



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 02:06 PM GMT

PDB ID : 3OQ5
Title : Crystal structure of the 3-MBT domain from human L3MBTL1 in complex with p53K382me1
Authors : Roy, S.; West, L.E.; Weiner, K.L.; Hayashi, R.; Shi, X.; Appella, E.; Gozani, O.; Kutateladze, T.
Deposited on : 2010-09-02
Resolution : 2.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

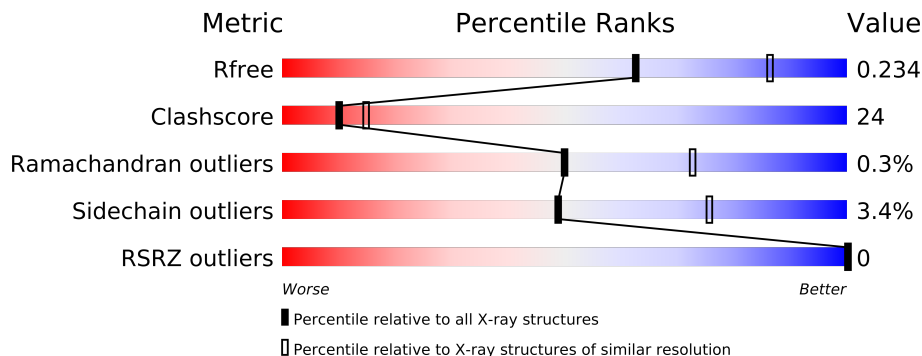
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	
1	C	345	
2	D	10	
2	E	10	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8043 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lethal(3)malignant brain tumor-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2509	1617	427	453	12			
1	B	309	Total	C	N	O	S	0	0	0
			2509	1617	427	453	12			
1	C	309	Total	C	N	O	S	0	0	0
			2509	1617	427	453	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLY	-	EXPRESSION TAG	UNP Q9Y468
A	187	PRO	-	EXPRESSION TAG	UNP Q9Y468
A	188	LEU	-	EXPRESSION TAG	UNP Q9Y468
A	189	GLY	-	EXPRESSION TAG	UNP Q9Y468
A	190	SER	-	EXPRESSION TAG	UNP Q9Y468
B	186	GLY	-	EXPRESSION TAG	UNP Q9Y468
B	187	PRO	-	EXPRESSION TAG	UNP Q9Y468
B	188	LEU	-	EXPRESSION TAG	UNP Q9Y468
B	189	GLY	-	EXPRESSION TAG	UNP Q9Y468
B	190	SER	-	EXPRESSION TAG	UNP Q9Y468
C	186	GLY	-	EXPRESSION TAG	UNP Q9Y468
C	187	PRO	-	EXPRESSION TAG	UNP Q9Y468
C	188	LEU	-	EXPRESSION TAG	UNP Q9Y468
C	189	GLY	-	EXPRESSION TAG	UNP Q9Y468
C	190	SER	-	EXPRESSION TAG	UNP Q9Y468

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	1	Total	C	N	O	0	0	0
			10	7	2	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	1	Total	C	N	O	0	0	0
			10	7	2	1			

- Molecule 3 is water.

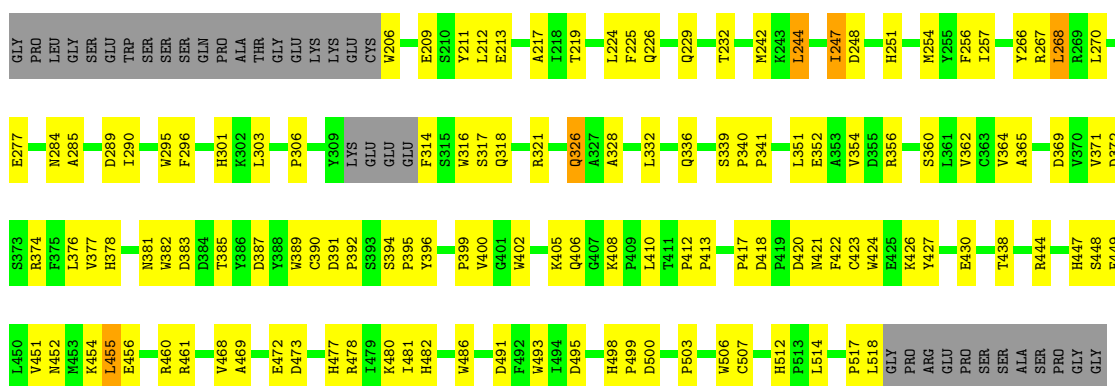
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	149	Total	O	0	0
			149	149		
3	B	155	Total	O	0	0
			155	155		
3	C	189	Total	O	0	0
			189	189		
3	D	3	Total	O	0	0
			3	3		

3 Residue-property plots

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.

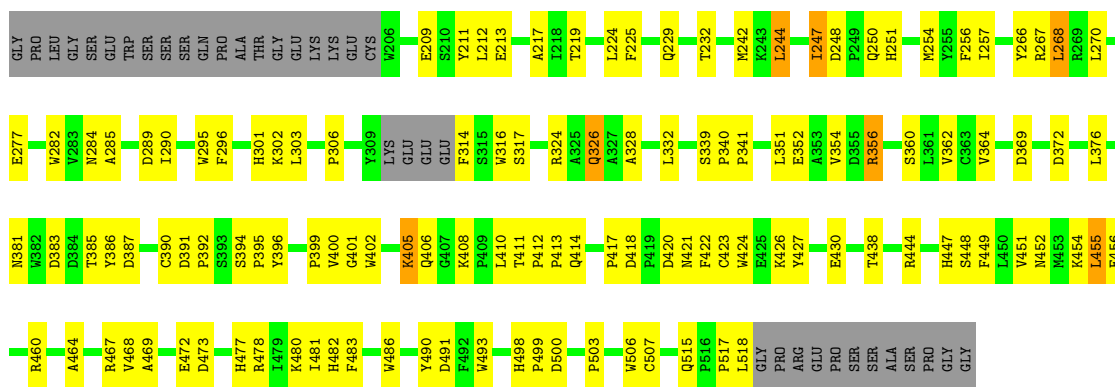
- Molecule 1: Lethal(3)malignant brain tumor-like protein

Chain A:



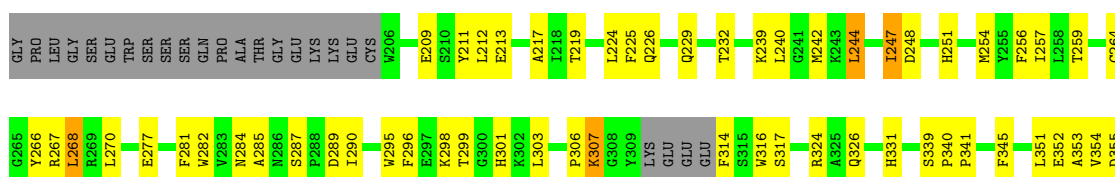
- Molecule 1: Lethal(3)malignant brain tumor-like protein

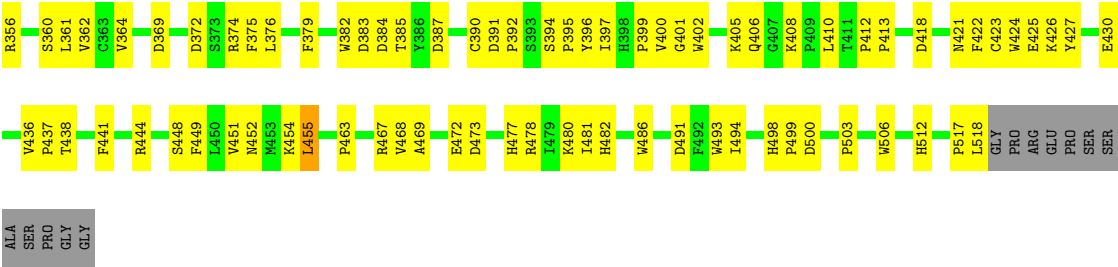
Chain B:



- Molecule 1: Lethal(3)malignant brain tumor-like protein

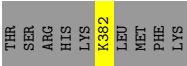
Chain C:





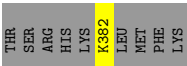
- Molecule 2: Cellular tumor antigen p53

Chain D:



- Molecule 2: Cellular tumor antigen p53

Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	109.08Å 109.08Å 90.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.65 – 2.50 46.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.65-2.50) 100.0 (46.65-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1.357)	Depositor
R, R_{free}	0.205 , 0.234 0.204 , 0.234	Depositor DCC
R_{free} test set	2084 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	EDS
Estimated twinning fraction	0.469 for -h,-k,l 0.406 for h,-h-k,-l 0.406 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 41472 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8043	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLZ

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	0.31	0/2607	0.43	0/3564
1	B	0.32	0/2607	0.46	2/3564 (0.1%)
1	C	0.32	0/2607	0.46	2/3564 (0.1%)
All	All	0.32	0/7821	0.45	4/10692 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	356	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	C	356	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	C	356	ARG	NE-CZ-NH2	-5.75	117.42	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2509	0	2348	109	0
1	B	2509	0	2348	114	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2509	0	2348	128	0
2	D	10	0	15	3	0
2	E	10	0	15	4	0
3	A	149	0	0	14	0
3	B	155	0	0	22	0
3	C	189	0	0	35	0
3	D	3	0	0	0	0
All	All	8043	0	7074	346	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

The worst 5 of 346 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:401:GLY:HA2	3:C:664:HOH:O	1.45	1.12
1:C:298:LYS:HB2	3:C:576:HOH:O	1.70	0.91
1:B:506:TRP:HB3	3:B:590:HOH:O	1.72	0.88
1:A:374:ARG:HD2	3:A:109:HOH:O	1.81	0.81
1:C:339:SER:HB2	1:C:340:PRO:HD2	1.63	0.80

There are no symmetry-related clashes.

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	
1	A	305/345 (88%)	289 (95%)	15 (5%)	1 (0%)	50	73
1	B	305/345 (88%)	292 (96%)	12 (4%)	1 (0%)	50	73
1	C	305/345 (88%)	291 (95%)	13 (4%)	1 (0%)	50	73
All	All	915/1035 (88%)	872 (95%)	40 (4%)	3 (0%)	50	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	383	ASP
1	A	383	ASP
1	B	383	ASP

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	273/301 (91%)	264 (97%)	9 (3%)	50	76
1	B	273/301 (91%)	263 (96%)	10 (4%)	45	72
1	C	273/301 (91%)	264 (97%)	9 (3%)	50	76
All	All	819/903 (91%)	791 (97%)	28 (3%)	49	75

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	317	SER
1	B	360	SER
1	C	360	SER
1	B	326	GLN
1	B	351	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	284	ASN
1	B	421	ASN
1	C	421	ASN
1	B	326	GLN
1	A	336	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLZ	D	382	-	9,9,10	5.88	1 (11%)	7,9,11	1.42	2 (28%)
2	MLZ	E	382	-	9,9,10	5.96	1 (11%)	7,9,11	1.41	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLZ	D	382	-	-	0/6/8/10	0/0/0/0
2	MLZ	E	382	-	-	0/6/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	382	MLZ	O-C	17.79	1.23	1.11
2	D	382	MLZ	O-C	17.53	1.23	1.11

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	382	MLZ	CM-NZ-CE	2.80	120.14	112.18
2	D	382	MLZ	CM-NZ-CE	2.49	119.26	112.18
2	D	382	MLZ	C-CA-N	-2.42	111.41	113.83
2	E	382	MLZ	C-CA-N	-2.20	111.63	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	A	309/345 (89%)	-0.17	0 100 100	27, 44, 62, 72	0
1	B	309/345 (89%)	-0.23	0 100 100	26, 44, 62, 71	0
1	C	309/345 (89%)	-0.22	0 100 100	27, 45, 63, 73	0
2	D	1/10 (10%)	-0.86	0 100 100	40, 40, 40, 40	0
2	E	1/10 (10%)	-1.18	0 100 100	47, 47, 47, 47	0
All	All	929/1055 (88%)	-0.21	0 100 100	26, 44, 62, 73	0

There are no RSRZ outliers to report.

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MLZ	D	382	10/11	0.16	2.28	27,36,49,53	0
2	MLZ	E	382	10/11	0.14	0.19	30,44,62,68	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.