



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:44 AM GMT

PDB ID : 2Q8S  
Title : X-ray Crystal structure of the nuclear hormone receptor PPAR-gamma in a complex with a PPAR gamma/alpha dual agonist  
Authors : Ohren, J.F.  
Deposited on : 2007-06-11  
Resolution : 2.30 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>

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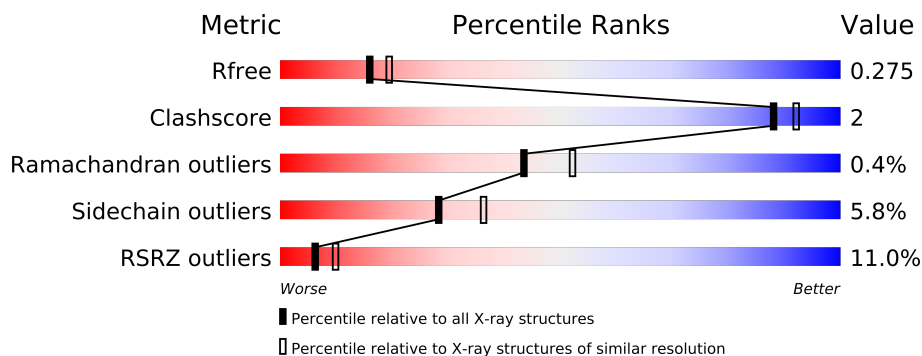
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	271	
1	B	271	

## 2 Entry composition i

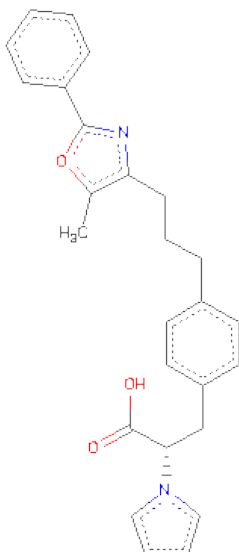
There are 3 unique types of molecules in this entry. The entry contains 4153 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Peroxisome proliferator-activatedreceptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	3	0
			2033	1313	330	380	10			
1	B	254	Total	C	N	O	S	0	1	0
			2030	1314	328	378	10			

- Molecule 2 is (2S)-3-{4-[3-(5-METHYL-2-PHENYL-1,3-OXAZOL-4-YL)PROPYL]PHENYL}-2-(1H-PYRROL-1-YL)PROPANOICACID (three-letter code: L92) (formula: C<sub>26</sub>H<sub>26</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	26	2	3		

- Molecule 3 is water.

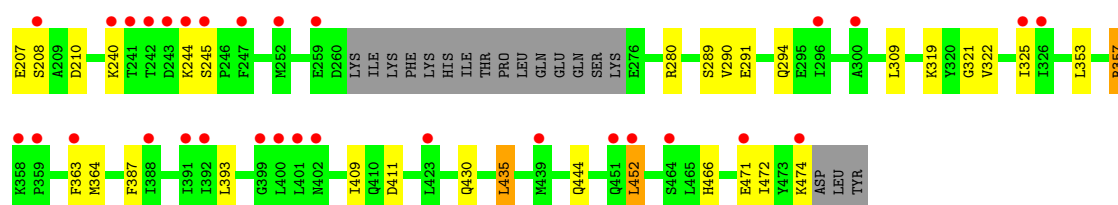
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total 34	O 34	0	0
3	B	25	Total 25	O 25	0	0

### 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 errors 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.

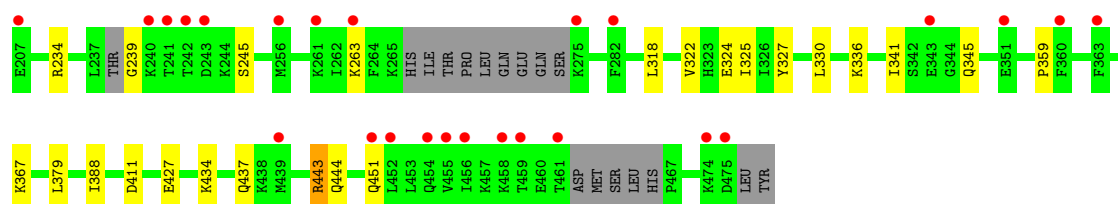
- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain A: 



- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.45Å 62.02Å 118.66Å 90.00° 102.54° 90.00°	Depositor
Resolution (Å)	35.00 – 2.30 33.24 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (35.00-2.30) 92.8 (33.24-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.222 , 0.282 0.218 , 0.275	Depositor DCC
$R_{free}$ test set	1420 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 100.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 27570 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4153	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: L92

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	0.44	0/2082	0.55	0/2804
1	B	0.44	0/2066	0.53	0/2777
All	All	0.44	0/4148	0.54	0/5581

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	2033	0	2085	12	0
1	B	2030	0	2089	7	0
2	A	31	0	25	2	0
3	A	34	0	0	0	0
3	B	25	0	0	1	0
All	All	4153	0	4199	20	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 2.

All (20) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:363[B]:PHE:CE1	1:A:452:LEU:HB3	2.34	0.63
1:A:387:PHE:CE1	1:A:435:LEU:HD22	2.38	0.59
2:A:1001:L92:H8	2:A:1001:L92:H162	1.89	0.54
1:B:327:TYR:CZ	1:B:367:LYS:NZ	2.76	0.52
1:B:434:LYS:HA	1:B:437:GLN:HE21	1.73	0.52
1:A:363[B]:PHE:CZ	1:A:452:LEU:HB3	2.48	0.48
1:B:345:GLN:HA	1:B:345:GLN:HE21	1.78	0.47
1:B:324:GLU:OE2	1:B:443:ARG:HD2	2.15	0.46
1:B:234:ARG:O	1:B:239:GLY:HA3	2.16	0.46
1:A:207:GLU:HB3	1:A:210:ASP:OD2	2.16	0.45
1:A:321:GLY:O	1:A:325:ILE:HG12	2.17	0.45
1:A:291:GLU:O	1:A:294:GLN:HG2	2.20	0.42
1:A:319:LYS:NZ	1:A:472:ILE:O	2.49	0.42
1:A:244[B]:LYS:HG3	1:A:245:SER:N	2.35	0.41
1:B:325:ILE:HD12	1:B:388:ILE:HG23	2.01	0.41
1:A:353:LEU:HD21	2:A:1001:L92:H261	2.03	0.41
1:B:411:ASP:HB3	3:B:483:HOH:O	2.21	0.41
1:A:393:LEU:CD2	1:A:409:ILE:HG21	2.51	0.41
1:A:290:VAL:HG21	1:A:466:HIS:CG	2.56	0.40
1:A:363[A]:PHE:CE2	1:A:364:MET:HG2	2.56	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	252/271 (93%)	249 (99%)	2 (1%)	1 (0%)	43	52
1	B	247/271 (91%)	237 (96%)	9 (4%)	1 (0%)	43	52
All	All	499/542 (92%)	486 (97%)	11 (2%)	2 (0%)	43	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	ARG
1	B	359	PRO

### 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	228/244 (93%)	214 (94%)	14 (6%)	26	34
1	B	226/244 (93%)	214 (95%)	12 (5%)	32	41
All	All	454/488 (93%)	428 (94%)	26 (6%)	28	37

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	A	240	LYS
1	A	280	ARG
1	A	289	SER
1	A	309	LEU
1	A	322	VAL
1	A	357	ARG
1	A	411	ASP
1	A	430	GLN
1	A	435	LEU
1	A	444	GLN
1	A	452	LEU
1	A	471	GLU
1	A	474	LYS
1	B	245	SER
1	B	263	LYS
1	B	318	LEU
1	B	322	VAL
1	B	330	LEU
1	B	336	LYS
1	B	341	ILE
1	B	379	LEU
1	B	427	GLU
1	B	443	ARG

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Mol	Chain	Res	Type
1	B	444	GLN
1	B	451	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	308	ASN
1	A	375	ASN
1	A	430	GLN
1	B	308	ASN
1	B	345	GLN
1	B	375	ASN
1	B	437	GLN
1	B	444	GLN
1	B	451	GLN
1	B	470	GLN

### 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 ⓘ

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	L92	A	1001	-	34,34,34	1.87	3 (8%)	44,46,46	1.66	8 (18%)

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	L92	A	1001	-	-	1/20/22/22	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	L92	C20-C18	-8.48	1.39	1.47
2	A	1001	L92	C10-N1	-4.46	1.34	1.37
2	A	1001	L92	C13-N1	-4.02	1.34	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	L92	C15-C16-C17	7.05	124.30	113.38
2	A	1001	L92	C1-C2-N1	-2.68	108.14	111.14
2	A	1001	L92	C20-C18-N2	2.58	128.36	122.73
2	A	1001	L92	O3-C18-N2	-2.53	109.98	117.79
2	A	1001	L92	C12-C13-N1	2.38	108.88	107.69
2	A	1001	L92	O3-C18-C20	2.35	121.66	119.23
2	A	1001	L92	C4-C3-C2	-2.30	107.55	114.15
2	A	1001	L92	C11-C10-N1	2.26	108.82	107.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	L92	C19-C17-C16-C15

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	253/271 (93%)	0.66	31 (12%) 5 8	61, 72, 93, 95	0
1	B	254/271 (93%)	0.62	25 (9%) 8 13	60, 75, 114, 125	0
All	All	507/542 (93%)	0.64	56 (11%) 6 10	60, 73, 111, 125	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	PHE	6.4
1	B	242	THR	6.1
1	B	451	GLN	5.1
1	A	241	THR	4.9
1	B	456	ILE	4.8
1	A	243	ASP	4.3
1	B	263	LYS	3.8
1	A	363[A]	PHE	3.8
1	B	275	LYS	3.8
1	A	359	PRO	3.7
1	A	423	LEU	3.7
1	B	459	THR	3.6
1	B	360	PHE	3.5
1	B	455	VAL	3.4
1	B	261	LYS	3.2
1	B	458	LYS	3.2
1	A	240	LYS	3.1
1	A	402	ASN	3.0
1	A	326	ILE	2.8
1	B	256	MET	2.8
1	A	247	PHE	2.8
1	B	475	ASP	2.8
1	A	242	THR	2.8
1	A	208	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	296	ILE	2.7
1	B	454	GLN	2.7
1	A	464	SER	2.7
1	B	343	GLU	2.6
1	A	358	LYS	2.6
1	B	452	LEU	2.6
1	A	400	LEU	2.5
1	A	391	ILE	2.5
1	B	241	THR	2.4
1	B	243	ASP	2.4
1	B	351	GLU	2.4
1	B	439[A]	MET	2.4
1	A	399	GLY	2.4
1	B	461	THR	2.4
1	A	300	ALA	2.3
1	A	259	GLU	2.3
1	A	244[A]	LYS	2.3
1	A	439	MET	2.3
1	A	451	GLN	2.3
1	B	282	PHE	2.3
1	A	245	SER	2.3
1	A	325	ILE	2.2
1	A	401	LEU	2.2
1	A	452	LEU	2.2
1	A	471	GLU	2.2
1	A	392	ILE	2.1
1	A	388	ILE	2.1
1	A	474	LYS	2.1
1	A	252	MET	2.1
1	B	207	GLU	2.0
1	B	240	LYS	2.0
1	B	474	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	L92	A	1001	31/31	0.20	0.19	81,83,83,84	0

## 6.5 Other polymers

There are no such residues in this entry.