



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:02 am BST

PDB ID : 3VD0  
Title : structure of p73 DNA binding domain tetramer modulates p73 transactivation  
Authors : Ethayathulla, A.S.; Tse, P.W.; Nguyen, S.; Viadiu, H.  
Deposited on : 2012-01-04  
Resolution : 2.95 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

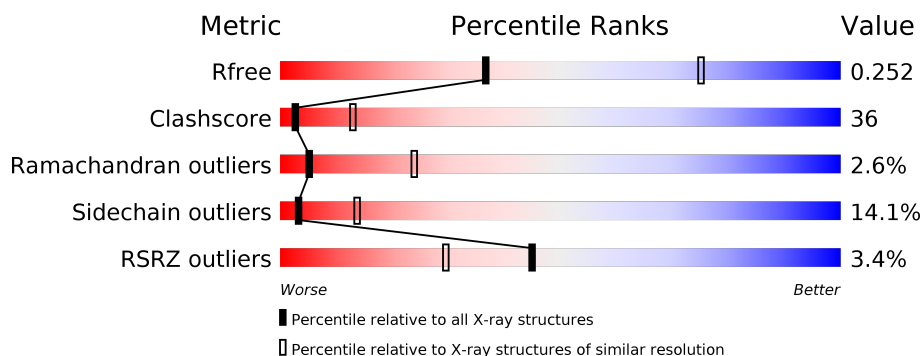
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	210	<div> <div>5%</div> <div>34% 48% 14%</div> </div>
1	B	210	<div> <div>3%</div> <div>35% 49% 11%</div> </div>
1	C	210	<div> <div>4%</div> <div>42% 49% 5%</div> </div>
1	D	210	<div> <div>2%</div> <div>40% 47% 9% 5%</div> </div>
1	I	210	<div> <div>2%</div> <div>45% 43% 7% 5%</div> </div>
1	J	210	<div> <div>6%</div> <div>31% 51% 11% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	210	<div><div></div><div>2%</div><div>44%</div><div>44%</div><div>9%</div><div></div></div>
1	L	210	<div><div></div><div>%</div><div>52%</div><div>40%</div><div></div><div></div></div>
2	E	12	<div><div></div><div>42%</div><div>50%</div><div>8%</div></div>
2	F	12	<div><div></div><div>8%</div><div>50%</div><div>33%</div><div>8%</div><div>8%</div></div>
2	G	12	<div><div></div><div>8%</div><div>42%</div><div>50%</div><div>8%</div></div>
2	H	12	<div><div></div><div>33%</div><div>50%</div><div>8%</div><div>8%</div></div>
2	M	12	<div><div></div><div>8%</div><div>8%</div><div>92%</div></div>
2	N	12	<div><div></div><div>25%</div><div>75%</div></div>
2	O	12	<div><div></div><div>42%</div><div>58%</div></div>
2	P	12	<div><div></div><div>33%</div><div>67%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14734 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 Tumor protein p73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1596	999	288	298	11			
1	B	201	Total	C	N	O	S	0	0	0
			1580	987	285	297	11			
1	C	202	Total	C	N	O	S	0	0	0
			1596	999	288	298	11			
1	D	200	Total	C	N	O	S	2	0	0
			1572	985	282	294	11			
1	I	199	Total	C	N	O	S	0	0	0
			1567	982	281	293	11			
1	J	199	Total	C	N	O	S	1	0	0
			1561	976	281	293	11			
1	K	206	Total	C	N	O	S	0	0	0
			1631	1020	298	302	11			
1	L	201	Total	C	N	O	S	1	0	0
			1586	993	285	297	11			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	INITIATING METHIONINE	UNP O15350
A	104	GLY	-	EXPRESSION TAG	UNP O15350
A	105	HIS	-	EXPRESSION TAG	UNP O15350
A	106	HIS	-	EXPRESSION TAG	UNP O15350
A	107	HIS	-	EXPRESSION TAG	UNP O15350
A	108	HIS	-	EXPRESSION TAG	UNP O15350
A	109	HIS	-	EXPRESSION TAG	UNP O15350
A	110	HIS	-	EXPRESSION TAG	UNP O15350
A	111	HIS	-	EXPRESSION TAG	UNP O15350
A	112	HIS	-	EXPRESSION TAG	UNP O15350
A	113	GLU	-	EXPRESSION TAG	UNP O15350
A	114	PHE	-	EXPRESSION TAG	UNP O15350
B	103	MET	-	INITIATING METHIONINE	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
B	104	GLY	-	EXPRESSION TAG	UNP 015350
B	105	HIS	-	EXPRESSION TAG	UNP 015350
B	106	HIS	-	EXPRESSION TAG	UNP 015350
B	107	HIS	-	EXPRESSION TAG	UNP 015350
B	108	HIS	-	EXPRESSION TAG	UNP 015350
B	109	HIS	-	EXPRESSION TAG	UNP 015350
B	110	HIS	-	EXPRESSION TAG	UNP 015350
B	111	HIS	-	EXPRESSION TAG	UNP 015350
B	112	HIS	-	EXPRESSION TAG	UNP 015350
B	113	GLU	-	EXPRESSION TAG	UNP 015350
B	114	PHE	-	EXPRESSION TAG	UNP 015350
C	103	MET	-	INITIATING METHIONINE	UNP 015350
C	104	GLY	-	EXPRESSION TAG	UNP 015350
C	105	HIS	-	EXPRESSION TAG	UNP 015350
C	106	HIS	-	EXPRESSION TAG	UNP 015350
C	107	HIS	-	EXPRESSION TAG	UNP 015350
C	108	HIS	-	EXPRESSION TAG	UNP 015350
C	109	HIS	-	EXPRESSION TAG	UNP 015350
C	110	HIS	-	EXPRESSION TAG	UNP 015350
C	111	HIS	-	EXPRESSION TAG	UNP 015350
C	112	HIS	-	EXPRESSION TAG	UNP 015350
C	113	GLU	-	EXPRESSION TAG	UNP 015350
C	114	PHE	-	EXPRESSION TAG	UNP 015350
D	103	MET	-	INITIATING METHIONINE	UNP 015350
D	104	GLY	-	EXPRESSION TAG	UNP 015350
D	105	HIS	-	EXPRESSION TAG	UNP 015350
D	106	HIS	-	EXPRESSION TAG	UNP 015350
D	107	HIS	-	EXPRESSION TAG	UNP 015350
D	108	HIS	-	EXPRESSION TAG	UNP 015350
D	109	HIS	-	EXPRESSION TAG	UNP 015350
D	110	HIS	-	EXPRESSION TAG	UNP 015350
D	111	HIS	-	EXPRESSION TAG	UNP 015350
D	112	HIS	-	EXPRESSION TAG	UNP 015350
D	113	GLU	-	EXPRESSION TAG	UNP 015350
D	114	PHE	-	EXPRESSION TAG	UNP 015350
I	103	MET	-	INITIATING METHIONINE	UNP 015350
I	104	GLY	-	EXPRESSION TAG	UNP 015350
I	105	HIS	-	EXPRESSION TAG	UNP 015350
I	106	HIS	-	EXPRESSION TAG	UNP 015350
I	107	HIS	-	EXPRESSION TAG	UNP 015350
I	108	HIS	-	EXPRESSION TAG	UNP 015350
I	109	HIS	-	EXPRESSION TAG	UNP 015350

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Chain	Residue	Modelled	Actual	Comment	Reference
I	110	HIS	-	EXPRESSION TAG	UNP 015350
I	111	HIS	-	EXPRESSION TAG	UNP 015350
I	112	HIS	-	EXPRESSION TAG	UNP 015350
I	113	GLU	-	EXPRESSION TAG	UNP 015350
I	114	PHE	-	EXPRESSION TAG	UNP 015350
J	103	MET	-	INITIATING METHIONINE	UNP 015350
J	104	GLY	-	EXPRESSION TAG	UNP 015350
J	105	HIS	-	EXPRESSION TAG	UNP 015350
J	106	HIS	-	EXPRESSION TAG	UNP 015350
J	107	HIS	-	EXPRESSION TAG	UNP 015350
J	108	HIS	-	EXPRESSION TAG	UNP 015350
J	109	HIS	-	EXPRESSION TAG	UNP 015350
J	110	HIS	-	EXPRESSION TAG	UNP 015350
J	111	HIS	-	EXPRESSION TAG	UNP 015350
J	112	HIS	-	EXPRESSION TAG	UNP 015350
J	113	GLU	-	EXPRESSION TAG	UNP 015350
J	114	PHE	-	EXPRESSION TAG	UNP 015350
K	103	MET	-	INITIATING METHIONINE	UNP 015350
K	104	GLY	-	EXPRESSION TAG	UNP 015350
K	105	HIS	-	EXPRESSION TAG	UNP 015350
K	106	HIS	-	EXPRESSION TAG	UNP 015350
K	107	HIS	-	EXPRESSION TAG	UNP 015350
K	108	HIS	-	EXPRESSION TAG	UNP 015350
K	109	HIS	-	EXPRESSION TAG	UNP 015350
K	110	HIS	-	EXPRESSION TAG	UNP 015350
K	111	HIS	-	EXPRESSION TAG	UNP 015350
K	112	HIS	-	EXPRESSION TAG	UNP 015350
K	113	GLU	-	EXPRESSION TAG	UNP 015350
K	114	PHE	-	EXPRESSION TAG	UNP 015350
L	103	MET	-	INITIATING METHIONINE	UNP 015350
L	104	GLY	-	EXPRESSION TAG	UNP 015350
L	105	HIS	-	EXPRESSION TAG	UNP 015350
L	106	HIS	-	EXPRESSION TAG	UNP 015350
L	107	HIS	-	EXPRESSION TAG	UNP 015350
L	108	HIS	-	EXPRESSION TAG	UNP 015350
L	109	HIS	-	EXPRESSION TAG	UNP 015350
L	110	HIS	-	EXPRESSION TAG	UNP 015350
L	111	HIS	-	EXPRESSION TAG	UNP 015350
L	112	HIS	-	EXPRESSION TAG	UNP 015350
L	113	GLU	-	EXPRESSION TAG	UNP 015350
L	114	PHE	-	EXPRESSION TAG	UNP 015350

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*GP\*CP\*CP\*

TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			
2	F	11	Total	C	N	O	P	0	0	0
			227	107	43	66	11			
2	G	11	Total	C	N	O	P	0	0	0
			227	107	43	66	11			
2	H	11	Total	C	N	O	P	0	0	0
			221	106	41	64	10			
2	M	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	N	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	O	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	P	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		

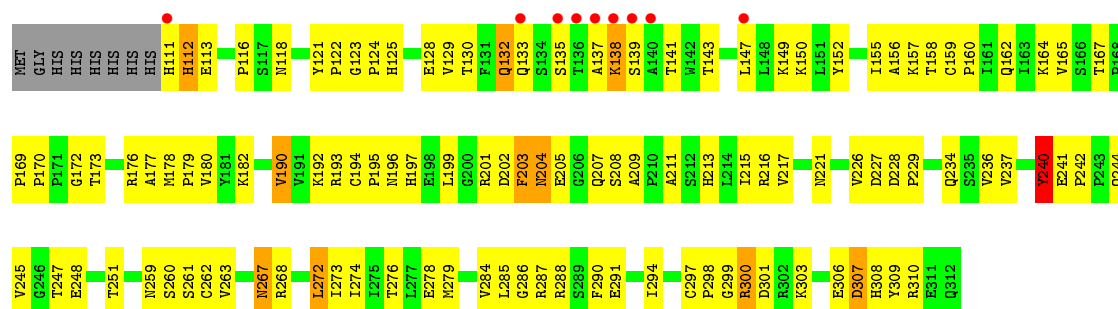
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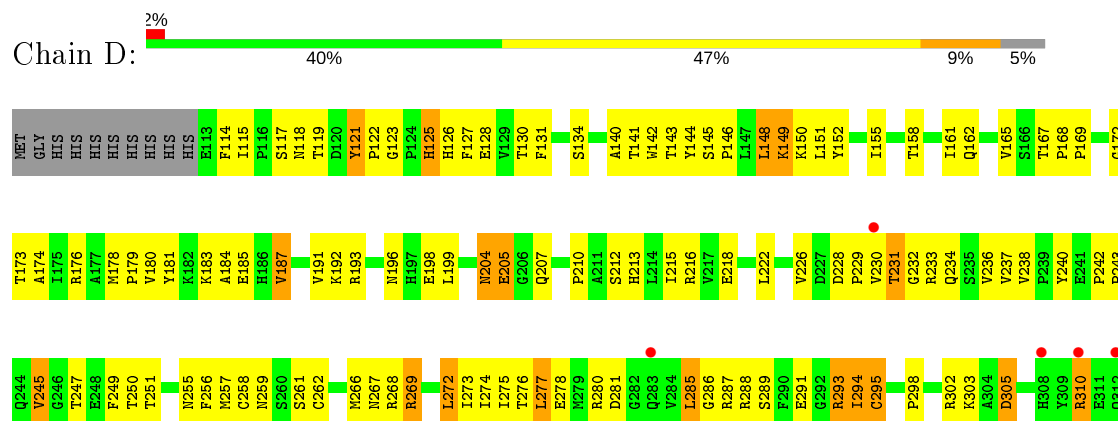
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	19	Total 19	O 19	0	0
4	C	19	Total 19	O 19	0	0
4	D	13	Total 13	O 13	0	0
4	I	19	Total 19	O 19	0	0
4	J	14	Total 14	O 14	0	0
4	K	34	Total 34	O 34	0	0
4	L	30	Total 30	O 30	0	0
4	E	1	Total 1	O 1	0	0
4	N	1	Total 1	O 1	0	0
4	O	1	Total 1	O 1	0	0



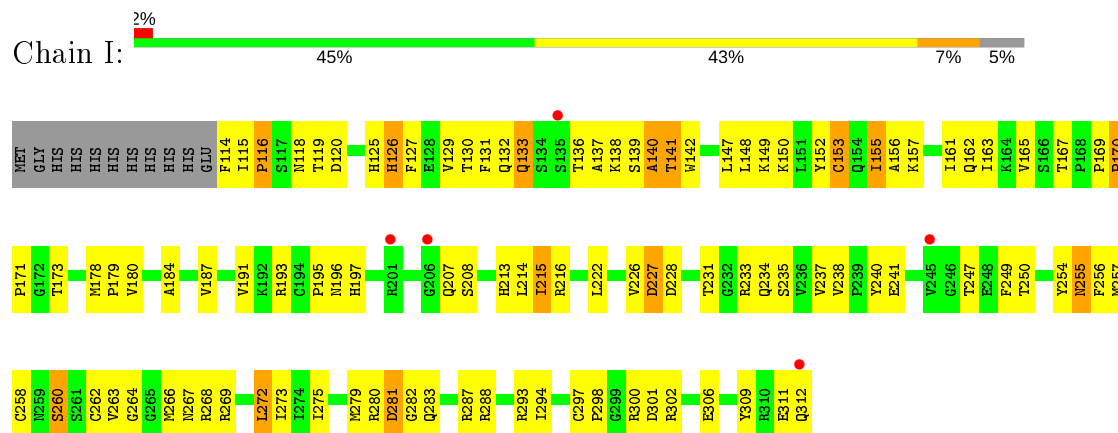




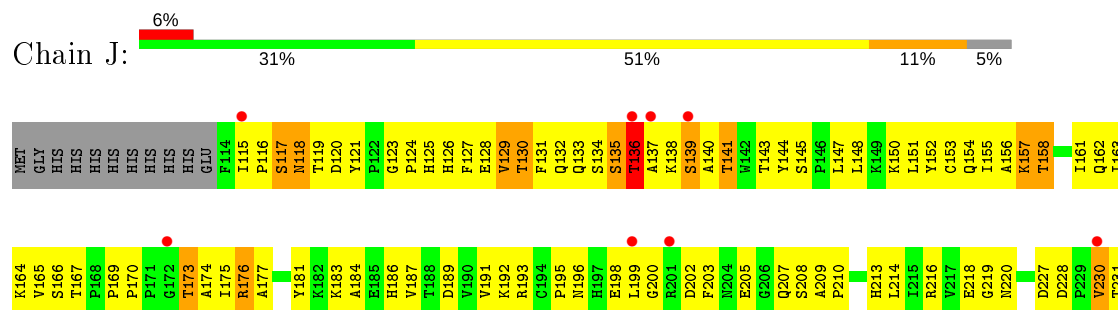
• Molecule 1: Tumor protein p73

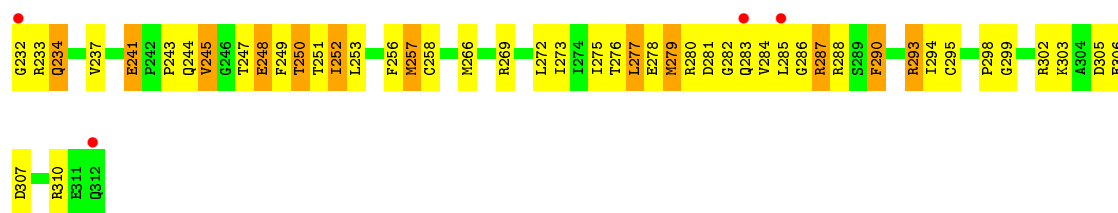


• Molecule 1: Tumor protein p73

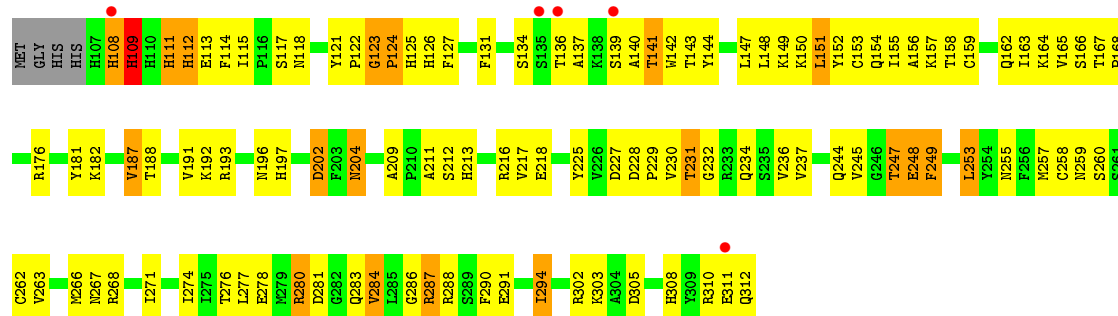
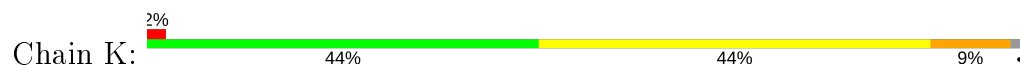


• Molecule 1: Tumor protein p73

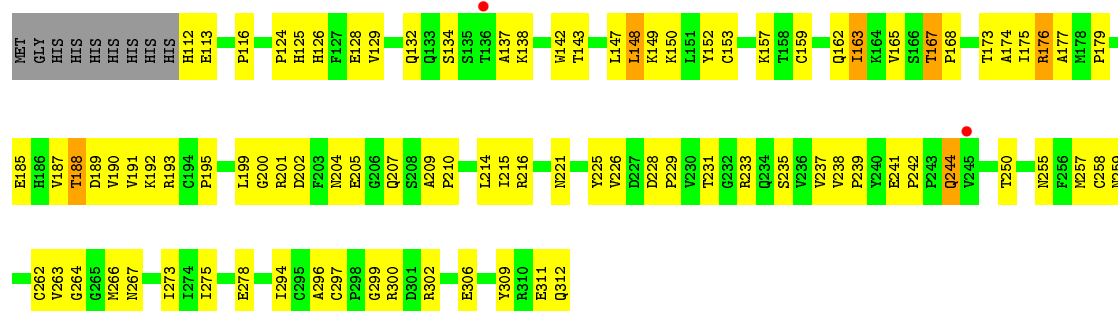




• Molecule 1: Tumor protein p73



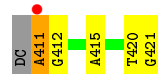
• Molecule 1: Tumor protein p73



• Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*GP\*CP\*CP\*TP\*G)-3')



• Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*GP\*CP\*CP\*TP\*G)-3')



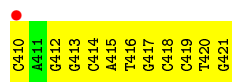
- Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*GP\*CP\*CP\*TP\*G)-3')



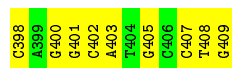
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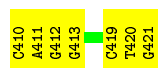
- Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*GP\*CP\*CP\*TP\*G)-3')



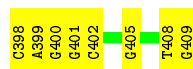
- Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*GP\*CP\*CP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*GP\*CP\*CP\*TP\*G)-3')



- Molecule 2: DNA (5'-D(\*CP\*AP\*GP\*GP\*CP\*AP\*TP\*GP\*CP\*CP\*TP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.09Å 104.52Å 122.99Å 90.00° 96.18° 90.00°	Depositor
Resolution (Å)	19.92 – 2.95 19.92 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.92-2.95) 99.7 (19.92-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 2.93Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.235 , 0.254 0.234 , 0.252	Depositor DCC
$R_{free}$ test set	877 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/1638	0.77	1/2225 (0.0%)
1	B	0.44	0/1620	0.77	0/2201
1	C	0.55	2/1638 (0.1%)	0.75	0/2225
1	D	0.41	0/1612	0.71	1/2190 (0.0%)
1	I	0.48	0/1607	0.77	1/2183 (0.0%)
1	J	0.41	0/1600	0.73	0/2174
1	K	0.44	0/1676	0.74	1/2277 (0.0%)
1	L	0.49	0/1627	0.79	1/2210 (0.0%)
2	E	0.43	0/247	0.81	0/379
2	F	0.68	0/254	0.97	1/390 (0.3%)
2	G	0.75	0/254	0.81	0/390
2	H	0.84	0/247	0.91	1/379 (0.3%)
2	M	0.65	0/272	0.89	0/418
2	N	0.60	0/272	1.08	0/418
2	O	0.50	0/272	0.86	0/418
2	P	0.52	0/272	0.81	0/418
All	All	0.49	2/15108 (0.0%)	0.78	7/20895 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	240	TYR	CB-CG	-5.84	1.42	1.51
1	C	240	TYR	CE2-CZ	-5.46	1.31	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	109	HIS	N-CA-C	-5.47	96.23	111.00
1	D	125	HIS	N-CA-C	-5.26	96.80	111.00
1	L	250	THR	N-CA-C	-5.24	96.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	411	DA	OP1-P-OP2	-5.24	111.74	119.60
1	A	207	GLN	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	1596	0	1558	155	0
1	B	1580	0	1544	148	0
1	C	1596	0	1558	113	0
1	D	1572	0	1540	132	0
1	I	1567	0	1538	107	0
1	J	1561	0	1531	145	0
1	K	1631	0	1581	123	0
1	L	1586	0	1551	65	0
2	E	221	0	125	8	0
2	F	227	0	124	8	0
2	G	227	0	124	5	0
2	H	221	0	125	6	0
2	M	243	0	136	11	0
2	N	243	0	136	14	0
2	O	243	0	136	10	0
2	P	243	0	136	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	18	0	0	2	0
4	B	19	0	0	1	0
4	C	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	13	0	0	0	0
4	E	1	0	0	0	0
4	I	19	0	0	3	0
4	J	14	0	0	2	0
4	K	34	0	0	0	0
4	L	30	0	0	3	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
All	All	14734	0	13443	1008	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 36.

The worst 5 of 1008 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:K:280:ARG:HH11	1:K:280:ARG:HG2	1.02	1.13
1:I:231:THR:CG2	1:I:233:ARG:HG2	1.83	1.08
2:N:401:DG:H2"	2:N:402:DC:H5"	1.33	1.08
1:C:240:TYR:C	1:C:240:TYR:CD2	2.30	1.01
1:B:169:PRO:HG2	1:B:170:PRO:HD3	1.43	1.00

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	200/210 (95%)	168 (84%)	23 (12%)	9 (4%)	2	12
1	B	199/210 (95%)	173 (87%)	20 (10%)	6 (3%)	4	20
1	C	200/210 (95%)	180 (90%)	18 (9%)	2 (1%)	15	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	198/210 (94%)	177 (89%)	20 (10%)	1 (0%)	29	64
1	I	197/210 (94%)	172 (87%)	18 (9%)	7 (4%)	3	16
1	J	197/210 (94%)	164 (83%)	26 (13%)	7 (4%)	3	16
1	K	204/210 (97%)	180 (88%)	16 (8%)	8 (4%)	3	14
1	L	199/210 (95%)	174 (87%)	24 (12%)	1 (0%)	29	64
All	All	1594/1680 (95%)	1388 (87%)	165 (10%)	41 (3%)	5	24

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	PRO
1	A	207	GLN
1	B	169	PRO
1	C	202	ASP
1	I	282	GLY

### 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	179/186 (96%)	146 (82%)	33 (18%)	1	7
1	B	177/186 (95%)	146 (82%)	31 (18%)	2	8
1	C	179/186 (96%)	155 (87%)	24 (13%)	4	15
1	D	176/186 (95%)	154 (88%)	22 (12%)	4	17
1	I	176/186 (95%)	162 (92%)	14 (8%)	12	37
1	J	175/186 (94%)	142 (81%)	33 (19%)	1	7
1	K	182/186 (98%)	158 (87%)	24 (13%)	4	16
1	L	178/186 (96%)	159 (89%)	19 (11%)	6	23
All	All	1422/1488 (96%)	1222 (86%)	200 (14%)	3	14

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	148	LEU
1	I	153	CYS
1	L	163	ILE
1	D	205	GLU
1	D	269	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	224	GLN
1	I	196	ASN
1	L	132	GLN
1	C	267	ASN
1	D	255	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	202/210 (96%)	0.30	10 (4%) 28 18	43, 89, 123, 127	3 (1%)
1	B	201/210 (95%)	0.06	7 (3%) 44 29	40, 75, 108, 136	1 (0%)
1	C	202/210 (96%)	-0.01	9 (4%) 33 21	41, 71, 108, 135	1 (0%)
1	D	200/210 (95%)	0.16	5 (2%) 57 40	49, 82, 112, 144	2 (1%)
1	I	199/210 (94%)	-0.03	5 (2%) 57 40	47, 70, 105, 114	1 (0%)
1	J	199/210 (94%)	0.40	12 (6%) 21 13	53, 88, 121, 129	1 (0%)
1	K	206/210 (98%)	-0.04	5 (2%) 59 42	32, 60, 108, 128	0
1	L	201/210 (95%)	-0.36	2 (0%) 82 68	26, 49, 80, 95	1 (0%)
2	E	11/12 (91%)	-0.02	0 100 100	59, 76, 97, 100	0
2	F	11/12 (91%)	0.06	1 (9%) 9 5	50, 80, 122, 133	0
2	G	11/12 (91%)	1.01	1 (9%) 9 5	91, 117, 128, 148	0
2	H	11/12 (91%)	0.29	0 100 100	76, 98, 129, 130	0
2	M	12/12 (100%)	0.10	1 (8%) 11 6	43, 75, 126, 136	0
2	N	12/12 (100%)	-0.11	0 100 100	50, 80, 93, 94	0
2	O	12/12 (100%)	-0.18	0 100 100	53, 66, 132, 133	0
2	P	12/12 (100%)	-0.19	0 100 100	49, 65, 121, 124	0
All	All	1702/1776 (95%)	0.06	58 (3%) 45 29	26, 73, 117, 148	10 (0%)

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	CYS	7.3
1	C	137	ALA	6.0
1	C	139	SER	5.8
1	B	312	GLN	5.5
1	J	172	GLY	5.3

## 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
3	ZN	I	401	1/1	0.97	0.10	74,74,74,74	0
3	ZN	A	401	1/1	0.98	0.10	72,72,72,72	0
3	ZN	D	401	1/1	0.98	0.11	62,62,62,62	0
3	ZN	C	401	1/1	0.99	0.13	50,50,50,50	0
3	ZN	J	401	1/1	0.99	0.10	70,70,70,70	0
3	ZN	L	401	1/1	0.99	0.15	50,50,50,50	0
3	ZN	B	401	1/1	0.99	0.09	49,49,49,49	0
3	ZN	K	401	1/1	1.00	0.08	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.