



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:59 PM GMT

PDB ID : 4GUQ
Title : Structure of mutS139F p73 DNA binding domain complexed with 20BP DNA response element
Authors : Ethayathulla, A.S.; Nguyen, H.T.; Viadiu, H.
Deposited on : 2012-08-29
Resolution : 3.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

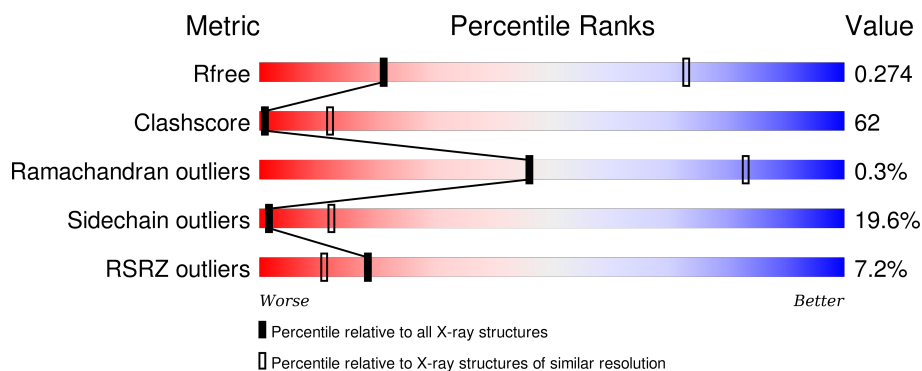
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	E	10	<div> <div>60%</div> <div>40%</div> </div>
1	F	10	<div> <div>90%</div> <div>10%</div> </div>
2	A	210	<div> <div>8%</div> <div>30%</div> <div>50%</div> <div>14%</div> <div>5%</div> </div>
2	B	210	<div> <div>7%</div> <div>31%</div> <div>50%</div> <div>11%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3533 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 DNA chain called DNA (5'-D(P*GP*AP*AP*CP*AP*TP*GP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	10	Total	C	N	O	P	0	0	0
			205	98	37	60	10			
1	F	10	Total	C	N	O	P	0	0	0
			205	98	37	60	10			

- Molecule 2 is a protein called Tumor protein p73.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	200	Total	C	N	O	S	0	0	0
			1566	982	280	293	11			
2	B	198	Total	C	N	O	S	0	0	0
			1555	977	279	288	11			

There are 26 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
A	139	PHE	SER	ENGINEERED MUTATION	UNP O15350
B	103	MET	-	INITIATING METHIONINE	UNP O15350
B	104	GLY	-	EXPRESSION TAG	UNP O15350

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	139	PHE	SER	ENGINEERED MUTATION	UNP O15350

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

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

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: DNA (5'-D(P*GP*AP*AP*CP*AP*TP*GP*TP*TP*C)-3')

Chain E: 



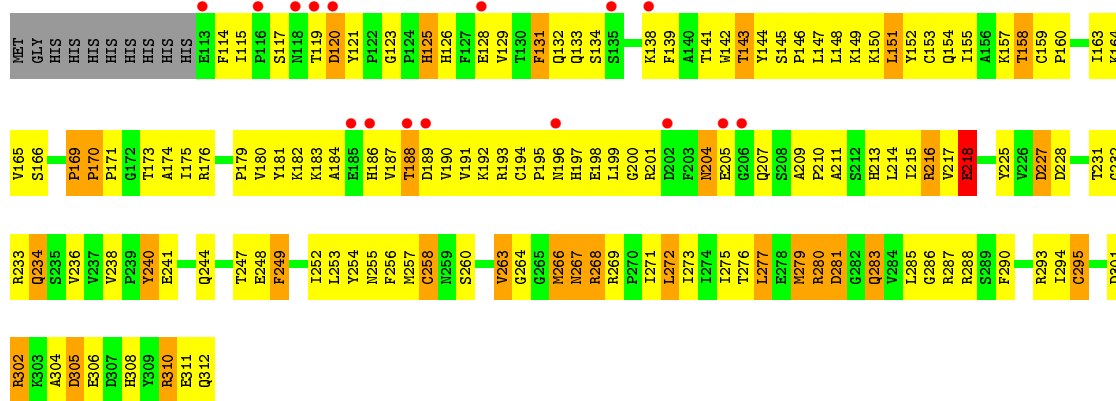
- Molecule 1: DNA (5'-D(P*GP*AP*AP*CP*AP*TP*GP*TP*TP*C)-3')

Chain F: 



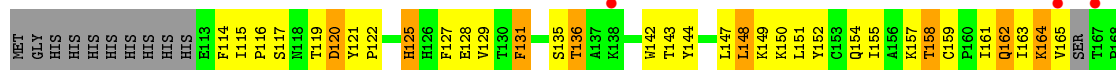
- Molecule 2: Tumor protein p73

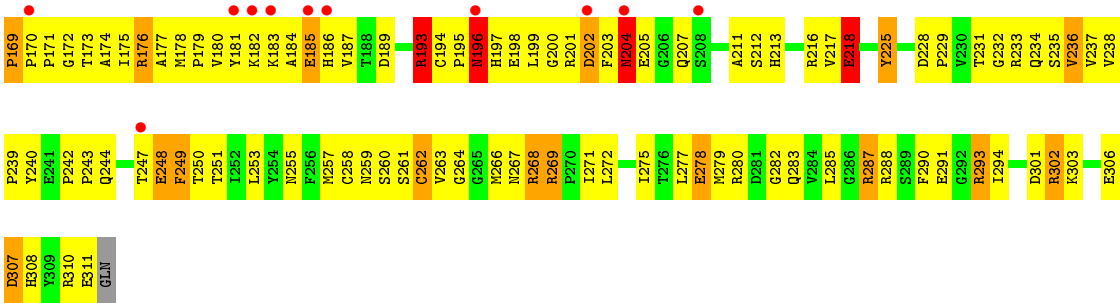
Chain A: 



- Molecule 2: Tumor protein p73

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	172.50 Å 172.50 Å 34.09 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 3.70 37.35 – 3.59	Depositor EDS
% Data completeness (in resolution range)	98.5 (100.00-3.70) 98.3 (37.35-3.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.56 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.302 , 0.316 0.302 , 0.274	Depositor DCC
R_{free} test set	301 reflections (4.89%)	DCC
Wilson B-factor (Å ²)	90.5	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 25.3	EDS
Estimated twinning fraction	0.068 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 7024 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	3533	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	E	0.39	0/229	0.79	0/351
1	F	0.49	0/229	0.81	0/351
2	A	0.82	2/1605 (0.1%)	0.89	2/2181 (0.1%)
2	B	0.90	4/1594 (0.3%)	0.95	8/2166 (0.4%)
All	All	0.82	6/3657 (0.2%)	0.91	10/5049 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	225	TYR	CE1-CZ	-5.91	1.30	1.38
2	B	193	ARG	CZ-NH2	5.70	1.40	1.33
2	B	218	GLU	CD-OE2	-5.64	1.19	1.25
2	A	218	GLU	CD-OE2	-5.28	1.19	1.25
2	B	243	PRO	N-CD	5.14	1.55	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	198	GLU	OE1-CD-OE2	-5.90	116.22	123.30
2	B	242	PRO	C-N-CD	5.85	140.68	128.40
2	B	250	THR	CA-CB-CG2	-5.70	104.42	112.40
2	A	169	PRO	C-N-CD	5.65	140.27	128.40
2	B	293	ARG	NE-CZ-NH1	-5.53	117.53	120.30

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	E	205	0	114	2	1
1	F	205	0	114	1	0
2	A	1566	0	1532	224	0
2	B	1555	0	1523	213	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	3533	0	3283	426	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 62.

The worst 5 of 426 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)
2:B:147:LEU:HD22	2:B:148:LEU:CD2	1.57	1.34
2:A:248:GLU:HB2	2:A:249:PHE:CE1	1.66	1.29
2:A:190:VAL:HG21	2:A:192:LYS:HE3	1.29	1.13
2:B:147:LEU:HD22	2:B:148:LEU:HD23	1.27	1.12
2:A:179:PRO:HB2	2:A:191:VAL:HG11	1.19	1.10

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:E:400:DG:O5'	1:E:409:DC:O3'[1_556]	2.04	0.16

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	198/210 (94%)	182 (92%)	16 (8%)	0	100	100
2	B	194/210 (92%)	176 (91%)	17 (9%)	1 (0%)	34	77
All	All	392/420 (93%)	358 (91%)	33 (8%)	1 (0%)	46	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	169	PRO

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	
2	A	174/186 (94%)	138 (79%)	36 (21%)	1	10
2	B	173/186 (93%)	141 (82%)	32 (18%)	2	14
All	All	347/372 (93%)	279 (80%)	68 (20%)	1	12

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	281	ASP
2	B	131	PHE
2	B	278	GLU
2	A	283	GLN
2	A	305	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	125	HIS
2	B	154	GLN

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Mol	Chain	Res	Type
2	B	259	ASN
2	A	267	ASN
2	B	213	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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 ⓘ

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 [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	E	10/10 (100%)	-0.20	0	100 100	73, 77, 85, 91	0
1	F	10/10 (100%)	-0.45	0	100 100	76, 81, 99, 105	0
2	A	200/210 (95%)	0.30	16 (8%)	15 9	50, 75, 107, 175	46 (23%)
2	B	198/210 (94%)	0.31	14 (7%)	19 11	51, 77, 131, 168	58 (29%)
All	All	418/440 (95%)	0.28	30 (7%)	18 11	50, 76, 123, 175	104 (24%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	186	HIS	4.4
2	B	138	LYS	4.0
2	A	189	ASP	4.0
2	A	202	ASP	3.9
2	B	167	THR	3.6

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ZN	A	401	1/1	0.99	0.15	-0.89	88,88,88,88	0
3	ZN	B	401	1/1	0.96	0.14	-1.32	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.