



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:17 AM GMT

PDB ID : 3BC5
Title : X-ray crystal structure of human ppar gamma with 2-(5-(3-(2-(5-methyl-2-phenyloxazol-4-yl)ethoxy)benzyl)-2-phenyl-2h-1,2,3-triazol-4-yl)aceticacid
Authors : Muckelbauer, J.K.
Deposited on : 2007-11-12
Resolution : 2.27 Å(reported)

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

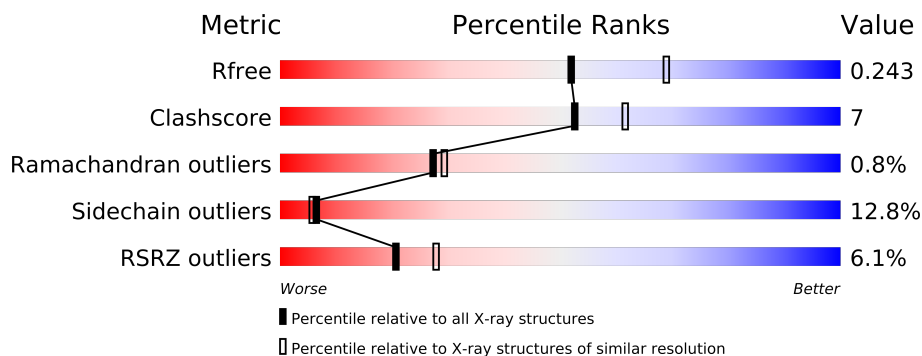
The following versions of software and data (see [references](#)) were used in the production of this report:

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

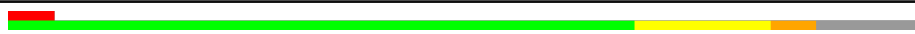
The reported resolution of this entry is 2.27 Å.

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	3861 (2.30-2.26)
Clashscore	79885	4801 (2.30-2.26)
Ramachandran outliers	78287	4729 (2.30-2.26)
Sidechain outliers	78261	4728 (2.30-2.26)
RSRZ outliers	66119	3864 (2.30-2.26)

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. 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	296	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2264 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.

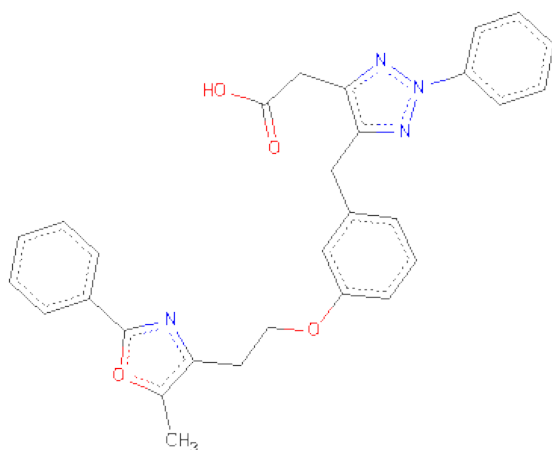
- Molecule 1 is a protein called Peroxisome proliferator-activatedreceptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2072	1341	339	382	10	14	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	182	MET	-	expression tag	UNP P37231
A	183	GLY	-	expression tag	UNP P37231
A	184	SER	-	expression tag	UNP P37231
A	185	SER	-	expression tag	UNP P37231
A	186	HIS	-	expression tag	UNP P37231
A	187	HIS	-	expression tag	UNP P37231
A	188	HIS	-	expression tag	UNP P37231
A	189	HIS	-	expression tag	UNP P37231
A	190	HIS	-	expression tag	UNP P37231
A	191	HIS	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	SER	-	expression tag	UNP P37231
A	194	GLY	-	expression tag	UNP P37231
A	195	LEU	-	expression tag	UNP P37231
A	196	VAL	-	expression tag	UNP P37231
A	197	PRO	-	expression tag	UNP P37231
A	198	ARG	-	expression tag	UNP P37231
A	199	GLY	-	expression tag	UNP P37231
A	200	SER	-	expression tag	UNP P37231
A	201	HIS	-	expression tag	UNP P37231
A	202	MET	-	expression tag	UNP P37231

- Molecule 2 is (5-{3-[2-(5-METHYL-2-PHENYL-1,3-OXAZOL-4-YL)ETHOXY]BENZYL}-2-PHENYL-2H-1,2,3-TRIAZOL-4-YL)ACETICACID (three-letter code: ZAA) (formula: C₂₉H₂₆N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	37	29	4	4	0	0

- Molecule 3 is water.

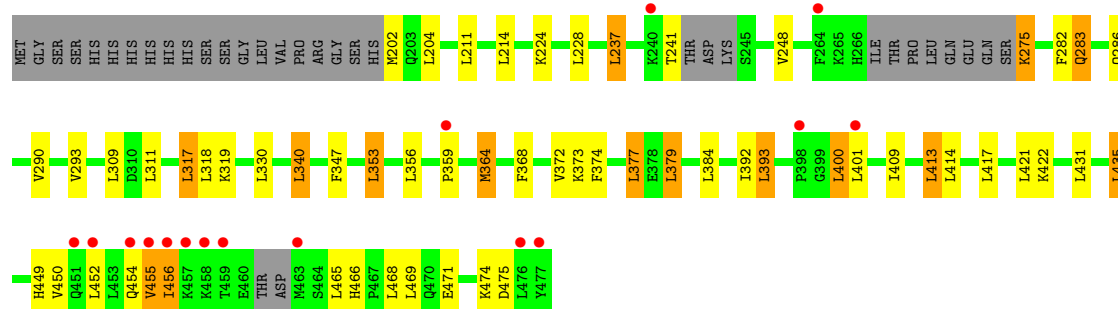
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	155	Total	O	0	0
			155	155		

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: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	66.30Å 66.30Å 156.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.27 34.85 – 2.27	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.27) 95.1 (34.85-2.27)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.76 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.249 0.211 , 0.243	Depositor DCC
R_{free} test set	632 reflections (4.12%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.5	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	0 of 15977 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2264	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: ZAA

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	1.92	4/2105 (0.2%)	1.05	8/2836 (0.3%)

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	1	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	GLN	CD-NE2	61.48	2.86	1.32
1	A	275	LYS	CA-CB	55.61	2.76	1.53
1	A	373	LYS	CE-NZ	10.48	1.75	1.49
1	A	224	LYS	CD-CE	6.29	1.67	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	LYS	N-CA-CB	-30.85	55.07	110.60
1	A	275	LYS	CB-CA-C	-19.16	72.07	110.40
1	A	373	LYS	CD-CE-NZ	-11.26	85.80	111.70
1	A	283	GLN	OE1-CD-NE2	-6.88	106.08	121.90
1	A	393	LEU	CA-CB-CG	-6.63	100.05	115.30
1	A	353	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	283	GLN	CG-CD-OE1	-5.15	111.29	121.60
1	A	237	LEU	CA-CB-CG	5.09	127.00	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	275	LYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	GLN	Sidechain

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	2072	0	2106	30	0
2	A	37	0	25	2	0
3	A	155	0	0	2	0
All	All	2264	0	2131	30	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 7.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:275:LYS:HA	3:A:519:HOH:O	1.66	0.96
1:A:286:GLN:HE22	1:A:465:LEU:HD23	1.43	0.83
1:A:319:LYS:HE2	1:A:475:ASP:HB2	1.74	0.69
1:A:359:PRO:CG	1:A:456:ILE:HG12	2.23	0.68
1:A:364:MET:CE	1:A:364:MET:HA	2.30	0.62
1:A:286:GLN:NE2	1:A:465:LEU:HD23	2.15	0.61
1:A:359:PRO:HG2	1:A:456:ILE:HG12	1.86	0.57
1:A:466:HIS:HD2	1:A:468:LEU:H	1.54	0.55
1:A:452:LEU:O	1:A:456:ILE:HD12	2.06	0.54
1:A:450:VAL:O	1:A:454:GLN:HG2	2.08	0.54
1:A:202:MET:HE3	1:A:422:LYS:HD3	1.90	0.53
1:A:466:HIS:CD2	1:A:468:LEU:H	2.29	0.50
1:A:379:LEU:HD21	1:A:435:LEU:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:409:ILE:HG22	1:A:413:LEU:HD22	1.95	0.48
1:A:290:VAL:HA	1:A:293:VAL:HG22	1.94	0.48
1:A:359:PRO:HG3	1:A:456:ILE:HG12	1.96	0.46
1:A:202:MET:CE	1:A:422:LYS:HD3	2.47	0.45
1:A:290:VAL:O	1:A:293:VAL:HG22	2.16	0.45
1:A:449:HIS:NE2	2:A:1:ZAA:O37	2.48	0.45
1:A:455:VAL:O	1:A:456:ILE:HG13	2.17	0.45
1:A:374:PHE:O	1:A:377:LEU:HB2	2.17	0.44
1:A:317:LEU:HG	1:A:392:ILE:O	2.17	0.44
1:A:340:LEU:HD13	1:A:347:PHE:HD2	1.83	0.44
1:A:364:MET:HE3	1:A:364:MET:HA	2.00	0.43
1:A:282:PHE:HD1	2:A:1:ZAA:H29	1.83	0.43
1:A:435:LEU:HA	1:A:435:LEU:HD12	1.91	0.42
1:A:471:GLU:O	1:A:474:LYS:HG2	2.21	0.41
1:A:317:LEU:HD13	1:A:400:LEU:HD11	2.03	0.40
1:A:372:VAL:HG22	3:A:524:HOH:O	2.21	0.40
1:A:368:PHE:O	1:A:372:VAL:HG13	2.21	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	255/296 (86%)	248 (97%)	5 (2%)	2 (1%)	27	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	VAL
1	A	456	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	226/266 (85%)	197 (87%)	29 (13%)	6 6

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	A	211	LEU
1	A	214	LEU
1	A	228	LEU
1	A	237	LEU
1	A	241	THR
1	A	248	VAL
1	A	309	LEU
1	A	311	LEU
1	A	317	LEU
1	A	318	LEU
1	A	330	LEU
1	A	340	LEU
1	A	353	LEU
1	A	356	LEU
1	A	364	MET
1	A	377	LEU
1	A	379	LEU
1	A	384	LEU
1	A	393	LEU
1	A	400	LEU
1	A	401	LEU
1	A	413	LEU
1	A	414	LEU
1	A	417	LEU
1	A	421	LEU
1	A	431	LEU
1	A	435	LEU
1	A	469	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN
1	A	424	ASN
1	A	451	GLN
1	A	466	HIS
1	A	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	ZAA	A	1	-	41,41,41	1.59	4 (9%)	54,56,56	3.15	17 (31%)

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	ZAA	A	1	-	-	0/22/22/22	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ZAA	C28-N26	-8.07	1.35	1.44
2	A	1	ZAA	C7-C5	2.82	1.49	1.47
2	A	1	ZAA	O6-C2	-2.45	1.30	1.36
2	A	1	ZAA	C1-C2	2.36	1.52	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ZAA	O6-C5-C7	14.92	134.64	119.23
2	A	1	ZAA	N27-N26-N25	-7.86	105.44	117.45
2	A	1	ZAA	C28-N26-N25	7.51	130.28	123.40
2	A	1	ZAA	C2-C3-N4	-5.31	104.23	111.04
2	A	1	ZAA	C16-C21-C20	5.29	125.20	119.73
2	A	1	ZAA	C13-C3-C2	4.07	133.79	126.87
2	A	1	ZAA	C23-N27-N26	4.04	112.56	106.55
2	A	1	ZAA	O6-C5-N4	-3.74	106.23	117.79
2	A	1	ZAA	O37-C35-C34	3.31	122.11	113.80
2	A	1	ZAA	C24-N25-N26	3.18	111.29	106.55
2	A	1	ZAA	C34-C24-C23	3.13	134.22	127.07
2	A	1	ZAA	O37-C35-O36	-2.44	117.08	123.30
2	A	1	ZAA	C17-C16-C21	-2.44	117.05	120.56
2	A	1	ZAA	C19-C20-C21	-2.22	115.18	118.53
2	A	1	ZAA	C1-C2-C3	2.18	131.83	127.69
2	A	1	ZAA	C22-C23-C24	2.09	131.84	127.07
2	A	1	ZAA	C8-C7-C12	2.06	121.42	117.58

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, 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	263/296 (88%)	0.19	16 (6%)	21 28	23, 36, 64, 88	5 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	VAL	5.3
1	A	456	ILE	4.6
1	A	458	LYS	4.3
1	A	459	THR	4.3
1	A	477	TYR	3.1
1	A	463	MET	3.1
1	A	454	GLN	2.6
1	A	264	PHE	2.5
1	A	451	GLN	2.4
1	A	359	PRO	2.3
1	A	401	LEU	2.2
1	A	457	LYS	2.2
1	A	240	LYS	2.1
1	A	452	LEU	2.1
1	A	476	LEU	2.1
1	A	398	PRO	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZAA	A	1	37/37	0.15	0.07	32,38,46,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.