



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2020 – 02:35 am BST

PDB ID : 6GYR  
Title : Transcription factor dimerization activates the p300 acetyltransferase  
Authors : Panne, D.; Ortega, E.  
Deposited on : 2018-07-01  
Resolution : 3.10 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](mailto: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.

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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	:	2.11
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)	:	2.11

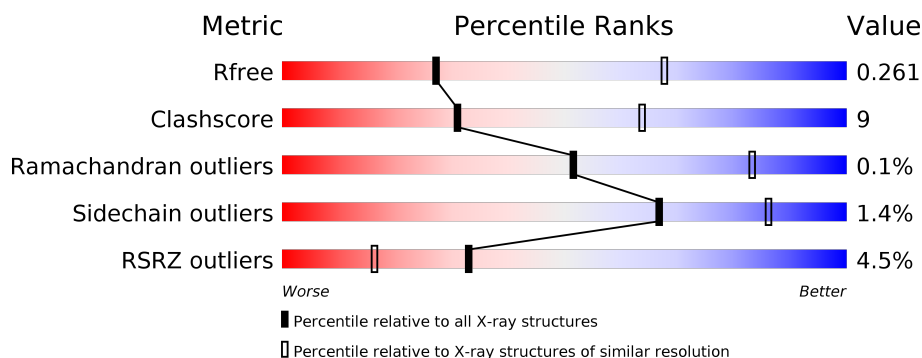
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	588	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
1	B	588	<div> <div>3%</div> <div>77%</div> <div>22%</div> <div>••</div> </div>
1	C	588	<div> <div>5%</div> <div>70%</div> <div>27%</div> <div>••</div> </div>
1	D	588	<div> <div>6%</div> <div>78%</div> <div>21%</div> <div>••</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	1705	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 38191 atoms, of which 18821 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 Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	588	Total	C	H	N	O	S	0	0	0
			9514	3063	4699	824	894	34			
1	B	583	Total	C	H	N	O	S	0	0	0
			9440	3042	4660	816	888	34			
1	C	575	Total	C	H	N	O	S	0	0	0
			9323	3007	4601	804	878	33			
1	D	584	Total	C	H	N	O	S	0	0	0
			9448	3045	4665	815	889	34			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1045	ALA	-	expression tag	UNP Q09472
A	1467	PHE	TYR	engineered mutation	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472
A	?	-	GLU	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	THR	deletion	UNP Q09472
A	?	-	ASP	deletion	UNP Q09472
A	?	-	VAL	deletion	UNP Q09472
A	?	-	THR	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	GLY	deletion	UNP Q09472
A	?	-	ASP	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472
A	?	-	ALA	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	THR	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	LEU	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	ARG	deletion	UNP Q09472
B	1045	ALA	-	expression tag	UNP Q09472
B	1467	PHE	TYR	engineered mutation	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	GLU	deletion	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	THR	deletion	UNP Q09472
B	?	-	ASP	deletion	UNP Q09472
B	?	-	VAL	deletion	UNP Q09472
B	?	-	THR	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	GLY	deletion	UNP Q09472
B	?	-	ASP	deletion	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	ALA	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	THR	deletion	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	LEU	deletion	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	ARG	deletion	UNP Q09472
C	1045	ALA	-	expression tag	UNP Q09472
C	1467	PHE	TYR	engineered mutation	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	GLU	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	THR	deletion	UNP Q09472
C	?	-	ASP	deletion	UNP Q09472
C	?	-	VAL	deletion	UNP Q09472
C	?	-	THR	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	GLY	deletion	UNP Q09472
C	?	-	ASP	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	ALA	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	THR	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	LEU	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	ARG	deletion	UNP Q09472
D	1045	ALA	-	expression tag	UNP Q09472
D	1467	PHE	TYR	engineered mutation	UNP Q09472
D	?	-	SER	deletion	UNP Q09472

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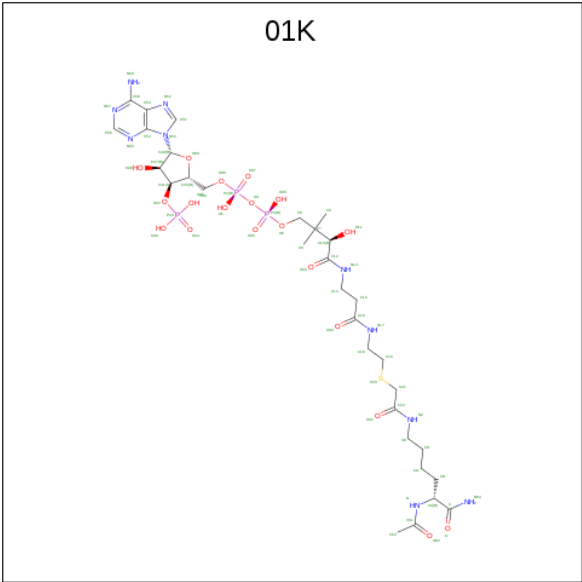
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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASN	deletion	UNP Q09472
D	?	-	GLU	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	THR	deletion	UNP Q09472
D	?	-	ASP	deletion	UNP Q09472
D	?	-	VAL	deletion	UNP Q09472
D	?	-	THR	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	GLY	deletion	UNP Q09472
D	?	-	ASP	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	ALA	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	THR	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	LEU	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	ARG	deletion	UNP Q09472

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Zn 4 4	0	0
2	A	4	Total Zn 4 4	0	0
2	D	3	Total Zn 3 3	0	0
2	C	3	Total Zn 3 3	0	0

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonooxy)tetrahydrofuran-2-yl]methyl (3R,20R)-20-carbamoyl-3-hydroxy-2,2-dimethyl-4,8,14,22-tetraoxo-12-thia-5,9,15,21-tetraazatricos-1-yl dihydrogen diphosphate (three-letter code: 01K) (formula: C<sub>31</sub>H<sub>53</sub>N<sub>10</sub>O<sub>19</sub>P<sub>3</sub>S).



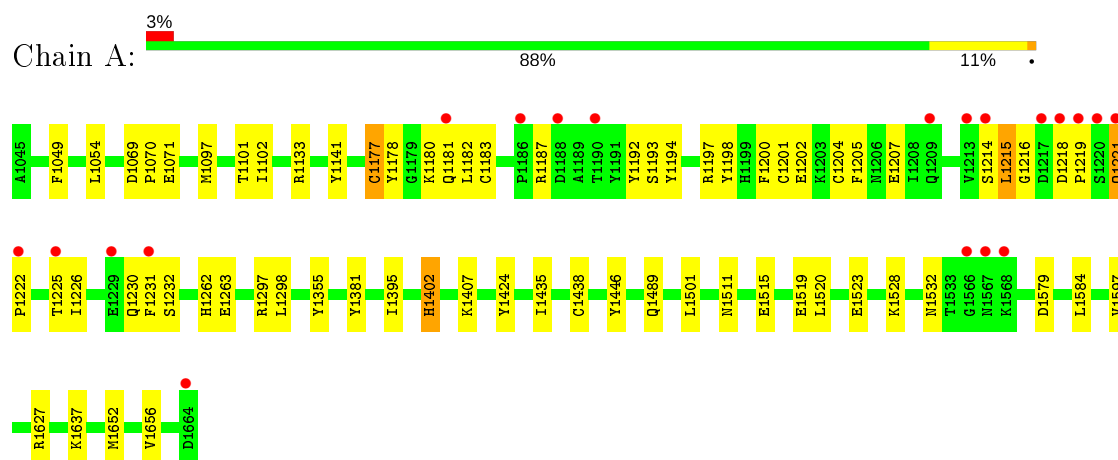
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			113	31	49	10	19	3	1		
3	B	1	Total	C	H	N	O	P	S	0	0
			113	31	49	10	19	3	1		
3	C	1	Total	C	H	N	O	P	S	0	0
			113	31	49	10	19	3	1		
3	D	1	Total	C	H	N	O	P	S	0	0
			113	31	49	10	19	3	1		



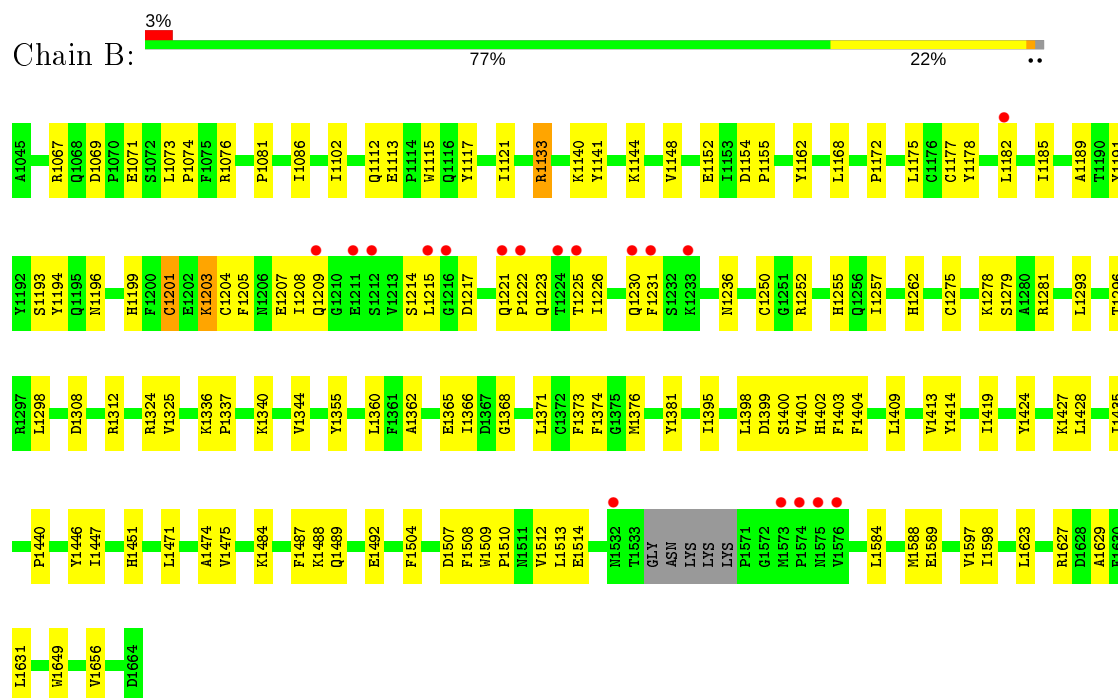
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

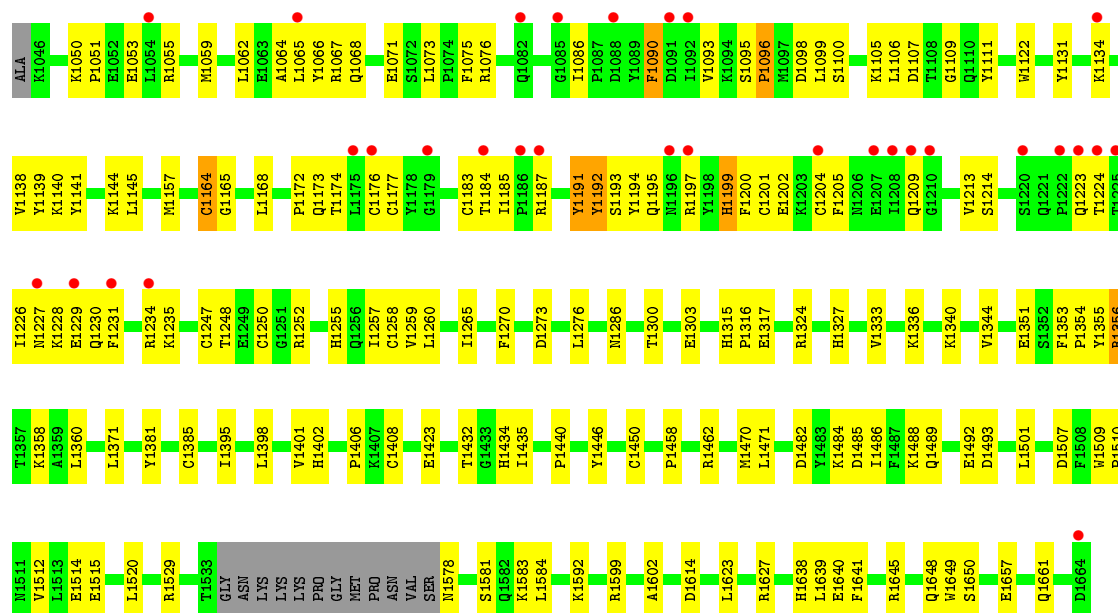
- Molecule 1: Histone acetyltransferase p300



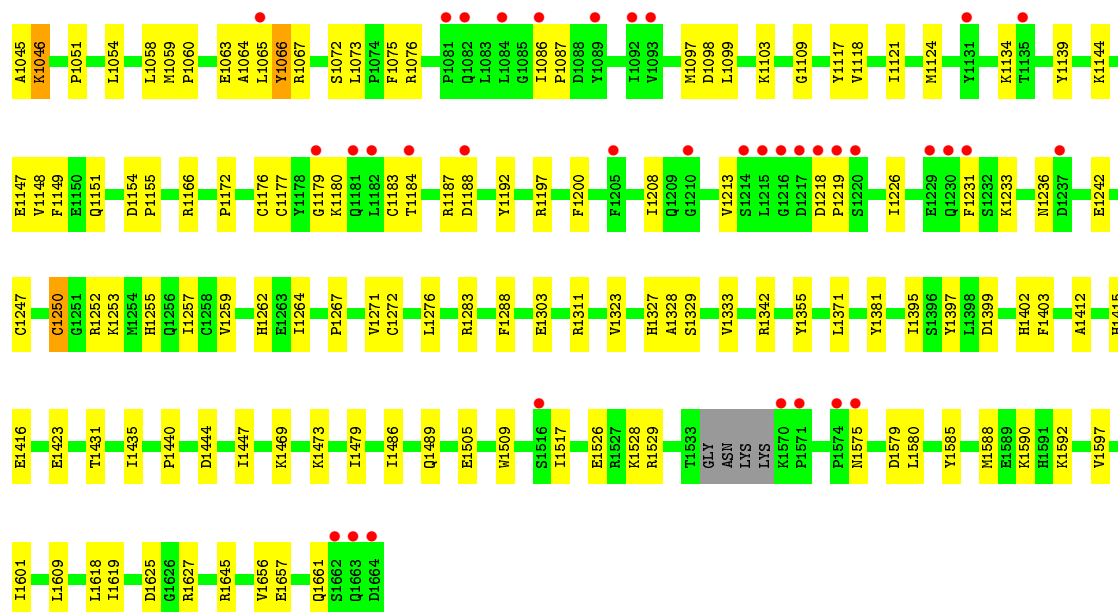
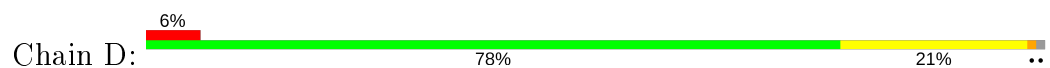
- Molecule 1: Histone acetyltransferase p300



- Molecule 1: Histone acetyltransferase p300



• Molecule 1: Histone acetyltransferase p300



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.83Å 146.72Å 116.48Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 75.07 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.10) 99.0 (75.07-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.209 , 0.265 0.207 , 0.261	Depositor DCC
$R_{free}$ test set	2967 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.4	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 63.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	38191	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 01K

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	0.38	0/4941	0.50	1/6679 (0.0%)
1	B	0.44	2/4906 (0.0%)	0.55	0/6633
1	C	0.50	2/4846 (0.0%)	0.57	1/6552 (0.0%)
1	D	0.39	2/4909 (0.0%)	0.52	1/6638 (0.0%)
All	All	0.43	6/19602 (0.0%)	0.54	3/26502 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1528	LYS	CB-CG	-7.37	1.32	1.52
1	B	1201	CYS	CB-SG	-6.95	1.70	1.82
1	B	1203	LYS	CB-CG	-6.47	1.35	1.52
1	C	1164	CYS	CB-SG	-6.01	1.72	1.82
1	C	1122	TRP	CE3-CZ3	-5.84	1.28	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1528	LYS	CG-CD-CE	-6.87	91.29	111.90
1	A	1215	LEU	CA-CB-CG	-5.37	102.95	115.30
1	C	1164	CYS	CA-CB-SG	-5.13	104.77	114.00

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	4815	4699	4696	50	0
1	B	4780	4660	4660	91	3
1	C	4722	4601	4601	123	4
1	D	4783	4665	4663	84	0
2	A	4	0	0	0	2
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	64	49	48	1	0
3	B	64	49	49	6	0
3	C	64	49	49	1	0
3	D	64	49	48	2	0
All	All	19370	18821	18814	346	5

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 9.

The worst 5 of 346 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:B:1201:CYS:SG	1:B:1204:CYS:HB2	2.01	1.00
1:C:1599:ARG:HD3	1:C:1602:ALA:HB2	1.49	0.95
1:C:1172:PRO:HB2	1:C:1187:ARG:HD2	1.49	0.92
1:D:1097:MET:HG3	1:D:1124:MET:HB2	1.53	0.90
1:C:1164:CYS:SG	1:C:1255:HIS:ND1	2.45	0.90

All (5) 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)
1:C:1315:HIS:HE2	2:A:1705:ZN:ZN[1_455]	1.14	0.46
1:C:1408:CYS:HG	2:A:1705:ZN:ZN[1_455]	1.25	0.35
1:B:1203:LYS:NZ	1:C:1194:TYR:OH[1_556]	1.98	0.22
1:B:1112:GLN:HE22	1:B:1492:GLU:OE1[2_546]	1.51	0.09
1:B:1203:LYS:HZ3	1:C:1194:TYR:OH[1_556]	1.58	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	
1	A	584/588 (99%)	568 (97%)	16 (3%)	0	100	100
1	B	579/588 (98%)	547 (94%)	32 (6%)	0	100	100
1	C	571/588 (97%)	536 (94%)	34 (6%)	1 (0%)	47	79
1	D	580/588 (99%)	535 (92%)	44 (8%)	1 (0%)	47	79
All	All	2314/2352 (98%)	2186 (94%)	126 (5%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1096	PRO
1	D	1046	LYS

### 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	536/537 (100%)	529 (99%)	7 (1%)	69	87
1	B	533/537 (99%)	527 (99%)	6 (1%)	73	89
1	C	526/537 (98%)	516 (98%)	10 (2%)	57	81
1	D	533/537 (99%)	526 (99%)	7 (1%)	69	87
All	All	2128/2148 (99%)	2098 (99%)	30 (1%)	67	86

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1065	LEU
1	C	1191	TYR
1	D	1272	CYS
1	C	1090	PHE
1	C	1192	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 14 are monoatomic - leaving 4 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	$\# Z  > 2$
3	01K	D	1704	-	58,66,66	2.08	12 (20%)	71,95,95	3.13	24 (33%)
3	01K	C	1704	-	58,66,66	1.45	9 (15%)	71,95,95	3.64	24 (33%)
3	01K	B	1704	-	58,66,66	1.50	8 (13%)	71,95,95	3.73	26 (36%)
3	01K	A	1704	-	58,66,66	2.95	12 (20%)	71,95,95	3.29	25 (35%)

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
3	01K	D	1704	-	-	15/64/84/84	0/3/3/3
3	01K	C	1704	-	-	9/64/84/84	0/3/3/3
3	01K	B	1704	-	-	10/64/84/84	0/3/3/3
3	01K	A	1704	-	-	15/64/84/84	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1704	01K	C47-C49	-14.24	1.32	1.53
3	A	1704	01K	O60-C49	9.50	1.54	1.41
3	A	1704	01K	C47-C41	9.08	1.73	1.52
3	D	1704	01K	P43-O42	6.00	1.70	1.59
3	D	1704	01K	O60-C49	5.51	1.48	1.41

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1704	01K	O60-C49-C47	-23.17	73.06	106.93
3	C	1704	01K	O60-C49-C47	-22.14	74.58	106.93
3	A	1704	01K	C49-N50-C54	16.94	156.41	126.64
3	D	1704	01K	C49-N50-C54	13.01	149.49	126.64
3	A	1704	01K	C39-C40-C41	-9.88	81.66	114.40

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1704	01K	C6-O5-P4-O35
3	A	1704	01K	O-C-CA-CB
3	A	1704	01K	N64-C-CA-CB
3	A	1704	01K	O38-C39-C40-C41
3	A	1704	01K	C41-O42-P43-O44

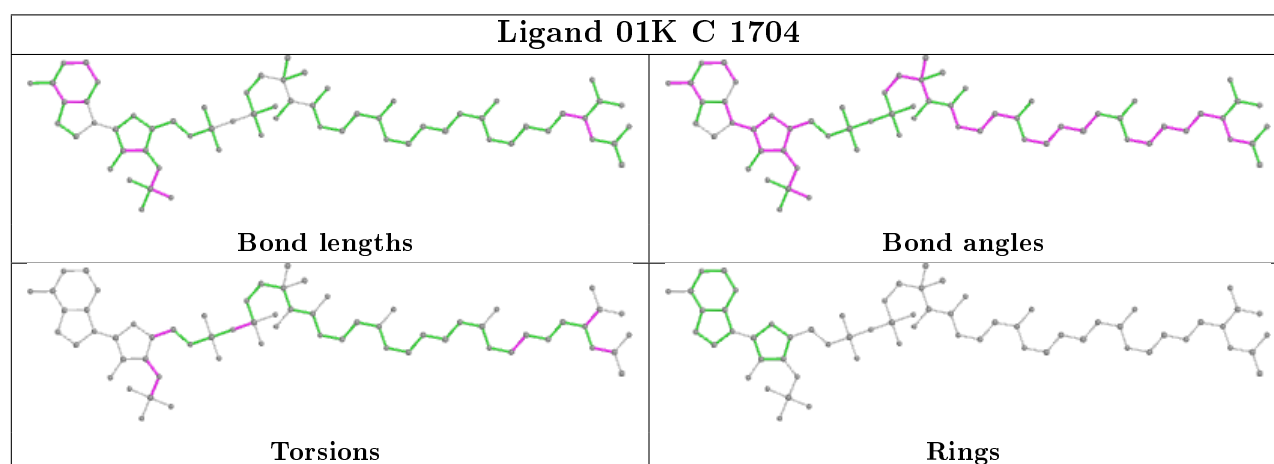
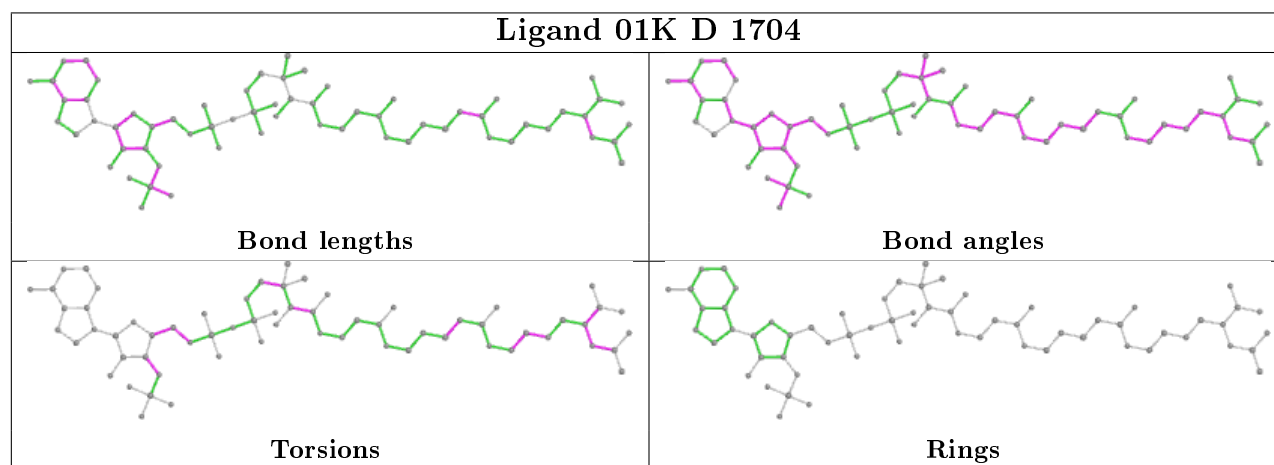
There are no ring outliers.

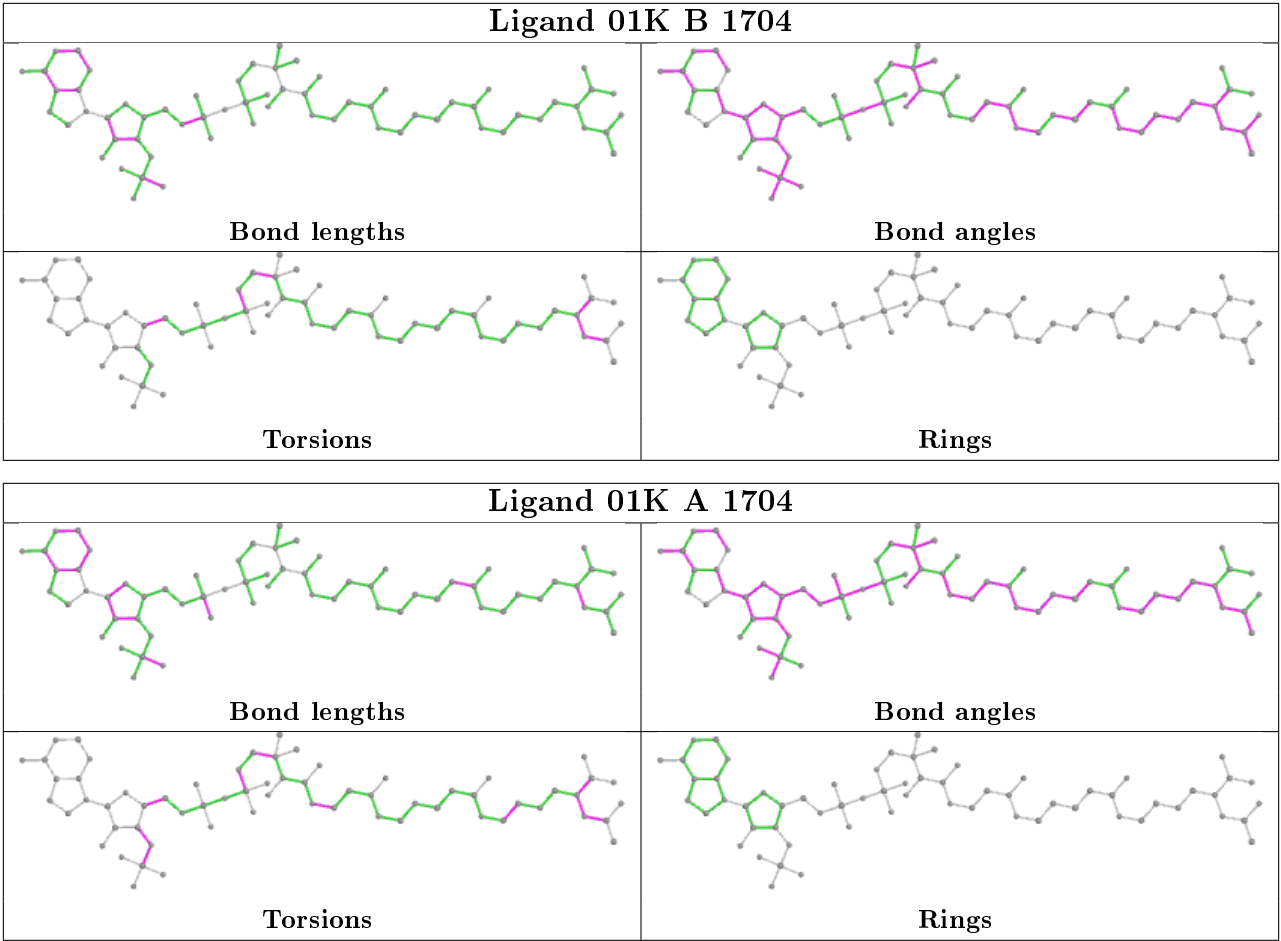
4 monomers are involved in 10 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1704	01K	2	0
3	C	1704	01K	1	0
3	B	1704	01K	6	0
3	A	1704	01K	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1533:THR	C	1566:GLY	N	39.28

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	588/588 (100%)	0.11	20 (3%)	45	24	35, 62, 174, 217	0
1	B	583/588 (99%)	0.08	18 (3%)	49	26	32, 70, 182, 211	0
1	C	575/588 (97%)	0.22	31 (5%)	25	12	42, 104, 188, 249	0
1	D	584/588 (99%)	0.17	36 (6%)	20	9	42, 96, 172, 228	0
All	All	2330/2352 (99%)	0.14	105 (4%)	33	16	32, 78, 180, 249	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1220	SER	8.5
1	A	1221	GLN	8.1
1	B	1231	PHE	7.3
1	D	1219	PRO	6.0
1	A	1218	ASP	5.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

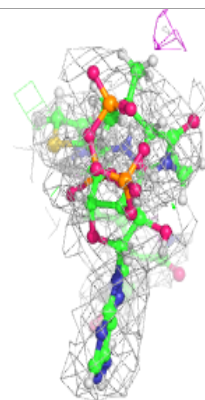
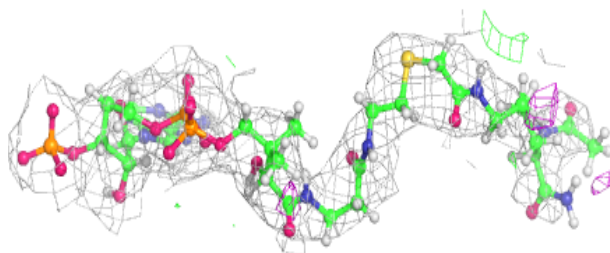
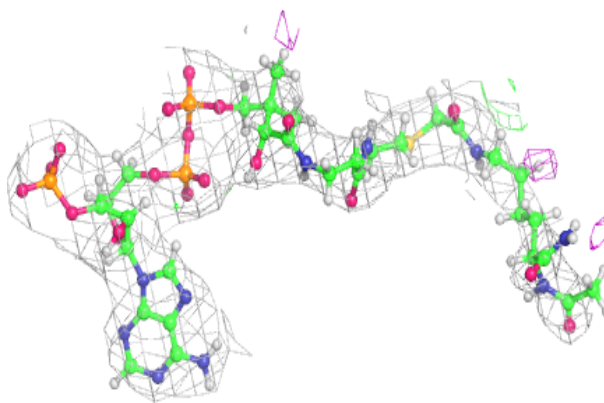
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	1703	1/1	0.48	0.07	205,205,205,205	0
2	ZN	B	1703	1/1	0.68	0.06	215,215,215,215	0
2	ZN	C	1702	1/1	0.68	0.11	166,166,166,166	0
2	ZN	D	1703	1/1	0.73	0.07	216,216,216,216	0
2	ZN	C	1701	1/1	0.93	0.13	88,88,88,88	0
3	01K	D	1704	64/64	0.93	0.29	38,69,95,108	0
3	01K	C	1704	64/64	0.94	0.25	44,73,108,127	0
2	ZN	A	1703	1/1	0.95	0.11	153,153,153,153	0
3	01K	B	1704	64/64	0.95	0.23	36,59,89,108	0
3	01K	A	1704	64/64	0.96	0.24	33,54,74,76	0
2	ZN	B	1705	1/1	0.97	0.23	92,92,92,92	0
2	ZN	A	1705	1/1	0.97	0.19	78,78,78,78	0
2	ZN	A	1702	1/1	0.98	0.21	78,78,78,78	0
2	ZN	D	1702	1/1	0.98	0.16	125,125,125,125	0
2	ZN	B	1702	1/1	0.99	0.19	83,83,83,83	0
2	ZN	B	1701	1/1	0.99	0.22	83,83,83,83	0
2	ZN	D	1701	1/1	0.99	0.17	89,89,89,89	0
2	ZN	A	1701	1/1	0.99	0.24	78,78,78,78	0

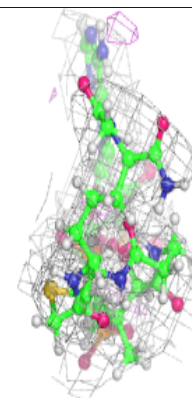
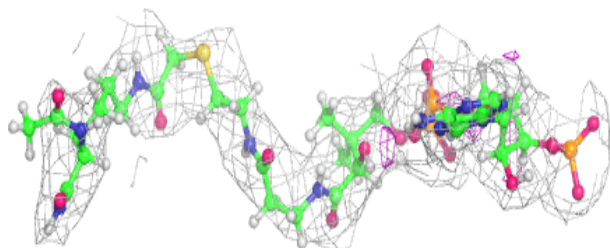
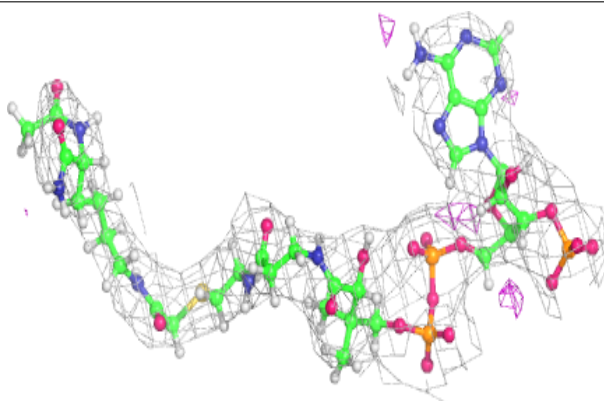
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 01K D 1704:**

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

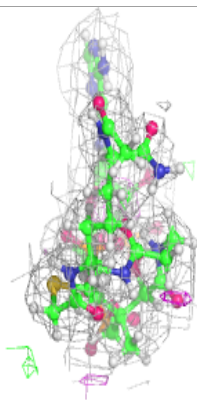
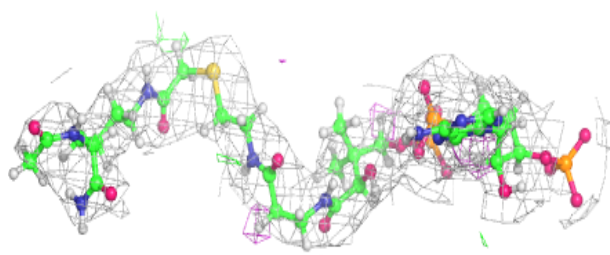
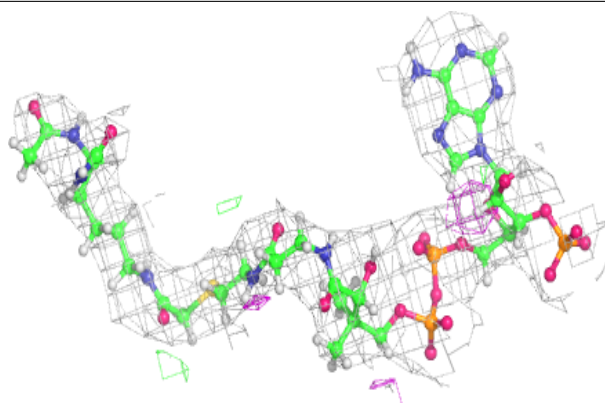
**Electron density around 01K C 1704:**

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

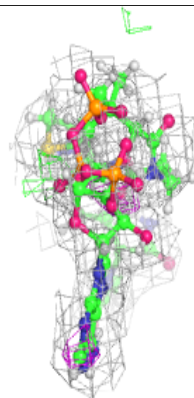
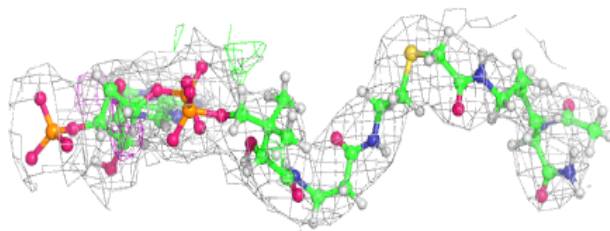
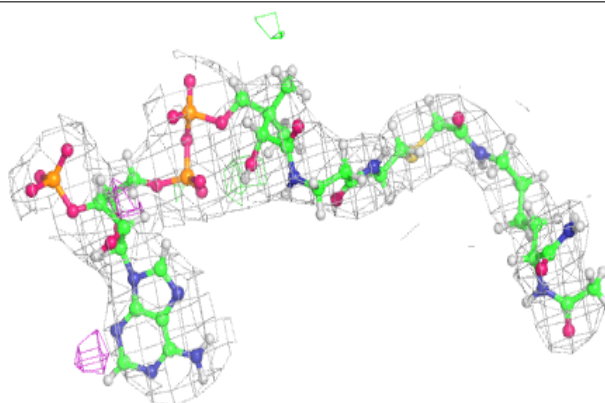


**Electron density around 01K B 1704:**

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

**Electron density around 01K A 1704:**

$2mF_o-DF_c$  (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.