



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2016 – 11:14 AM GMT

PDB ID : 4YT1  
Title : Human PPAR Gamma Ligand Binding Domain in complex with a Gamma Selective Synthetic Partial Agonist MEKT76  
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Deposited on : 2015-03-17  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20026982

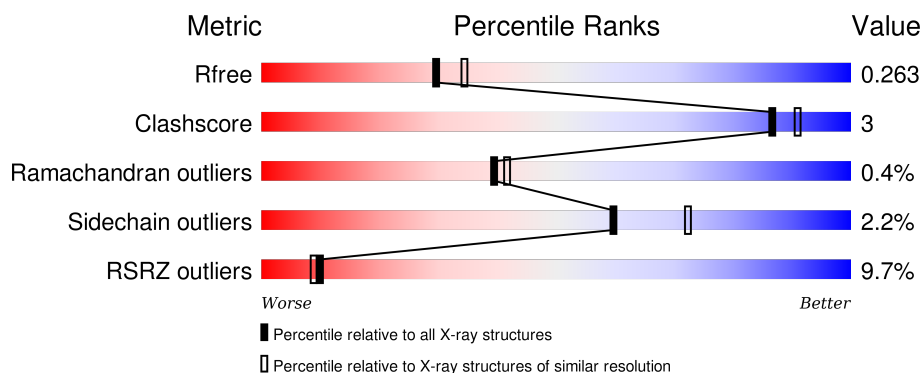
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	286	<div> <div>7%</div> <div>83% 7% • 9%</div> </div>
1	B	286	<div> <div>10%</div> <div>79% 10% 10%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4199 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.

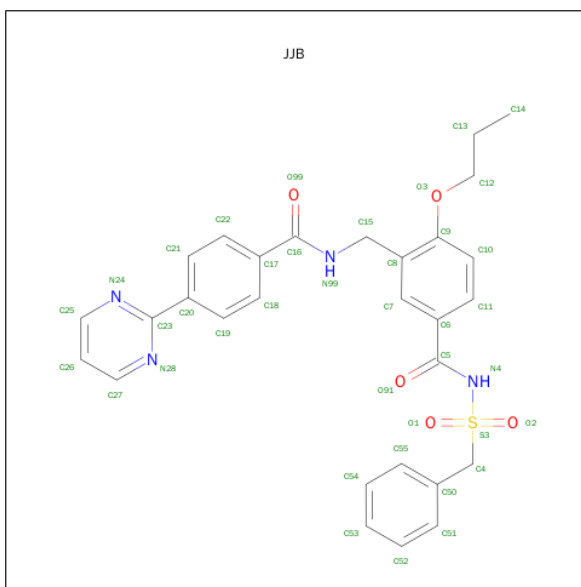
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2084	1343	340	391	10			
1	B	257	Total	C	N	O	S	0	0	0
			2046	1321	336	379	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	MET	-	expression tag	UNP P37231
B	191	GLY	-	expression tag	UNP P37231
B	192	SER	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	UNP P37231
B	194	MET	-	expression tag	UNP P37231

- Molecule 2 is N-(benzylsulfonyl)-4-propoxy-3-({[4-(pyrimidin-2-yl)benzoyl]amino}methyl)benzamide (three-letter code: JJB) (formula: C<sub>29</sub>H<sub>28</sub>N<sub>4</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			39	29	4	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	15	Total	O	0	0
			15	15		



- Molecule 1: Peroxisome proliferator-activated receptor gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.28Å 60.81Å 118.94Å 90.00° 103.74° 90.00°	Depositor
Resolution (Å)	38.51 – 2.20 48.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.51-2.20) 99.7 (48.70-2.20)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.237 , 0.256 0.244 , 0.263	Depositor DCC
$R_{free}$ test set	1673 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 33111 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.21	0/2118	0.36	0/2853
1	B	0.21	0/2079	0.35	0/2799
All	All	0.21	0/4197	0.35	0/5652

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

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	2084	0	2141	12	0
1	B	2046	0	2094	12	0
2	B	39	0	0	0	0
3	A	15	0	0	1	0
3	B	15	0	0	0	0
All	All	4199	0	4235	23	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 3.

All (23) 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:B:466:HIS:HB3	1:B:469:LEU:HB2	1.68	0.74
1:B:259:GLU:HA	1:B:262:ILE:HG22	1.76	0.66
1:B:288:ARG:NH1	1:B:291:GLU:OE1	2.29	0.65
1:B:325:ILE:HG23	1:B:388:ILE:HD12	1.78	0.65
1:A:322:VAL:HG21	1:A:472:ILE:HD13	1.89	0.55
1:A:353:LEU:HD13	1:A:364:MET:HG2	1.91	0.52
1:A:363:PHE:CE2	1:A:452:LEU:HB3	2.47	0.50
1:A:430:GLN:NE2	3:A:503:HOH:O	2.45	0.49
1:B:266:HIS:HB3	1:B:284:GLY:HA2	1.94	0.48
1:B:299:TYR:OH	1:B:385:ALA:O	2.29	0.48
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.96	0.47
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.98	0.45
1:B:334:MET:HG2	1:B:339:VAL:HB	1.97	0.45
1:B:247:PHE:HZ	1:B:257:MET:HE2	1.82	0.45
1:A:357:ARG:HD2	1:A:358:LYS:O	2.19	0.43
1:A:276:GLU:HB3	1:A:279:ILE:HG12	2.01	0.42
1:A:350:ARG:NH2	1:A:365:GLU:OE1	2.47	0.42
1:B:251:ASP:H	1:B:254:SER:HG	1.67	0.42
1:A:235:ALA:HA	1:A:240:LYS:HE2	2.01	0.42
1:B:230:LYS:NZ	1:B:379:LEU:O	2.39	0.41
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.82	0.41
1:A:443:ARG:HG3	1:B:440:THR:HG23	2.03	0.40
1:A:229:THR:HG23	1:A:232:LYS:H	1.86	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	257/286 (90%)	252 (98%)	5 (2%)	0	100	100
1	B	251/286 (88%)	241 (96%)	8 (3%)	2 (1%)	24	22
All	All	508/572 (89%)	493 (97%)	13 (3%)	2 (0%)	39	42



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	PRO
1	B	460	GLU

### 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	233/257 (91%)	230 (99%)	3 (1%)	76	87
1	B	226/257 (88%)	219 (97%)	7 (3%)	47	59
All	All	459/514 (89%)	449 (98%)	10 (2%)	60	72

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	THR
1	A	362	ASP
1	A	363	PHE
1	B	261	LYS
1	B	343	GLU
1	B	357	ARG
1	B	358	LYS
1	B	363	PHE
1	B	459	THR
1	B	469	LEU

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 molecules 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 ⓘ

1 ligand is 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	JJB	B	901	-	42,42,42	1.30	4 (9%)	55,57,57	1.72	11 (20%)

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	JJB	B	901	-	-	0/31/31/31	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	JJB	O2-S3	2.78	1.47	1.43
2	B	901	JJB	O1-S3	2.84	1.47	1.43
2	B	901	JJB	C5-N4	4.40	1.44	1.39
2	B	901	JJB	C16-N99	4.52	1.43	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	901	JJB	O1-S3-O2	-5.80	109.20	119.31
2	B	901	JJB	N28-C23-N24	-3.30	119.68	125.81
2	B	901	JJB	O3-C9-C10	-2.03	119.87	124.03
2	B	901	JJB	O3-C12-C13	2.11	119.76	109.83
2	B	901	JJB	C20-C23-N24	2.38	120.00	117.31
2	B	901	JJB	C20-C23-N28	2.65	120.31	117.31
2	B	901	JJB	C6-C5-N4	2.87	119.58	116.05
2	B	901	JJB	O3-C9-C8	3.08	119.66	115.66
2	B	901	JJB	C27-N28-C23	4.16	120.61	115.99
2	B	901	JJB	C25-N24-C23	4.21	120.67	115.99
2	B	901	JJB	C8-C15-N99	4.26	121.33	113.06

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 ⓘ

### 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	261/286 (91%)	0.60	20 (7%) 16 16	40, 59, 88, 97	0
1	B	257/286 (89%)	0.85	30 (11%) 6 6	39, 58, 97, 120	0
All	All	518/572 (90%)	0.72	50 (9%) 10 9	39, 59, 93, 120	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	SER	6.8
1	B	240	LYS	6.6
1	A	363	PHE	6.1
1	B	363	PHE	5.2
1	B	256	MET	4.9
1	B	458	LYS	3.9
1	A	360	PHE	3.8
1	A	362	ASP	3.8
1	B	465	LEU	3.8
1	A	359	PRO	3.6
1	B	238	THR	3.5
1	B	463	MET	3.4
1	A	356	LEU	3.3
1	B	260	ASP	3.3
1	B	352	PHE	3.0
1	A	253	ASN	3.0
1	B	462	ASP	3.0
1	B	452	LEU	3.0
1	B	275	LYS	3.0
1	B	358	LYS	2.9
1	A	261	LYS	2.8
1	B	207	GLU	2.8
1	A	452	LEU	2.8
1	B	287	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	456	ILE	2.7
1	B	318	LEU	2.7
1	B	259	GLU	2.6
1	B	360	PHE	2.5
1	A	257	MET	2.4
1	B	252	MET	2.4
1	B	290	VAL	2.4
1	B	266	HIS	2.4
1	B	456	ILE	2.4
1	A	476	LEU	2.3
1	A	457	LYS	2.3
1	A	252	MET	2.3
1	B	357	ARG	2.3
1	A	242	THR	2.2
1	A	282	PHE	2.2
1	A	454	GLN	2.2
1	A	343	GLU	2.2
1	B	354	LYS	2.2
1	B	261	LYS	2.1
1	B	461	THR	2.1
1	B	277	VAL	2.1
1	B	311	LEU	2.1
1	A	207	GLU	2.0
1	A	286	GLN	2.0
1	A	240	LYS	2.0
1	B	257	MET	2.0

## 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](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	JJB	B	901	39/39	0.80	0.23	0.45	67,80,105,186	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.