



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:08 AM GMT

PDB ID : 1ILH
Title : Crystal Structure of Human Pregnane X Receptor Ligand Binding Domain
Bound to SR12813
Authors : Watkins, R.E.; Redinbo, M.R.
Deposited on : 2001-05-08
Resolution : 2.76 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

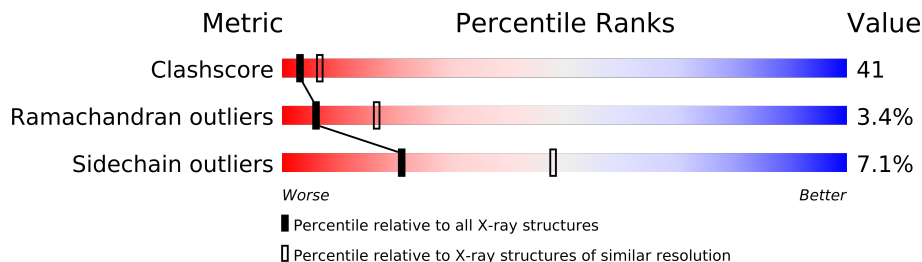
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.76 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))
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	316	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2406 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

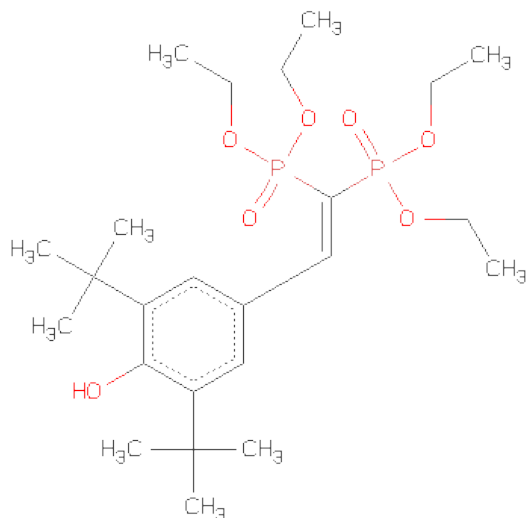
- Molecule 1 is a protein called ORPHAN NUCLEAR RECEPTOR PXR.

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 [2-(3,5-DI-TERT-BUTYL-4-HYDROXY-PHENYL)-1-(DIETHOXY-PHOSPHORYL)-VINYL]-PHOSPHONICACID DIETHYL ESTER (three-letter code: SRL) (formula: C₂₄H₄₂O₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	99	72	21	6	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total	O	0	0
			166	166		

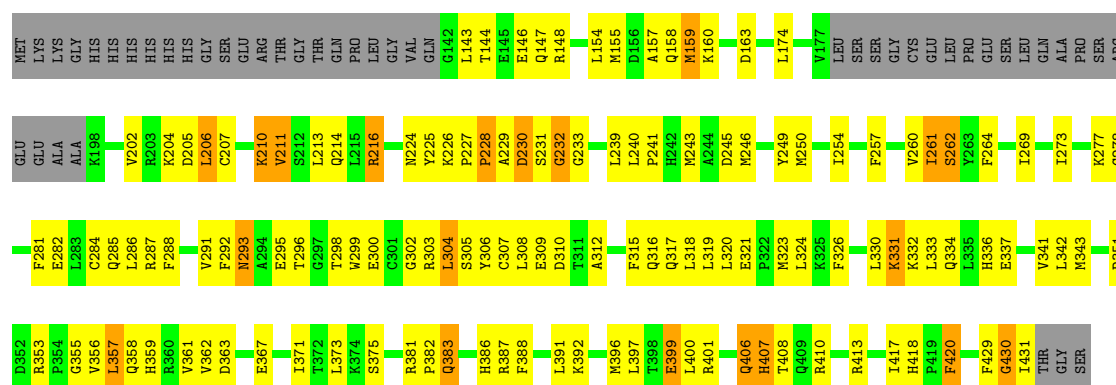
3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: ORPHAN NUCLEAR RECEPTOR PXR

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.34Å 91.34Å 85.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.76	Depositor
% Data completeness (in resolution range)	99.2 (19.86-2.76)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2406	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SRL

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	0.40	0/2189	0.62	1/2954 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	232	GLY	N-CA-C	-6.99	95.63	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	HIS	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2141	0	2109	179	1
2	A	99	0	123	50	0
3	A	166	0	0	11	1
All	All	2406	0	2232	184	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

The worst 5 of 184 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:MET:CG	2:A:1[C]:SRL:H161	1.72	1.18
1:A:323:MET:HG2	2:A:1[C]:SRL:C16	1.77	1.14
1:A:281:PHE:HD1	2:A:1[A]:SRL:H153	1.17	1.08
1:A:243:MET:HB3	2:A:1[C]:SRL:H263	1.07	1.04
1:A:243:MET:SD	2:A:1[A]:SRL:H303	2.02	0.99

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:358:GLN:OE1	3:A:1600:HOH:O[6_465]	2.16	0.04

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	266/316 (84%)	232 (87%)	25 (9%)	9 (3%)	6 17

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ILE
1	A	316	GLN
1	A	233	GLY

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Mol	Chain	Res	Type
1	A	262	SER
1	A	430	GLY

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	225/279 (81%)	209 (93%)	16 (7%)	21	48

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	304	LEU
1	A	383	GLN
1	A	224	ASN
1	A	391	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	407	HIS
1	A	368	GLN
1	A	224	ASN
1	A	344	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	SRL	A	1[A]	-	33,33,33	1.98	6 (18%)	49,50,50	2.71	19 (38%)
2	SRL	A	1[B]	-	33,33,33	2.49	10 (30%)	49,50,50	2.66	19 (38%)
2	SRL	A	1[C]	-	33,33,33	2.22	11 (33%)	49,50,50	2.78	18 (36%)

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	SRL	A	1[A]	-	-	4/44/44/44	0/1/1/1
2	SRL	A	1[B]	-	-	3/44/44/44	0/1/1/1
2	SRL	A	1[C]	-	-	2/44/44/44	0/1/1/1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1[B]	SRL	P9-C8	7.31	1.91	1.79
2	A	1[C]	SRL	C2-C3	6.30	1.49	1.41
2	A	1[A]	SRL	P9-C8	4.66	1.87	1.79
2	A	1[B]	SRL	C2-C3	4.61	1.47	1.41
2	A	1[A]	SRL	P9-O20	4.57	1.52	1.46

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1[C]	SRL	C13-C3-C2	10.42	132.48	121.96
2	A	1[B]	SRL	C13-C3-C2	9.14	131.18	121.96
2	A	1[A]	SRL	C13-C3-C2	9.11	131.15	121.96
2	A	1[B]	SRL	O21-P9-O20	-5.30	103.40	115.07
2	A	1[C]	SRL	C4-C3-C2	-5.29	111.83	116.77

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1[C]	SRL	O20-P9-C8-C7
2	A	1[B]	SRL	O20-P9-C8-C7
2	A	1[A]	SRL	O21-P9-C8-C7
2	A	1[A]	SRL	O20-P9-C8-C7
2	A	1[B]	SRL	O21-P9-C8-C7

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.