Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 06:33 PM EDT

PDB ID	:	1ILG
Title	:	Crystal Structure of Apo Human Pregnane X Receptor Ligand Binding Domain
Authors	:	Watkins, R.E.; Redinbo, M.R.
Deposited on	:	2001-05-08
Resolution	:	2.52 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:

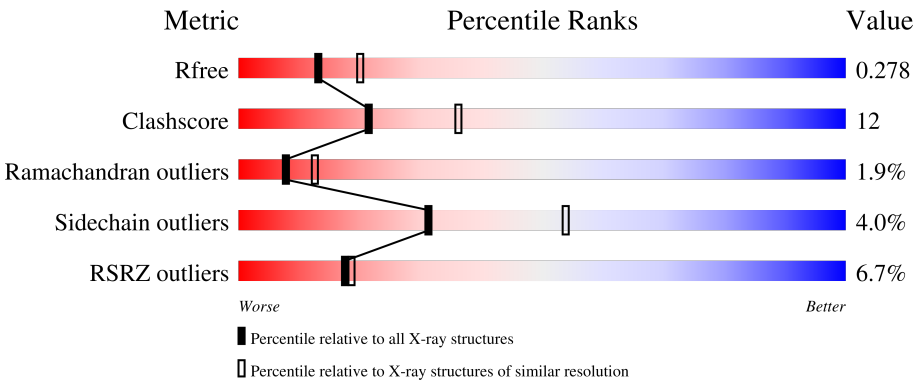
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.52 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 <=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	316	6% 62% 22% • 15%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2391 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 ORPHAN NUCLEAR RECEPTOR PXR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2141	1383	364	377	17	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	expression tag	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

- Molecule 2 is water.

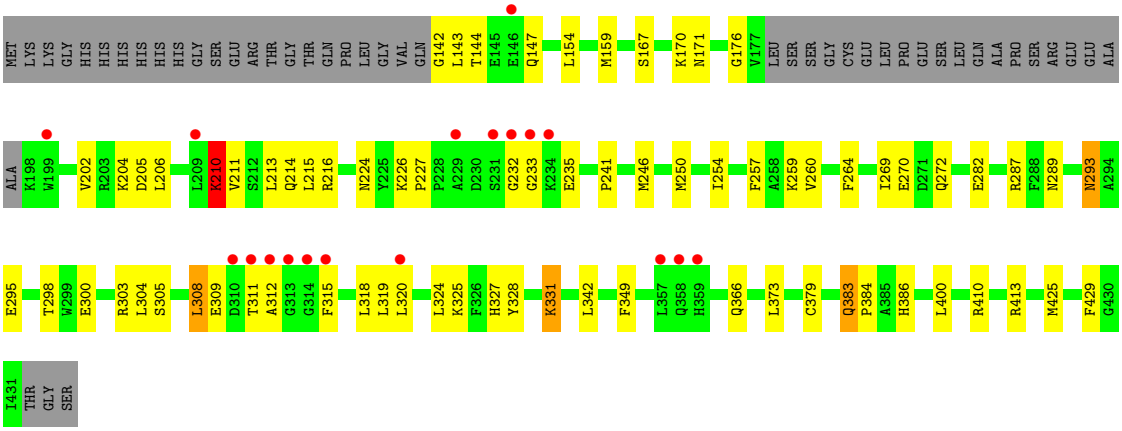
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	250	250	250	0	0

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: ORPHAN NUCLEAR RECEPTOR PXR

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.59Å 91.59Å 84.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.52 19.91 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.91-2.52) 99.4 (19.91-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.18 (at 2.53Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.279 0.215 , 0.278	Depositor DCC
R_{free} test set	1295 reflections (10.33%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2391	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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.

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	0.36	0/2189	0.68	3/2954 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	311	THR	N-CA-C	15.69	153.36	111.00
1	A	312	ALA	N-CA-CB	-11.72	93.69	110.10
1	A	311	THR	CB-CA-C	-9.99	84.61	111.60

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	2141	0	2109	51	0
2	A	250	0	0	10	0
All	All	2391	0	2109	51	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 12.

All (51) 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:282:GLU:HG2	1:A:400:LEU:HG	1.64	0.77
1:A:206:LEU:H	1:A:206:LEU:HD12	1.55	0.71
1:A:205:ASP:HB3	1:A:410:ARG:HD3	1.75	0.68
1:A:214:GLN:HE21	1:A:216:ARG:HH11	1.45	0.63
1:A:303:ARG:HG3	1:A:303:ARG:HH11	1.66	0.59
1:A:167:SER:HB2	2:A:660:HOH:O	2.03	0.59
1:A:319:LEU:HD12	2:A:437:HOH:O	2.04	0.57
1:A:319:LEU:HA	2:A:437:HOH:O	2.05	0.57
1:A:246:MET:O	1:A:246:MET:HE2	2.05	0.57
1:A:293:ASN:HD21	1:A:295:GLU:HB2	1.70	0.56
1:A:144:THR:H	1:A:147:GLN:NE2	2.03	0.56
1:A:293:ASN:HD22	1:A:295:GLU:H	1.54	0.56
1:A:215:LEU:CD2	1:A:304:LEU:HD13	2.35	0.56
1:A:315:PHE:HD1	1:A:318:LEU:HD12	1.71	0.55
1:A:210:LYS:HG3	1:A:309:GLU:HG3	1.87	0.55
1:A:293:ASN:HD22	1:A:293:ASN:C	2.10	0.55
1:A:257:PHE:O	1:A:260:VAL:HG12	2.07	0.55
1:A:289:ASN:HD22	1:A:327:HIS:HD1	1.55	0.55
1:A:293:ASN:ND2	1:A:295:GLU:H	2.06	0.54
1:A:259:LYS:NZ	2:A:441:HOH:O	2.42	0.53
1:A:383:GLN:HG2	1:A:386:HIS:ND1	2.23	0.53
1:A:300:GLU:HG2	2:A:529:HOH:O	2.09	0.52
1:A:142:GLY:HA2	1:A:379:CYS:SG	2.50	0.52
1:A:425:MET:O	1:A:429:PHE:HD1	1.93	0.51
1:A:320:LEU:HB3	2:A:662:HOH:O	2.11	0.51
1:A:215:LEU:HD23	1:A:304:LEU:HD13	1.94	0.50
1:A:170:LYS:O	1:A:171:ASN:HB2	2.12	0.49
1:A:202:VAL:C	1:A:204:LYS:H	2.16	0.49
1:A:206:LEU:HD12	1:A:206:LEU:N	2.25	0.48
1:A:211:VAL:HG12	1:A:308:LEU:HD13	1.95	0.48
1:A:384:PRO:HB3	2:A:455:HOH:O	2.13	0.47
1:A:325:LYS:HD3	2:A:492:HOH:O	2.14	0.47
1:A:205:ASP:OD2	1:A:413:ARG:NH1	2.45	0.47
1:A:342:LEU:HD13	1:A:373:LEU:HA	1.97	0.46
1:A:260:VAL:HG22	1:A:260:VAL:O	2.16	0.45
1:A:269:ILE:HG22	1:A:270:GLU:OE1	2.16	0.45
1:A:226:LYS:HD3	1:A:227:PRO:O	2.17	0.45
1:A:383:GLN:CD	1:A:383:GLN:H	2.20	0.45
1:A:213:LEU:HD21	1:A:215:LEU:HG	2.00	0.44
1:A:331:LYS:HE2	2:A:472:HOH:O	2.17	0.43
1:A:254:ILE:HD11	1:A:287:ARG:HD2	2.01	0.43
1:A:264:PHE:CZ	1:A:272:GLN:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:H	1:A:147:GLN:HE21	1.67	0.42
1:A:214:GLN:HB3	1:A:305:SER:HB2	2.01	0.42
1:A:246:MET:HE2	1:A:250:MET:HG2	2.01	0.42
1:A:241:PRO:HD2	2:A:454:HOH:O	2.20	0.41
1:A:269:ILE:HG23	1:A:270:GLU:N	2.34	0.41
1:A:349:PHE:O	1:A:366:GLN:HB2	2.21	0.41
1:A:324:LEU:HD12	1:A:328:TYR:HE1	1.85	0.40
1:A:143:LEU:HA	1:A:147:GLN:NE2	2.36	0.40
1:A:383:GLN:HA	1:A:384:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	266/316 (84%)	246 (92%)	15 (6%)	5 (2%)	8 12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	GLU
1	A	176	GLY
1	A	210	LYS
1	A	233	GLY
1	A	232	GLY

5.3.2 Protein sidechains (i)

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	225/279 (81%)	216 (96%)	9 (4%)	31 54

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LEU
1	A	159	MET
1	A	210	LYS
1	A	224	ASN
1	A	293	ASN
1	A	298	THR
1	A	308	LEU
1	A	331	LYS
1	A	383	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	171	ASN
1	A	214	GLN
1	A	224	ASN
1	A	272	GLN
1	A	285	GLN
1	A	293	ASN
1	A	364	GLN
1	A	380	ASN
1	A	383	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	270/316 (85%)	0.06	18 (6%) 17 18	19, 37, 91, 103	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	ALA	11.9
1	A	311	THR	10.8
1	A	313	GLY	4.9
1	A	233	GLY	4.7
1	A	232	GLY	4.3
1	A	359	HIS	3.8
1	A	310	ASP	3.4
1	A	231	SER	3.0
1	A	229	ALA	3.0
1	A	357	LEU	2.8
1	A	315	PHE	2.6
1	A	358	GLN	2.5
1	A	146	GLU	2.5
1	A	234	LYS	2.3
1	A	199	TRP	2.3
1	A	320	LEU	2.3
1	A	209	LEU	2.2
1	A	314	GLY	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 monosaccharides 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.