



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 07:28 AM UTC

PDB ID : 7KEF / pdb_00007kef
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 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

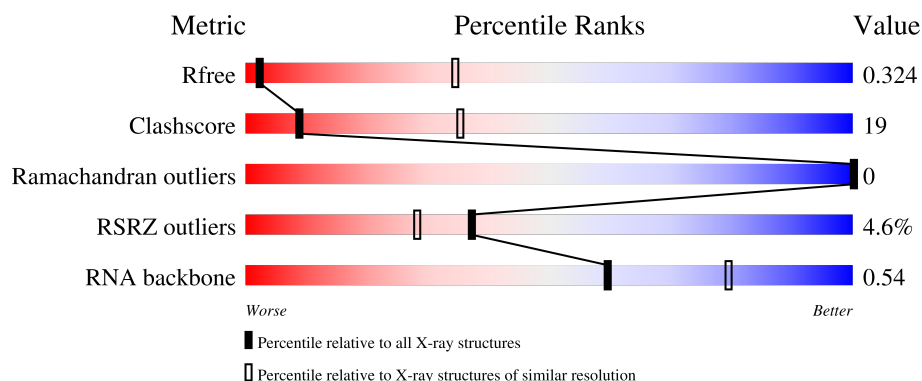
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 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.



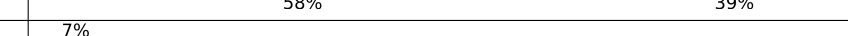
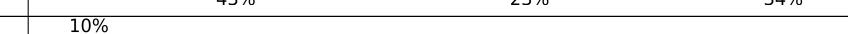
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

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	A	1733	4% 50% 30% 20%
2	B	1224	5% 53% 37% 10%
3	C	318	3% 54% 30% 16%
4	E	215	5% 69% 31%
5	F	155	2% 34% 21% 46%

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Mol	Chain	Length	Quality of chain
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			

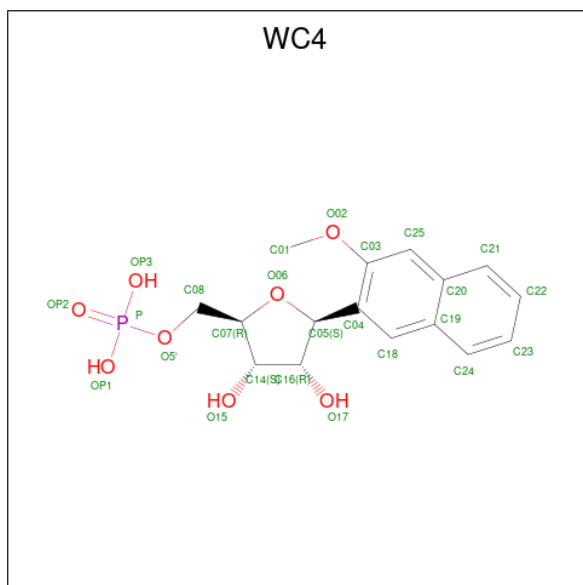
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (1S)-1,4-anhydro-1-(3-methoxynaphthalen-2-yl)-5-O-phosphono-D-ribitol (CCD ID: WC4) (formula: C₁₆H₁₉O₈P) (labeled as "Ligand of Interest" by depositor).

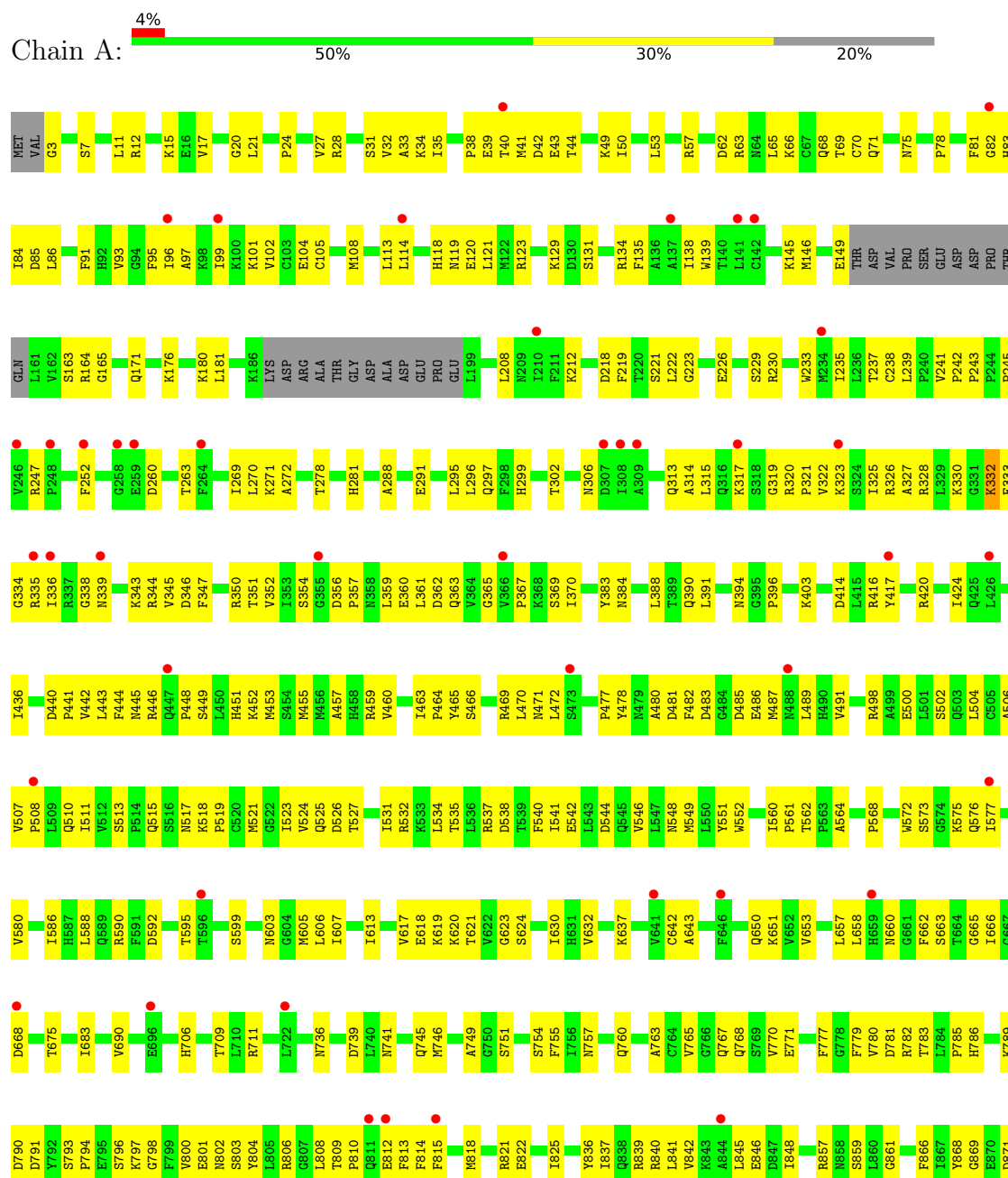


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	R	1	Total 24	C 16	O 7	P 1	0	0

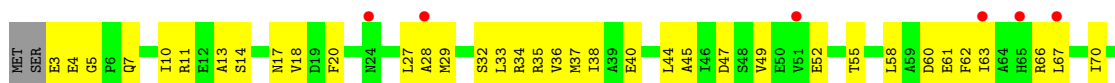
3 Residue-property plots

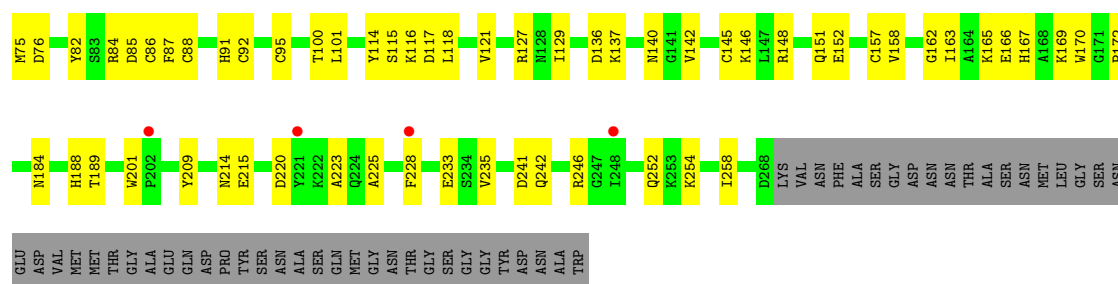
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA-directed RNA polymerase II subunit RPB1

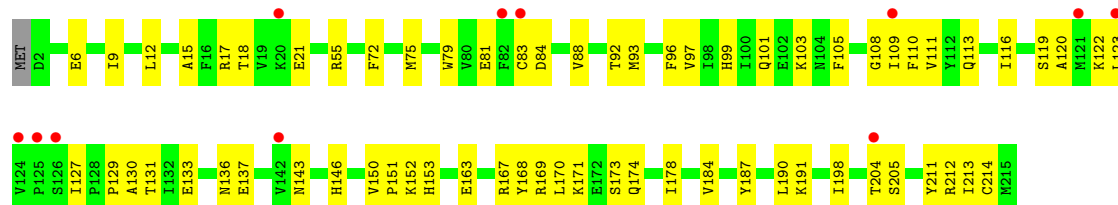




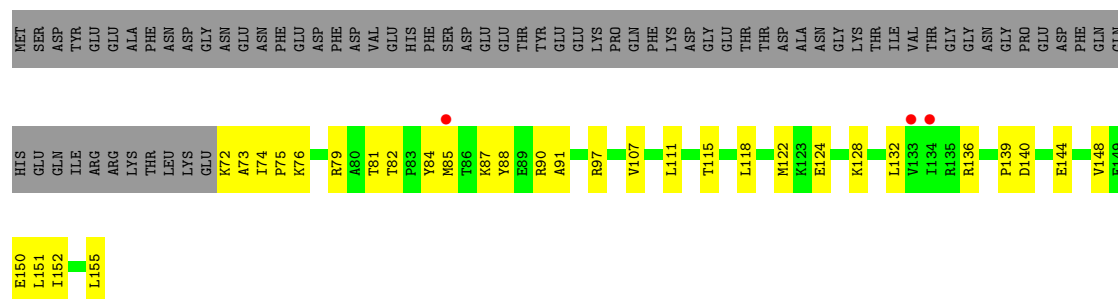
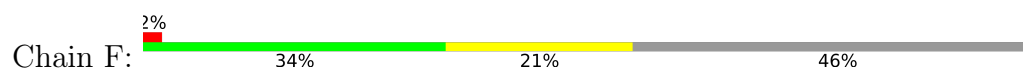




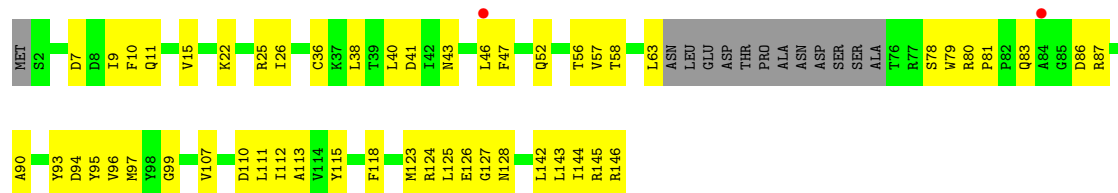
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1



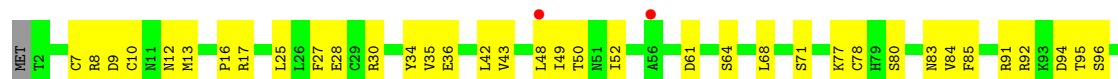
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



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

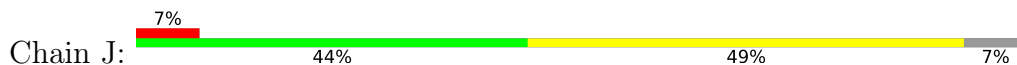


- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

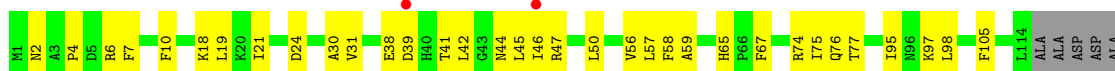




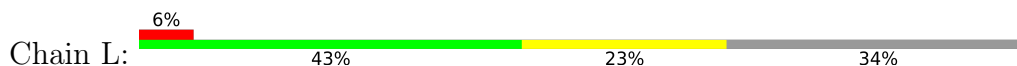
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



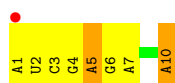
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



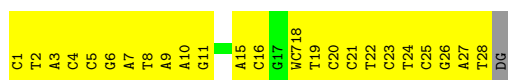
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



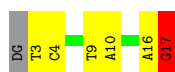
- Molecule 11: RNA



- Molecule 12: Template strand DNA



- Molecule 13: Non-template strand DNA



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 0.270 , 0.324	Depositor DCC
R_{free} test set	2000 reflections (3.15%)	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)	0.28 , 84.0	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	0.88	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: WC4, WC7, 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	A	0.18	0/11113	0.45	0/15025
2	B	0.18	0/8963	0.44	0/12086
3	C	0.16	0/2129	0.44	0/2886
4	E	0.16	0/1784	0.41	0/2402
5	F	0.17	0/691	0.41	0/933
6	H	0.16	0/1086	0.43	0/1470
7	I	0.17	0/989	0.42	0/1331
8	J	0.19	0/541	0.46	0/727
9	K	0.18	0/937	0.40	0/1265
10	L	0.16	0/361	0.49	0/481
11	R	0.19	0/244	0.33	0/380
12	T	0.26	0/609	0.55	0/934
13	N	0.20	0/342	0.57	1/526 (0.2%)
All	All	0.18	0/29789	0.44	1/40446 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	N	17	DG	C5-C6-O6	-8.01	116.29	128.30

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

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	454	0
2	B	8792	0	8823	415	0
3	C	2091	0	2049	83	0
4	E	1748	0	1765	53	0
5	F	679	0	701	27	0
6	H	1068	0	1040	42	0
7	I	971	0	929	33	0
8	J	532	0	543	37	0
9	K	919	0	929	38	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
All	All	29202	0	28747	1080	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 19.

The worst 5 of 1080 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:CE	1.65	1.10
2:B:1094:ARG:NH1	2:B:1098:MET:HE1	1.69	1.06
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
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 [i](#)

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

5.3.3 RNA [i](#)

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 [i](#)

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	18,23,24	2.14	4 (22%)	23,33,36	1.88	5 (21%)

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	-	3/7/21/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	T	18	WC7	C3-C4	7.15	1.46	1.38
12	T	18	WC7	C4-S3	-3.13	1.67	1.72
12	T	18	WC7	C5-S1	-2.68	1.59	1.67
12	T	18	WC7	C1-C2	2.25	1.40	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	18	WC7	C8-S3-C4	4.48	95.97	91.38
12	T	18	WC7	C5-C4-S3	4.45	130.10	123.13
12	T	18	WC7	C3-C4-S3	-3.74	109.00	111.42
12	T	18	WC7	C3-C4-C5	-3.21	120.90	124.02
12	T	18	WC7	C3'-C2'-C1'	2.04	107.60	102.60

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 [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	WC4	R	11	15,11	23,26,27	7.30	18 (78%)	31,37,40	1.57	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	15,11	-	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	-15.54	1.35	1.54
16	R	11	WC4	O06-C05	15.12	1.66	1.44
16	R	11	WC4	C25-C03	11.09	1.56	1.36
16	R	11	WC4	C18-C04	10.71	1.54	1.36
16	R	11	WC4	C23-C24	9.02	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	4.29	106.70	101.89
16	R	11	WC4	O02-C03-C25	-3.89	120.23	125.16
16	R	11	WC4	O02-C03-C04	3.68	119.49	115.84
16	R	11	WC4	C01-O02-C03	-2.57	113.74	117.51

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

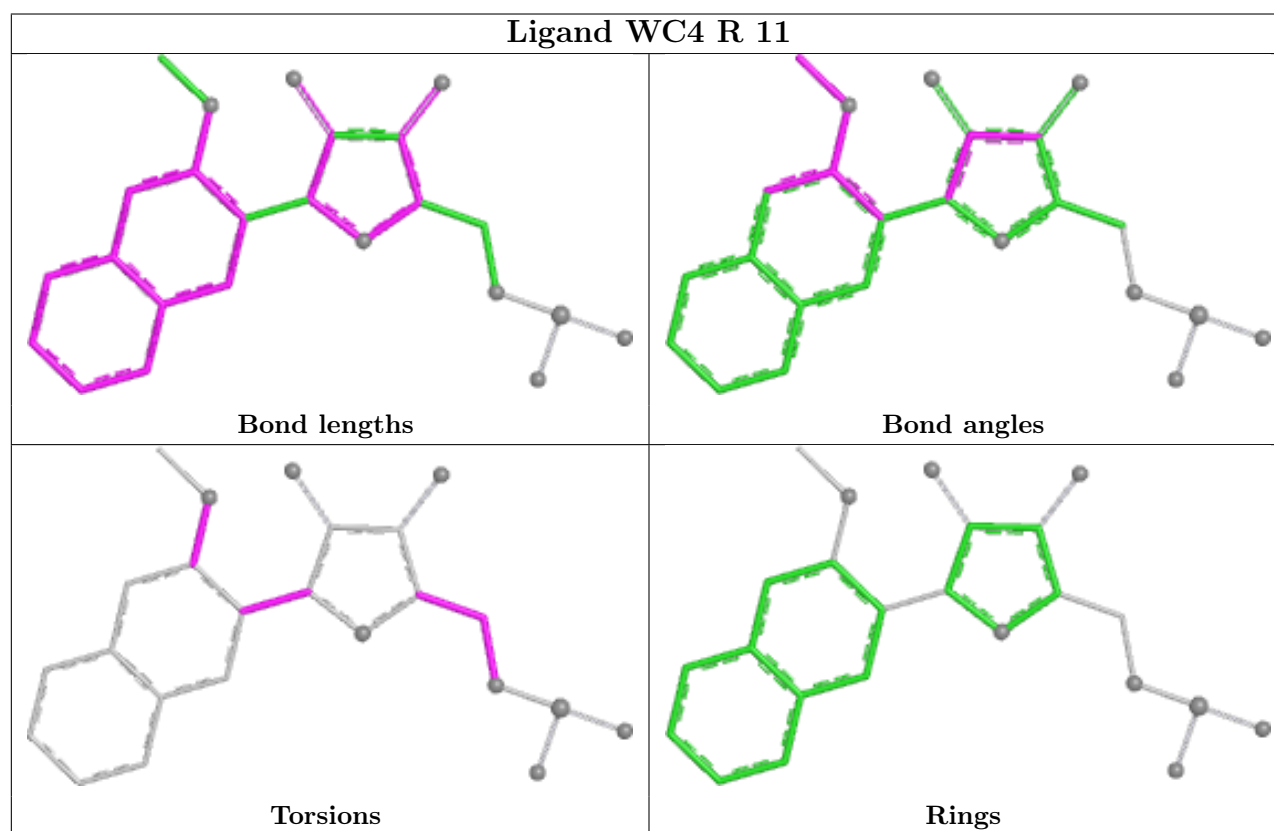
Mol	Chain	Res	Type	Atoms
16	R	11	WC4	C03-C04-C05-C16
16	R	11	WC4	C18-C04-C05-C16
16	R	11	WC4	O06-C07-C08-O5'
16	R	11	WC4	C14-C07-C08-O5'
16	R	11	WC4	C25-C03-O02-C01

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 [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	A	1390/1733 (80%)	0.50	62 (4%) 38 28	56, 105, 169, 216	0
2	B	1106/1224 (90%)	0.58	63 (5%) 29 24	65, 108, 158, 199	0
3	C	266/318 (83%)	0.41	10 (3%) 44 32	66, 105, 134, 156	0
4	E	214/215 (99%)	0.37	11 (5%) 33 26	68, 126, 185, 214	0
5	F	84/155 (54%)	0.29	3 (3%) 46 33	81, 107, 128, 139	0
6	H	133/146 (91%)	0.38	2 (1%) 72 50	95, 126, 164, 190	0
7	I	119/122 (97%)	0.35	2 (1%) 69 48	83, 117, 144, 172	0
8	J	65/70 (92%)	0.69	5 (7%) 19 18	74, 101, 130, 149	0
9	K	114/120 (95%)	0.28	2 (1%) 67 47	75, 107, 132, 142	0
10	L	46/70 (65%)	0.58	4 (8%) 16 17	90, 143, 170, 183	0
11	R	10/10 (100%)	1.23	1 (10%) 12 15	101, 121, 165, 172	0
12	T	27/29 (93%)	0.65	0 100 100	109, 164, 257, 265	0
13	N	15/16 (93%)	0.59	0 100 100	149, 224, 246, 252	0
All	All	3589/4228 (84%)	0.50	165 (4%) 37 28	56, 109, 167, 265	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1113	VAL	4.9
2	B	708	GLU	4.7
10	L	27	LEU	4.6
2	B	816	GLU	4.4
1	A	811	GLN	4.3

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	0.77	0.14	110,121,135,140	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

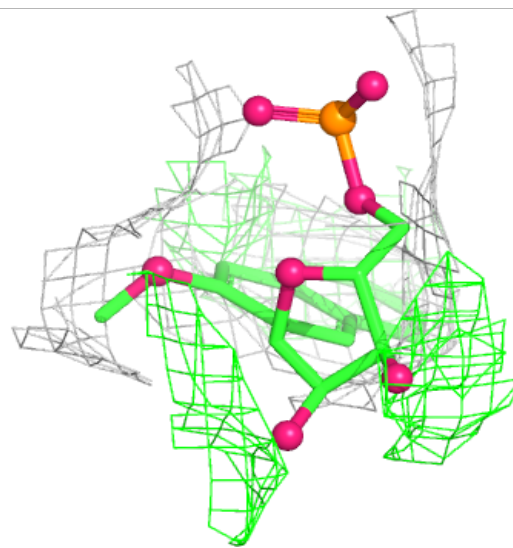
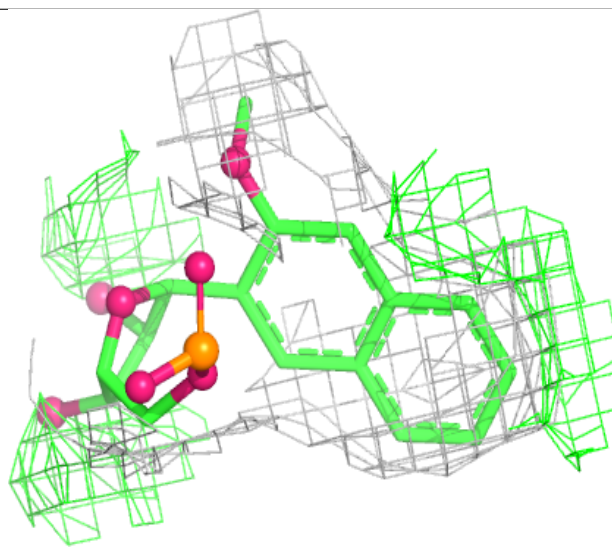
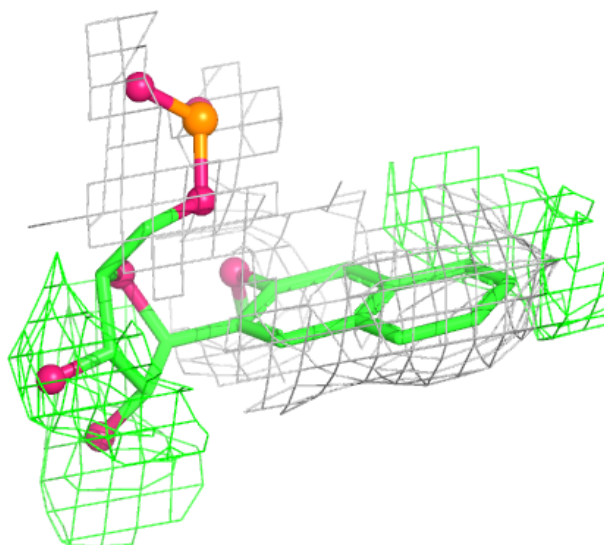
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	WC4	R	11	24/25	0.85	0.17	96,109,119,123	0
14	ZN	L	105	1/1	0.91	0.07	179,179,179,179	0
14	ZN	A	1734	1/1	0.93	0.09	206,206,206,206	0
14	ZN	B	1307	1/1	0.93	0.05	179,179,179,179	0
14	ZN	C	319	1/1	0.95	0.06	91,91,91,91	0
14	ZN	A	1735	1/1	0.97	0.04	134,134,134,134	0
14	ZN	J	101	1/1	0.98	0.06	107,107,107,107	0
14	ZN	I	203	1/1	0.98	0.04	98,98,98,98	0
14	ZN	I	204	1/1	0.98	0.04	131,131,131,131	0
15	MG	A	2001	1/1	0.99	0.03	88,88,88,88	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.