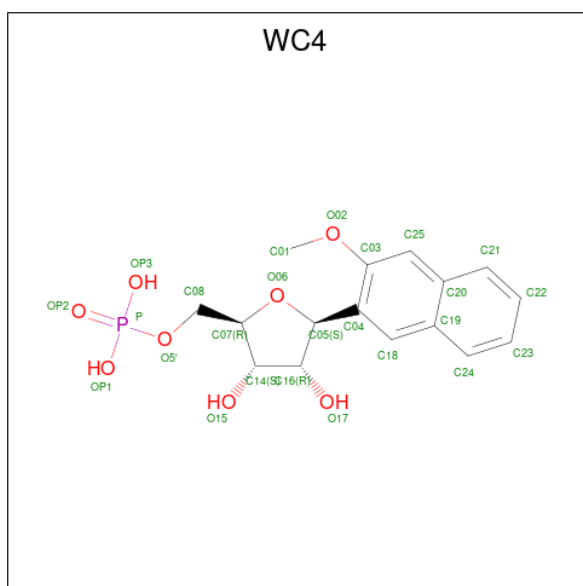
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is (1S)-1,4-anhydro-1-(3-methoxynaphthalen-2-yl)-5-O-phosphono-D-riitol (three-letter code: WC4) (formula: C₁₆H₁₉O₈P) (labeled as "Ligand of Interest" by depositor).

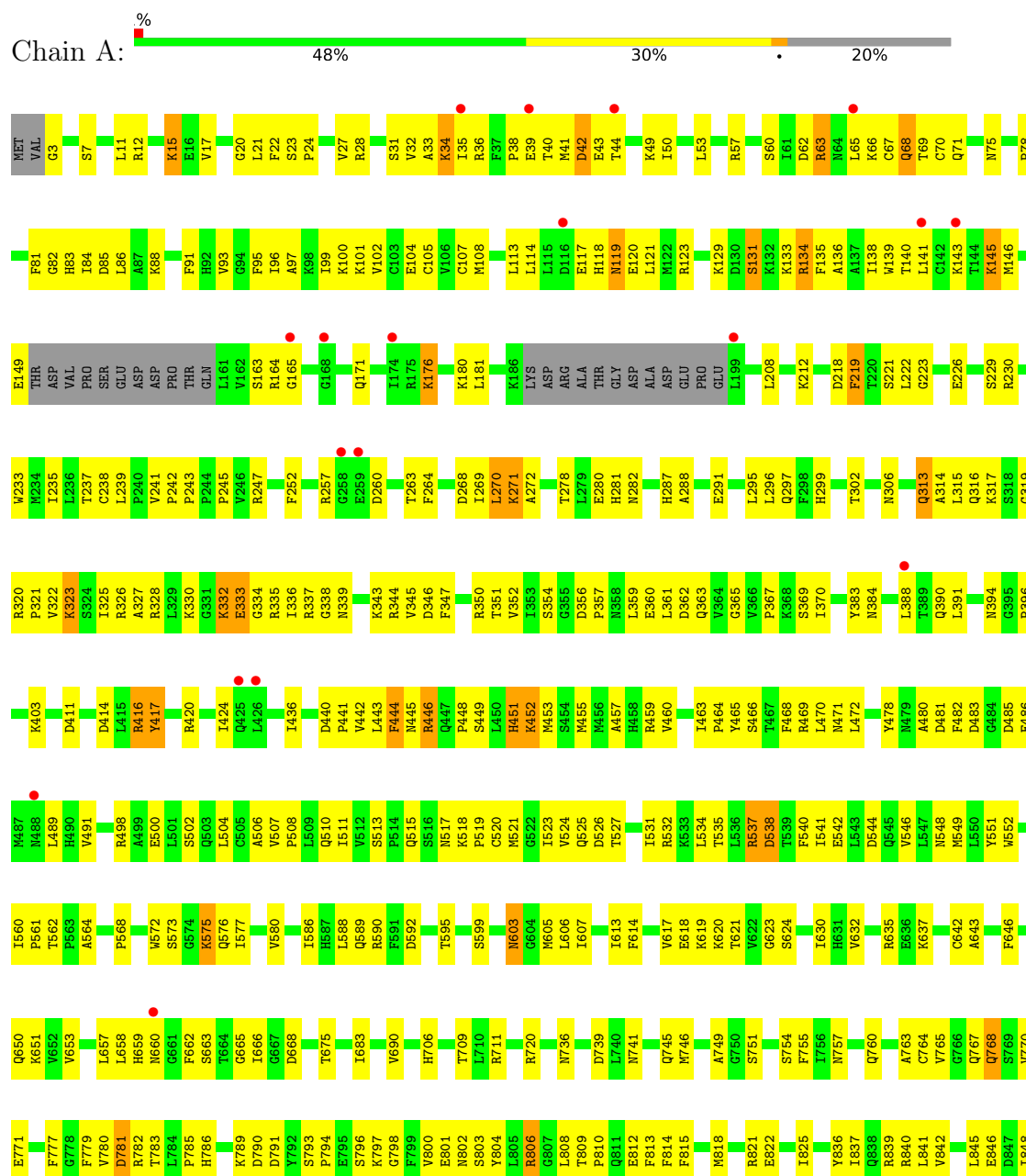


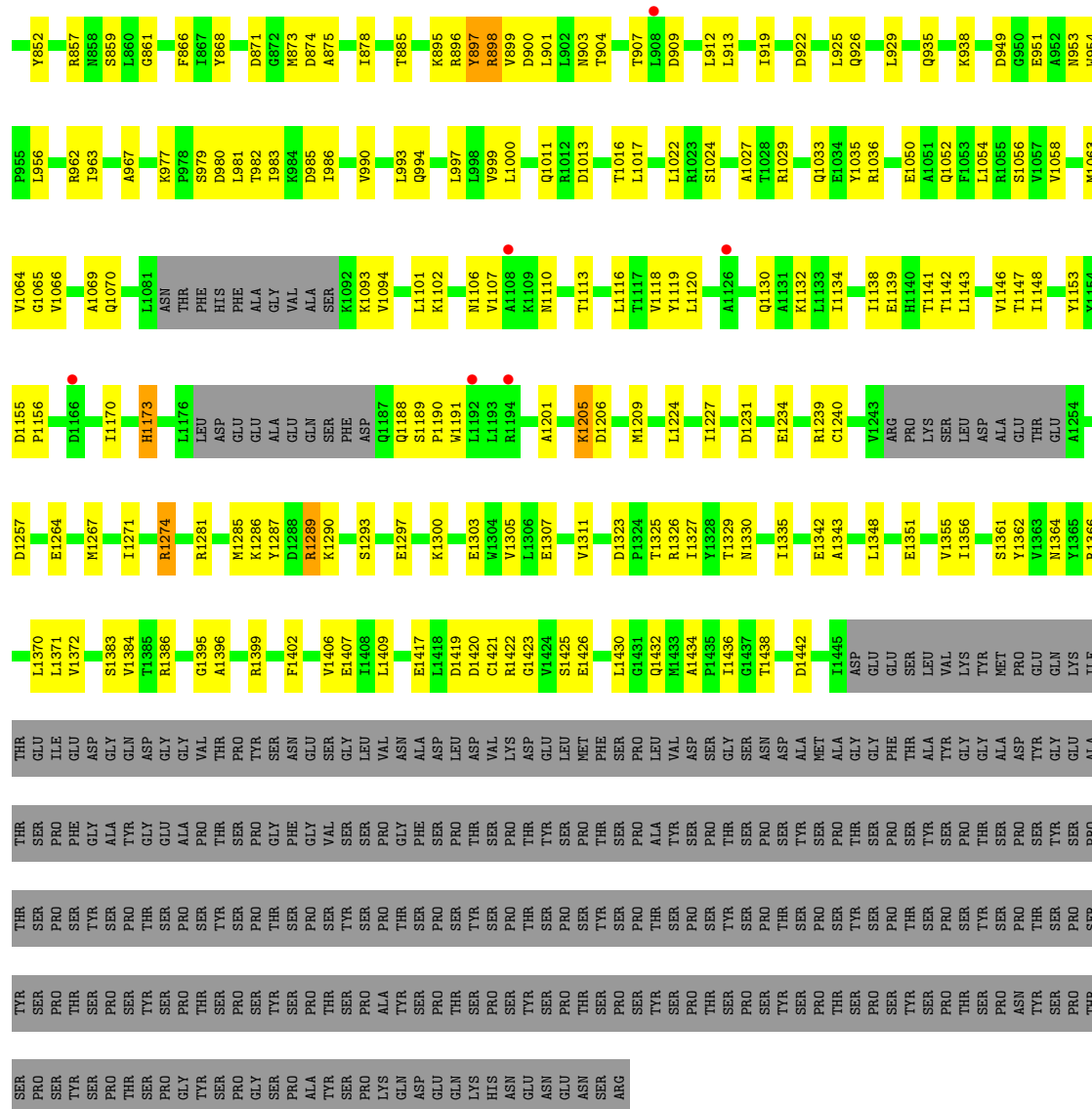
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	R	1	Total	C	O	P	0	0
			24	16	7	1		

3 Residue-property plots

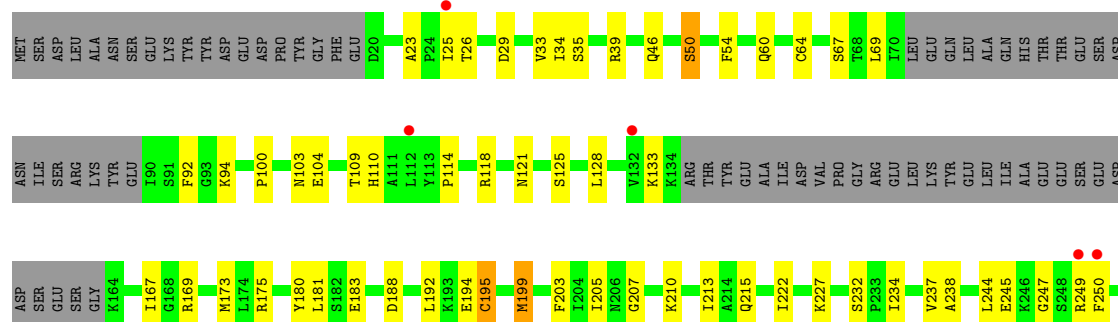
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

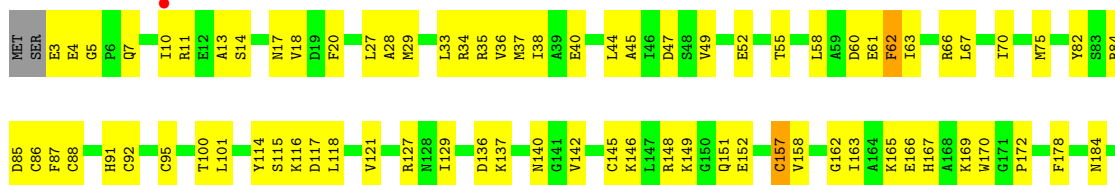
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

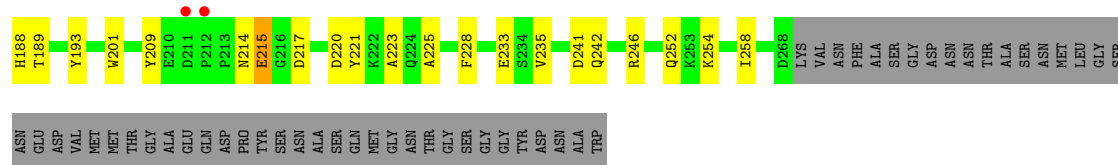




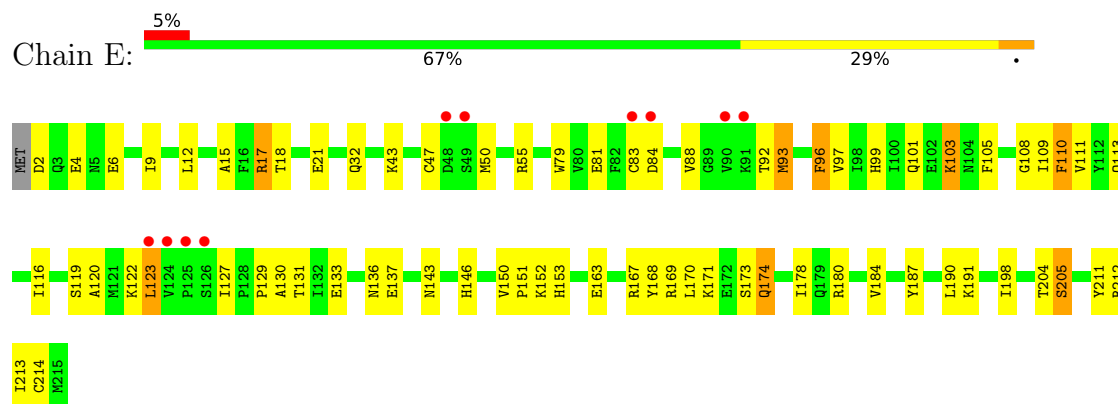
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2



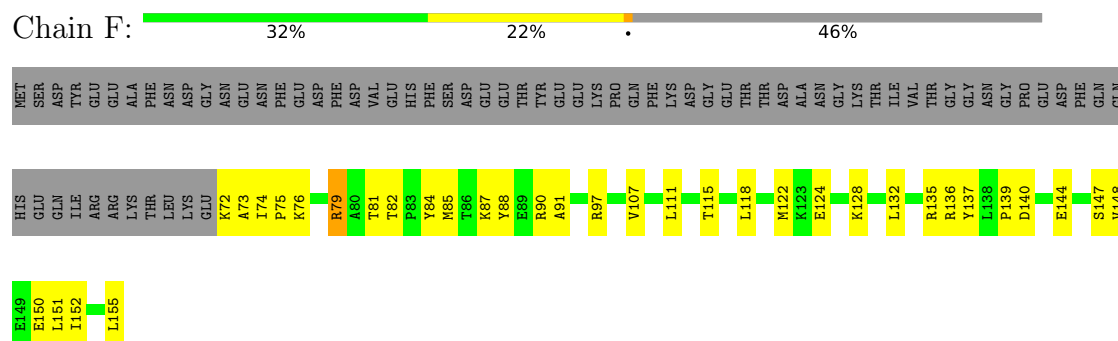




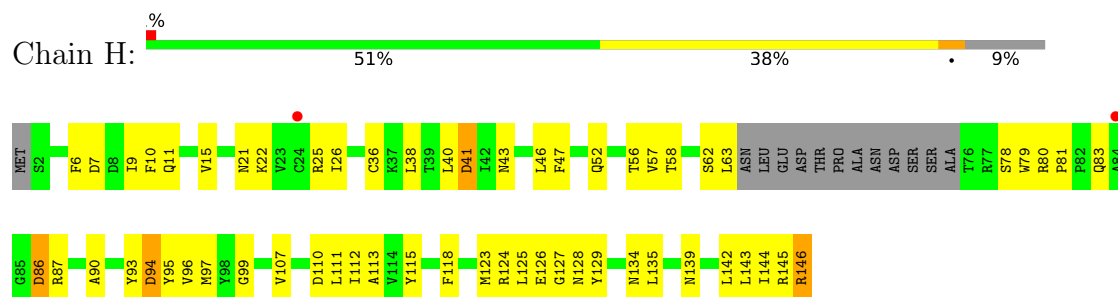
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



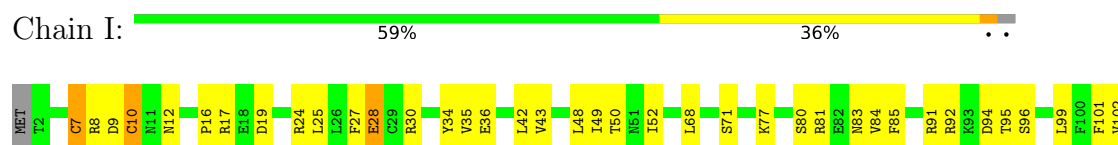
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

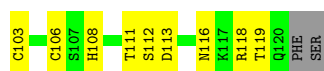


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 7: DNA-directed RNA polymerase II subunit RPB9





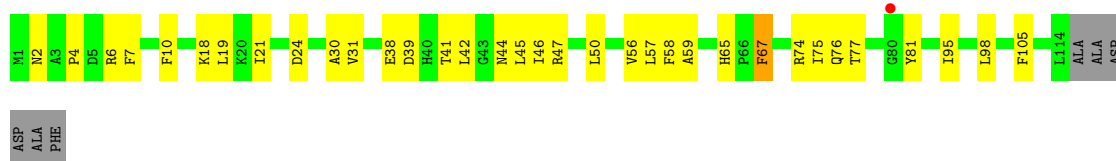
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 41% 46% 6% 7%



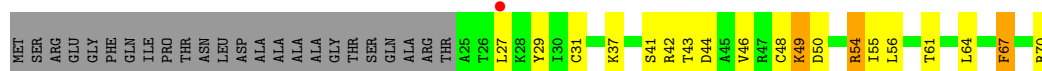
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K: 67% 28% 5%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 39% 23% 34%



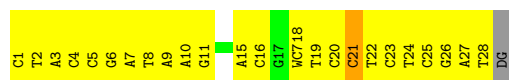
- Molecule 11: RNA

Chain R: 10% 70% 20%



- Molecule 12: Template strand DNA

Chain T: 14% 79% 6% 6%



- Molecule 13: Non-template strand DNA

Chain N: 56% 31% 6% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.71Å 221.71Å 193.25Å 90.00° 101.78° 90.00°	Depositor
Resolution (Å)	48.70 – 3.89 48.70 – 3.89	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.70-3.89) 98.6 (48.70-3.89)	Depositor EDS
R_{merge}	1.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.268 , 0.326 0.268 , 0.325	Depositor DCC
R_{free} test set	1979 reflections (3.17%)	wwPDB-VP
Wilson B-factor (Å ²)	107.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	29202	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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, WC4, MG, WC7

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	0.26	0/11113	0.48	1/15025 (0.0%)
2	B	0.26	0/8963	0.49	0/12086
3	C	0.26	0/2129	0.48	0/2886
4	E	0.26	0/1784	0.46	0/2402
5	F	0.26	0/691	0.43	0/933
6	H	0.26	0/1086	0.50	0/1470
7	I	0.27	0/989	0.47	0/1331
8	J	0.28	0/541	0.51	0/727
9	K	0.27	0/937	0.46	0/1265
10	L	0.25	0/361	0.57	0/481
11	R	0.41	0/244	1.08	1/380 (0.3%)
12	T	0.62	0/609	1.06	1/934 (0.1%)
13	N	0.55	0/342	1.35	1/526 (0.2%)
All	All	0.28	0/29789	0.53	4/40446 (0.0%)

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	A	0	2
13	N	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	17	DG	C5-C6-O6	-20.52	116.29	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	21	DC	O4'-C4'-C3'	-5.52	102.29	104.50
11	R	8	G	N3-C2-N2	-5.51	116.04	119.90
1	A	997	LEU	CA-CB-CG	5.40	127.71	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	LYS	Peptide
1	A	895	LYS	Peptide
13	N	17	DG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10920	0	11003	438	0
2	B	8792	0	8823	397	0
3	C	2091	0	2049	77	0
4	E	1748	0	1765	50	0
5	F	679	0	701	27	0
6	H	1068	0	1040	41	0
7	I	971	0	929	29	0
8	J	532	0	543	36	0
9	K	919	0	929	35	0
10	L	359	0	378	13	0
11	R	217	0	110	13	0
12	T	566	0	305	34	0
13	N	307	0	172	6	1
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	R	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29202	0	28747	1036	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 18.

The worst 5 of 1036 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:B:1094:ARG:NH2	2:B:1098:MET:SD	2.09	1.23
16:R:11:WC4:O06	16:R:11:WC4:C05	1.66	1.19
2:B:1094:ARG:HH12	2:B:1098:MET:HE2	0.98	1.11
2:B:1094:ARG:HH12	2:B:1098:MET:CE	1.65	1.10
1:A:508:PRO:HA	1:A:511:ILE:HG13	1.35	1.05

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)
13:N:17:DG:C6	13:N:17:DG:O6[2_856]	1.25	0.95

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	1378/1733 (80%)	1285 (93%)	93 (7%)	0	100	100
2	B	1088/1224 (89%)	1021 (94%)	67 (6%)	0	100	100
3	C	264/318 (83%)	242 (92%)	22 (8%)	0	100	100
4	E	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
5	F	82/155 (53%)	80 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
7	I	117/122 (96%)	111 (95%)	6 (5%)	0	100	100
8	J	63/70 (90%)	62 (98%)	1 (2%)	0	100	100
9	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
10	L	44/70 (63%)	43 (98%)	1 (2%)	0	100	100
All	All	3489/4173 (84%)	3279 (94%)	210 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	1210/1520 (80%)	1123 (93%)	87 (7%)	14	44
2	B	960/1061 (90%)	898 (94%)	62 (6%)	17	46
3	C	233/274 (85%)	225 (97%)	8 (3%)	37	62
4	E	195/197 (99%)	180 (92%)	15 (8%)	13	42
5	F	74/137 (54%)	70 (95%)	4 (5%)	22	52
6	H	117/128 (91%)	105 (90%)	12 (10%)	7	30
7	I	113/116 (97%)	106 (94%)	7 (6%)	18	48
8	J	60/65 (92%)	54 (90%)	6 (10%)	7	30
9	K	99/102 (97%)	97 (98%)	2 (2%)	55	74
10	L	39/57 (68%)	33 (85%)	6 (15%)	2	17
All	All	3100/3657 (85%)	2891 (93%)	209 (7%)	16	46

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	560	GLU
2	B	1148	LYS

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Mol	Chain	Res	Type
8	J	48	ARG
2	B	678	GLU
2	B	935	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
6	H	52	GLN
9	K	112	GLN
7	I	22	ASN
2	B	1025	HIS
6	H	11	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	9/10 (90%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	5	A
11	R	10	A

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
12	WC7	T	18	12	17,23,24	1.82	3 (17%)	17,33,36	1.60	4 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	WC7	T	18	12	-	3/4/21/22	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	WC7	C5-C4	4.97	1.48	1.40
12	T	18	WC7	C5-S1	-4.23	1.59	1.67
12	T	18	WC7	C1-C2	2.70	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	18	WC7	C3-C4-S3	-4.59	109.00	111.74
12	T	18	WC7	C6-C3-C4	2.33	113.60	108.07
12	T	18	WC7	C6-C3-C2	-2.16	129.19	136.72
12	T	18	WC7	C3'-C2'-C1'	2.02	107.60	102.54

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	T	18	WC7	C3'-C4'-C5'-O5'
12	T	18	WC7	O4'-C4'-C5'-O5'
12	T	18	WC7	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	WC4	R	11	11,15	23,26,27	7.11	18 (78%)	33,37,40	1.53	4 (12%)

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	WC4	R	11	11,15	-	9/9/27/28	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)
16	R	11	WC4	C16-C05	-16.02	1.35	1.54
16	R	11	WC4	O06-C05	14.76	1.66	1.44
16	R	11	WC4	C25-C03	11.16	1.56	1.36
16	R	11	WC4	C18-C04	10.46	1.54	1.36
16	R	11	WC4	C23-C24	8.24	1.55	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	R	11	WC4	C14-C16-C05	4.14	106.70	101.93
16	R	11	WC4	O02-C03-C25	-3.87	120.23	125.24
16	R	11	WC4	O02-C03-C04	3.83	119.49	115.83
16	R	11	WC4	C01-O02-C03	-2.51	113.74	117.53

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

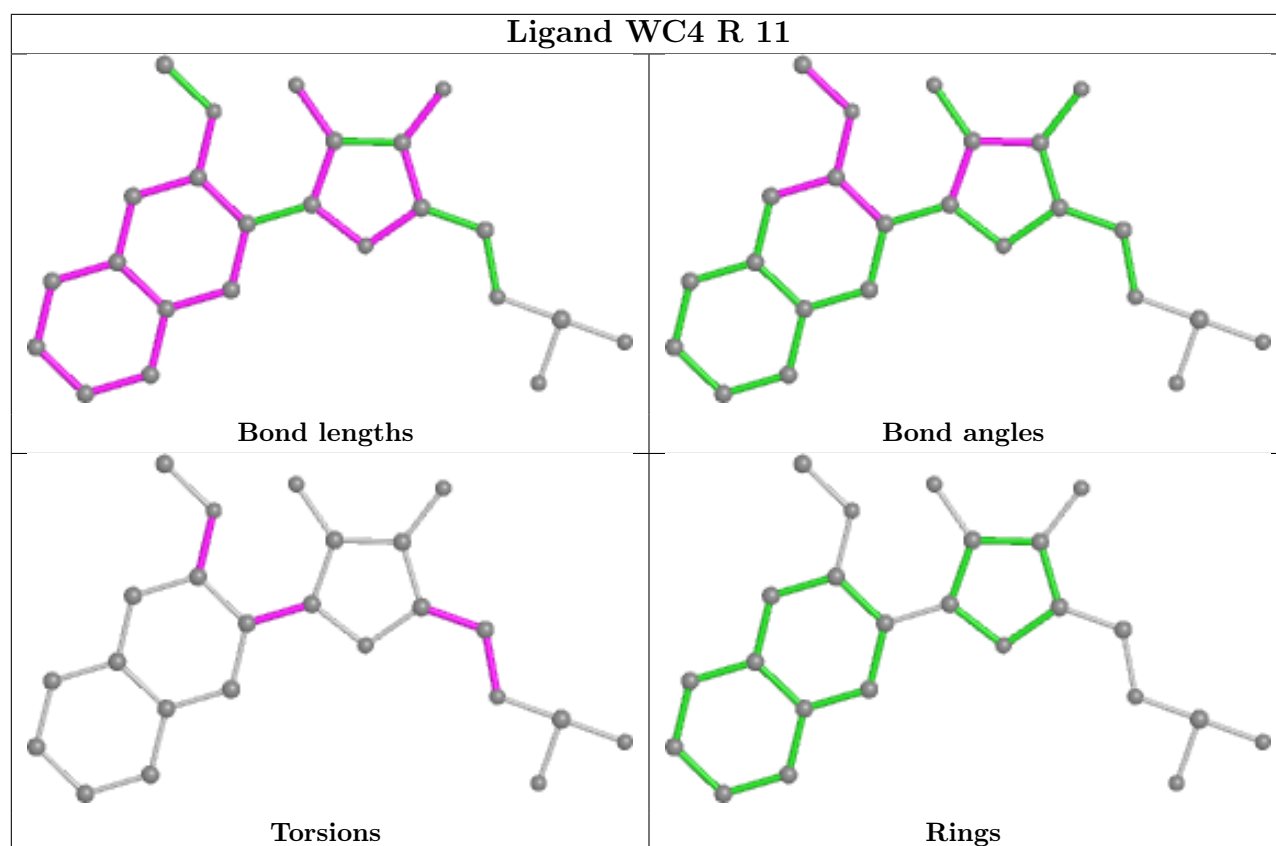
Mol	Chain	Res	Type	Atoms
16	R	11	WC4	C03-C04-C05-C16
16	R	11	WC4	C18-C04-C05-C16
16	R	11	WC4	C14-C07-C08-O5'
16	R	11	WC4	O06-C07-C08-O5'
16	R	11	WC4	C25-C03-O02-C01

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	R	11	WC4	1	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

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	1390/1733 (80%)	-0.05	24 (1%) 70 60	56, 105, 169, 216	0
2	B	1106/1224 (90%)	-0.04	22 (1%) 65 55	65, 108, 158, 199	0
3	C	266/318 (83%)	-0.17	3 (1%) 80 73	66, 105, 134, 156	0
4	E	214/215 (99%)	-0.03	10 (4%) 31 25	68, 126, 185, 214	0
5	F	84/155 (54%)	-0.25	0 100 100	81, 107, 128, 139	0
6	H	133/146 (91%)	-0.05	2 (1%) 73 64	95, 126, 164, 190	0
7	I	119/122 (97%)	-0.13	0 100 100	83, 117, 144, 172	0
8	J	65/70 (92%)	-0.14	0 100 100	74, 101, 130, 149	0
9	K	114/120 (95%)	-0.17	1 (0%) 84 77	75, 107, 132, 142	0
10	L	46/70 (65%)	0.13	1 (2%) 62 51	90, 143, 170, 183	0
11	R	10/10 (100%)	0.38	0 100 100	101, 121, 165, 172	0
12	T	27/29 (93%)	-0.10	0 100 100	109, 164, 257, 265	0
13	N	15/16 (93%)	-0.09	0 100 100	149, 224, 249, 252	0
All	All	3589/4228 (84%)	-0.07	63 (1%) 68 59	56, 109, 167, 265	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	GLY	5.9
4	E	126	SER	5.6
4	E	125	PRO	4.6
4	E	83	CYS	4.5
4	E	123	LEU	4.5

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
12	WC7	T	18	21/22	0.88	0.21	110,121,135,140	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

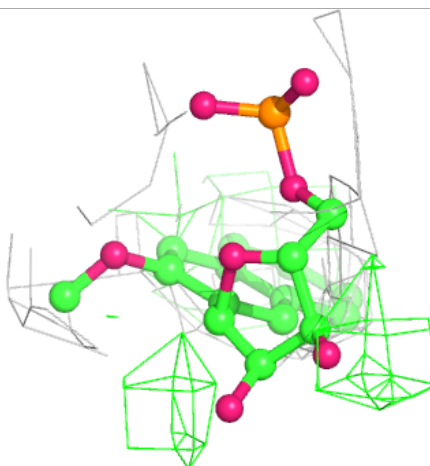
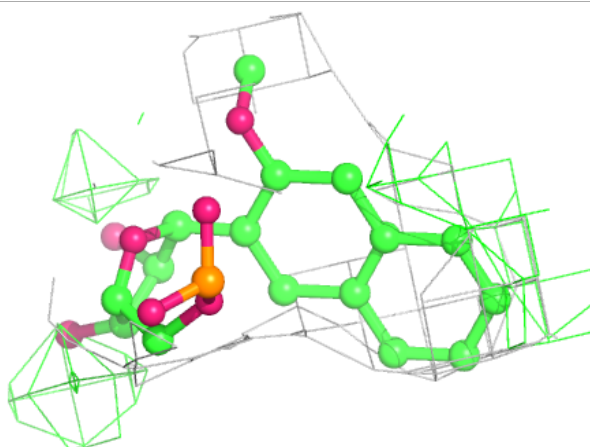
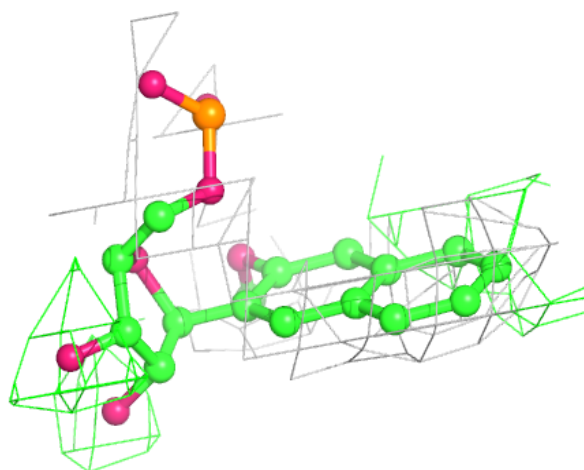
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	ZN	B	1307	1/1	0.79	0.10	179,179,179,179	0
14	ZN	L	105	1/1	0.79	0.08	179,179,179,179	0
16	WC4	R	11	24/25	0.90	0.25	96,109,119,123	0
14	ZN	C	319	1/1	0.92	0.10	91,91,91,91	0
14	ZN	J	101	1/1	0.92	0.21	107,107,107,107	0
14	ZN	A	1735	1/1	0.93	0.04	134,134,134,134	0
14	ZN	I	204	1/1	0.94	0.08	131,131,131,131	0
14	ZN	I	203	1/1	0.97	0.07	98,98,98,98	0
15	MG	A	2001	1/1	0.98	0.09	88,88,88,88	0
14	ZN	A	1734	1/1	0.98	0.21	206,206,206,206	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 WC4 R 11:

$2mF_o-DF_c$ (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.