



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 05:58 PM BST

PDB ID : 6QFI
Title : Structure of human Mcl-1 in complex with BIM BH3 peptide
Authors : Dokurno, P.; Murray, J.; Davidson, J.; Chen, I.; Davis, B.; Graham, C.J.; Harris, R.; Jordan, A.M.; Matassova, N.; Pedder, C.; Ray, S.; Roughley, S.; Smith, J.; Walmsley, C.; Wang, Y.; Whitehead, N.; Williamson, D.S.; Casara, P.; Le Diguarher, T.; Hickman, J.; Stark, J.; Kotschy, A.; Geneste, O.; Hubbard, R.E.
Deposited on : 2019-01-10
Resolution : 2.40 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

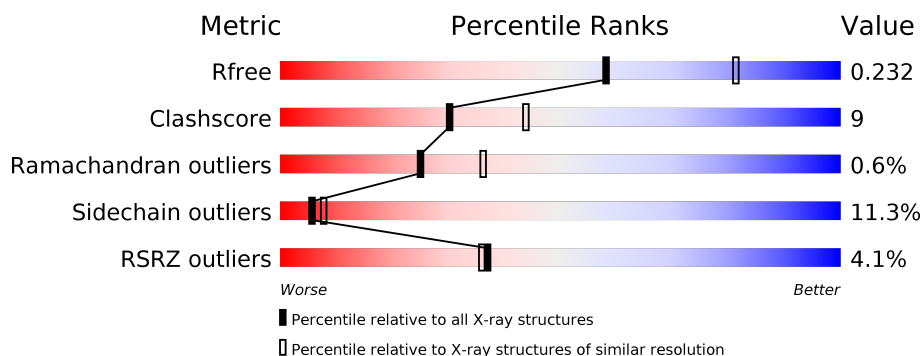
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	A	162	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>20%</div> <div>5%</div> <div>9%</div> </div> </div>
2	B	26	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>8%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1410 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	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1165	733	211	218	3			

There are 5 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

- Molecule 2 is a protein called Bcl-2-like protein 11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	0	0	0
			191	124	32	35			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Zn	0	0
			4	4		

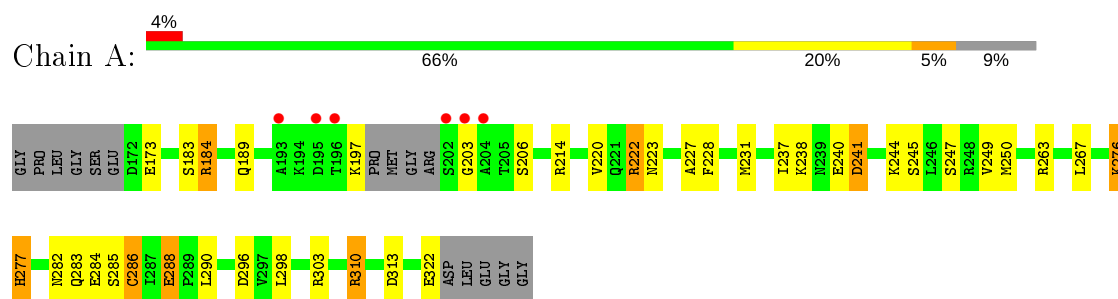
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	10	Total	O	0	0
			10	10		

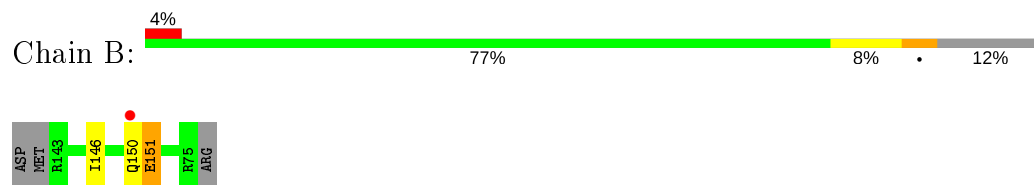
3 Residue-property plots [i](#)

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: Induced myeloid leukemia cell differentiation protein Mcl-1



- Molecule 2: Bcl-2-like protein 11



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	52.75Å 71.70Å 117.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.1 (20.00-2.40) 88.4 (19.98-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.186 , 0.236 0.190 , 0.232	Depositor DCC
R_{free} test set	359 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1410	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.56	0/1183	0.69	0/1594
2	B	0.63	0/196	0.75	0/266
All	All	0.57	0/1379	0.70	0/1860

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	ARG	Sidechain
1	A	222	ARG	Sidechain
1	A	263	ARG	Sidechain
1	A	303	ARG	Sidechain
1	A	310	ARG	Sidechain

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	1165	0	1150	24	2
2	B	191	0	171	1	2
3	A	4	0	0	0	1
4	A	40	0	0	7	0
4	B	10	0	0	0	0
All	All	1410	0	1321	25	3

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 9.

All (25) 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:241:ASP:OD2	4:A:501:HOH:O	1.81	0.99
1:A:203:GLY:HA2	1:A:206:SER:HB2	1.76	0.68
2:B:146:ILE:HD13	2:B:146:ILE:N	2.13	0.64
1:A:184:ARG:HH22	1:A:197:LYS:C	2.01	0.63
1:A:240:GLU:OE1	1:A:285:SER:HA	2.00	0.62
1:A:240:GLU:OE1	1:A:285:SER:CA	2.48	0.62
1:A:228:PHE:CD1	1:A:231:MET:CE	2.85	0.60
1:A:277:HIS:CE1	4:A:528:HOH:O	2.56	0.58
1:A:237:ILE:HG22	4:A:522:HOH:O	2.03	0.57
1:A:222:ARG:HD3	4:A:529:HOH:O	2.07	0.54
1:A:240:GLU:OE1	1:A:285:SER:HB3	2.08	0.53
1:A:228:PHE:HD1	1:A:231:MET:CE	2.23	0.52
1:A:240:GLU:OE1	1:A:286:CYS:N	2.42	0.52
1:A:228:PHE:CD1	1:A:231:MET:HE3	2.45	0.52
1:A:277:HIS:HB3	4:A:537:HOH:O	2.10	0.50
1:A:310:ARG:NH2	1:A:313:ASP:OD2	2.45	0.50
1:A:288:GLU:OE2	1:A:288:GLU:HA	2.11	0.49
1:A:227:ALA:O	1:A:231:MET:HG3	2.14	0.48
1:A:245:SER:O	1:A:249:VAL:HG23	2.17	0.44
1:A:223:ASN:HB2	4:A:515:HOH:O	2.18	0.44
1:A:240:GLU:OE1	1:A:285:SER:CB	2.66	0.43
1:A:189:GLN:NE2	1:A:276:LYS:HE3	2.33	0.43
1:A:282:ASN:OD1	1:A:284:GLU:N	2.54	0.41
1:A:214:ARG:NH1	4:A:503:HOH:O	2.39	0.41
1:A:250:MET:HG2	1:A:267:LEU:HD13	2.03	0.41

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:GLU:OE1	3:A:404:ZN:ZN[8_544]	1.50	0.70
1:A:286:CYS:SG	1:A:286:CYS:SG[3_455]	1.66	0.54
1:A:322:GLU:OE2	2:B:151:GLU:OE2[8_444]	2.16	0.04

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	143/162 (88%)	136 (95%)	6 (4%)	1 (1%)	22	32
2	B	21/26 (81%)	21 (100%)	0	0	100	100
All	All	164/188 (87%)	157 (96%)	6 (4%)	1 (1%)	25	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	GLN

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	124/139 (89%)	110 (89%)	14 (11%)	6	8
2	B	17/22 (77%)	15 (88%)	2 (12%)	5	7
All	All	141/161 (88%)	125 (89%)	16 (11%)	6	8

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	GLU
1	A	183	SER
1	A	220	VAL
1	A	238	LYS
1	A	241	ASP
1	A	244	LYS
1	A	247	SER
1	A	276	LYS
1	A	277	HIS
1	A	286	CYS
1	A	288	GLU
1	A	290	LEU
1	A	296	ASP
1	A	298	LEU
2	B	150	GLN
2	B	151	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	221	GLN

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 4 ligands modelled in this entry, 4 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	147/162 (90%)	-0.03	6 (4%) 37 36	27, 44, 90, 113	0
2	B	23/26 (88%)	-0.07	1 (4%) 35 33	30, 44, 70, 84	0
All	All	170/188 (90%)	-0.04	7 (4%) 37 36	27, 44, 86, 113	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	THR	6.1
1	A	202	SER	4.6
1	A	203	GLY	3.6
1	A	193	ALA	3.5
1	A	204	ALA	2.6
1	A	195	ASP	2.5
2	B	150	GLN	2.1

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(\AA^2)	Q<0.9
3	ZN	A	403	1/1	0.81	0.28	88,88,88,88	1
3	ZN	A	402	1/1	0.99	0.07	42,42,42,42	0
3	ZN	A	404	1/1	0.99	0.04	63,63,63,63	0
3	ZN	A	401	1/1	1.00	0.05	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.