



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 05:12 AM BST

PDB ID : 5W51
Title : Pol II elongation complex with an N6-methyladenine-containing template and a matched UMPNPP
Authors : Wang, W.; Wang, D.
Deposited on : 2017-06-13
Resolution : 3.40 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 : 2.13.1
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) : 2.13.1

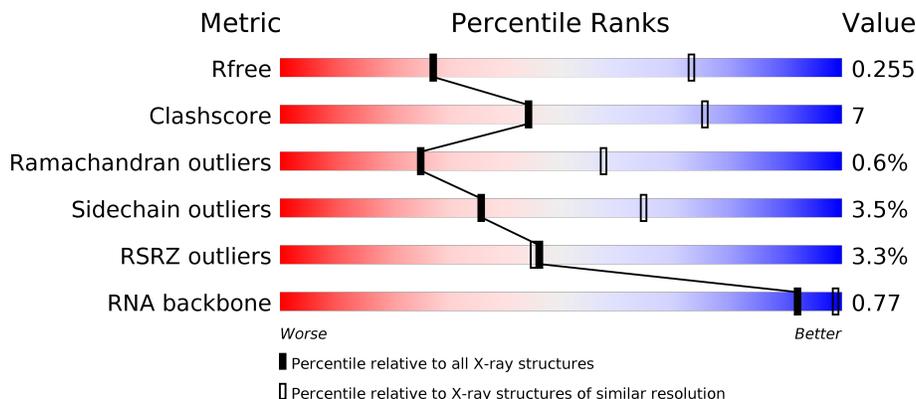
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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 on 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	 3% 63% 16% 11% 7%
2	B	1224	 % 69% 19% 11% 1%
3	C	318	 69% 14% 16% 1%
4	E	215	 11% 89% 8% 2%

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Mol	Chain	Length	Quality of chain
5	F	155	<p>%</p> <p>43% 11% 46%</p>
6	H	146	<p>12%</p> <p>72% 16% 11%</p>
7	I	122	<p>%</p> <p>80% 13% 6%</p>
8	J	70	<p>73% 17% 7%</p>
9	K	120	<p>%</p> <p>77% 18% 5%</p>
10	L	70	<p>4%</p> <p>46% 17% 37%</p>
11	T	29	<p>7%</p> <p>62% 31% 7%</p>
12	N	14	<p>14%</p> <p>71% 29%</p>
13	R	9	<p>44% 44% 11%</p>

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 28880 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
			Total	C	N	O	S			
1	A	1371	10787	6806	1886	2034	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1089	8657	5485	1517	1601	54	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	213	1744	1107	308	318	11	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	130	1043	660	173	206	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	115	935	575	170	180	10	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	44	351	217	70	60	4	0	0	0

- Molecule 11 is a DNA chain called 29mer template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	T	29	588	283	107	170	28	0	0	0

- Molecule 12 is a DNA chain called 14mer non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	N	14	284	137	49	85	13	0	0	0

- Molecule 13 is a RNA chain called 9mer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	R	9	198	89	42	59	8	0	0	0

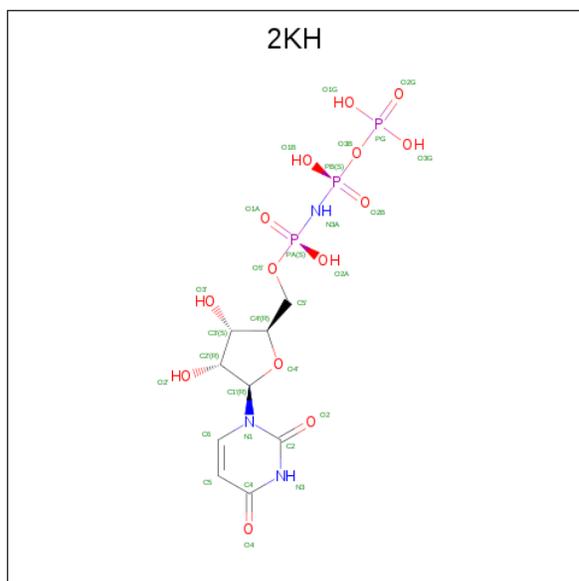
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	2	Total Mg 2 2	0	0

- Molecule 16 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonoxy)phosphoryl]amino}phosphoryl]uridine (three-letter code: 2KH) (formula: C₉H₁₆N₃O₁₄P₃).

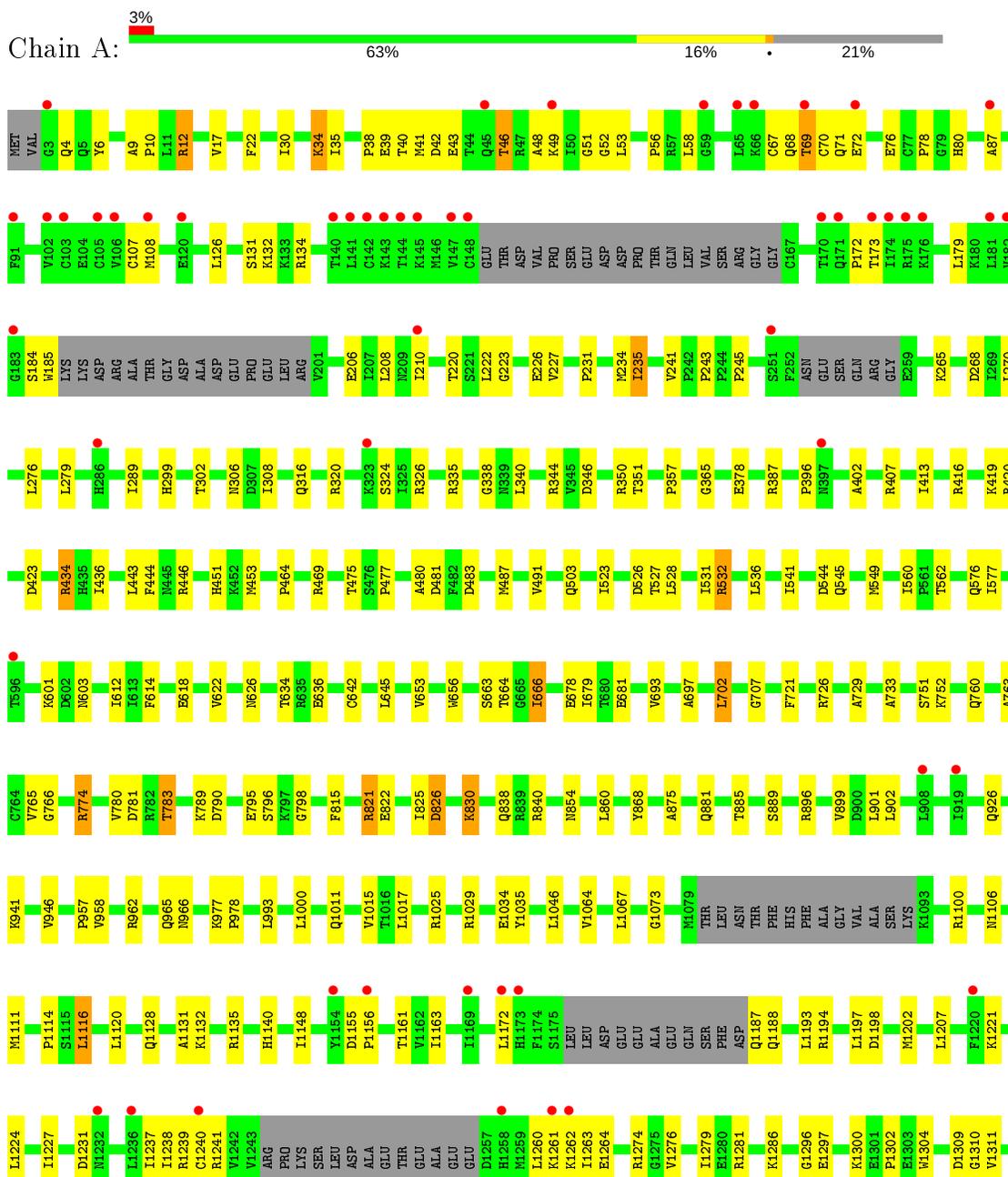


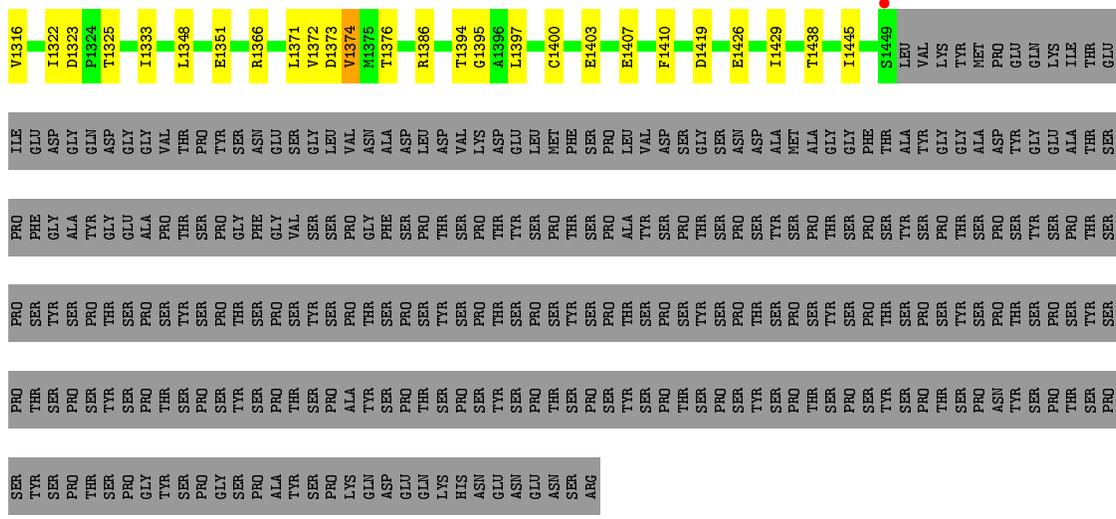
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total C N O P 58 18 6 28 6	0	1

3 Residue-property plots

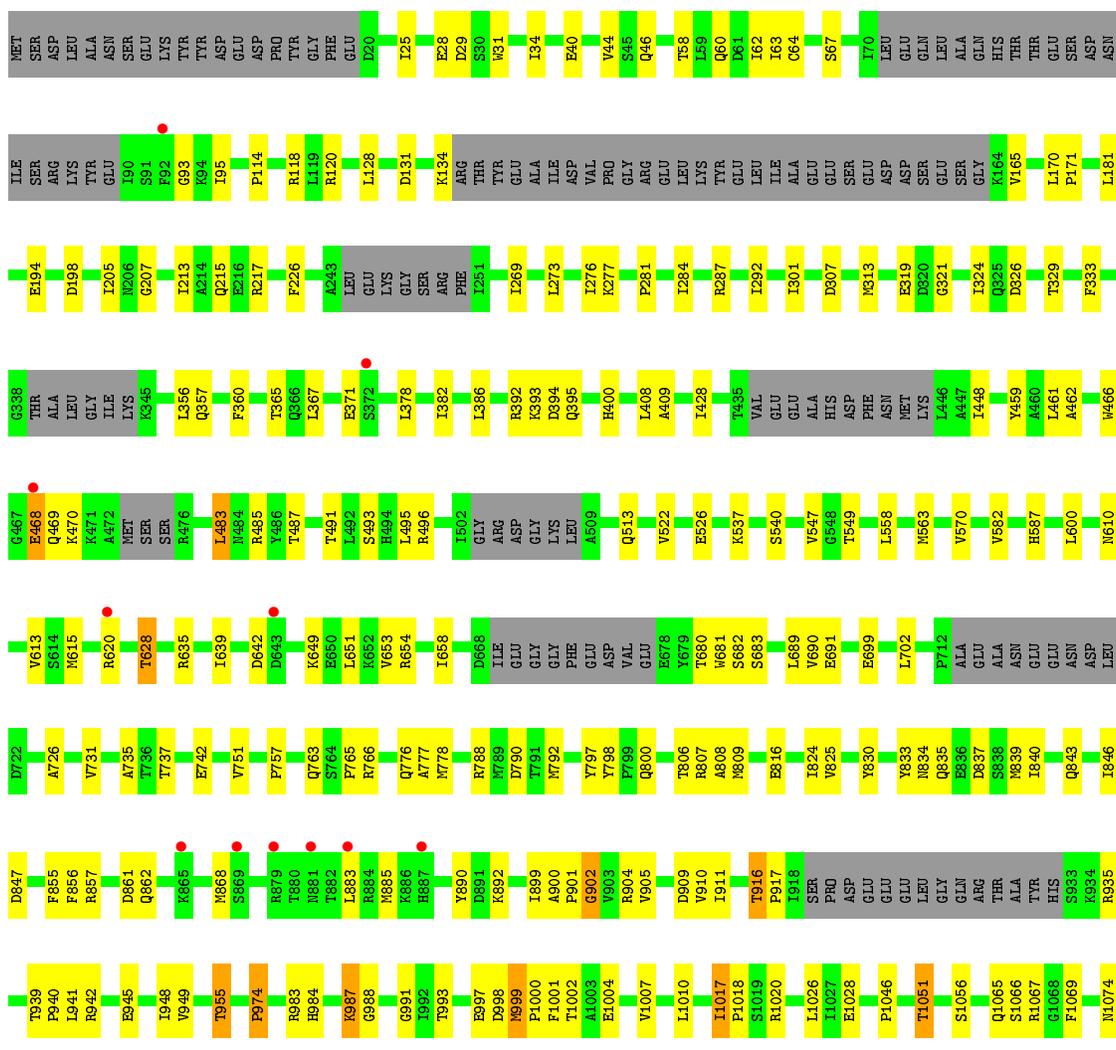
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

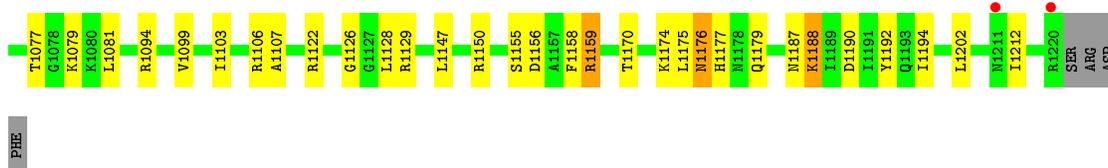
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1





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





PHE

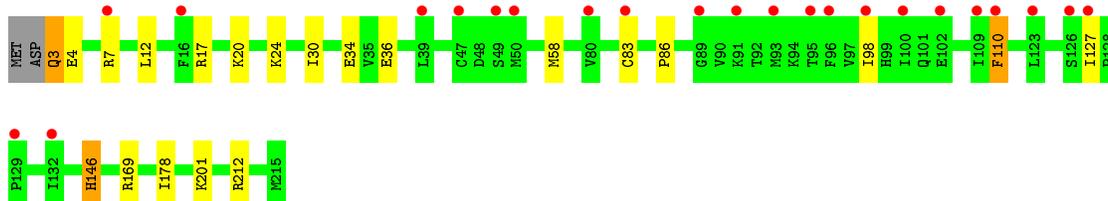
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:



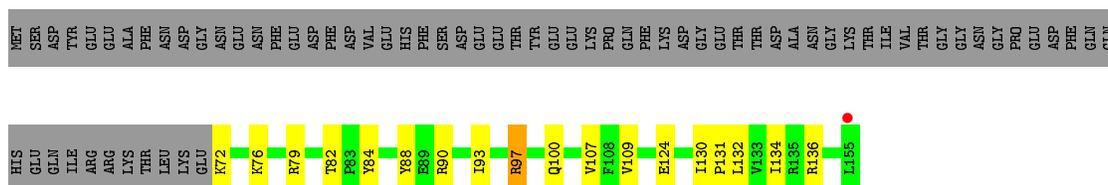
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



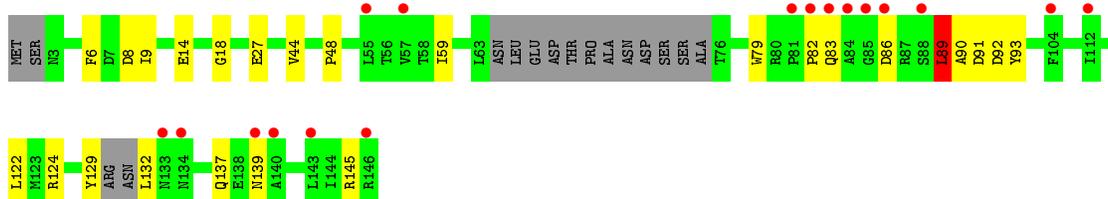
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

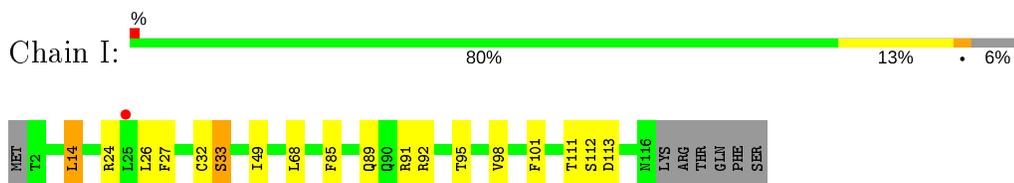


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

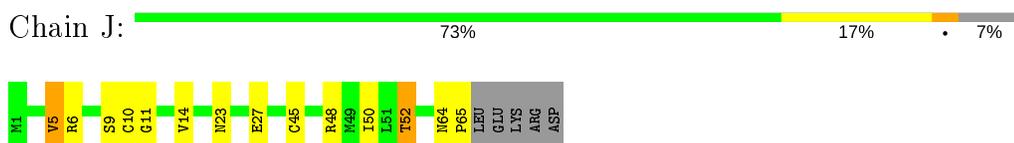
Chain H:



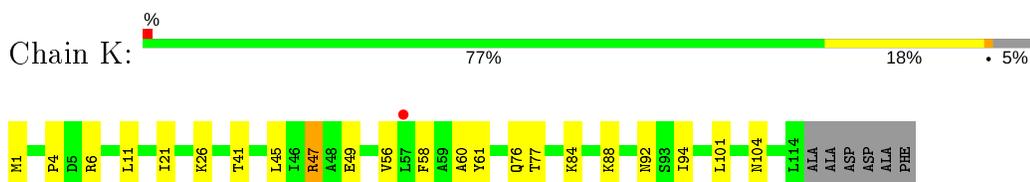
- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



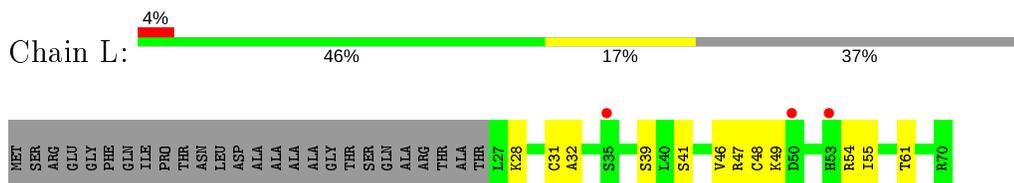
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



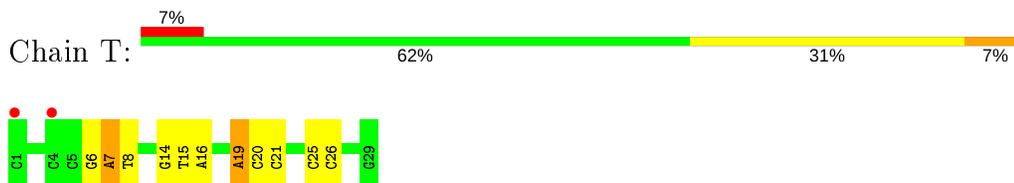
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



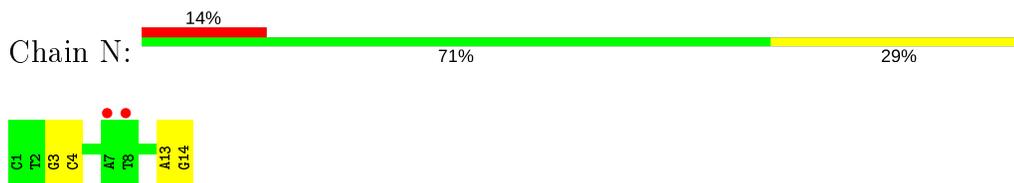
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 11: 29mer template DNA



- Molecule 12: 14mer non-template DNA



- Molecule 13: 9mer RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.70Å 224.00Å 193.06Å 90.00° 101.04° 90.00°	Depositor
Resolution (Å)	82.79 – 3.40 94.74 – 3.40	Depositor EDS
% Data completeness (in resolution range)	87.1 (82.79-3.40) 87.2 (94.74-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.41Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.227 , 0.254 0.229 , 0.255	Depositor DCC
R_{free} test set	4066 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtrriage
Anisotropy	0.015	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	28880	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, 2KH, MG, 6MA

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	0.21	0/10979	0.38	0/14843
2	B	0.21	0/8824	0.37	0/11898
3	C	0.21	0/2133	0.38	0/2891
4	E	0.21	0/1780	0.36	0/2395
5	F	0.21	0/691	0.38	0/933
6	H	0.21	0/1060	0.39	1/1434 (0.1%)
7	I	0.21	0/953	0.35	0/1284
8	J	0.21	0/541	0.36	0/727
9	K	0.22	0/937	0.35	0/1265
10	L	0.20	0/353	0.35	0/468
11	T	0.46	0/580	0.86	0/884
12	N	0.49	0/317	0.93	0/488
13	R	0.14	0/223	0.61	0/348
All	All	0.22	0/29371	0.40	1/39858 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	H	89	LEU	CA-CB-CG	5.38	127.67	115.30

There are no chirality outliers.

There are no planarity outliers.

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	10787	0	10872	164	0
2	B	8657	0	8693	144	0
3	C	2095	0	2051	29	0
4	E	1744	0	1772	10	0
5	F	679	0	701	11	0
6	H	1043	0	1015	14	0
7	I	935	0	887	11	0
8	J	532	0	542	9	0
9	K	919	0	929	16	0
10	L	351	0	375	7	0
11	T	588	0	333	8	0
12	N	284	0	161	2	0
13	R	198	0	99	5	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	2	0	0	0	0
16	A	58	0	32	3	0
All	All	28880	0	28462	376	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 7.

The worst 5 of 376 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)
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.29	0.78
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.67	0.76
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.69	0.73
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.72	0.72
1:A:42:ASP:HB3	1:A:46:THR:H	1.55	0.71

There are no symmetry-related clashes.

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	1357/1733 (78%)	1258 (93%)	95 (7%)	4 (0%)	41	72
2	B	1067/1224 (87%)	987 (92%)	71 (7%)	9 (1%)	19	51
3	C	264/318 (83%)	245 (93%)	18 (7%)	1 (0%)	34	67
4	E	211/215 (98%)	201 (95%)	9 (4%)	1 (0%)	29	61
5	F	82/155 (53%)	77 (94%)	5 (6%)	0	100	100
6	H	124/146 (85%)	113 (91%)	9 (7%)	2 (2%)	9	34
7	I	113/122 (93%)	101 (89%)	11 (10%)	1 (1%)	17	49
8	J	63/70 (90%)	58 (92%)	5 (8%)	0	100	100
9	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	17	49
10	L	42/70 (60%)	34 (81%)	7 (17%)	1 (2%)	6	28
All	All	3435/4173 (82%)	3181 (93%)	234 (7%)	20 (1%)	25	57

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
2	B	902	GLY
2	B	277	LYS
2	B	883	LEU
2	B	1046	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1198/1520 (79%)	1150 (96%)	48 (4%)	31	60
2	B	944/1061 (89%)	908 (96%)	36 (4%)	33	61
3	C	234/274 (85%)	227 (97%)	7 (3%)	41	68
4	E	195/197 (99%)	189 (97%)	6 (3%)	40	68
5	F	74/137 (54%)	72 (97%)	2 (3%)	44	70
6	H	114/128 (89%)	112 (98%)	2 (2%)	59	79
7	I	109/116 (94%)	107 (98%)	2 (2%)	59	79
8	J	60/65 (92%)	58 (97%)	2 (3%)	38	66
9	K	99/102 (97%)	97 (98%)	2 (2%)	55	77
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3066/3657 (84%)	2959 (96%)	107 (4%)	36	65

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	46	GLN
2	B	570	VAL
5	F	97	ARG
2	B	134	LYS
2	B	466	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	742	ASN
2	B	762	ASN
2	B	984	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	9	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

3 non-standard protein/DNA/RNA residues are 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
11	6MA	T	16	11	18,24,25	1.77	4 (22%)	15,34,37	1.42	2 (13%)
11	6MA	T	7	11,12	18,24,25	1.85	4 (22%)	15,34,37	1.30	2 (13%)
11	6MA	T	19	11	18,24,25	1.85	4 (22%)	15,34,37	1.19	1 (6%)

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
11	6MA	T	16	11	-	1/5/23/24	0/3/3/3
11	6MA	T	7	11,12	-	3/5/23/24	0/3/3/3
11	6MA	T	19	11	-	0/5/23/24	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	19	6MA	C6-N6	4.87	1.43	1.35
11	T	7	6MA	C6-N6	4.85	1.43	1.35
11	T	16	6MA	C6-N6	4.38	1.42	1.35
11	T	7	6MA	C1'-N9	-3.44	1.39	1.49
11	T	19	6MA	C1'-N9	-3.39	1.39	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	16	6MA	C1-N6-C6	-3.52	119.84	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	7	6MA	C2-N1-C6	3.22	119.35	116.59
11	T	19	6MA	C2-N1-C6	2.99	119.15	116.59
11	T	16	6MA	C2'-C3'-C4'	2.53	108.04	102.76
11	T	7	6MA	C1-N6-C6	2.09	124.67	122.87

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	7	6MA	C3'-C4'-C5'-O5'
11	T	7	6MA	O4'-C4'-C5'-O5'
11	T	16	6MA	C4'-C5'-O5'-P
11	T	7	6MA	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	7	6MA	2	0
11	T	19	6MA	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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	2KH	A	1805[B]	15	25,30,30	2.50	9 (36%)	30,47,47	1.93	8 (26%)
16	2KH	A	1805[A]	15	25,30,30	2.45	10 (40%)	30,47,47	1.96	7 (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
16	2KH	A	1805[B]	15	-	5/17/38/38	0/2/2/2
16	2KH	A	1805[A]	15	-	6/17/38/38	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	1805[A]	2KH	C4-N3	5.19	1.42	1.33
16	A	1805[B]	2KH	C4-N3	5.17	1.42	1.33
16	A	1805[A]	2KH	C6-N1	4.54	1.41	1.35
16	A	1805[B]	2KH	PB-O2B	4.48	1.53	1.46
16	A	1805[B]	2KH	C6-N1	4.48	1.41	1.35

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	1805[A]	2KH	O1G-PG-O3B	5.55	123.24	104.64
16	A	1805[B]	2KH	O1G-PG-O3B	5.51	123.10	104.64
16	A	1805[B]	2KH	O3B-PB-N3A	3.82	117.20	106.59
16	A	1805[B]	2KH	O3G-PG-O2G	-3.71	96.14	110.68
16	A	1805[A]	2KH	O3B-PB-N3A	3.65	116.72	106.59

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

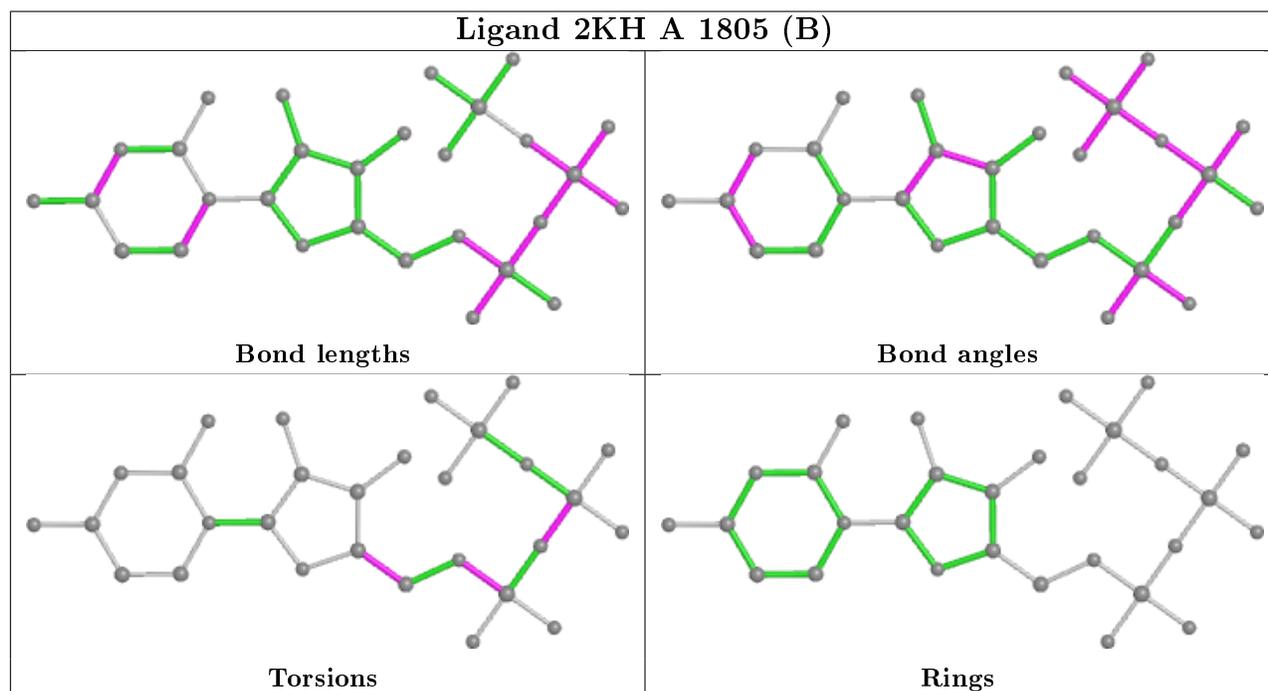
Mol	Chain	Res	Type	Atoms
16	A	1805[A]	2KH	C5'-O5'-PA-O1A
16	A	1805[A]	2KH	C5'-O5'-PA-O2A
16	A	1805[A]	2KH	C4'-C5'-O5'-PA
16	A	1805[A]	2KH	PB-O3B-PG-O1G
16	A	1805[B]	2KH	C5'-O5'-PA-O2A

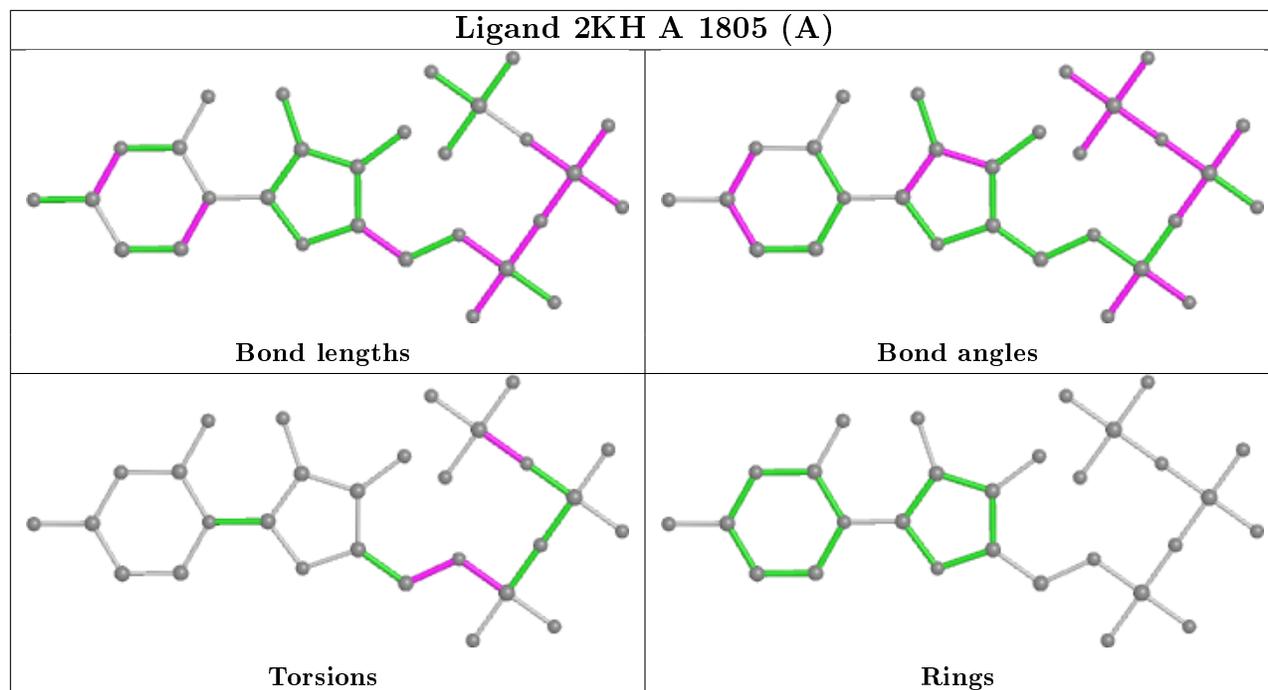
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	1805[B]	2KH	1	0
16	A	1805[A]	2KH	2	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	1371/1733 (79%)	0.23	54 (3%) 39 38	13, 68, 150, 221	0
2	B	1089/1224 (88%)	0.06	13 (1%) 79 77	13, 48, 115, 201	0
3	C	266/318 (83%)	0.04	1 (0%) 92 92	21, 50, 93, 148	0
4	E	213/215 (99%)	0.66	23 (10%) 5 7	44, 95, 174, 201	0
5	F	84/155 (54%)	0.06	1 (1%) 79 77	38, 66, 115, 154	0
6	H	130/146 (89%)	1.03	17 (13%) 3 4	41, 88, 155, 215	0
7	I	115/122 (94%)	0.24	1 (0%) 84 83	35, 70, 119, 149	0
8	J	65/70 (92%)	-0.17	0 100 100	17, 40, 78, 138	0
9	K	114/120 (95%)	0.01	1 (0%) 84 83	16, 50, 91, 105	0
10	L	44/70 (62%)	0.94	3 (6%) 17 19	37, 119, 176, 195	0
11	T	26/29 (89%)	0.85	2 (7%) 13 15	45, 185, 246, 273	0
12	N	14/14 (100%)	1.19	2 (14%) 2 3	157, 216, 265, 267	0
13	R	9/9 (100%)	0.13	0 100 100	30, 43, 91, 92	0
All	All	3540/4225 (83%)	0.22	118 (3%) 46 45	13, 62, 145, 273	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	84	ALA	7.7
1	A	105	CYS	6.2
2	B	643	ASP	5.1
10	L	50	ASP	5.1
6	H	83	GLN	5.0

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
11	6MA	T	7	22/23	0.76	0.24	227,229,235,237	0
11	6MA	T	16	22/23	0.79	0.24	138,145,158,168	0
11	6MA	T	19	22/23	0.93	0.23	63,79,96,101	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

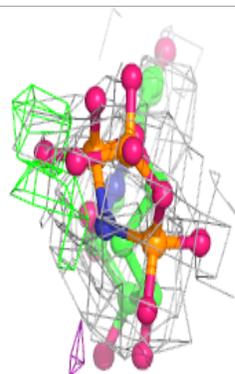
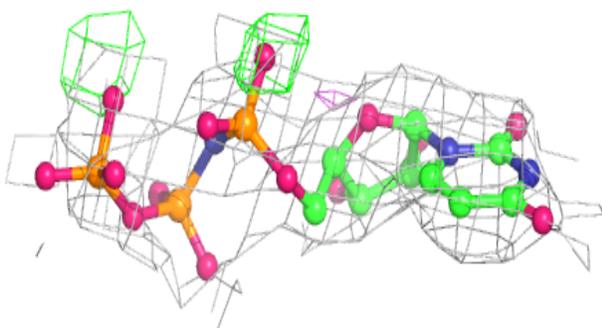
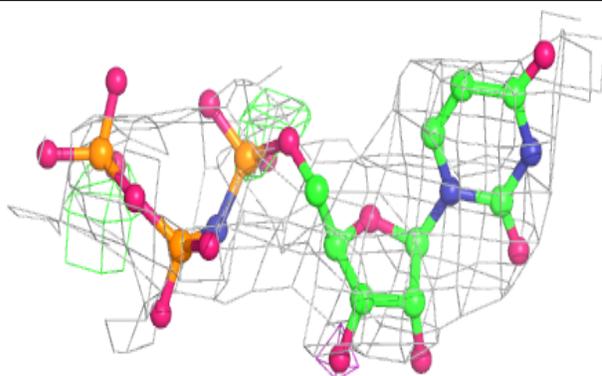
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	2KH	A	1805[A]	29/29	0.84	0.32	79,110,128,143	29
16	2KH	A	1805[B]	29/29	0.84	0.32	113,115,127,136	29
14	ZN	L	101	1/1	0.91	0.07	120,120,120,120	0
14	ZN	A	1801	1/1	0.92	0.08	150,150,150,150	0
15	MG	A	1804	1/1	0.93	0.15	31,31,31,31	0
14	ZN	B	1301	1/1	0.94	0.10	83,83,83,83	0
14	ZN	A	1802	1/1	0.96	0.15	77,77,77,77	0
15	MG	A	1803	1/1	0.97	0.19	11,11,11,11	0
14	ZN	I	202	1/1	0.97	0.13	53,53,53,53	0
14	ZN	J	101	1/1	0.97	0.13	33,33,33,33	0
14	ZN	I	201	1/1	0.98	0.12	71,71,71,71	0
14	ZN	C	401	1/1	0.99	0.18	51,51,51,51	0

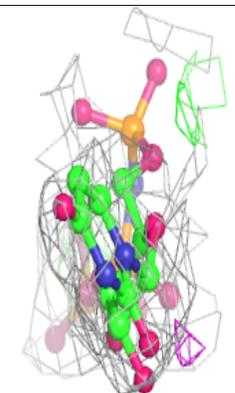
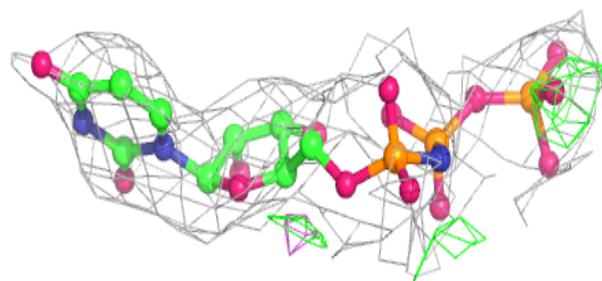
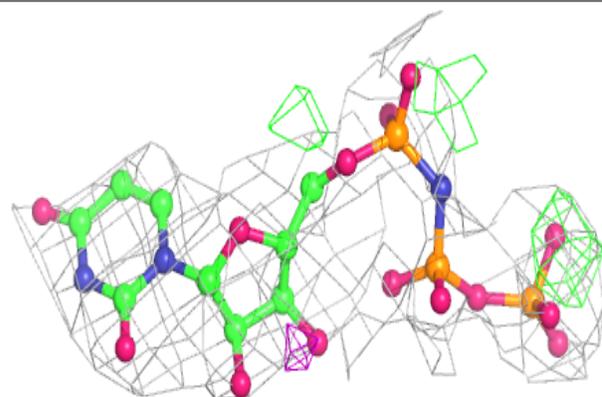
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2KH A 1805 (A):

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

**Electron density around 2KH A 1805 (B):**

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



6.5 Other polymers

There are no such residues in this entry.