Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 04:05 AM EDT

PDB ID	:	5KBD
Title	:	Structural Studies of Transcription Factor p73 DNA Binding Domain Bound to PA26 20-mer Response Element
Authors	:	Nguyen, H.T.; Huang, D.
Deposited on	:	2016-06-03
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (1)) were used in the production of this report:

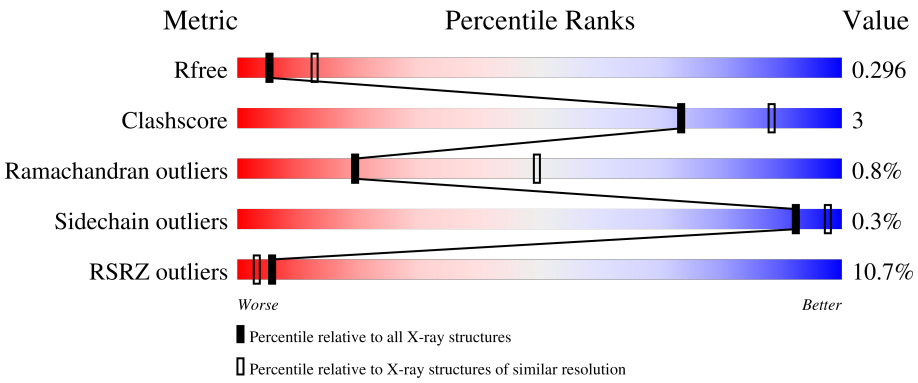
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	207	12% 87% 10% •
1	B	207	10% 86% 11% •
2	C	10	90% 10%
3	D	10	90% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6916 atoms, of which 3332 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
			Total	C	H	N	O	S			
1	A	201	3138	993	1552	285	297	11	0	0	0
1	B	201	3139	993	1553	285	297	11	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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

- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*GP*AP*CP*AP*AP*GP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	C	10	320	98	113	40	59	10	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*AP*CP*TP*TP*GP*TP*CP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
3	D	10	317	97	114	35	61	10	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

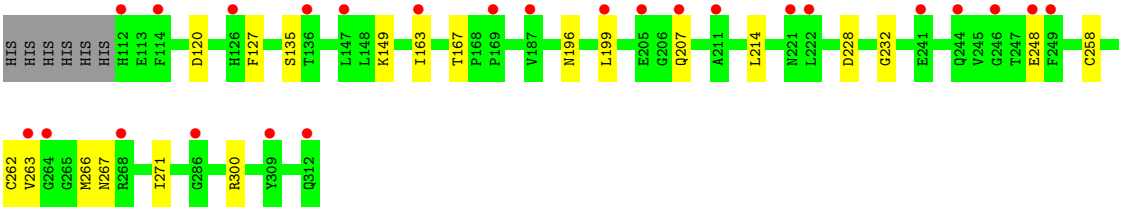
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	1	1	1	0	0
			Total	Zn		
4	B	1	1	1	0	0

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.

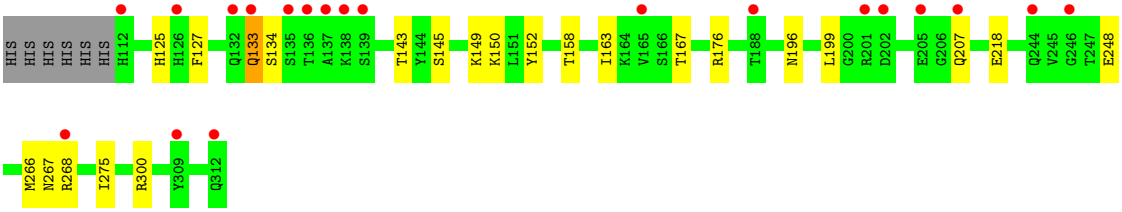
• Molecule 1: Tumor protein p73

Chain A:



• Molecule 1: Tumor protein p73

Chain B:



• Molecule 2: DNA (5'-D(P*GP*GP*AP*CP*AP*AP*GP*TP*CP*T)-3')

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	174.88Å 174.88Å 34.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.41 – 2.80 34.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.41-2.80) 99.1 (34.74-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.279 , 0.308 0.283 , 0.296	Depositor DCC
R_{free} test set	782 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 72.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.020 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6916	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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 (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	0.26	0/1627	0.42	0/2210
1	B	0.26	0/1627	0.42	0/2210
2	C	0.55	0/232	0.87	0/356
3	D	0.52	0/226	0.92	0/346
All	All	0.31	0/3712	0.51	0/5122

There are no bond length outliers.

There are no bond angle outliers.

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	1586	1552	1552	11	1
1	B	1586	1553	1553	14	1
2	C	207	113	113	1	0
3	D	203	114	114	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	3584	3332	3332	23	1

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 3.

All (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:CYS:O	1:A:267:ASN:ND2	2.09	0.84
1:B:300:ARG:NH1	3:D:17:DG:N7	2.38	0.71
1:B:158:THR:OG1	1:B:218:GLU:OE1	2.09	0.70
1:A:120:ASP:OD2	1:A:149:LYS:NZ	2.38	0.56
1:B:207:GLN:OE1	1:B:207:GLN:N	2.42	0.52
1:A:263:VAL:O	1:B:196:ASN:ND2	2.44	0.51
1:A:228:ASP:O	1:A:232:GLY:N	2.43	0.49
1:B:125:HIS:ND1	1:B:167:THR:O	2.46	0.47
1:B:134:SER:CB	1:B:143:THR:HA	2.45	0.46
1:B:248:GLU:N	1:B:248:GLU:OE1	2.48	0.46
1:B:127:PHE:CE1	1:B:163:ILE:HD11	2.51	0.46
1:A:207:GLN:N	1:A:207:GLN:OE1	2.49	0.45
1:A:127:PHE:CE1	1:A:163:ILE:HD11	2.53	0.44
1:B:176:ARG:O	1:B:275:ILE:HA	2.18	0.43
1:A:199:LEU:HD11	1:B:199:LEU:HD11	2.02	0.42
1:A:300:ARG:NH1	2:C:7:DG:N7	2.68	0.42
1:B:133:GLN:O	1:B:134:SER:C	2.58	0.41
1:A:214:LEU:CD1	1:A:258:CYS:HB3	2.50	0.41
1:A:248:GLU:OE1	1:A:248:GLU:N	2.54	0.41
1:A:266:MET:HE3	1:A:271:ILE:HG23	2.01	0.41
1:B:145:SER:O	1:B:149:LYS:N	2.53	0.41
1:B:266:MET:O	1:B:268:ARG:N	2.54	0.41
1:B:150:LYS:HD2	1:B:152:TYR:CZ	2.56	0.40

All (1) 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:A:167:THR:OG1	1:B:133:GLN:OE1[5_555]	2.15	0.05

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	199/207 (96%)	186 (94%)	12 (6%)	1 (0%)	29	61
1	B	199/207 (96%)	179 (90%)	18 (9%)	2 (1%)	15	44
All	All	398/414 (96%)	365 (92%)	30 (8%)	3 (1%)	19	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	SER
1	B	133	GLN
1	B	267	ASN

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	178/184 (97%)	177 (99%)	1 (1%)	86	96
1	B	178/184 (97%)	178 (100%)	0	100	100
All	All	356/368 (97%)	355 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASN

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

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 2 ligands modelled in this entry, 2 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	201/207 (97%)	0.76	25 (12%) 4 2	26, 92, 165, 201	0
1	B	201/207 (97%)	0.68	20 (9%) 7 4	30, 88, 168, 266	0
2	C	10/10 (100%)	0.23	0 100 100	47, 70, 80, 92	0
3	D	10/10 (100%)	0.14	0 100 100	45, 70, 79, 114	0
All	All	422/434 (97%)	0.69	45 (10%) 6 3	26, 88, 166, 266	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	HIS	7.2
1	B	136	THR	5.8
1	B	138	LYS	5.1
1	B	137	ALA	5.0
1	B	112	HIS	4.5
1	A	199	LEU	4.2
1	B	133	GLN	4.0
1	B	135	SER	4.0
1	A	136	THR	3.8
1	A	169	PRO	3.7
1	A	205	GLU	3.6
1	A	263	VAL	3.4
1	B	139	SER	3.3
1	A	246	GLY	3.3
1	A	126	HIS	3.3
1	A	248	GLU	3.2
1	B	312	GLN	3.1
1	A	244	GLN	3.1
1	B	201	ARG	3.0
1	B	165	VAL	3.0
1	A	268	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	241	GLU	2.8
1	B	205	GLU	2.8
1	A	249	PHE	2.6
1	B	132	GLN	2.6
1	B	202	ASP	2.6
1	B	309	TYR	2.6
1	B	244	GLN	2.5
1	A	264	GLY	2.5
1	B	246	GLY	2.5
1	A	163	ILE	2.5
1	A	309	TYR	2.5
1	B	188	THR	2.4
1	A	222	LEU	2.4
1	A	114	PHE	2.4
1	A	221	ASN	2.4
1	B	268	ARG	2.4
1	B	207	GLN	2.4
1	A	312	GLN	2.3
1	A	286	GLY	2.3
1	B	126	HIS	2.3
1	A	207	GLN	2.2
1	A	211	ALA	2.1
1	A	147	LEU	2.0
1	A	187	VAL	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	B	401	1/1	0.95	0.18	89,89,89,89	0
4	ZN	A	401	1/1	0.96	0.19	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.