WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 7, 2023 – 12:58 AM EDT

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
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:

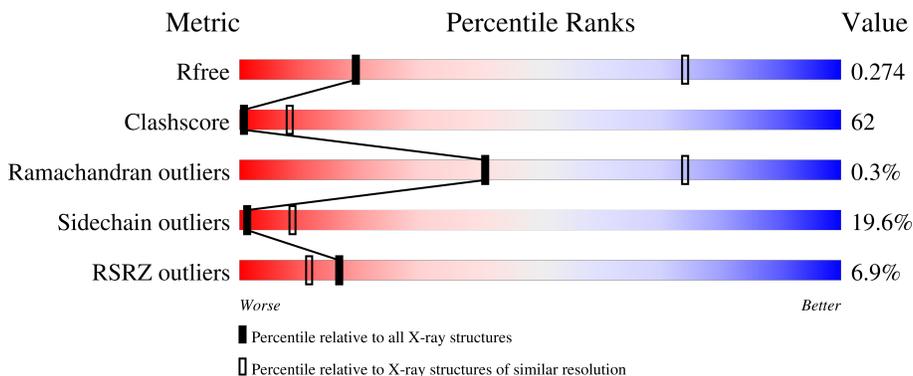|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.274
Clashscore		62
Ramachandran outliers		0.3%
Sidechain outliers		19.6%
RSRZ outliers		6.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (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 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	E	10	60% 40%
1	F	10	90% 10%
2	A	210	7% / 30% 50% 14% 5%
2	B	210	7% / 31% 50% 11% · 6%

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	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

3 Residue-property plots ⓘ

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: 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:

P169 P170 P171 G172 T173 A174 I175 R176 A177 M178 P179 V180 Y181 K182 K183 A184 E185 H186 V187 T188 D189 R193 C194 P195 N196 H197 E198 L199 G200 R201 D202 F203 N204 E205 G206 Q207 S208 A211 S212 H213 R216 V217 E218 Y225 D228 P229 V230 T231 G232 R233 Q234 S235 V236 V237 V238

P239 Y240 E241 P242 P243 Q244 T247 E248 F249 T250 T251 I252 L253 Y254 N255 F256 M257 C258 N259 S260 S261 C262 V263 G264 G265 M266 N267 R268 R269 P270 I271 L272 I275 T276 L277 E278 M279 R280 D281 G282 Q283 V284 L285 G286 R287 R288 S289 F290 E291 G292 R293 I294 D301 R302 K303 E306

D307 H308 Y309 R310 E311 GLN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	172.50Å 172.50Å 34.09Å 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
$< I/\sigma(I) >$ [1]	1.82 (at 3.56Å)	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	330 reflections (4.70%)	wwPDB-VP
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 , 26.2	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.068 for h,-h-k,-l	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.*

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[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	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(^{o})	Ideal(^{o})
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%)	29	66
All	All	392/420 (93%)	358 (91%)	33 (8%)	1 (0%)	41	74

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	7
2	B	173/186 (93%)	141 (82%)	32 (18%)	1	10
All	All	347/372 (93%)	279 (80%)	68 (20%)	1	9

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

Mol	Chain	Res	Type
2	B	258	CYS
2	B	268	ARG
2	B	307	ASP
2	A	267	ASN
2	A	266	MET

Sometimes 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	213	HIS
2	B	259	ASN

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Mol	Chain	Res	Type
2	B	308	HIS
2	B	283	GLN
2	B	125	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 monosaccharides 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 ⓘ

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, 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%)	-0.22	0	100	100	73, 77, 85, 91	0
1	F	10/10 (100%)	-0.47	0	100	100	76, 81, 99, 105	0
2	A	200/210 (95%)	0.27	15 (7%)	14	10	50, 75, 107, 175	46 (23%)
2	B	198/210 (94%)	0.29	14 (7%)	16	11	51, 77, 131, 168	58 (29%)
All	All	418/440 (95%)	0.25	29 (6%)	16	11	50, 76, 123, 175	104 (24%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	186	HIS	4.6
2	B	138	LYS	4.1
2	A	189	ASP	3.9
2	A	202	ASP	3.8
2	B	167	THR	3.6

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	ZN	B	401	1/1	0.96	0.14	83,83,83,83	0
3	ZN	A	401	1/1	0.99	0.15	88,88,88,88	0

6.5 Other polymers ⓘ

There are no such residues in this entry.

W O R L D W I D E
PDB
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