Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 03:44 AM EDT

PDB ID	:	6VZM
Title	:	Crystal structure of human PPARgamma ligand binding domain Y473E mutant in complex with Darglitazone
Authors	:	Shang, J.; Kojetin, D.J.
Deposited on	:	2020-02-28
Resolution	:	2.40 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4340 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.

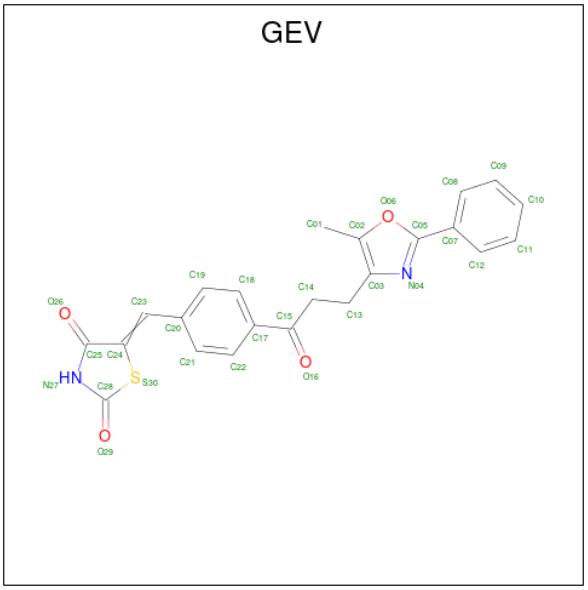
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	2026	1307	331	378	10	0	0	0
1	B	255	2049	1324	336	380	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	473	GLU	TYR	engineered mutation	UNP P37231
B	473	GLU	TYR	engineered mutation	UNP P37231

- Molecule 2 is (5Z)-5-({4-[3-(5-methyl-2-phenyl-1,3-oxazol-4-yl)propanoyl]phenyl}methylidene)-1,3-thiazolidine-2,4-dione (three-letter code: GEV) (formula: $C_{23}H_{18}N_2O_4S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	30	23	2	4	1	0	0
			Total	C	N	O	S		
2	B	1	30	23	2	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	98	98	98	0	0
			Total	O		
3	B	107	107	107	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.07Å 61.59Å 120.53Å 90.00° 102.17° 90.00°	Depositor
Resolution (Å)	33.41 – 2.40	Depositor
% Data completeness (in resolution range)	98.2 (33.41-2.40)	Depositor
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.217 , 0.278	Depositor
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.000	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4340	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
2	GEV	A	501	-	29,33,33	5.18	10 (34%)	37,46,46	5.14	11 (29%)
2	GEV	B	501	-	29,33,33	5.23	9 (31%)	37,46,46	4.26	14 (37%)

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	GEV	A	501	-	-	7/15/29/29	0/4/4/4
2	GEV	B	501	-	-	4/15/29/29	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	GEV	C23-C24	17.75	1.54	1.34
2	A	501	GEV	C23-C24	17.63	1.54	1.34
2	A	501	GEV	O29-C28	12.83	1.41	1.22
2	B	501	GEV	O29-C28	12.70	1.41	1.22
2	B	501	GEV	O16-C15	11.71	1.41	1.22
2	A	501	GEV	O16-C15	11.18	1.40	1.22
2	A	501	GEV	O26-C25	8.89	1.40	1.23
2	B	501	GEV	O26-C25	8.76	1.40	1.23
2	B	501	GEV	C28-S30	-6.21	1.70	1.78
2	A	501	GEV	C28-S30	-6.14	1.70	1.78
2	B	501	GEV	C25-C24	-4.14	1.41	1.48
2	B	501	GEV	C20-C23	3.95	1.54	1.46
2	A	501	GEV	C25-C24	-3.93	1.41	1.48
2	A	501	GEV	C01-C02	3.88	1.53	1.48
2	B	501	GEV	C01-C02	3.81	1.53	1.48
2	A	501	GEV	C20-C23	3.45	1.53	1.46
2	B	501	GEV	C17-C15	2.78	1.53	1.49
2	A	501	GEV	C17-C15	2.55	1.53	1.49
2	A	501	GEV	C28-N27	-2.00	1.34	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	GEV	C24-S30-C28	22.43	98.17	91.69
2	B	501	GEV	C24-S30-C28	18.07	96.91	91.69
2	A	501	GEV	C20-C23-C24	-10.38	116.75	130.94
2	A	501	GEV	C23-C24-C25	9.29	127.82	120.47
2	B	501	GEV	O16-C15-C17	-8.75	108.36	120.74
2	A	501	GEV	O16-C15-C17	-8.50	108.71	120.74
2	B	501	GEV	C20-C23-C24	-7.99	120.01	130.94
2	A	501	GEV	C25-C24-S30	-7.55	104.20	109.84
2	B	501	GEV	O16-C15-C14	-7.12	108.22	120.38
2	B	501	GEV	C25-C24-S30	-6.95	104.65	109.84
2	A	501	GEV	O16-C15-C14	-6.57	109.16	120.38
2	B	501	GEV	C24-C25-N27	5.76	115.02	110.22
2	A	501	GEV	C24-C25-N27	5.50	114.81	110.22
2	A	501	GEV	C14-C15-C17	-5.37	111.69	119.13
2	A	501	GEV	S30-C28-N27	-3.36	106.06	109.19
2	B	501	GEV	C23-C24-C25	3.28	123.06	120.47
2	B	501	GEV	O26-C25-C24	-3.07	122.14	126.01
2	B	501	GEV	C14-C15-C17	-2.80	115.25	119.13
2	B	501	GEV	C25-N27-C28	-2.79	116.27	117.79
2	B	501	GEV	C13-C14-C15	-2.53	107.69	113.14
2	A	501	GEV	O29-C28-S30	2.39	127.69	124.64
2	B	501	GEV	C23-C24-S30	2.39	132.28	129.22
2	B	501	GEV	S30-C28-N27	-2.20	107.15	109.19
2	A	501	GEV	O26-C25-C24	-2.07	123.40	126.01
2	B	501	GEV	O29-C28-S30	2.02	127.21	124.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

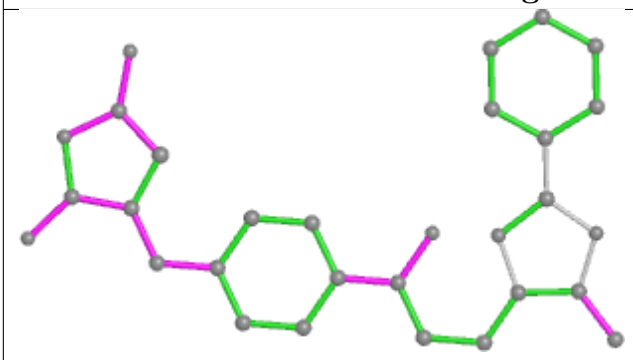
Mol	Chain	Res	Type	Atoms
2	A	501	GEV	C02-C03-C13-C14
2	A	501	GEV	C20-C23-C24-C25
2	A	501	GEV	C20-C23-C24-S30
2	B	501	GEV	C21-C20-C23-C24
2	B	501	GEV	C19-C20-C23-C24
2	B	501	GEV	C14-C15-C17-C18
2	A	501	GEV	O16-C15-C17-C22
2	B	501	GEV	C14-C15-C17-C22
2	A	501	GEV	O16-C15-C17-C18
2	A	501	GEV	C13-C14-C15-C17
2	A	501	GEV	C19-C20-C23-C24

There are no ring outliers.

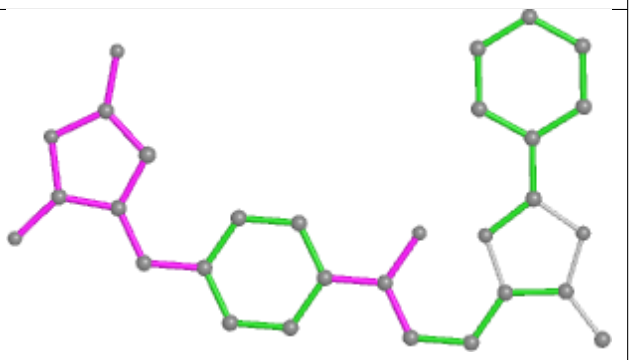
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

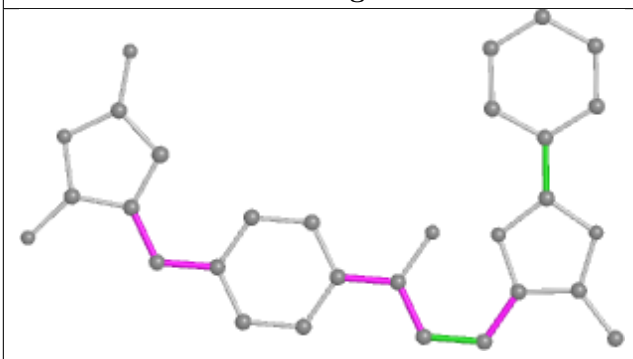
Ligand GEV A 501



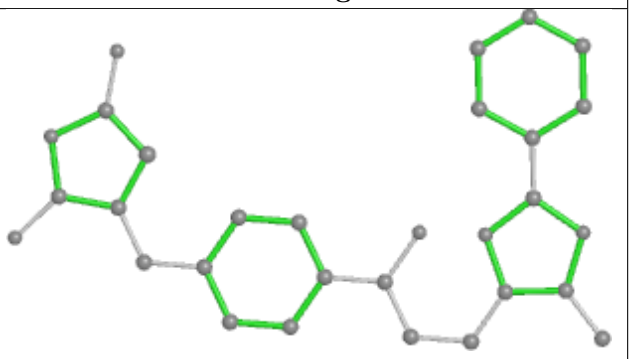
Bond lengths



Bond angles

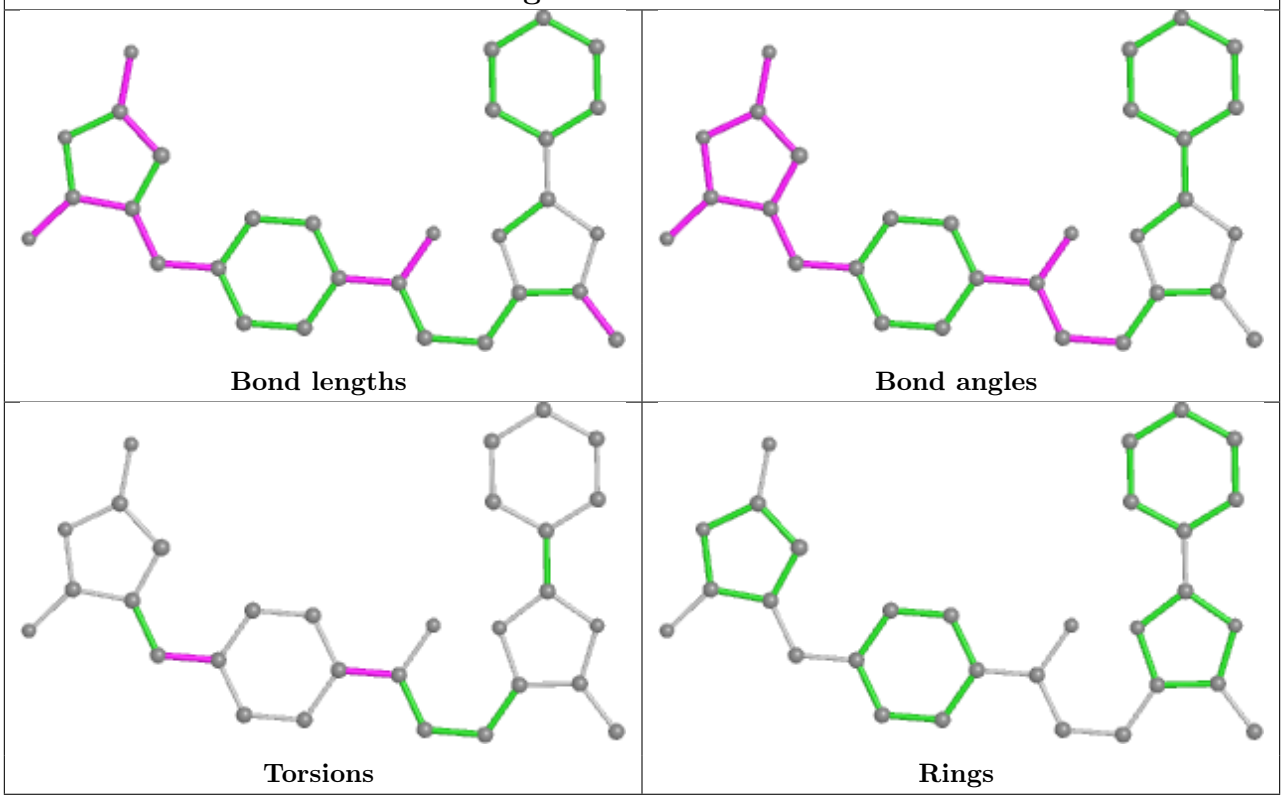


Torsions



Rings

Ligand GEV B 501



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.