



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2022 – 06:10 PM JST

PDB ID : 7EZJ  
Title : Crystal structure of p73 DNA binding domain complex bound with 1 bp and 2 bp spacer DNA response elements.  
Authors : Koley, T.; Roy Chowdhury, S.; Kumar, M.; Kaur, P.; Singh, T.P.; Viadiu, H.; Ethayathulla, A.S.  
Deposited on : 2021-06-01  
Resolution : 2.90 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	:	2.27
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)	:	2.27

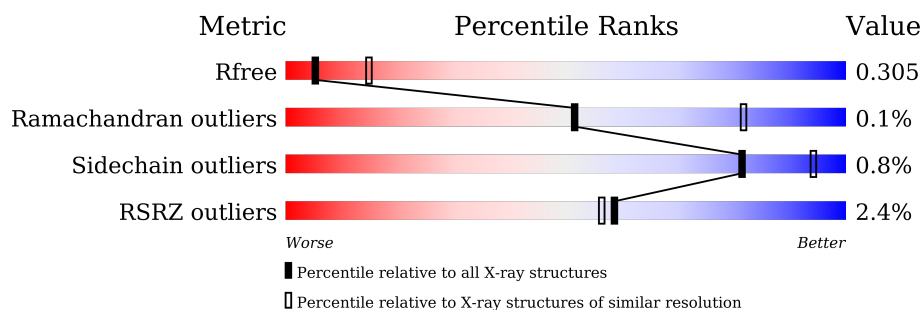
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.



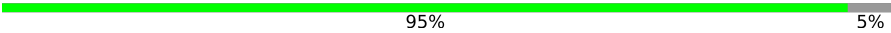


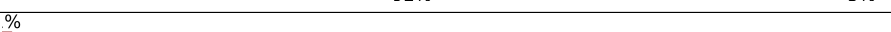
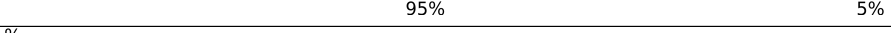
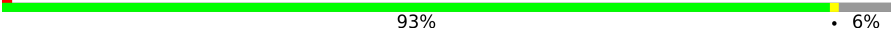
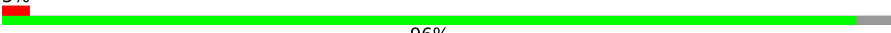

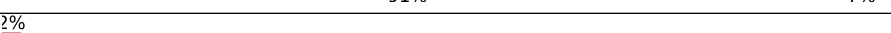
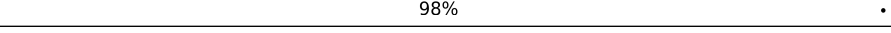
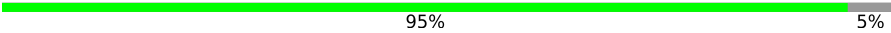


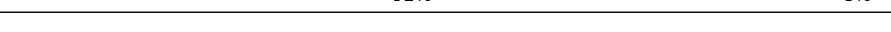
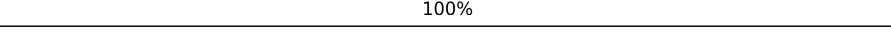
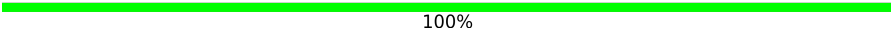
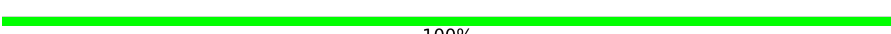

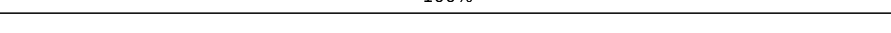
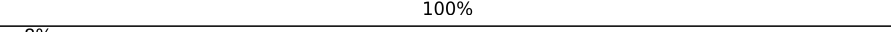
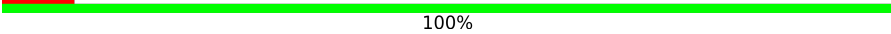


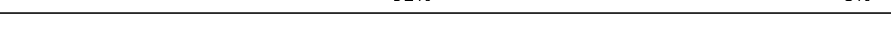
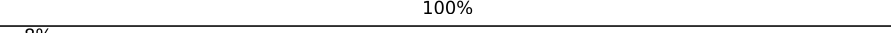
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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></div> <div>95%</div> <div>..</div> </div>
1	B	210	<div> <div>3%</div> <div>94%</div> <div>..</div> </div>
1	C	210	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	D	210	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>
1	I	210	<div> <div>2%</div> <div>95%</div> <div>5%</div> </div>
1	J	210	<div> <div>7%</div> <div>92%</div> <div>6%</div> </div>
1	K	210	<div> <div>2%</div> <div>95%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	L	210	 95% 5%
1	a	210	 94% 5%
1	b	210	 92% 5%
1	c	210	 95% 5%
1	d	210	 93% 6%
1	i	210	 96%
1	j	210	 91% 7%
1	k	210	 98%
1	l	210	 95% 5%
2	E	12	 92% 8%
2	F	12	 92% 8%
2	G	12	 100%
2	H	12	 100%
2	M	12	 100%
2	N	12	 100%
2	O	12	 100%
2	P	12	 100%
2	e	12	 92% 8%
2	f	12	 92% 8%
2	g	12	 100%
2	h	12	 100%
2	m	12	 100%
2	n	12	 100%
2	o	12	 100%
2	p	12	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29062 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
			1591	996	286	298	11			
1	B	201	Total	C	N	O	S	0	0	0
			1580	987	285	297	11			
1	C	201	Total	C	N	O	S	0	0	0
			1586	993	285	297	11			
1	D	199	Total	C	N	O	S	0	0	0
			1558	978	280	289	11			
1	I	199	Total	C	N	O	S	0	0	0
			1559	979	280	289	11			
1	J	197	Total	C	N	O	S	0	0	0
			1542	966	278	287	11			
1	K	201	Total	C	N	O	S	0	0	0
			1586	993	285	297	11			
1	L	200	Total	C	N	O	S	0	0	0
			1576	988	283	294	11			
1	a	199	Total	C	N	O	S	0	0	0
			1566	982	280	293	11			
1	b	199	Total	C	N	O	S	0	0	0
			1561	977	282	291	11			
1	c	200	Total	C	N	O	S	0	0	0
			1577	989	285	292	11			
1	d	198	Total	C	N	O	S	0	0	0
			1553	975	279	288	11			
1	i	201	Total	C	N	O	S	0	0	0
			1577	988	283	295	11			
1	j	196	Total	C	N	O	S	0	0	0
			1536	960	277	288	11			
1	k	206	Total	C	N	O	S	0	0	0
			1626	1018	297	300	11			
1	l	200	Total	C	N	O	S	0	0	0
			1576	988	283	294	11			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	expression tag	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	-	expression tag	UNP O15350
B	104	GLY	-	expression tag	UNP O15350
B	105	HIS	-	expression tag	UNP O15350
B	106	HIS	-	expression tag	UNP O15350
B	107	HIS	-	expression tag	UNP O15350
B	108	HIS	-	expression tag	UNP O15350
B	109	HIS	-	expression tag	UNP O15350
B	110	HIS	-	expression tag	UNP O15350
B	111	HIS	-	expression tag	UNP O15350
B	112	HIS	-	expression tag	UNP O15350
B	113	GLU	-	expression tag	UNP O15350
B	114	PHE	-	expression tag	UNP O15350
C	103	MET	-	expression tag	UNP O15350
C	104	GLY	-	expression tag	UNP O15350
C	105	HIS	-	expression tag	UNP O15350
C	106	HIS	-	expression tag	UNP O15350
C	107	HIS	-	expression tag	UNP O15350
C	108	HIS	-	expression tag	UNP O15350
C	109	HIS	-	expression tag	UNP O15350
C	110	HIS	-	expression tag	UNP O15350
C	111	HIS	-	expression tag	UNP O15350
C	112	HIS	-	expression tag	UNP O15350
C	113	GLU	-	expression tag	UNP O15350
C	114	PHE	-	expression tag	UNP O15350
D	103	MET	-	expression tag	UNP O15350
D	104	GLY	-	expression tag	UNP O15350
D	105	HIS	-	expression tag	UNP O15350
D	106	HIS	-	expression tag	UNP O15350
D	107	HIS	-	expression tag	UNP O15350
D	108	HIS	-	expression tag	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
D	109	HIS	-	expression tag	UNP O15350
D	110	HIS	-	expression tag	UNP O15350
D	111	HIS	-	expression tag	UNP O15350
D	112	HIS	-	expression tag	UNP O15350
D	113	GLU	-	expression tag	UNP O15350
D	114	PHE	-	expression tag	UNP O15350
I	103	MET	-	expression tag	UNP O15350
I	104	GLY	-	expression tag	UNP O15350
I	105	HIS	-	expression tag	UNP O15350
I	106	HIS	-	expression tag	UNP O15350
I	107	HIS	-	expression tag	UNP O15350
I	108	HIS	-	expression tag	UNP O15350
I	109	HIS	-	expression tag	UNP O15350
I	110	HIS	-	expression tag	UNP O15350
I	111	HIS	-	expression tag	UNP O15350
I	112	HIS	-	expression tag	UNP O15350
I	113	GLU	-	expression tag	UNP O15350
I	114	PHE	-	expression tag	UNP O15350
J	103	MET	-	expression tag	UNP O15350
J	104	GLY	-	expression tag	UNP O15350
J	105	HIS	-	expression tag	UNP O15350
J	106	HIS	-	expression tag	UNP O15350
J	107	HIS	-	expression tag	UNP O15350
J	108	HIS	-	expression tag	UNP O15350
J	109	HIS	-	expression tag	UNP O15350
J	110	HIS	-	expression tag	UNP O15350
J	111	HIS	-	expression tag	UNP O15350
J	112	HIS	-	expression tag	UNP O15350
J	113	GLU	-	expression tag	UNP O15350
J	114	PHE	-	expression tag	UNP O15350
K	103	MET	-	expression tag	UNP O15350
K	104	GLY	-	expression tag	UNP O15350
K	105	HIS	-	expression tag	UNP O15350
K	106	HIS	-	expression tag	UNP O15350
K	107	HIS	-	expression tag	UNP O15350
K	108	HIS	-	expression tag	UNP O15350
K	109	HIS	-	expression tag	UNP O15350
K	110	HIS	-	expression tag	UNP O15350
K	111	HIS	-	expression tag	UNP O15350
K	112	HIS	-	expression tag	UNP O15350
K	113	GLU	-	expression tag	UNP O15350
K	114	PHE	-	expression tag	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
L	103	MET	-	expression tag	UNP O15350
L	104	GLY	-	expression tag	UNP O15350
L	105	HIS	-	expression tag	UNP O15350
L	106	HIS	-	expression tag	UNP O15350
L	107	HIS	-	expression tag	UNP O15350
L	108	HIS	-	expression tag	UNP O15350
L	109	HIS	-	expression tag	UNP O15350
L	110	HIS	-	expression tag	UNP O15350
L	111	HIS	-	expression tag	UNP O15350
L	112	HIS	-	expression tag	UNP O15350
L	113	GLU	-	expression tag	UNP O15350
L	114	PHE	-	expression tag	UNP O15350
a	103	MET	-	expression tag	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	-	expression tag	UNP O15350
b	104	GLY	-	expression tag	UNP O15350
b	105	HIS	-	expression tag	UNP O15350
b	106	HIS	-	expression tag	UNP O15350
b	107	HIS	-	expression tag	UNP O15350
b	108	HIS	-	expression tag	UNP O15350
b	109	HIS	-	expression tag	UNP O15350
b	110	HIS	-	expression tag	UNP O15350
b	111	HIS	-	expression tag	UNP O15350
b	112	HIS	-	expression tag	UNP O15350
b	113	GLU	-	expression tag	UNP O15350
b	114	PHE	-	expression tag	UNP O15350
c	103	MET	-	expression tag	UNP O15350
c	104	GLY	-	expression tag	UNP O15350
c	105	HIS	-	expression tag	UNP O15350
c	106	HIS	-	expression tag	UNP O15350
c	107	HIS	-	expression tag	UNP O15350
c	108	HIS	-	expression tag	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
c	109	HIS	-	expression tag	UNP O15350
c	110	HIS	-	expression tag	UNP O15350
c	111	HIS	-	expression tag	UNP O15350
c	112	HIS	-	expression tag	UNP O15350
c	113	GLU	-	expression tag	UNP O15350
c	114	PHE	-	expression tag	UNP O15350
d	103	MET	-	expression tag	UNP O15350
d	104	GLY	-	expression tag	UNP O15350
d	105	HIS	-	expression tag	UNP O15350
d	106	HIS	-	expression tag	UNP O15350
d	107	HIS	-	expression tag	UNP O15350
d	108	HIS	-	expression tag	UNP O15350
d	109	HIS	-	expression tag	UNP O15350
d	110	HIS	-	expression tag	UNP O15350
d	111	HIS	-	expression tag	UNP O15350
d	112	HIS	-	expression tag	UNP O15350
d	113	GLU	-	expression tag	UNP O15350
d	114	PHE	-	expression tag	UNP O15350
i	103	MET	-	expression tag	UNP O15350
i	104	GLY	-	expression tag	UNP O15350
i	105	HIS	-	expression tag	UNP O15350
i	106	HIS	-	expression tag	UNP O15350
i	107	HIS	-	expression tag	UNP O15350
i	108	HIS	-	expression tag	UNP O15350
i	109	HIS	-	expression tag	UNP O15350
i	110	HIS	-	expression tag	UNP O15350
i	111	HIS	-	expression tag	UNP O15350
i	112	HIS	-	expression tag	UNP O15350
i	113	GLU	-	expression tag	UNP O15350
i	114	PHE	-	expression tag	UNP O15350
j	103	MET	-	expression tag	UNP O15350
j	104	GLY	-	expression tag	UNP O15350
j	105	HIS	-	expression tag	UNP O15350
j	106	HIS	-	expression tag	UNP O15350
j	107	HIS	-	expression tag	UNP O15350
j	108	HIS	-	expression tag	UNP O15350
j	109	HIS	-	expression tag	UNP O15350
j	110	HIS	-	expression tag	UNP O15350
j	111	HIS	-	expression tag	UNP O15350
j	112	HIS	-	expression tag	UNP O15350
j	113	GLU	-	expression tag	UNP O15350
j	114	PHE	-	expression tag	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
k	103	MET	-	expression tag	UNP O15350
k	104	GLY	-	expression tag	UNP O15350
k	105	HIS	-	expression tag	UNP O15350
k	106	HIS	-	expression tag	UNP O15350
k	107	HIS	-	expression tag	UNP O15350
k	108	HIS	-	expression tag	UNP O15350
k	109	HIS	-	expression tag	UNP O15350
k	110	HIS	-	expression tag	UNP O15350
k	111	HIS	-	expression tag	UNP O15350
k	112	HIS	-	expression tag	UNP O15350
k	113	GLU	-	expression tag	UNP O15350
k	114	PHE	-	expression tag	UNP O15350
l	103	MET	-	expression tag	UNP O15350
l	104	GLY	-	expression tag	UNP O15350
l	105	HIS	-	expression tag	UNP O15350
l	106	HIS	-	expression tag	UNP O15350
l	107	HIS	-	expression tag	UNP O15350
l	108	HIS	-	expression tag	UNP O15350
l	109	HIS	-	expression tag	UNP O15350
l	110	HIS	-	expression tag	UNP O15350
l	111	HIS	-	expression tag	UNP O15350
l	112	HIS	-	expression tag	UNP O15350
l	113	GLU	-	expression tag	UNP O15350
l	114	PHE	-	expression tag	UNP O15350

- Molecule 2 is a DNA chain called 12-mer DNA.

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	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	H	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
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	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
2	h	12	Total	C	N	O	P	0	0	0
			243	116	46	70	11			
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	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		
3	K	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	a	1	Total	Zn	0	0
			1	1		
3	b	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	c	1	Total 1	Zn 1	0	0
3	d	1	Total 1	Zn 1	0	0
3	i	1	Total 1	Zn 1	0	0
3	j	1	Total 1	Zn 1	0	0
3	k	1	Total 1	Zn 1	0	0
3	l	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

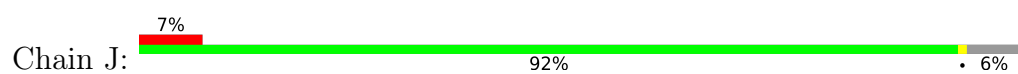
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	O 4	0	0
4	B	5	Total 5	O 5	0	0
4	C	5	Total 5	O 5	0	0
4	D	2	Total 2	O 2	0	0
4	I	3	Total 3	O 3	0	0
4	J	2	Total 2	O 2	0	0
4	K	1	Total 1	O 1	0	0
4	L	14	Total 14	O 14	0	0
4	a	2	Total 2	O 2	0	0
4	b	4	Total 4	O 4	0	0
4	c	6	Total 6	O 6	0	0
4	d	5	Total 5	O 5	0	0
4	i	9	Total 9	O 9	0	0

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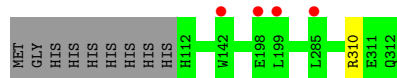
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	j	1	Total 1	O 1	0	0
4	k	11	Total 11	O 11	0	0
4	l	7	Total 7	O 7	0	0
4	H	1	Total 1	O 1	0	0
4	h	1	Total 1	O 1	0	0
4	o	1	Total 1	O 1	0	0

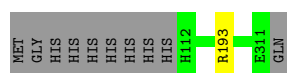




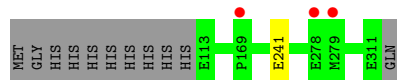
- Molecule 1: Tumor protein p73



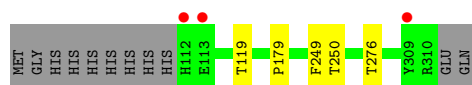
- Molecule 1: Tumor protein p73



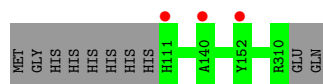
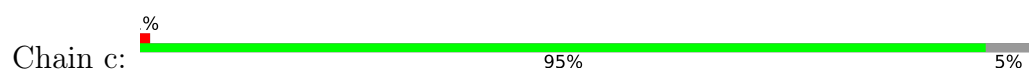
- Molecule 1: Tumor protein p73



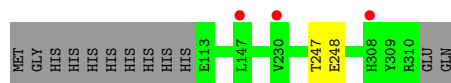
- Molecule 1: Tumor protein p73



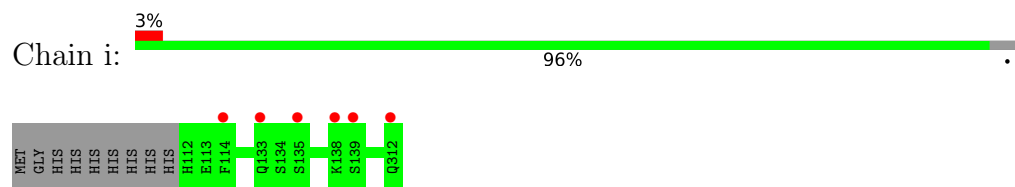
- Molecule 1: Tumor protein p73



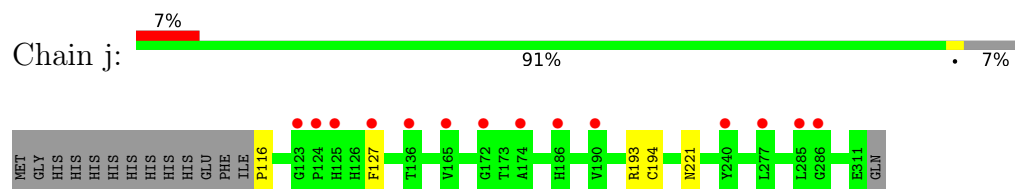
- Molecule 1: Tumor protein p73



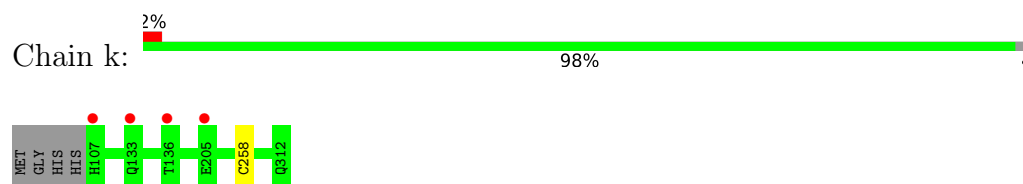
- Molecule 1: Tumor protein p73



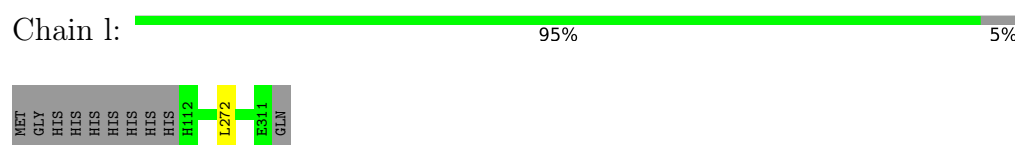
- Molecule 1: Tumor protein p73



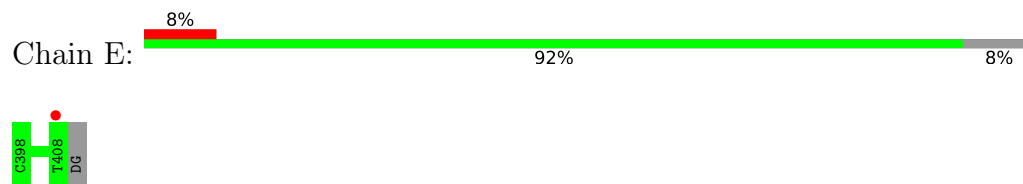
- Molecule 1: Tumor protein p73



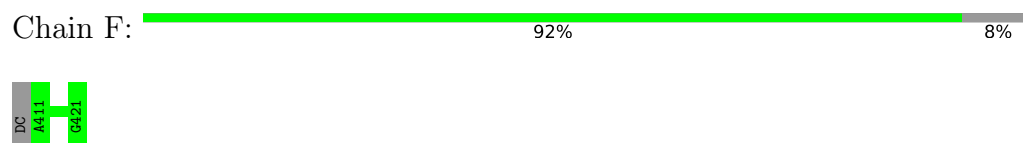
- Molecule 1: Tumor protein p73



- Molecule 2: 12-mer DNA



- Molecule 2: 12-mer DNA



- Molecule 2: 12-mer DNA



There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain P:  100%




- Molecule 2: 12-mer DNA

Chain e:  92% 8%



- Molecule 2: 12-mer DNA

Chain f:  92% 8%



- Molecule 2: 12-mer DNA

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain h:  100%



- Molecule 2: 12-mer DNA

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: 12-mer DNA

Chain p:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.70Å 105.50Å 155.50Å 90.00° 112.36° 90.00°	Depositor
Resolution (Å)	40.93 – 2.90 46.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (40.93-2.90) 95.4 (46.64-2.90)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.241 , 0.306 0.256 , 0.305	Depositor DCC
$R_{free}$ test set	4387 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	29062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 86.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5269e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

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	0.54	0/1632	0.70	0/2217
1	B	0.57	0/1620	0.71	0/2201
1	C	0.56	0/1627	0.73	0/2210
1	D	0.58	1/1598 (0.1%)	0.70	0/2173
1	I	0.52	0/1599	0.71	0/2174
1	J	0.49	0/1581	0.68	0/2150
1	K	0.50	0/1627	0.67	0/2210
1	L	0.59	0/1617	0.75	0/2198
1	a	0.54	0/1606	0.75	0/2183
1	b	0.53	0/1601	0.70	0/2177
1	c	0.55	0/1619	0.70	0/2201
1	d	0.54	0/1593	0.69	0/2166
1	i	0.52	0/1617	0.71	0/2197
1	j	0.57	0/1574	0.77	1/2139 (0.0%)
1	k	0.56	0/1671	0.76	0/2272
1	l	0.60	0/1617	0.74	0/2198
2	E	0.63	0/247	0.79	0/379
2	F	0.57	0/254	0.79	0/390
2	G	0.54	0/272	0.74	0/418
2	H	0.66	0/272	0.73	0/418
2	M	0.70	0/272	0.80	0/418
2	N	0.49	0/272	0.76	0/418
2	O	0.70	0/272	0.82	0/418
2	P	0.61	0/272	0.78	0/418
2	e	0.72	0/247	0.78	0/379
2	f	0.64	0/254	0.82	0/390
2	g	0.63	0/272	0.77	0/418
2	h	0.56	0/272	0.79	0/418
2	m	0.38	0/272	0.76	0/418
2	n	0.63	0/272	0.76	0/418
2	o	0.36	0/272	0.73	0/418
2	p	0.54	0/272	0.75	0/418

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.55	1/30065 (0.0%)	0.73	1/41620 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	PRO	C-N	8.51	1.50	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	j	116	PRO	N-CA-CB	5.63	110.06	103.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	189 (94%)	11 (6%)	0	100	100
1	B	199/210 (95%)	186 (94%)	12 (6%)	1 (0%)	29	61
1	C	199/210 (95%)	190 (96%)	9 (4%)	0	100	100
1	D	197/210 (94%)	188 (95%)	9 (5%)	0	100	100
1	I	197/210 (94%)	184 (93%)	13 (7%)	0	100	100
1	J	195/210 (93%)	188 (96%)	6 (3%)	1 (0%)	29	61
1	K	199/210 (95%)	195 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	198/210 (94%)	186 (94%)	12 (6%)	0	100	100
1	a	197/210 (94%)	193 (98%)	4 (2%)	0	100	100
1	b	197/210 (94%)	188 (95%)	8 (4%)	1 (0%)	29	61
1	c	198/210 (94%)	194 (98%)	4 (2%)	0	100	100
1	d	196/210 (93%)	188 (96%)	8 (4%)	0	100	100
1	i	199/210 (95%)	192 (96%)	7 (4%)	0	100	100
1	j	194/210 (92%)	182 (94%)	12 (6%)	0	100	100
1	k	204/210 (97%)	200 (98%)	4 (2%)	0	100	100
1	l	198/210 (94%)	185 (93%)	13 (7%)	0	100	100
All	All	3167/3360 (94%)	3028 (96%)	136 (4%)	3 (0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	124	PRO
1	b	179	PRO
1	B	232	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	178/186 (96%)	176 (99%)	2 (1%)	73	92
1	B	177/186 (95%)	175 (99%)	2 (1%)	73	92
1	C	178/186 (96%)	176 (99%)	2 (1%)	73	92
1	D	174/186 (94%)	174 (100%)	0	100	100
1	I	174/186 (94%)	174 (100%)	0	100	100
1	J	173/186 (93%)	171 (99%)	2 (1%)	71	91
1	K	178/186 (96%)	177 (99%)	1 (1%)	86	96
1	L	177/186 (95%)	176 (99%)	1 (1%)	86	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	176/186 (95%)	175 (99%)	1 (1%)	86	96
1	b	175/186 (94%)	171 (98%)	4 (2%)	50	80
1	c	177/186 (95%)	177 (100%)	0	100	100
1	d	174/186 (94%)	172 (99%)	2 (1%)	73	92
1	i	176/186 (95%)	176 (100%)	0	100	100
1	j	172/186 (92%)	168 (98%)	4 (2%)	50	80
1	k	181/186 (97%)	180 (99%)	1 (1%)	86	96
1	l	177/186 (95%)	176 (99%)	1 (1%)	86	96
All	All	2817/2976 (95%)	2794 (99%)	23 (1%)	81	94

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	276	THR
1	j	127	PHE
1	d	248	GLU
1	j	193	ARG
1	J	132	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	132	GLN
1	a	255	ASN
1	k	255	ASN
1	L	213	HIS
1	a	259	ASN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 16 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%)	0.04	3 (1%) 73 73	54, 86, 126, 174	0
1	B	201/210 (95%)	0.04	7 (3%) 44 38	53, 84, 120, 150	0
1	C	201/210 (95%)	-0.11	4 (1%) 65 63	53, 76, 109, 155	0
1	D	199/210 (94%)	-0.05	5 (2%) 57 55	57, 80, 120, 201	0
1	I	199/210 (94%)	-0.01	4 (2%) 65 63	56, 76, 120, 144	0
1	J	197/210 (93%)	0.29	14 (7%) 16 12	63, 105, 167, 196	0
1	K	201/210 (95%)	0.31	4 (1%) 65 63	80, 110, 151, 210	0
1	L	200/210 (95%)	-0.27	0 100 100	45, 63, 94, 120	0
1	a	199/210 (94%)	0.06	3 (1%) 73 73	61, 95, 141, 163	0
1	b	199/210 (94%)	0.01	3 (1%) 73 73	59, 92, 131, 169	0
1	c	200/210 (95%)	-0.02	3 (1%) 73 73	58, 81, 119, 144	0
1	d	198/210 (94%)	0.04	3 (1%) 73 73	68, 93, 133, 157	0
1	i	201/210 (95%)	0.06	6 (2%) 50 45	56, 78, 119, 150	0
1	j	196/210 (93%)	0.20	14 (7%) 16 12	62, 93, 143, 179	0
1	k	206/210 (98%)	-0.05	4 (1%) 66 65	52, 72, 123, 170	0
1	l	200/210 (95%)	-0.17	0 100 100	49, 71, 98, 128	0
2	E	11/12 (91%)	-0.07	1 (9%) 9 6	81, 92, 103, 117	0
2	F	11/12 (91%)	-0.37	0 100 100	72, 94, 115, 119	0
2	G	12/12 (100%)	-0.01	0 100 100	78, 97, 120, 121	0
2	H	12/12 (100%)	-0.12	0 100 100	72, 101, 113, 120	0
2	M	12/12 (100%)	-0.40	0 100 100	70, 95, 109, 110	0
2	N	12/12 (100%)	-0.24	0 100 100	77, 95, 112, 119	0
2	O	12/12 (100%)	-0.15	0 100 100	93, 113, 165, 165	0
2	P	12/12 (100%)	0.22	1 (8%) 11 8	87, 101, 171, 178	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	e	11/12 (91%)	-0.34	0 100 100	81, 96, 113, 148	0
2	f	11/12 (91%)	-0.34	0 100 100	79, 103, 124, 129	0
2	g	12/12 (100%)	-0.06	0 100 100	87, 107, 148, 152	0
2	h	12/12 (100%)	0.39	1 (8%) 11 8	44, 88, 143, 156	0
2	m	12/12 (100%)	-0.22	0 100 100	67, 86, 109, 109	0
2	n	12/12 (100%)	-0.21	0 100 100	74, 97, 114, 121	0
2	o	12/12 (100%)	-0.10	0 100 100	74, 86, 108, 110	0
2	p	12/12 (100%)	0.21	0 100 100	69, 89, 114, 124	0
All	All	3387/3552 (95%)	0.01	80 (2%) 59 56	44, 85, 134, 210	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	i	139	SER	7.0
1	b	112	HIS	6.4
1	I	135	SER	5.8
2	h	523	DG	5.5
1	k	107	HIS	5.1

## 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 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, 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(Å <sup>2</sup> )	Q<0.9
3	ZN	L	401	1/1	0.90	0.15	63,63,63,63	0
3	ZN	B	401	1/1	0.94	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	a	401	1/1	0.94	0.14	85,85,85,85	0
3	ZN	i	401	1/1	0.94	0.18	86,86,86,86	0
3	ZN	d	401	1/1	0.95	0.17	76,76,76,76	0
3	ZN	K	401	1/1	0.96	0.15	101,101,101,101	0
3	ZN	l	401	1/1	0.97	0.14	68,68,68,68	0
3	ZN	I	401	1/1	0.98	0.14	76,76,76,76	0
3	ZN	b	401	1/1	0.98	0.12	59,59,59,59	0
3	ZN	J	401	1/1	0.98	0.18	81,81,81,81	0
3	ZN	A	401	1/1	0.98	0.11	84,84,84,84	0
3	ZN	j	401	1/1	0.98	0.13	79,79,79,79	0
3	ZN	k	401	1/1	0.98	0.17	69,69,69,69	0
3	ZN	D	401	1/1	0.98	0.13	63,63,63,63	0
3	ZN	c	401	1/1	0.99	0.21	65,65,65,65	0
3	ZN	C	401	1/1	0.99	0.20	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.