



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:06 AM UTC

PDB ID : 9O44 / pdb_00009o44
Title : Crystal structure of the L411W mutant of pregnane X receptor ligand binding domain (apo form)
Authors : Huber, A.D.; Garcia-Maldonado, E.; Miller, D.J.; Chen, T.
Deposited on : 2025-04-08
Resolution : 2.30 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:

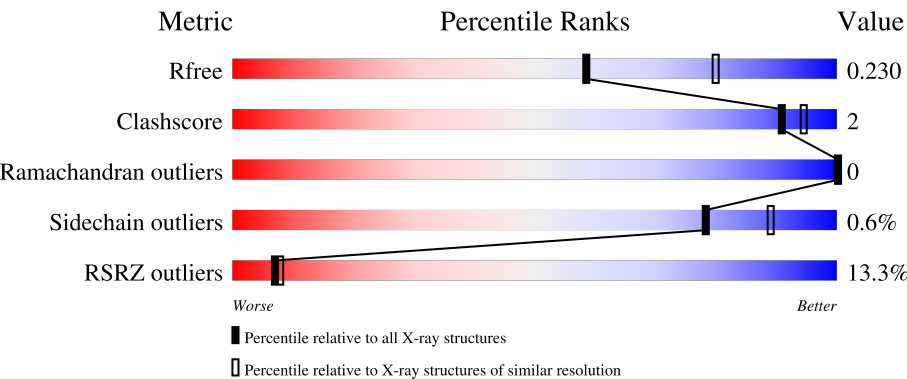
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	355	10% 76% 5% • 18%
1	B	355	12% 81% • 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4847 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 Pregnane X receptor ligand binding domain tethered to steroid receptor coactivator-1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	2	0
			2365	1521	409	417	18			
1	B	296	Total	C	N	O	S	0	1	0
			2346	1511	400	417	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	initiating methionine	UNP O75469
A	120	LYS	-	expression tag	UNP O75469
A	121	LYS	-	expression tag	UNP O75469
A	122	GLY	-	expression tag	UNP O75469
A	123	HIS	-	expression tag	UNP O75469
A	124	HIS	-	expression tag	UNP O75469
A	125	HIS	-	expression tag	UNP O75469
A	126	HIS	-	expression tag	UNP O75469
A	127	HIS	-	expression tag	UNP O75469
A	128	HIS	-	expression tag	UNP O75469
A	129	GLY	-	expression tag	UNP O75469
A	411	TRP	LEU	engineered mutation	UNP O75469
A	431D	SER	-	linker	UNP O75469
A	431E	GLY	-	linker	UNP O75469
A	431F	GLY	-	linker	UNP O75469
A	431G	SER	-	linker	UNP O75469
A	431H	GLY	-	linker	UNP O75469
A	431I	GLY	-	linker	UNP O75469
A	431J	SER	-	linker	UNP O75469
A	431K	SER	-	linker	UNP O75469
A	431L	HIS	-	linker	UNP O75469
A	431M	SER	-	linker	UNP O75469
B	119	MET	-	initiating methionine	UNP O75469
B	120	LYS	-	expression tag	UNP O75469

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Chain	Residue	Modelled	Actual	Comment	Reference
B	121	LYS	-	expression tag	UNP O75469
B	122	GLY	-	expression tag	UNP O75469
B	123	HIS	-	expression tag	UNP O75469
B	124	HIS	-	expression tag	UNP O75469
B	125	HIS	-	expression tag	UNP O75469
B	126	HIS	-	expression tag	UNP O75469
B	127	HIS	-	expression tag	UNP O75469
B	128	HIS	-	expression tag	UNP O75469
B	129	GLY	-	expression tag	UNP O75469
B	411	TRP	LEU	engineered mutation	UNP O75469
B	431D	SER	-	linker	UNP O75469
B	431E	GLY	-	linker	UNP O75469
B	431F	GLY	-	linker	UNP O75469
B	431G	SER	-	linker	UNP O75469
B	431H	GLY	-	linker	UNP O75469
B	431I	GLY	-	linker	UNP O75469
B	431J	SER	-	linker	UNP O75469
B	431K	SER	-	linker	UNP O75469
B	431L	HIS	-	linker	UNP O75469
B	431M	SER	-	linker	UNP O75469

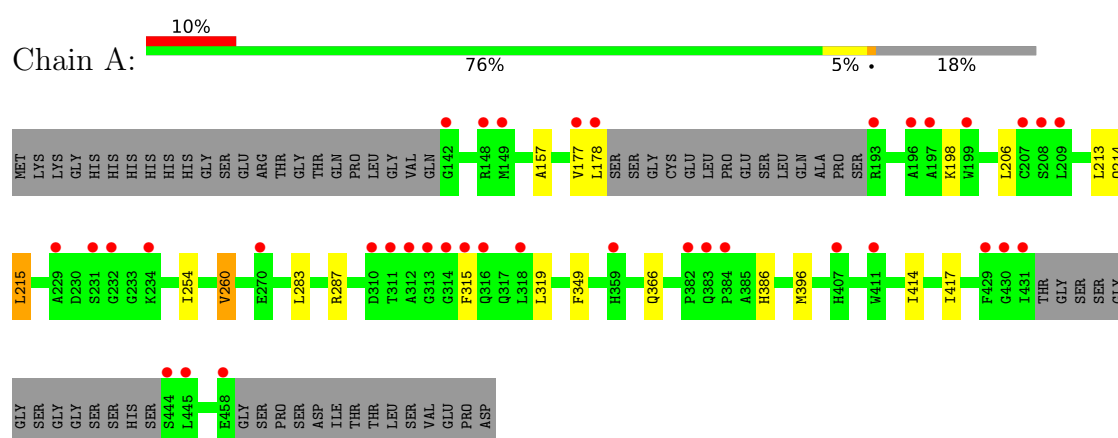
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	76	Total O 76 76	0	0
2	B	60	Total O 60 60	0	0

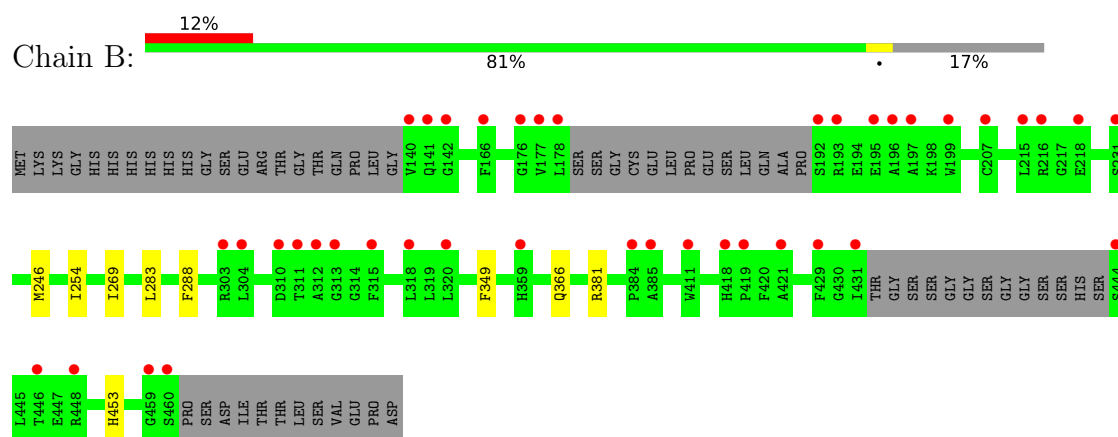
3 Residue-property plots

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: Pregnane X receptor ligand binding domain tethered to steroid receptor coactivator-1 peptide



- Molecule 1: Pregnane X receptor ligand binding domain tethered to steroid receptor coactivator-1 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.39Å 89.09Å 105.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.74 – 2.30 44.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.74-2.30) 99.3 (44.74-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.203 , 0.228 (Not available) , 0.230	Depositor DCC
R_{free} test set	1787 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4847	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

5.1 Standard geometry

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	0.32	0/2419	0.40	0/3260
1	B	0.35	0/2399	0.46	0/3241
All	All	0.34	0/4818	0.43	0/6501

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

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	2365	0	2341	12	0
1	B	2346	0	2288	4	0
2	A	76	0	0	1	0
2	B	60	0	0	0	0
All	All	4847	0	4629	16	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 2.

All (16) 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:396:MET:HA	1:A:396:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:O	1:A:178:LEU:CB	2.55	0.54
1:A:386:HIS:HD2	2:A:567:HOH:O	1.92	0.52
1:A:315:PHE:O	1:A:319:LEU:HG	2.12	0.50
1:B:254:ILE:HD12	1:B:283:LEU:HB3	1.94	0.49
1:A:198:LYS:HB3	1:A:417:ILE:HD11	1.94	0.49
1:A:213:LEU:CD2	1:A:215:LEU:HD12	2.43	0.48
1:A:213:LEU:HD23	1:A:214:GLN:N	2.28	0.48
1:A:254:ILE:HD12	1:A:283:LEU:HB3	1.96	0.46
1:A:254:ILE:HD11	1:A:287:ARG:HD2	1.99	0.44
1:B:246:MET:SD	1:B:288:PHE:HZ	2.41	0.43
1:A:157:ALA:HB2	1:A:260:VAL:HG22	2.01	0.42
1:B:269:ILE:HD13	1:B:453:HIS:CE1	2.55	0.42
1:A:349:PHE:O	1:A:366:GLN:HB2	2.21	0.41
1:B:349:PHE:O	1:B:366:GLN:HB2	2.21	0.41
1:A:206:LEU:HD21	1:A:414:ILE:HD13	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	109/355 (31%)	107 (98%)	2 (2%)	0	100	100
1	B	254/355 (72%)	250 (98%)	4 (2%)	0	100	100
All	All	363/710 (51%)	357 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	253/313 (81%)	251 (99%)	2 (1%)	73	86
1	B	246/313 (79%)	245 (100%)	1 (0%)	84	92
All	All	499/626 (80%)	496 (99%)	3 (1%)	78	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	LEU
1	A	260	VAL
1	B	381	ARG

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	158	GLN
1	A	201	GLN
1	A	214	GLN
1	A	224	ASN
1	A	317	GLN
1	A	344	GLN
1	B	380	ASN

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	291/355 (81%)	0.63	37 (12%)	8 8	14, 45, 86, 109	2 (0%)
1	B	296/355 (83%)	0.65	41 (13%)	6 7	15, 47, 82, 110	1 (0%)
All	All	587/710 (82%)	0.64	78 (13%)	7 8	14, 46, 84, 110	3 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	6.3
1	B	177	VAL	5.2
1	A	315	PHE	5.1
1	A	207	CYS	5.0
1	A	383	GLN	5.0
1	B	178	LEU	4.8
1	B	431	ILE	4.8
1	A	177	VAL	4.7
1	A	431	ILE	4.2
1	B	199	TRP	4.1
1	B	460	SER	4.1
1	A	384	PRO	4.0
1	B	142	GLY	3.8
1	B	192	SER	3.7
1	A	231	SER	3.5
1	A	359[A]	HIS	3.5
1	A	445	LEU	3.5
1	B	411	TRP	3.3
1	B	196	ALA	3.3
1	A	196	ALA	3.2
1	B	140	VAL	3.2
1	A	199	TRP	3.2
1	B	429	PHE	3.1
1	B	197	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	311	THR	3.0
1	A	193	ARG	3.0
1	A	208	SER	3.0
1	B	193	ARG	2.9
1	B	320	LEU	2.9
1	B	195	GLU	2.9
1	B	359	HIS	2.9
1	B	312	ALA	2.9
1	B	318	LEU	2.8
1	B	303	ARG	2.8
1	A	444	SER	2.8
1	B	141	GLN	2.8
1	B	315	PHE	2.7
1	B	418	HIS	2.7
1	A	313	GLY	2.7
1	A	318	LEU	2.7
1	A	229	ALA	2.7
1	B	218	GLU	2.7
1	B	385	ALA	2.7
1	B	215	LEU	2.7
1	A	197	ALA	2.6
1	A	310	ASP	2.6
1	A	312	ALA	2.5
1	A	314	GLY	2.5
1	A	458	GLU	2.5
1	B	310	ASP	2.5
1	A	382	PRO	2.5
1	B	304	LEU	2.5
1	B	207	CYS	2.4
1	B	311	THR	2.4
1	A	429	PHE	2.4
1	A	209	LEU	2.4
1	A	316	GLN	2.4
1	A	149	MET	2.3
1	A	232	GLY	2.3
1	A	270	GLU	2.3
1	B	166	PHE	2.3
1	B	459	GLY	2.2
1	B	421	ALA	2.2
1	B	176	GLY	2.2
1	B	216	ARG	2.1
1	B	384	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	313	GLY	2.1
1	A	407	HIS	2.1
1	A	430	GLY	2.1
1	B	231	SER	2.1
1	B	444	SER	2.1
1	A	411	TRP	2.1
1	A	142	GLY	2.0
1	B	446	THR	2.0
1	A	148	ARG	2.0
1	B	419	PRO	2.0
1	B	448	ARG	2.0
1	A	234	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.