



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:49 PM GMT

PDB ID : 4M1M  
Title : Corrected Structure of Mouse P-glycoprotein  
Authors : Li, J.; Jaimes, K.F.; Aller, S.G.  
Deposited on : 2013-08-03  
Resolution : 3.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

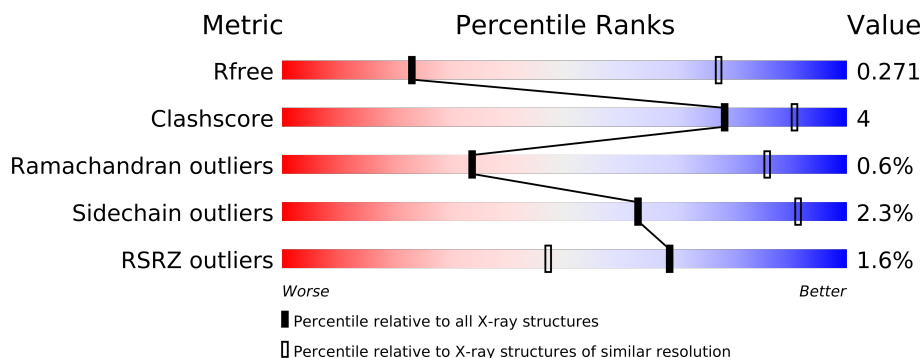
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.80 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	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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  $\geq 3$ , 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	1282	
1	B	1282	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	HG	A	1302	-	X
2	HG	A	1305	-	X
2	HG	A	1307	-	X
2	HG	B	1305	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18378 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1188	Total	C	N	O	S	0	0	0
			9213	5923	1559	1694	37			
1	B	1180	Total	C	N	O	S	0	0	0
			9152	5887	1550	1678	37			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	CONFLICT	UNP P21447
A	87	GLN	ASN	CONFLICT	UNP P21447
A	90	GLN	ASN	CONFLICT	UNP P21447
A	952	ALA	CYS	CONFLICT	UNP P21447
A	1277	HIS	-	EXPRESSION TAG	UNP P21447
A	1278	HIS	-	EXPRESSION TAG	UNP P21447
A	1279	HIS	-	EXPRESSION TAG	UNP P21447
A	1280	HIS	-	EXPRESSION TAG	UNP P21447
A	1281	HIS	-	EXPRESSION TAG	UNP P21447
A	1282	HIS	-	EXPRESSION TAG	UNP P21447
B	83	GLN	ASN	CONFLICT	UNP P21447
B	87	GLN	ASN	CONFLICT	UNP P21447
B	90	GLN	ASN	CONFLICT	UNP P21447
B	952	ALA	CYS	CONFLICT	UNP P21447
B	1277	HIS	-	EXPRESSION TAG	UNP P21447
B	1278	HIS	-	EXPRESSION TAG	UNP P21447
B	1279	HIS	-	EXPRESSION TAG	UNP P21447
B	1280	HIS	-	EXPRESSION TAG	UNP P21447
B	1281	HIS	-	EXPRESSION TAG	UNP P21447
B	1282	HIS	-	EXPRESSION TAG	UNP P21447

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total 6	Hg 6	0	0
2	A	7	Total 7	Hg 7	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.54Å 115.43Å 378.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 3.80 42.33 – 3.79	Depositor EDS
% Data completeness (in resolution range)	95.9 (24.89-3.80) 95.5 (42.33-3.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.19 (at 3.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, $R_{free}$	0.212 , 0.267 0.223 , 0.271	Depositor DCC
$R_{free}$ test set	4243 reflections (10.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	132.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 80.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 41573 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: HG

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	0/9382	0.51	0/12684
1	B	0.30	0/9321	0.50	0/12601
All	All	0.31	0/18703	0.51	0/25285

There are no bond length outliers.

There are no bond angle outliers.

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	9213	0	27	39	0
1	B	9152	0	17	30	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
All	All	18378	0	44	67	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 4.

All (67) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1149:ASN:O	1:A:1179:ARG:NH2	2.14	0.79
1:A:966:THR:OG1	1:A:967:PHE:N	2.15	0.77
1:A:239:GLU:OE1	1:A:287:LYS:NZ	2.20	0.75
1:B:272:ARG:NH2	1:B:1125:GLU:OE2	2.27	0.68
1:B:160:ASP:OD1	1:B:901:ARG:NH2	2.29	0.66
1:B:396:SER:OG	1:B:403:VAL:O	2.14	0.65
1:A:34:SER:OG	1:A:37:THR:OG1	2.13	0.65
1:B:1096:GLU:OE1	1:B:1098:LYS:N	2.32	0.62
1:A:1110:GLY:O	1:A:1194:LEU:N	2.33	0.61
1:A:1096:GLU:OE1	1:A:1098:LYS:N	2.36	0.59
1:B:206:ARG:O	1:B:326:GLN:NE2	2.36	0.59
1:A:1039:ASN:ND2	1:A:1086:MET:SD	2.76	0.59
1:A:337:GLY:O	1:A:340:SER:OG	2.21	0.58
1:B:312:TYR:O	1:B:315:SER:OG	2.21	0.57
1:A:1199:THR:OG1	1:A:1229:ARG:NH2	2.37	0.57
1:B:291:ALA:O	1:B:294:SER:OG	2.22	0.57
1:B:1149:ASN:O	1:B:1179:ARG:NH2	2.38	0.56
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.38	0.56
1:A:215:LEU:O	1:A:218:SER:OG	2.23	0.56
1:A:510:MET:SD	1:A:515:GLN:NE2	2.79	0.56
1:B:510:MET:SD	1:B:515:GLN:NE2	2.80	0.55
1:B:381:PRO:O	1:B:461:TYR:OH	2.24	0.55
1:B:1035:GLY:N	1:B:1053:SER:OG	2.40	0.54
1:B:292:ASN:ND2	1:B:766:PHE:O	2.41	0.54
1:A:1020:GLN:O	1:A:1101:ASN:ND2	2.40	0.54
1:A:453:ASP:OD1	1:A:454:ILE:N	2.41	0.53
1:A:485:ARG:NH2	1:B:914:THR:OG1	2.42	0.53
1:A:43:GLY:N	1:A:46:ASP:OD2	2.42	0.53
1:A:291:ALA:O	1:A:294:SER:OG	2.27	0.52
1:B:379:HIS:ND1	1:B:456:THR:O	2.42	0.52
1:B:907:THR:O	1:B:908:ARG:NE	2.42	0.52
1:A:46:ASP:OD1	1:A:138:ARG:NH1	2.43	0.52
1:B:1204:THR:OG1	1:B:1205:GLU:N	2.43	0.51
1:B:507:ASP:OD1	1:B:508:PHE:N	2.44	0.51
1:A:382:ASP:OD1	1:A:382:ASP:N	2.43	0.51
1:A:1159:ASP:N	1:A:1159:ASP:OD1	2.43	0.51
1:A:794:ARG:NH1	1:A:1015:ASP:OD2	2.46	0.49
1:A:260:VAL:O	1:A:264:GLY:N	2.45	0.49
1:A:302:ILE:O	1:A:305:SER:OG	2.31	0.48
1:A:517:ASP:O	1:B:925:ARG:NH1	2.46	0.48
1:A:209:LYS:NZ	1:A:321:GLU:OE1	2.46	0.48
1:A:1110:GLY:N	1:A:1192:ILE:O	2.47	0.48
1:B:1045:SER:OG	1:B:1046:ILE:N	2.47	0.47

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:453:ASP:OD1	1:B:454:ILE:N	2.47	0.47
1:A:698:LYS:O	1:A:701:SER:OG	2.32	0.47
1:A:562:GLU:OE1	1:A:584:ARG:NH1	2.48	0.46
1:A:702:THR:OG1	1:A:783:ARG:NH2	2.48	0.46
1:A:381:PRO:O	1:A:461:TYR:OH	2.33	0.46
1:A:431:THR:O	1:A:435:LEU:N	2.49	0.45
1:A:906:LEU:O	1:A:907:THR:OG1	2.35	0.44
1:B:801:ASP:OD2	1:B:1083:TYR:OH	2.36	0.44
1:A:1131:ASP:OD2	1:A:1134:ARG:NE	2.51	0.44
1:B:314:THR:OG1	1:B:748:SER:OG	2.36	0.43
1:B:201:ILE:O	1:B:205:THR:OG1	2.36	0.43
1:B:203:GLY:O	1:B:207:GLY:N	2.52	0.43
1:A:73:ASP:O	1:A:110:TYR:OH	2.37	0.42
1:A:604:GLU:OE1	1:A:617:ILE:N	2.52	0.42
1:A:1122:SER:O	1:A:1126:ASN:ND2	2.52	0.42
1:B:610:GLU:OE1	1:B:610:GLU:N	2.52	0.42
1:A:1018:SER:OG	1:A:1020:GLN:OE1	2.37	0.41
1:B:46:ASP:OD1	1:B:138:ARG:NH1	2.54	0.41
1:B:825:THR:OG1	1:B:826:GLY:N	2.53	0.41
1:A:1004:ILE:O	1:A:1008:ILE:HG13	2.20	0.41
1:B:1096:GLU:OE1	1:B:1097:ILE:N	2.54	0.40
1:B:1189:GLN:OE1	1:B:1221:ARG:NH2	2.55	0.40
1:B:1028:GLU:OE2	1:B:1058:LYS:NZ	2.54	0.40
1:A:1101:ASN:OD1	1:A:1104:TRP:N	2.54	0.40

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	1184/1282 (92%)	1124 (95%)	54 (5%)	6 (0%)	38 88
1	B	1176/1282 (92%)	1111 (94%)	57 (5%)	8 (1%)	30 84
All	All	2360/2564 (92%)	2235 (95%)	111 (5%)	14 (1%)	33 86

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1036	VAL
1	B	32	ALA
1	B	1136	VAL
1	A	1070	CYS
1	A	1120	ASP
1	B	393	ILE
1	A	278	GLU
1	A	838	ASN
1	B	278	GLU
1	B	383	ASN
1	B	1172	LEU
1	B	128	GLN
1	B	33	VAL
1	A	1046	ILE

### 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	978/1062 (92%)	953 (97%)	25 (3%)	59	90
1	B	972/1062 (92%)	953 (98%)	19 (2%)	68	92
All	All	1950/2124 (92%)	1906 (98%)	44 (2%)	63	91

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	A	258	ARG
1	A	283	LEU
1	A	310	PHE
1	A	374	PHE
1	A	383	ASN
1	A	396	SER
1	A	435	LEU
1	A	478	THR
1	A	520	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	681	LYS
1	A	688	VAL
1	A	695	ARG
1	A	700	ASN
1	A	817	ASP
1	A	852	GLN
1	A	942	GLN
1	A	965	MET
1	A	966	THR
1	A	1020	GLN
1	A	1037	VAL
1	A	1111	ILE
1	A	1163	THR
1	A	1167	ASP
1	A	1168	LYS
1	B	258	ARG
1	B	310	PHE
1	B	335	LEU
1	B	373	SER
1	B	383	ASN
1	B	435	LEU
1	B	478	THR
1	B	603	VAL
1	B	755	PHE
1	B	817	ASP
1	B	828	ARG
1	B	886	LEU
1	B	908	ARG
1	B	944	MET
1	B	966	THR
1	B	967	PHE
1	B	1022	LEU
1	B	1111	ILE
1	B	1163	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 13 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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1188/1282 (92%)	0.00	11 (0%) 81 62	83, 141, 236, 375	0
1	B	1180/1282 (92%)	0.13	23 (1%) 64 42	86, 152, 247, 420	0
All	All	2368/2564 (92%)	0.06	34 (1%) 68 50	83, 146, 241, 420	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1212	GLU	3.9
1	B	1114	GLN	3.6
1	A	965	MET	3.5
1	B	598	ASP	3.4
1	A	963	GLN	3.2
1	B	423	GLY	3.2
1	B	1229	ARG	3.1
1	B	1020	GLN	3.0
1	B	1233	ILE	2.7
1	A	1123	ILE	2.7
1	B	1164	ARG	2.7
1	A	964	LEU	2.6
1	B	589	ARG	2.6
1	B	1230	LEU	2.6
1	A	36	LEU	2.6
1	A	1226	ILE	2.5
1	B	878	GLN	2.4
1	B	97	ARG	2.4
1	A	1161	TYR	2.4
1	A	443	LEU	2.4
1	A	1197	GLU	2.3
1	B	875	LEU	2.3
1	B	874	MET	2.3
1	A	1027	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1046	ILE	2.2
1	B	279	GLU	2.2
1	B	1169	GLY	2.2
1	B	443	LEU	2.1
1	B	93	GLU	2.1
1	B	1199	THR	2.1
1	B	1021	GLY	2.1
1	B	1172	LEU	2.0
1	B	932	HIS	2.0
1	B	96	LYS	2.0

## 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 carbohydrates 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. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	HG	A	1305	1/1	0.42	22.76	65,65,65,65	1
2	HG	A	1307	1/1	0.80	9.07	138,138,138,138	1
2	HG	B	1305	1/1	0.60	4.22	46,46,46,46	1
2	HG	A	1302	1/1	0.46	2.65	71,71,71,71	1
2	HG	A	1303	1/1	0.32	1.62	102,102,102,102	1
2	HG	B	1306	1/1	0.25	0.40	71,71,71,71	1
2	HG	A	1304	1/1	0.33	0.23	38,38,38,38	1
2	HG	B	1301	1/1	0.17	-0.43	129,129,129,129	1
2	HG	A	1301	1/1	0.12	-0.80	164,164,164,164	1
2	HG	B	1304	1/1	0.25	-0.87	107,107,107,107	1
2	HG	B	1303	1/1	0.09	-2.02	198,198,198,198	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HG	A	1306	1/1	0.44	-	96,96,96,96	1
2	HG	B	1302	1/1	0.23	-	189,189,189,189	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.