wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2023 – 06:52 PM EDT

PDB ID	:	3VD1
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

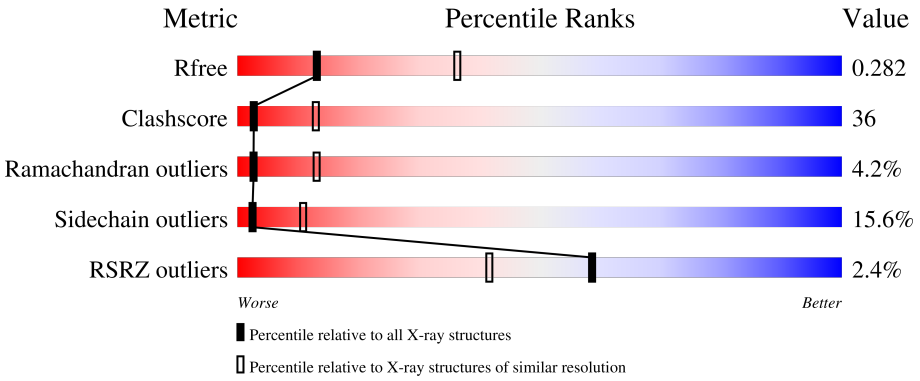
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 39% 48% 10% •
1	B	210	36% 47% 12% 5%
1	C	210	2% 46% 40% 10% •
1	D	210	2% 38% 45% 10% • 5%
1	I	210	2% 43% 44% 7% • 5%

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Mol	Chain	Length	Quality of chain
1	J	210	5% 42% 41% 11% 5%
1	K	210	4% 35% 44% 15%
1	L	210	37% 46% 13%
2	E	12	8% 67% 33%
2	F	12	17% 42% 50% 8%
2	G	12	58% 42%
2	H	12	42% 58%
2	M	12	67% 33%
2	N	12	25% 67% 8%
2	O	12	67% 33%
2	P	12	25% 75%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14716 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
			1581	991	284	295	11			
1	B	199	Total	C	N	O	S	0	0	0
			1560	976	281	292	11			
1	C	201	Total	C	N	O	S	0	0	0
			1575	985	285	294	11			
1	D	199	Total	C	N	O	S	0	0	0
			1560	976	281	292	11			
1	I	199	Total	C	N	O	S	0	0	0
			1560	976	281	292	11			
1	J	199	Total	C	N	O	S	0	0	0
			1560	976	281	292	11			
1	K	202	Total	C	N	O	S	0	0	0
			1590	996	286	297	11			
1	L	202	Total	C	N	O	S	0	0	0
			1590	996	286	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 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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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 DNA (5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*

CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
2	F	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
2	G	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
2	H	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
2	M	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
2	N	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
2	O	12	Total	C	N	O	P	0	0	0
			243	115	47	70	11			
2	P	12	Total	C	N	O	P	0	0	0
			243	115	47	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		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	25	Total	O	0	0
			25	25		

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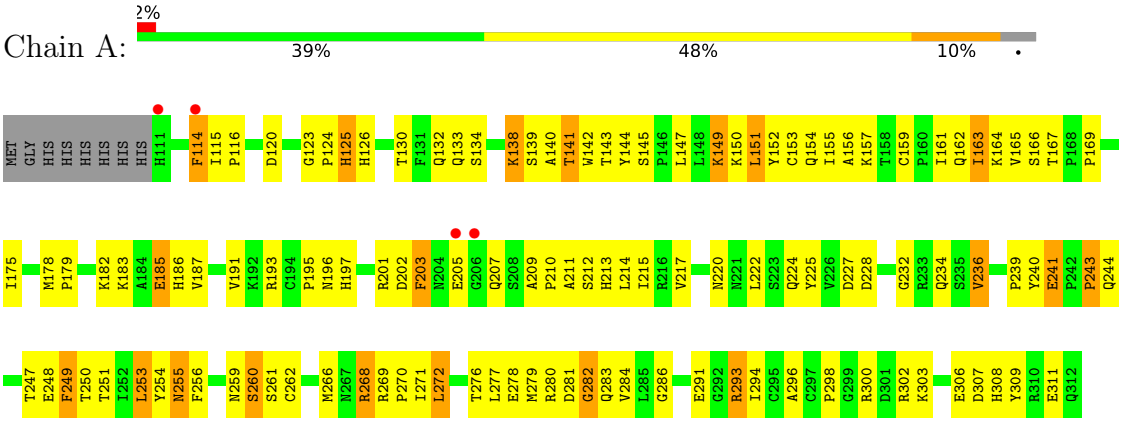
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	20	Total O 20 20	0	0
4	C	28	Total O 28 28	0	0
4	D	23	Total O 23 23	0	0
4	I	26	Total O 26 26	0	0
4	J	14	Total O 14 14	0	0
4	K	20	Total O 20 20	0	0
4	L	19	Total O 19 19	0	0
4	E	3	Total O 3 3	0	0
4	F	2	Total O 2 2	0	0
4	H	1	Total O 1 1	0	0
4	M	1	Total O 1 1	0	0
4	N	3	Total O 3 3	0	0
4	O	2	Total O 2 2	0	0
4	P	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

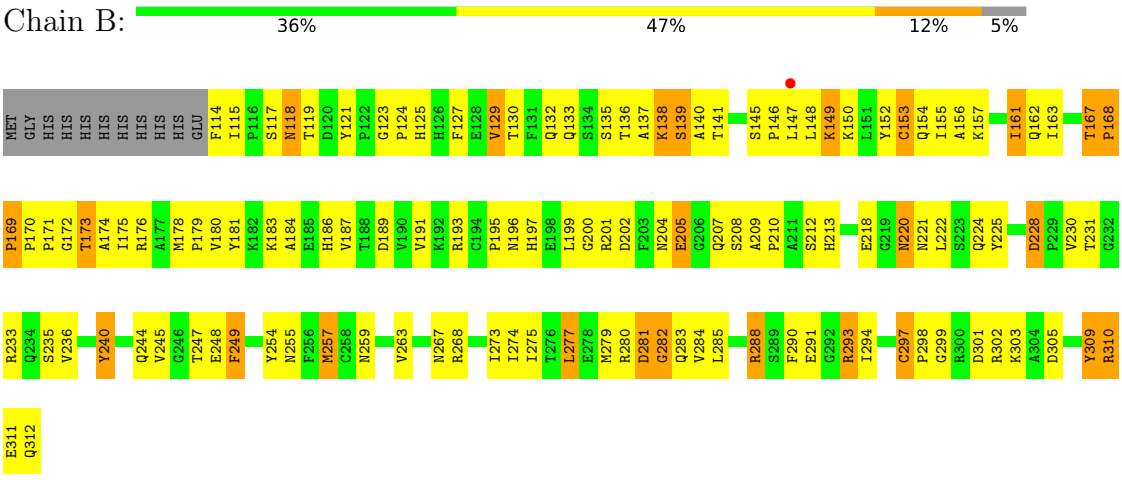
• Molecule 1: Tumor protein p73

Chain A:



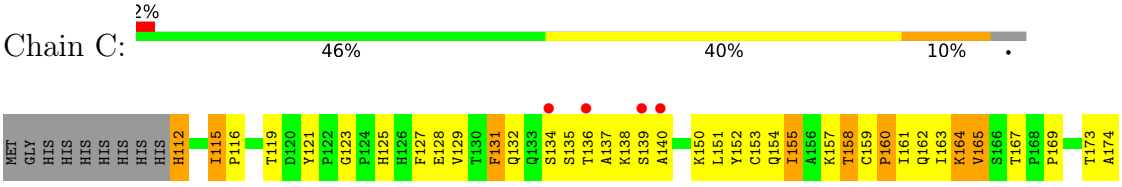
• Molecule 1: Tumor protein p73

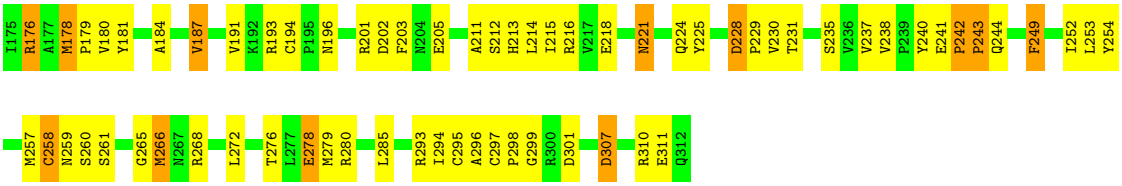
Chain B:



• Molecule 1: Tumor protein p73

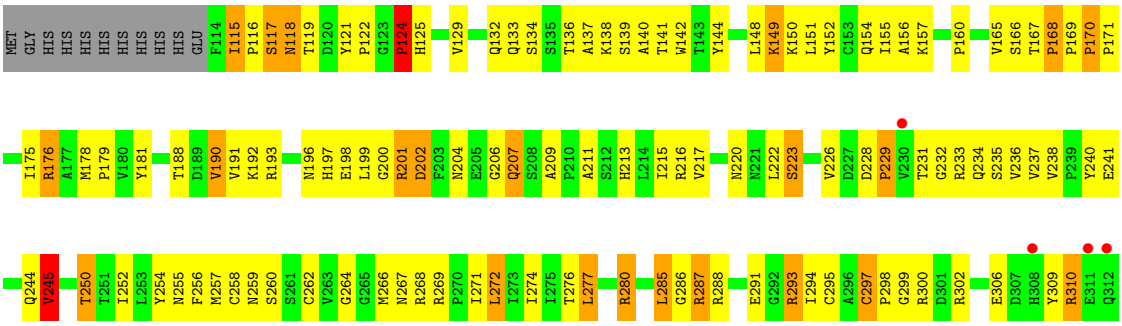
Chain C:





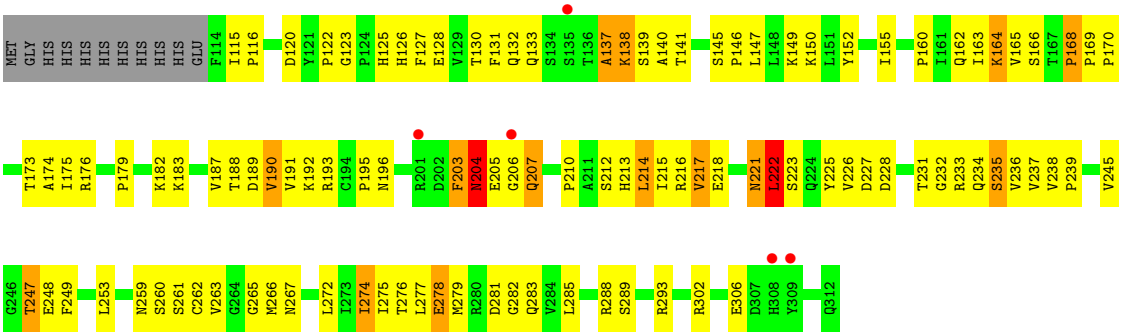
• Molecule 1: Tumor protein p73

Chain D:



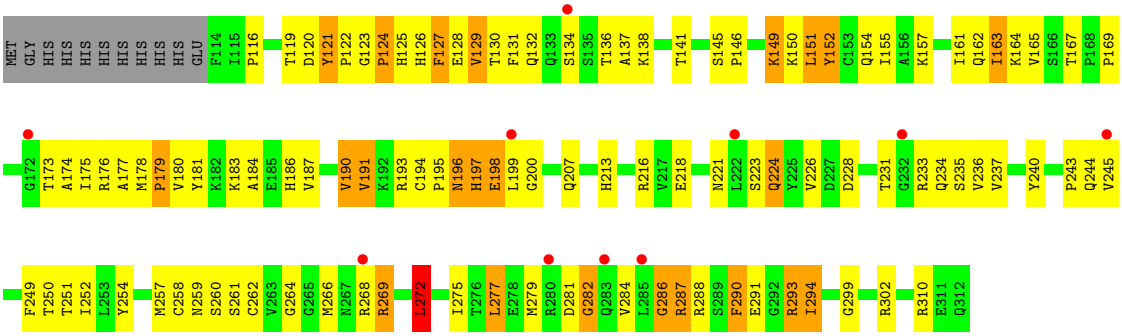
• Molecule 1: Tumor protein p73

Chain I:



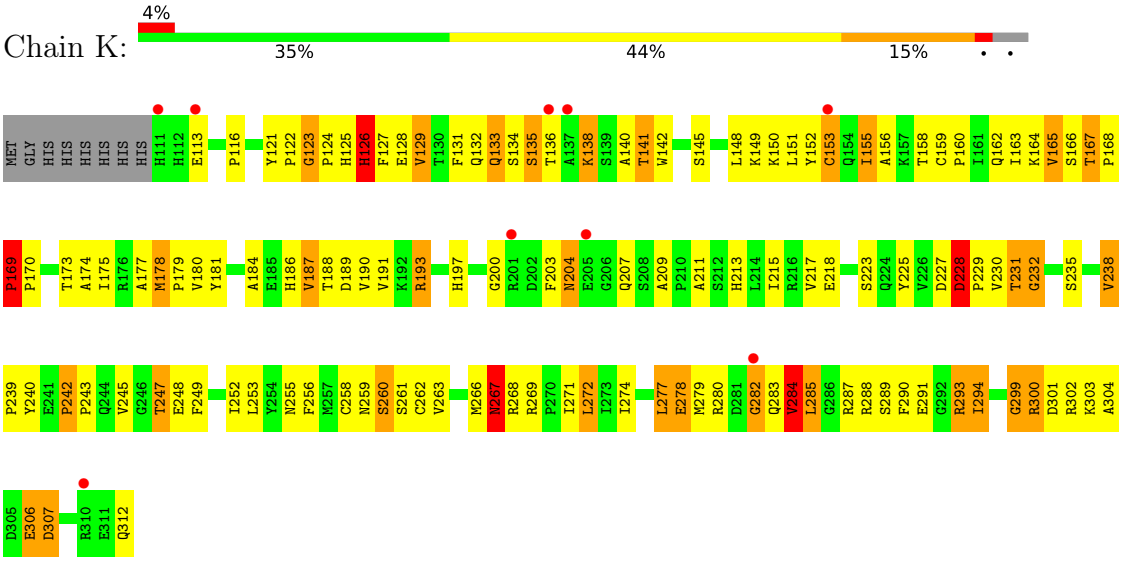
• Molecule 1: Tumor protein p73

Chain J:



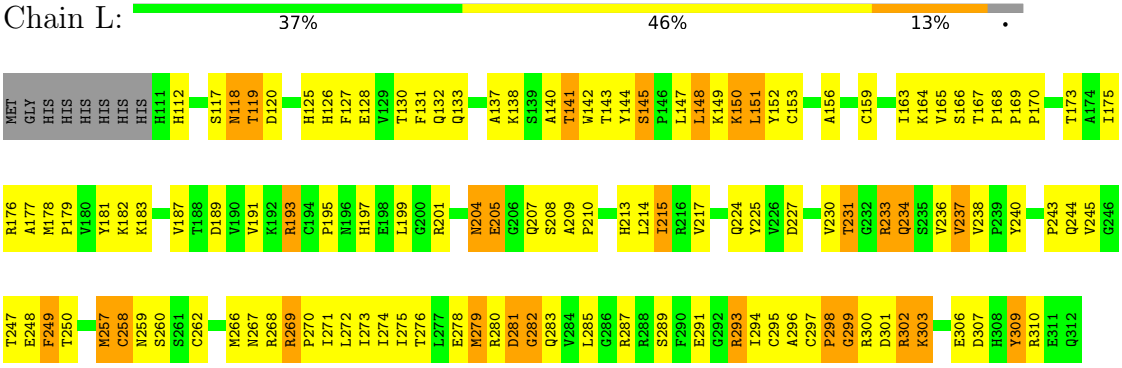
• Molecule 1: Tumor protein p73

Chain K:



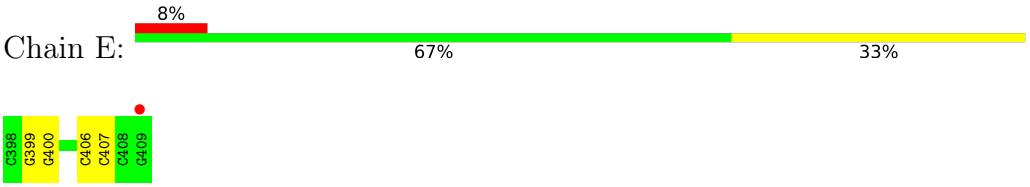
• Molecule 1: Tumor protein p73

Chain L:



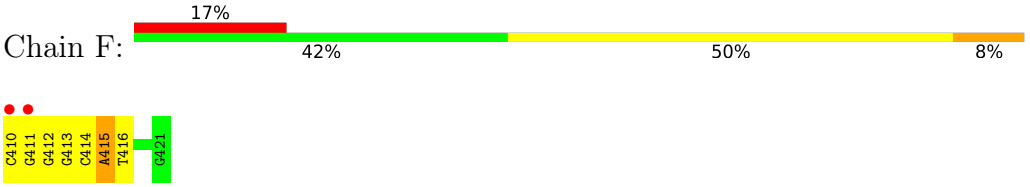
• Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3')

Chain E:



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

Chain F:

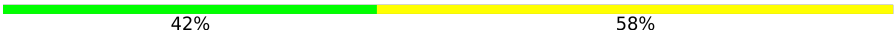


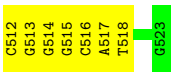
• Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3')

Chain G:

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

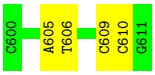
Chain H:





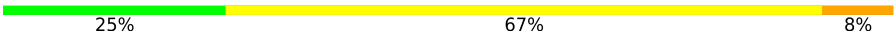
• Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3')

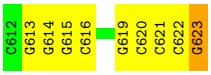
Chain M:



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

Chain N:



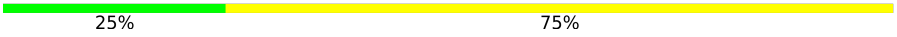


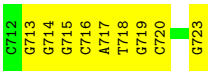
• Molecule 2: DNA (5'-D(*CP*GP*GP*GP*CP*AP*TP*GP*CP*CP*CP*G)-3')

Chain O:

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

Chain P:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.54Å 104.20Å 123.22Å 90.00° 96.55° 90.00°	Depositor
Resolution (Å)	19.99 – 2.95 19.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.99-2.95) 95.7 (19.99-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.93Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.239 , 0.285 0.238 , 0.282	Depositor DCC
R_{free} test set	843 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å^2)	68.6	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14716	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.45	0/1621	0.79	1/2204 (0.0%)
1	B	0.56	0/1599	0.81	3/2174 (0.1%)
1	C	0.50	0/1615	0.77	2/2196 (0.1%)
1	D	0.48	0/1599	0.75	0/2174
1	I	0.46	0/1599	0.72	0/2174
1	J	0.40	0/1599	0.73	1/2174 (0.0%)
1	K	0.52	0/1631	0.84	2/2217 (0.1%)
1	L	0.53	0/1631	0.85	1/2217 (0.0%)
2	E	0.54	0/272	0.84	0/418
2	F	0.77	0/272	1.29	2/418 (0.5%)
2	G	0.40	0/272	0.67	0/418
2	H	0.47	0/272	0.86	0/418
2	M	0.51	0/272	0.89	0/418
2	N	0.55	0/272	0.94	1/418 (0.2%)
2	O	0.51	0/272	0.88	0/418
2	P	0.45	0/272	0.84	0/418
All	All	0.50	0/15070	0.81	13/20874 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	415	DA	P-O3'-C3'	10.24	131.98	119.70
1	K	284	VAL	N-CA-C	5.80	126.65	111.00
1	B	168	PRO	C-N-CD	-5.70	108.07	120.60
2	N	623	DG	C4'-C3'-O3'	5.65	123.83	109.70
1	A	125	HIS	N-CA-C	-5.65	95.75	111.00

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	1581	0	1544	124	0
1	B	1560	0	1531	142	0
1	C	1575	0	1540	82	0
1	D	1560	0	1531	129	0
1	I	1560	0	1531	100	0
1	J	1560	0	1531	125	0
1	K	1590	0	1553	139	0
1	L	1590	0	1553	143	0
2	E	243	0	135	8	0
2	F	243	0	135	12	0
2	G	243	0	135	5	0
2	H	243	0	135	6	0
2	M	243	0	135	2	0
2	N	243	0	135	6	0
2	O	243	0	135	6	0
2	P	243	0	135	8	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	25	0	0	3	0
4	B	20	0	0	3	0
4	C	28	0	0	1	0
4	D	23	0	0	1	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
4	H	1	0	0	0	0
4	I	26	0	0	1	0
4	J	14	0	0	0	0
4	K	20	0	0	1	0
4	L	19	0	0	2	0
4	M	1	0	0	0	0
4	N	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	2	0	0	0	0
4	P	1	0	0	0	0
All	All	14716	0	13394	1003	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 1003 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:169:PRO:CD	1:B:170:PRO:HD3	1.62	1.28
1:D:115:ILE:CB	1:D:116:PRO:HD3	1.66	1.22
1:B:169:PRO:HD2	1:B:170:PRO:CD	1.75	1.15
1:D:310:ARG:HH11	1:D:310:ARG:HA	1.15	1.11
1:C:138:LYS:HA	1:C:299:GLY:HA3	1.34	1.10

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%)	173 (86%)	21 (10%)	6 (3%)	4 20
1	B	197/210 (94%)	165 (84%)	26 (13%)	6 (3%)	4 20
1	C	199/210 (95%)	170 (85%)	26 (13%)	3 (2%)	10 38
1	D	197/210 (94%)	153 (78%)	30 (15%)	14 (7%)	1 4
1	I	197/210 (94%)	166 (84%)	24 (12%)	7 (4%)	3 16
1	J	197/210 (94%)	161 (82%)	28 (14%)	8 (4%)	3 13
1	K	200/210 (95%)	158 (79%)	27 (14%)	15 (8%)	1 4
1	L	200/210 (95%)	167 (84%)	25 (12%)	8 (4%)	3 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1587/1680 (94%)	1313 (83%)	207 (13%)	67 (4%)	3 13

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PHE
1	B	168	PRO
1	B	169	PRO
1	C	243	PRO
1	D	115	ILE

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	176/186 (95%)	142 (81%)	34 (19%)	1 6
1	B	175/186 (94%)	147 (84%)	28 (16%)	2 10
1	C	176/186 (95%)	146 (83%)	30 (17%)	2 9
1	D	175/186 (94%)	151 (86%)	24 (14%)	3 15
1	I	175/186 (94%)	156 (89%)	19 (11%)	6 23
1	J	175/186 (94%)	148 (85%)	27 (15%)	2 11
1	K	178/186 (96%)	150 (84%)	28 (16%)	2 10
1	L	178/186 (96%)	148 (83%)	30 (17%)	2 9
All	All	1408/1488 (95%)	1188 (84%)	220 (16%)	2 11

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	310	ARG
1	J	151	LEU
1	L	309	TYR
1	L	193	ARG
1	I	168	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	186	HIS
1	J	213	HIS
1	I	196	ASN
1	I	255	ASN
1	J	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 monosaccharides 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

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^{th} 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	202/210 (96%)	0.13	4 (1%) 65 48	42, 74, 109, 114	2 (0%)
1	B	199/210 (94%)	0.00	1 (0%) 91 81	43, 73, 108, 129	2 (1%)
1	C	201/210 (95%)	-0.15	4 (1%) 65 48	41, 62, 99, 114	2 (0%)
1	D	199/210 (94%)	-0.06	4 (2%) 65 48	40, 69, 102, 120	1 (0%)
1	I	199/210 (94%)	-0.14	5 (2%) 57 40	42, 63, 102, 113	2 (1%)
1	J	199/210 (94%)	0.29	10 (5%) 28 18	52, 86, 112, 119	2 (1%)
1	K	202/210 (96%)	0.13	9 (4%) 33 21	42, 72, 100, 118	0
1	L	202/210 (96%)	-0.25	0 100 100	29, 53, 83, 96	1 (0%)
2	E	12/12 (100%)	0.71	1 (8%) 11 6	68, 79, 129, 155	0
2	F	12/12 (100%)	0.39	2 (16%) 1 1	57, 84, 126, 144	0
2	G	12/12 (100%)	0.14	0 100 100	66, 87, 99, 115	0
2	H	12/12 (100%)	-0.05	0 100 100	61, 85, 113, 121	0
2	M	12/12 (100%)	-0.01	0 100 100	51, 73, 100, 117	0
2	N	12/12 (100%)	-0.14	0 100 100	53, 76, 92, 95	0
2	O	12/12 (100%)	-0.17	0 100 100	64, 75, 108, 115	0
2	P	12/12 (100%)	-0.02	0 100 100	54, 70, 120, 128	0
All	All	1699/1776 (95%)	0.00	40 (2%) 59 42	29, 70, 107, 155	12 (0%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	409	DG	10.5
2	F	410	DC	5.4
1	K	205	GLU	5.3
1	A	111	HIS	4.6
1	C	139	SER	4.2

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^{th} 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
3	ZN	A	401	1/1	0.94	0.12	72,72,72,72	0
3	ZN	D	401	1/1	0.95	0.09	53,53,53,53	0
3	ZN	K	401	1/1	0.96	0.08	59,59,59,59	0
3	ZN	J	401	1/1	0.97	0.10	64,64,64,64	0
3	ZN	I	401	1/1	0.97	0.12	66,66,66,66	0
3	ZN	C	401	1/1	0.98	0.15	46,46,46,46	0
3	ZN	B	401	1/1	0.99	0.10	46,46,46,46	0
3	ZN	L	401	1/1	0.99	0.16	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.