

# wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 06:16 am BST

PDB ID : 6QB6

Title : Mcl1 in complex with a Fab

Authors : Hargreaves, D. Deposited on : 2018-12-20

Resolution : 2.24 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 following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} Mol Probity & : & 4.02 \text{b-}467 \\ Xtriage (Phenix) & : & 1.13 \end{array}$ 

henix) : 1.13 EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)
oteins) : Engh & Huber (200)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

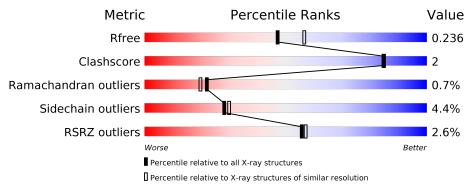
Validation Pipeline (wwPDB-VP) : 2.11

### 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 2.24 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 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	162	86%	10%
2	Н	230	83%	8% 9%
3	L	220	90%	7% •



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4583 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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	159	Total	C 700	N	0	S	0	0	0
			1265	793	231	238	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	GLY	-	expression tag	UNP Q07820
A	167	PRO	-	expression tag	UNP Q07820
A	168	LEU	-	expression tag	UNP Q07820
A	169	GLY	-	expression tag	UNP Q07820
A	170	SER	_	expression tag	UNP Q07820
A	171	GLU	-	expression tag	UNP Q07820
A	172	ASP	-	expression tag	UNP Q07820
A	173	ASP	-	expression tag	UNP Q07820
A	193	SER	ALA	conflict	UNP Q07820
A	196	SER	THR	conflict	UNP Q07820
A	199	LEU	MET	conflict	UNP Q07820
A	201	GLU	ARG	conflict	UNP Q07820
A	202	ALA	SER	conflict	UNP Q07820
A	205	ALA	THR	conflict	UNP Q07820
A	206	GLY	SER	conflict	UNP Q07820
A	208	ARG	LYS	conflict	UNP Q07820

• Molecule 2 is a protein called Fab Heavy Chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Н	210	Total 1565	C 992	N 260	O 306	S 7	0	0	0

• Molecule 3 is a protein called Fab Light Chain.



Mol	Chain	Residues					ZeroOcc	AltConf	Trace	
2	т	213	Total	С	N	О	S	0	0	0
3	L	∠13	1599	990	271	332	6	0	0	0

### • Molecule 4 is water.

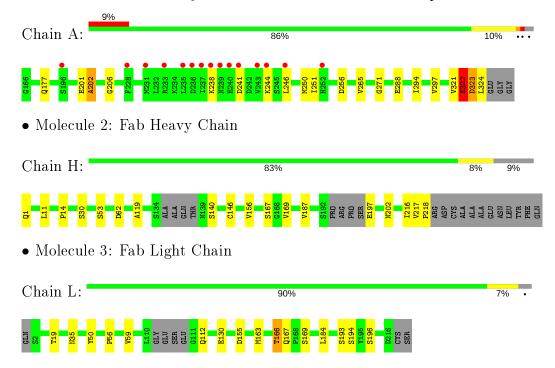
Mol	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	Н	52	Total O 52 52	0	0
4	L	73	Total O 73 73	0	0



# 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 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: Induced myeloid leukemia cell differentiation protein Mcl-1





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	148.05Å 42.46Å 106.23Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 113.19° 90.00°	Depositor
Resolution (Å)	47.71 - 2.24	Depositor
Resolution (A)	47.71 - 2.24	EDS
% Data completeness	99.2 (47.71-2.24)	Depositor
(in resolution range)	99.2 (47.71-2.24)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.23  (at  2.24Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
$R, R_{free}$	0.187 , $0.232$	Depositor
It, It free	0.190 , 0.236	DCC
$R_{free}$ test set	1497 reflections $(5.08\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.29 , 38.7	EDS
L-test for twinning <sup>2</sup>	$ < L >=0.46, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o$ , $F_c$ correlation	0.95	EDS
Total number of atoms	4583	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.21% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

#### 5.1 Standard geometry (i)

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		
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.50	0/1286	0.65	0/1731	
2	Н	0.52	0/1602	0.71	0/2184	
3	L	0.51	0/1636	0.71	0/2233	
All	All	0.51	0/4524	0.69	0/6148	

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	1265	0	1263	10	0
2	Н	1565	0	1539	5	0
3	L	1599	0	1526	5	0
4	A	29	0	0	0	0
4	Н	52	0	0	0	0
4	L	73	0	0	1	0
All	All	4583	0	4328	20	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 2.

The worst 5 of 20 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$egin{array}{c}  ext{Interatomic} \  ext{distance } ( ext{Å}) \end{array}$	Clash overlap (Å)	
3:L:35:ASN:HD22	3:L:50:TYR:HA	1.59	0.68	
1:A:177:GLN:HG3	1:A:202:ALA:HB2	1.78	0.65	
1:A:241:ASP:HA	1:A:244:LYS:HD3	1.80	0.61	
1:A:251:ILE:HG13	1:A:297:VAL:HG22	1.85	0.57	
3:L:19:THR:HG22	4:L:371:HOH:O	2.06	0.54	

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	Perce	ntiles
1	A	$157/162 \ (97\%)$	149 (95%)	5 (3%)	3 (2%)	8	3
2	Н	$204/230 \ (89\%)$	196 (96%)	7 (3%)	1 (0%)	29	28
3	L	$209/220 \ (95\%)$	205 (98%)	4 (2%)	0	100	100
All	All	570/612 (93%)	550 (96%)	16 (3%)	4 (1%)	22	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	ALA
1	A	201	GLU
1	A	322	GLU
2	Н	140	SER

#### 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	136/137~(99%)	129 (95%)	7 (5%)	24 23
2	Н	176/192 (92%)	169 (96%)	7 (4%)	31 34
3	L	183/189 (97%)	175 (96%)	8 (4%)	28 30
All	All	495/518 (96%)	473 (96%)	22 (4%)	28 30

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Н	62	ASP
2	Н	197	GLU
3	L	193	SER
2	Н	156	VAL
2	Н	167	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	35	ASN
3	L	112	GLN
3	L	201	HIS

#### 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 carbohydrates in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.



### 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	202:GLU	С	205:GLY	N	2.93



### 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,  $95^{th}$  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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	159/162~(98%)	0.23	15 (9%) 8 8	28, 54, 133, 140	0
2	Н	210/230 (91%)	-0.42	0 100 100	24, 39, 73, 100	0
3	L	213/220 (96%)	-0.51	0 100 100	24, 36, 54, 98	0
All	All	582/612 (95%)	-0.28	15 (2%) 56 57	24, 41, 94, 140	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ILE	8.7
1	A	235	LEU	5.5
1	A	246	LEU	5.4
1	A	243	VAL	5.3
1	A	236	ASP	4.3

#### 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)

There are no ligands in this entry.



# 6.5 Other polymers (i)

There are no such residues in this entry.

