



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:55 PM UTC

PDB ID : 9IWK / pdb_00009iwk
Title : X-ray structure of human PPARgamma ligand binding domain-NCOR2 corepressor peptide co-crystals obtained by co-crystallization
Authors : Kamata, S.; Honda, A.; Masuda, R.; Oota, M.; Namatame, R.; Machida, Y.; Uchii, K.; Shiiyama, Y.; Oyama, T.; Ishii, I.
Deposited on : 2024-07-25
Resolution : 2.43 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

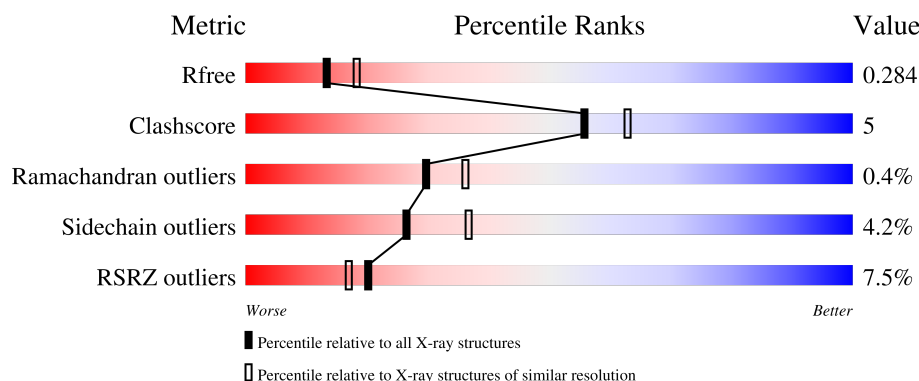
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	279	5% 74% 6% 19%
1	C	279	6% 74% 13% 11%
2	B	22	9% 18% 23% 59%
2	D	22	23% 27% 18% 55%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3881 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 Isoform 1 of Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1781	1148	288	336	9			
1	C	247	Total	C	N	O	S	0	0	0
			1958	1264	322	363	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLY	-	expression tag	UNP P37231-2
A	200	SER	-	expression tag	UNP P37231-2
A	201	HIS	-	expression tag	UNP P37231-2
A	202	MET	-	expression tag	UNP P37231-2
C	199	GLY	-	expression tag	UNP P37231-2
C	200	SER	-	expression tag	UNP P37231-2
C	201	HIS	-	expression tag	UNP P37231-2
C	202	MET	-	expression tag	UNP P37231-2

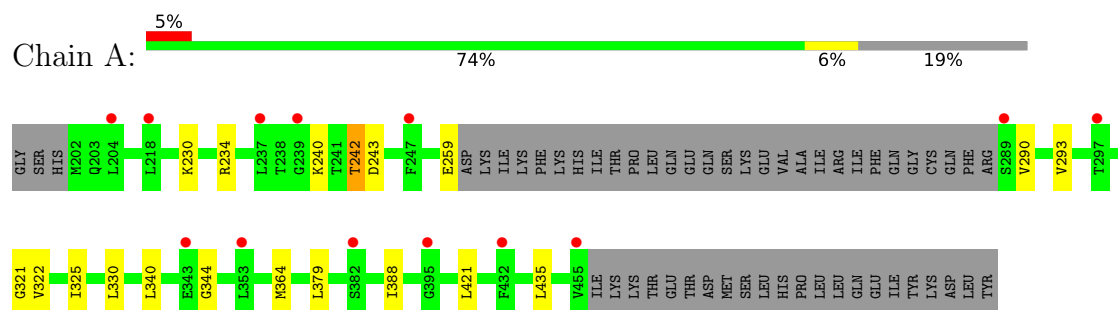
- Molecule 2 is a protein called Nuclear receptor corepressor 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			71	47	13	11			
2	D	10	Total	C	N	O	0	0	0
			71	46	13	12			

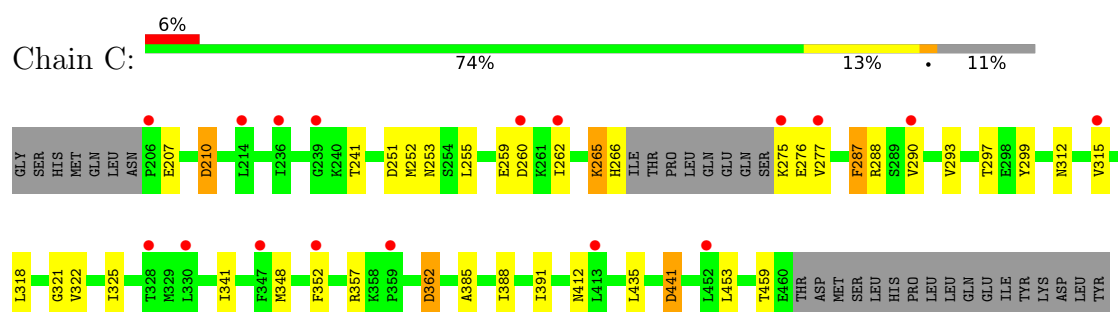
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

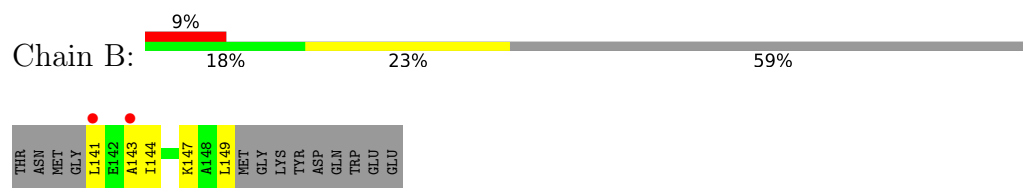
- Molecule 1: Isoform 1 of Peroxisome proliferator-activated receptor gamma



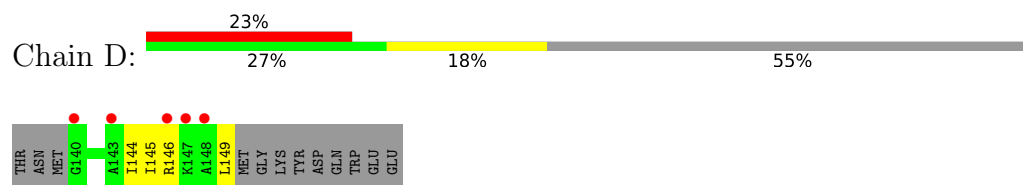
- Molecule 1: Isoform 1 of Peroxisome proliferator-activated receptor gamma



- Molecule 2: Nuclear receptor corepressor 2



- Molecule 2: Nuclear receptor corepressor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.30Å 60.05Å 92.83Å 90.00° 105.66° 90.00°	Depositor
Resolution (Å)	44.08 – 2.43 44.08 – 2.43	Depositor EDS
% Data completeness (in resolution range)	96.9 (44.08-2.43) 57.3 (44.08-2.43)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575-000)	Depositor
R, R_{free}	0.238 , 0.266 (Not available) , 0.284	Depositor DCC
R_{free} test set	1193 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3881	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.61% 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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.09	0/1810	0.23	0/2443
1	C	0.08	0/1990	0.23	0/2679
2	B	0.12	0/70	0.38	0/92
2	D	0.14	0/70	0.45	0/93
All	All	0.09	0/3940	0.24	0/5307

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 [i](#)

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	1781	0	1821	13	0
1	C	1958	0	2012	20	0
2	B	71	0	85	3	0
2	D	71	0	77	5	0
All	All	3881	0	3995	37	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 5.

All (37) 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:A:242:THR:OG1	1:A:243:ASP:N	2.11	0.79
1:C:362:ASP:N	1:C:362:ASP:OD1	2.23	0.70
1:A:379:LEU:HD11	1:A:435:LEU:HD21	1.73	0.69
1:C:288:ARG:HH22	1:C:341:ILE:HB	1.62	0.65
1:A:325:ILE:HD12	1:A:388:ILE:HG23	1.78	0.65
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.80	0.64
1:C:293:VAL:HG22	1:C:322:VAL:HG21	1.81	0.63
1:C:312:ASN:OD1	2:D:146:ARG:NH2	2.34	0.58
1:A:421:LEU:HD11	1:A:435:LEU:HD12	1.88	0.56
1:C:297:THR:HG23	1:C:318:LEU:HD13	1.86	0.56
2:D:145:ILE:O	2:D:146:ARG:HB2	2.07	0.54
1:C:325:ILE:HD12	1:C:388:ILE:HG13	1.90	0.52
1:C:290:VAL:HG13	2:D:144:ILE:HD13	1.92	0.52
1:A:340:LEU:HG	1:A:344:GLY:HA2	1.93	0.51
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.93	0.51
1:C:265:LYS:HB2	1:C:287:PHE:HB3	1.94	0.50
1:C:315:VAL:HG21	2:D:146:ARG:HG3	1.94	0.49
1:A:242:THR:HG1	1:A:243:ASP:H	1.57	0.48
1:A:330:LEU:HD21	1:A:364:MET:HE1	1.95	0.48
1:C:325:ILE:HG23	1:C:388:ILE:HG13	1.98	0.46
1:C:276:GLU:OE2	1:C:357:ARG:NH2	2.45	0.46
1:C:341:ILE:HD13	1:C:348:MET:HE3	1.98	0.46
1:C:259:GLU:HA	1:C:260:ASP:HA	1.57	0.45
1:A:321:GLY:O	1:A:325:ILE:HG12	2.17	0.44
1:C:207:GLU:HB3	1:C:210:ASP:HB2	1.99	0.44
1:A:290:VAL:HG13	2:B:144:ILE:HD13	2.00	0.43
1:C:255:LEU:HD22	1:C:352:PHE:HZ	1.84	0.43
2:B:141:LEU:C	2:B:143:ALA:H	2.27	0.43
1:C:325:ILE:HD11	1:C:391:ILE:HB	2.02	0.42
1:C:441:ASP:OD1	1:C:441:ASP:N	2.52	0.42
2:D:149:LEU:HD12	2:D:149:LEU:HA	1.86	0.41
1:A:230:LYS:O	1:A:234:ARG:HG2	2.20	0.41
1:A:435:LEU:HD23	1:A:435:LEU:HA	1.81	0.41
2:B:141:LEU:HD23	2:B:144:ILE:HG13	2.02	0.41
1:C:321:GLY:O	1:C:325:ILE:HG12	2.21	0.41
1:C:299:TYR:OH	1:C:385:ALA:O	2.30	0.41
1:C:252:MET:HE1	1:C:277:VAL:HG21	2.03	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	221/279 (79%)	214 (97%)	6 (3%)	1 (0%)	24	29
1	C	243/279 (87%)	238 (98%)	5 (2%)	0	100	100
2	B	7/22 (32%)	4 (57%)	2 (29%)	1 (14%)	0	0
2	D	8/22 (36%)	7 (88%)	1 (12%)	0	100	100
All	All	479/602 (80%)	463 (97%)	14 (3%)	2 (0%)	30	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	LYS
2	B	147	LYS

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	199/251 (79%)	197 (99%)	2 (1%)	68	77
1	C	216/251 (86%)	201 (93%)	15 (7%)	14	18
2	B	7/18 (39%)	6 (86%)	1 (14%)	3	2
2	D	6/18 (33%)	6 (100%)	0	100	100
All	All	428/538 (80%)	410 (96%)	18 (4%)	26	37

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	THR
1	A	259	GLU
2	B	149	LEU
1	C	210	ASP
1	C	241	THR
1	C	251	ASP
1	C	253	ASN
1	C	262	ILE
1	C	265	LYS
1	C	266	HIS
1	C	275	LYS
1	C	287	PHE
1	C	362	ASP
1	C	412	ASN
1	C	435	LEU
1	C	441	ASP
1	C	453	LEU
1	C	459	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	410	GLN
1	A	430	GLN
1	A	437	GLN
1	C	410	GLN
1	C	437	GLN
1	C	449	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	225/279 (80%)	0.57	13 (5%) 29 25	37, 59, 93, 107	0
1	C	247/279 (88%)	0.67	17 (6%) 23 19	39, 65, 101, 123	0
2	B	9/22 (40%)	1.67	2 (22%) 2 2	79, 82, 90, 90	0
2	D	10/22 (45%)	1.88	5 (50%) 0 0	77, 87, 96, 97	0
All	All	491/602 (81%)	0.67	37 (7%) 20 17	37, 63, 98, 123	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	SER	4.0
1	C	452	LEU	3.9
1	A	237	LEU	3.8
1	C	206	PRO	3.5
1	A	218	LEU	3.5
1	A	455	VAL	3.2
1	C	277	VAL	3.1
1	C	347	PHE	3.0
2	D	148	ALA	3.0
1	C	359	PRO	3.0
1	C	328	THR	2.9
1	C	214	LEU	2.8
1	A	353	LEU	2.8
1	C	262	ILE	2.7
1	A	432	PHE	2.6
1	A	239	GLY	2.6
1	A	382	SER	2.5
2	D	146	ARG	2.4
1	C	260	ASP	2.4
1	A	204	LEU	2.4
1	C	275	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	352	PHE	2.3
1	C	290	VAL	2.3
1	C	236	ILE	2.3
1	A	247	PHE	2.3
1	C	315	VAL	2.3
1	A	297	THR	2.3
2	B	141	LEU	2.3
1	C	330	LEU	2.2
1	A	395	GLY	2.2
1	A	343	GLU	2.1
2	D	143	ALA	2.1
1	C	413	LEU	2.1
2	B	143	ALA	2.1
1	C	239	GLY	2.0
2	D	140	GLY	2.0
2	D	147	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.