



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 1, 2018 – 09:18 AM EST

PDB ID : 6FN1  
EMDB ID: : EMD-4281  
Title : Zosuquidar and UIC2 Fab complex of human-mouse chimeric ABCB1 (ABCB1HM)  
Authors : Alam, A.; Locher, K.P.  
Deposited on : 2018-02-02  
Resolution : 3.58 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

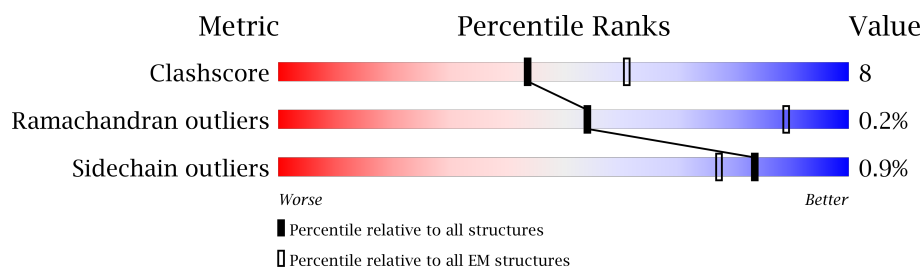
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.58 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1249	 74% 20% • 5%
2	B	220	 77% 21% •
3	C	225	 84% 16%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12739 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Human-mouse chimeric ABCB1 (ABCBHM).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0
			9186	5915	1553	1685	33		

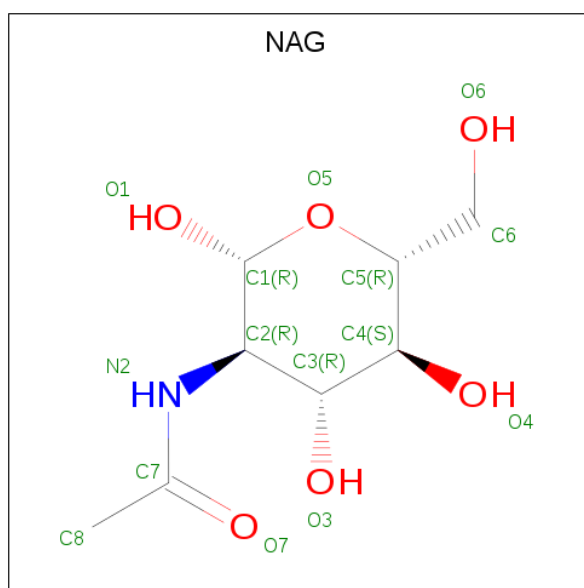
- Molecule 2 is a protein called UIC2 Antigen Binding Fragment Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	220	Total	C	N	O	S	1	0
			1713	1071	292	342	8		

- Molecule 3 is a protein called UIC2 Antigen Binding Fragment Heavy Chain.

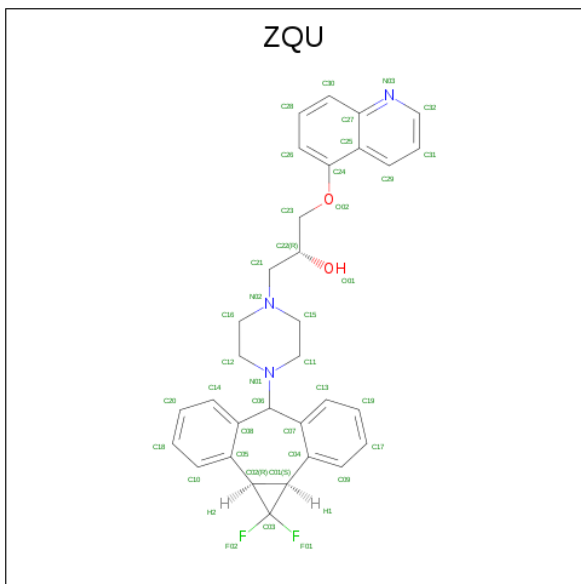
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	225	Total	C	N	O	S	1	0
			1720	1100	274	337	9		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 42	C 24	N 3	O 15	0
4	A	1	Total 42	C 24	N 3	O 15	0
4	A	1	Total 42	C 24	N 3	O 15	0

- Molecule 5 is Zosuquidar (three-letter code: ZQU) (formula:  $C_{32}H_{31}F_2N_3O_2$ ).

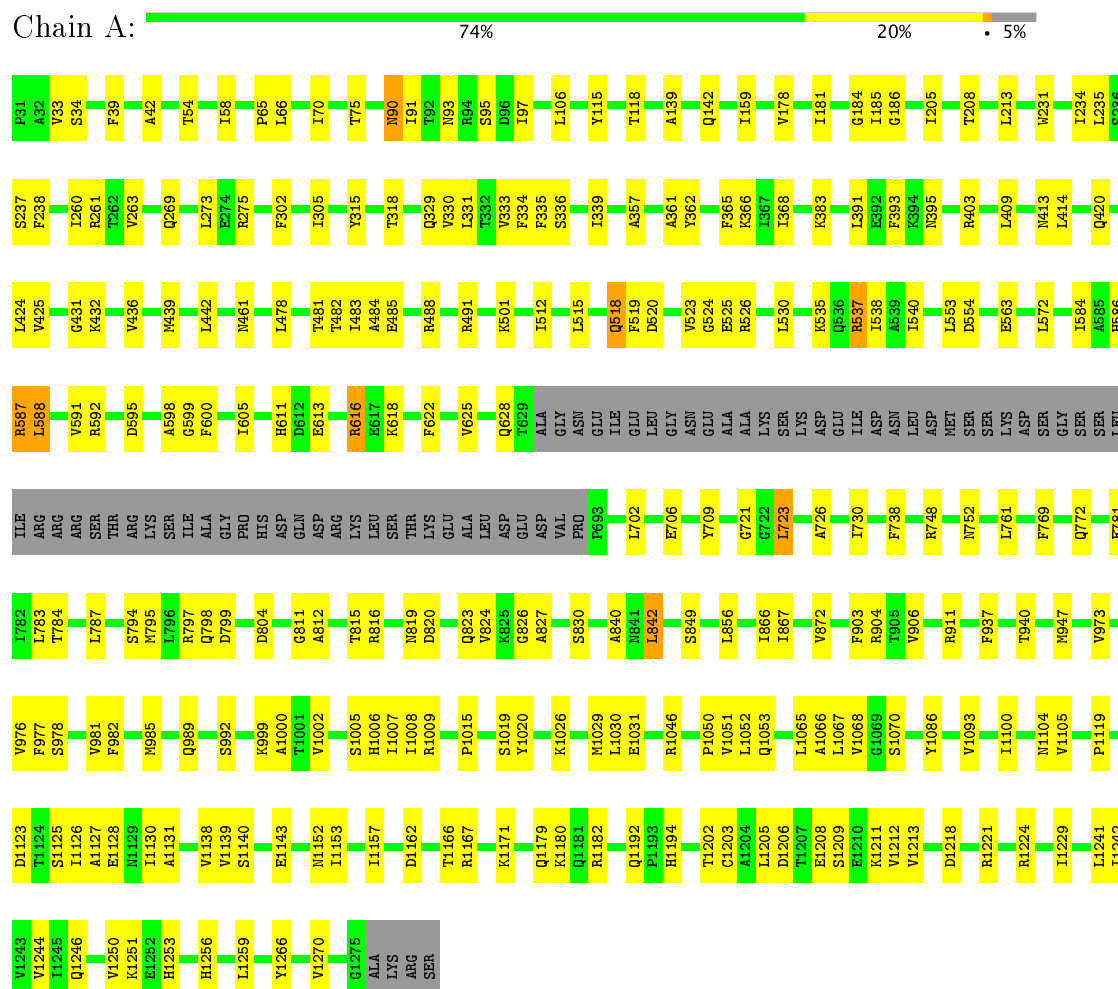


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 78	C 64	F 4	N 6	O 4	0
5	A	1	Total 78	C 64	F 4	N 6	O 4	0

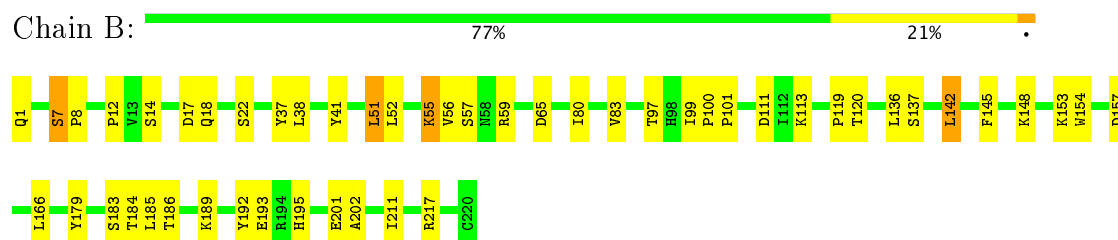
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

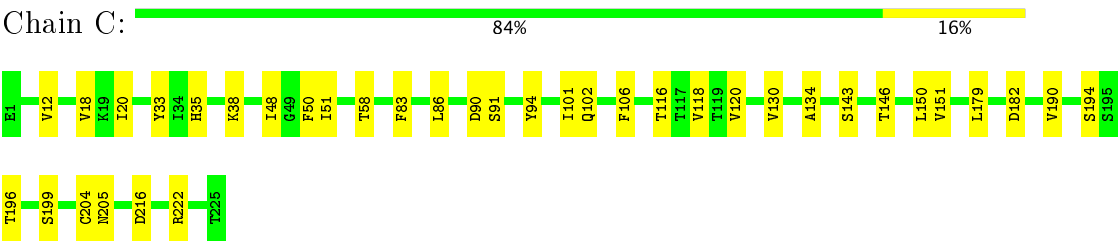
- Molecule 1: Human-mouse chimeric ABCB1 (ABCBHM)



- Molecule 2: UIC2 Antigen Binding Fragment Light chain



● Molecule 3: UIC2 Antigen Binding Fragment Heavy Chain



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	231969	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.54	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.41	0/9356	0.66	5/12650 (0.0%)
2	B	0.49	0/1757	0.75	5/2384 (0.2%)
3	C	0.50	0/1773	0.64	1/2420 (0.0%)
All	All	0.43	0/12886	0.67	11/17454 (0.1%)

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	2
2	B	0	3
All	All	0	5

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	723	LEU	CA-CB-CG	10.20	138.77	115.30
2	B	38	LEU	CA-CB-CG	7.52	132.59	115.30
1	A	723	LEU	CB-CG-CD2	-7.02	99.07	111.00
2	B	38	LEU	CB-CG-CD2	-6.48	99.98	111.00
1	A	106	LEU	CA-CB-CG	6.29	129.77	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	1138	VAL	Peptide
1	A	93	ASN	Peptide
2	B	55	LYS	Peptide
2	B	7	SER	Mainchain,Peptide

## 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	A	9186	0	9357	159	0
2	B	1713	0	1656	28	0
3	C	1720	0	1660	19	0
4	A	42	0	39	4	0
5	A	78	0	0	0	0
All	All	12739	0	12712	204	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 8.

The worst 5 of 204 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:90:ASN:ND2	4:A:1302:NAG:C1	2.28	0.97
1:A:90:ASN:HD21	4:A:1302:NAG:C1	1.79	0.95
2:B:18:GLN:HA	2:B:80:ILE:O	1.68	0.94
2:B:137:SER:HA	2:B:185:LEU:O	1.81	0.80
1:A:525:GLU:OE2	1:A:526:ARG:NH1	2.17	0.78

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 PDB entries followed by that with respect to all EM entries.

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	1178/1249 (94%)	1118 (95%)	58 (5%)	2 (0%)	51	85
2	B	219/220 (100%)	199 (91%)	18 (8%)	2 (1%)	20	64
3	C	224/225 (100%)	197 (88%)	27 (12%)	0	100	100
All	All	1621/1694 (96%)	1514 (93%)	103 (6%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	VAL
1	A	518	GLN
2	B	8	PRO
1	A	1139	VAL

### 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 PDB entries followed by that with respect to all EM entries.

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	972/1029 (94%)	961 (99%)	11 (1%)	78	91
2	B	200/199 (100%)	200 (100%)	0	100	100
3	C	196/195 (100%)	194 (99%)	2 (1%)	80	91
All	All	1368/1423 (96%)	1355 (99%)	13 (1%)	83	91

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	537	ARG
1	A	587	ARG
1	A	1211	LYS
1	A	515	LEU
1	A	1046	ARG

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	798	GLN
1	A	838	ASN
1	A	1053	GLN
1	A	611	HIS
1	A	989	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands 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	$\# Z  > 2$
4	NAG	A	1301	1	14,14,15	2.16	4 (28%)	15,19,21	1.41	2 (13%)
4	NAG	A	1302	-	14,14,15	2.17	4 (28%)	15,19,21	1.40	2 (13%)
4	NAG	A	1303	1	14,14,15	2.16	4 (28%)	15,19,21	1.41	2 (13%)
5	ZQU	A	1304	-	43,45,45	0.75	0	62,67,67	1.15	5 (8%)
5	ZQU	A	1305	-	43,45,45	0.68	0	62,67,67	1.11	5 (8%)

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
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	ZQU	A	1304	-	-	0/13/52/52	0/6/7/7
5	ZQU	A	1305	-	-	0/13/52/52	0/6/7/7

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1302	NAG	O7-C7	-2.74	1.16	1.23
4	A	1301	NAG	O7-C7	-2.72	1.16	1.23
4	A	1303	NAG	O7-C7	-2.70	1.16	1.23
4	A	1303	NAG	C2-N2	2.68	1.51	1.46
4	A	1302	NAG	C2-N2	2.68	1.51	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1303	NAG	C2-N2-C7	-3.00	118.56	122.94
4	A	1301	NAG	C2-N2-C7	-3.00	118.56	122.94
4	A	1302	NAG	C2-N2-C7	-2.98	118.60	122.94
5	A	1305	ZQU	O02-C24-C26	-2.79	118.09	124.41
5	A	1304	ZQU	O02-C24-C26	-2.29	119.22	124.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1302	NAG	2	0
4	A	1303	NAG	2	0

## 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.