



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:17 PM EDT

PDB ID : 6DCU / pdb_00006dcu
Title : Crystal structure of PPAR gamma co-crystallized with nTZDpa
Authors : Mou, T.C.; Chrisman, I.M.; Hughes, T.S.; Sprang, S.R.
Deposited on : 2018-05-08
Resolution : 2.95 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.95 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

There are 2 unique types of molecules in this entry. The entry contains 4045 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	254	Total	C	N	O	S	0	0	0
			2022	1303	331	378	10			
1	B	247	Total	C	N	O	S	0	0	0
			1967	1271	321	365	10			

There are 52 discrepancies between the modelled and reference sequences:

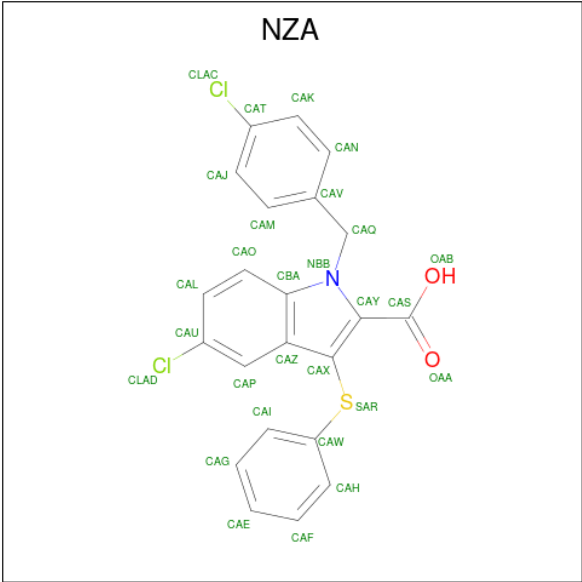
Chain	Residue	Modelled	Actual	Comment	Reference
A	181	MET	-	initiating methionine	UNP P37231
A	182	ALA	-	expression tag	UNP P37231
A	183	HIS	-	expression tag	UNP P37231
A	184	HIS	-	expression tag	UNP P37231
A	185	HIS	-	expression tag	UNP P37231
A	186	HIS	-	expression tag	UNP P37231
A	187	HIS	-	expression tag	UNP P37231
A	188	HIS	-	expression tag	UNP P37231
A	189	VAL	-	expression tag	UNP P37231
A	190	ASP	-	expression tag	UNP P37231
A	191	ASP	-	expression tag	UNP P37231
A	192	ASP	-	expression tag	UNP P37231
A	193	ASP	-	expression tag	UNP P37231
A	194	LYS	-	expression tag	UNP P37231
A	195	MET	-	expression tag	UNP P37231
A	196	GLU	-	expression tag	UNP P37231
A	197	ASN	-	expression tag	UNP P37231
A	198	LEU	-	expression tag	UNP P37231
A	199	TYR	-	expression tag	UNP P37231
A	200	PHE	-	expression tag	UNP P37231
A	201	GLN	-	expression tag	UNP P37231
A	202	GLY	-	expression tag	UNP P37231
A	478	LEU	-	expression tag	UNP P37231
A	479	VAL	-	expression tag	UNP P37231
A	480	PRO	-	expression tag	UNP P37231

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Chain	Residue	Modelled	Actual	Comment	Reference
A	481	ARG	-	expression tag	UNP P37231
B	181	MET	-	initiating methionine	UNP P37231
B	182	ALA	-	expression tag	UNP P37231
B	183	HIS	-	expression tag	UNP P37231
B	184	HIS	-	expression tag	UNP P37231
B	185	HIS	-	expression tag	UNP P37231
B	186	HIS	-	expression tag	UNP P37231
B	187	HIS	-	expression tag	UNP P37231
B	188	HIS	-	expression tag	UNP P37231
B	189	VAL	-	expression tag	UNP P37231
B	190	ASP	-	expression tag	UNP P37231
B	191	ASP	-	expression tag	UNP P37231
B	192	ASP	-	expression tag	UNP P37231
B	193	ASP	-	expression tag	UNP P37231
B	194	LYS	-	expression tag	UNP P37231
B	195	MET	-	expression tag	UNP P37231
B	196	GLU	-	expression tag	UNP P37231
B	197	ASN	-	expression tag	UNP P37231
B	198	LEU	-	expression tag	UNP P37231
B	199	TYR	-	expression tag	UNP P37231
B	200	PHE	-	expression tag	UNP P37231
B	201	GLN	-	expression tag	UNP P37231
B	202	GLY	-	expression tag	UNP P37231
B	478	LEU	-	expression tag	UNP P37231
B	479	VAL	-	expression tag	UNP P37231
B	480	PRO	-	expression tag	UNP P37231
B	481	ARG	-	expression tag	UNP P37231

- Molecule 2 is 5-CHLORO-1-(4-CHLOROBENZYL)-3-(PHENYLTHIO)-1H-INDOLE-2-CARBOXYLIC ACID (CCD ID: NZA) (formula: C₂₂H₁₅Cl₂NO₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			28	22	2	1	2	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			28	22	2	1	2	1		

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

3 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	94.08Å 94.08Å 192.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.93 – 2.95	Depositor
% Data completeness (in resolution range)	97.0 (37.93-2.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	379.46 (at 2.95Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.264 , 0.303	Depositor
Wilson B-factor (Å ²)	86.6	Xtriage
Anisotropy	0.054	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.399 for h,-h-k,-l	Xtriage
Total number of atoms	4045	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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 oligosaccharides 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	NZA	B	501	-	31,31,31	1.53	5 (16%)	42,44,44	2.61	8 (19%)
2	NZA	A	501	-	31,31,31	1.55	6 (19%)	42,44,44	2.57	8 (19%)

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	NZA	B	501	-	-	5/12/12/12	0/4/4/4
2	NZA	A	501	-	-	0/12/12/12	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NZA	CAZ-CAX	-4.25	1.36	1.44
2	A	501	NZA	CAZ-CAX	-3.72	1.37	1.44
2	A	501	NZA	CAX-SAR	3.64	1.82	1.76
2	B	501	NZA	CAX-SAR	3.24	1.81	1.76
2	A	501	NZA	CAW-SAR	3.23	1.82	1.78
2	B	501	NZA	CAW-SAR	3.18	1.82	1.78
2	B	501	NZA	CAZ-CBA	-2.92	1.37	1.41
2	A	501	NZA	CAZ-CBA	-2.92	1.37	1.41
2	A	501	NZA	CAY-NBB	-2.33	1.36	1.39
2	B	501	NZA	CAY-NBB	-2.25	1.36	1.39
2	A	501	NZA	CAY-CAS	2.12	1.53	1.48

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NZA	CAS-CAY-NBB	13.39	139.25	122.59
2	A	501	NZA	CAS-CAY-NBB	11.27	136.62	122.59
2	A	501	NZA	CAW-SAR-CAX	6.99	113.75	103.43
2	A	501	NZA	CAP-CAU-CLAD	4.78	125.16	119.17
2	B	501	NZA	CAQ-NBB-CBA	4.63	131.90	124.79
2	A	501	NZA	CAQ-NBB-CBA	4.24	131.31	124.79
2	B	501	NZA	CAQ-NBB-CAY	-4.16	120.36	126.93
2	B	501	NZA	CAP-CAU-CLAD	4.15	124.37	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NZA	CAQ-NBB-CAY	-4.11	120.44	126.93
2	A	501	NZA	CAL-CAU-CLAD	-3.40	114.33	119.36
2	B	501	NZA	CAW-SAR-CAX	2.97	107.82	103.43
2	B	501	NZA	CAZ-CAX-SAR	-2.94	120.32	125.55
2	A	501	NZA	CAZ-CAX-SAR	-2.72	120.71	125.55
2	B	501	NZA	CAL-CAU-CLAD	-2.49	115.69	119.36
2	B	501	NZA	CAO-CBA-CAZ	-2.14	119.56	121.95
2	A	501	NZA	CAX-CAY-NBB	-2.05	107.85	109.68

There are no chirality outliers.

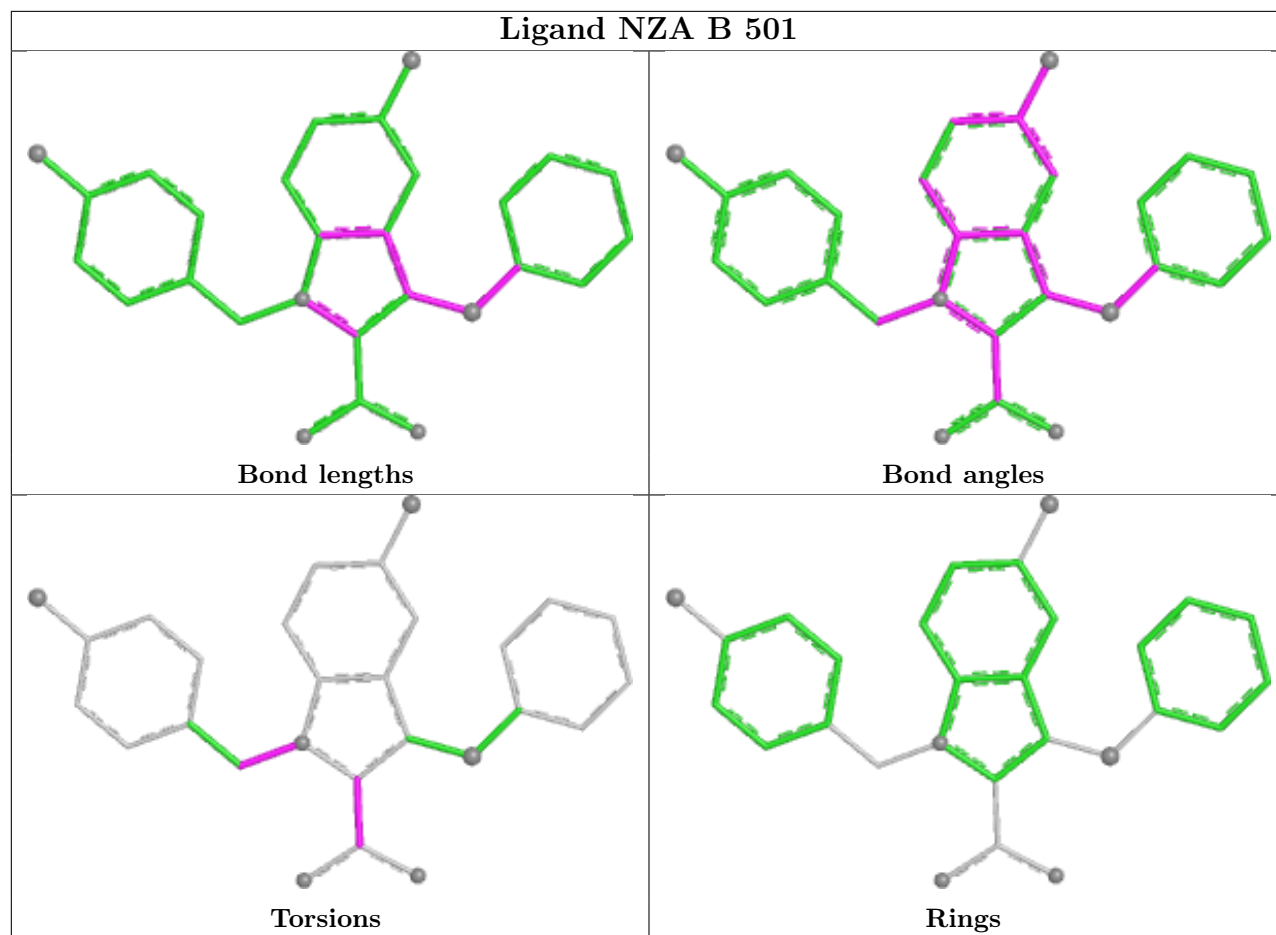
All (5) torsion outliers are listed below:

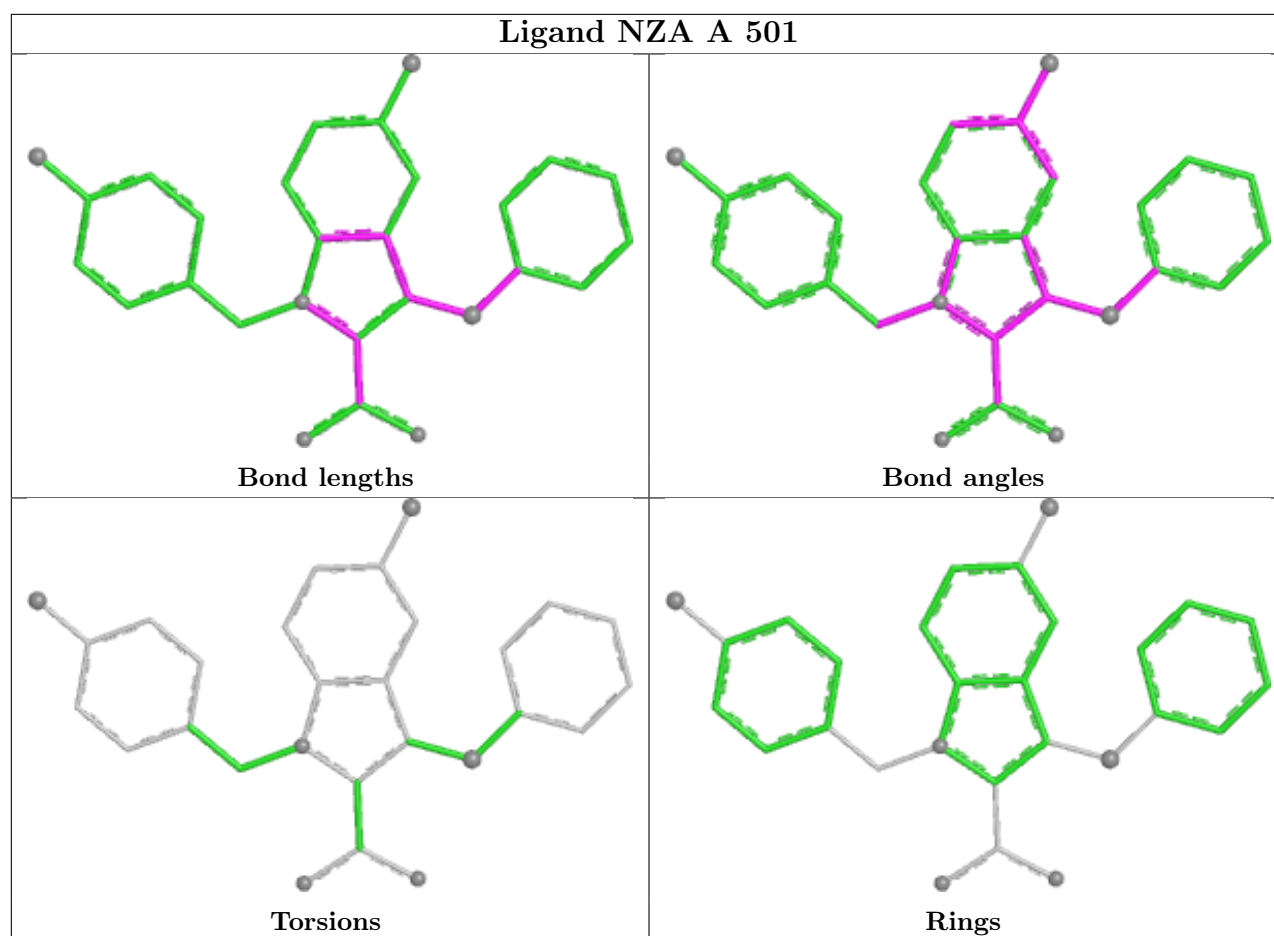
Mol	Chain	Res	Type	Atoms
2	B	501	NZA	OAB-CAS-CAY-NBB
2	B	501	NZA	OAA-CAS-CAY-NBB
2	B	501	NZA	OAB-CAS-CAY-CAX
2	B	501	NZA	OAA-CAS-CAY-CAX
2	B	501	NZA	CAV-CAQ-NBB-CBA

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 than 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.





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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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