



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 8SVN / pdb_00008svn
Title : Crystal structure of the apo form of pregnane X receptor ligand binding domain
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Deposited on : 2023-05-17
Resolution : 2.20 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

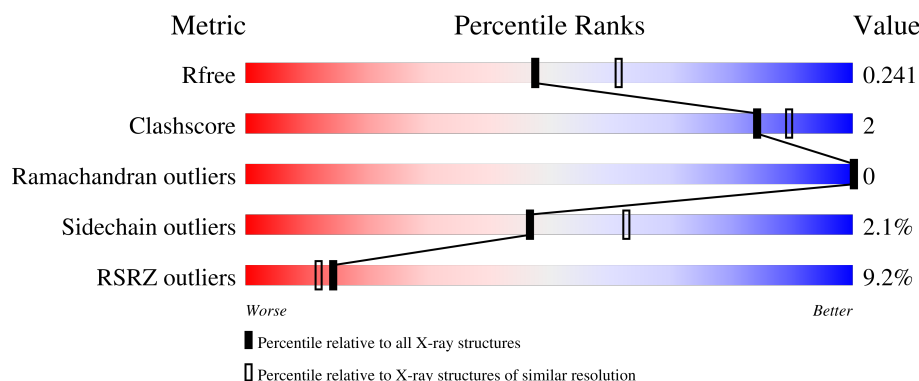
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	351	9% 75% 6% 18%
1	B	351	6% 77% 5% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4666 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 fused to SRC-1 coactivator peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	3	0
			2283	1465	394	406	18			
1	B	289	Total	C	N	O	S	0	2	0
			2311	1486	397	409	19			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	435	SER	-	linker	UNP O75469
A	436	GLY	-	linker	UNP O75469
A	437	GLY	-	linker	UNP O75469
A	438	SER	-	linker	UNP O75469
A	439	GLY	-	linker	UNP O75469
A	440	GLY	-	linker	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	435	SER	-	linker	UNP O75469
B	436	GLY	-	linker	UNP O75469
B	437	GLY	-	linker	UNP O75469
B	438	SER	-	linker	UNP O75469

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Chain	Residue	Modelled	Actual	Comment	Reference
B	439	GLY	-	linker	UNP O75469
B	440	GLY	-	linker	UNP O75469

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	36	Total O 36 36	0	0
2	B	36	Total O 36 36	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.99Å 89.65Å 106.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.44 – 2.20 53.44 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (53.44-2.20) 99.9 (53.44-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487)	Depositor
R, R_{free}	0.210 , 0.235 0.213 , 0.241	Depositor DCC
R_{free} test set	2133 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4666	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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	0.19	0/2338	0.34	0/3156
1	B	0.14	0/2363	0.29	0/3185
All	All	0.17	0/4701	0.32	0/6341

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	2283	0	2222	13	0
1	B	2311	0	2281	9	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
All	All	4666	0	4503	21	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 (21) 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:281:PHE:HZ	1:A:323:MET:HE1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LYS:HD2	1:B:450:HIS:NE2	2.23	0.53
1:A:383:GLN:CD	1:A:383:GLN:H	2.17	0.53
1:A:165:THR:OG1	1:A:167:SER:OG	2.21	0.50
1:B:155:MET:HE2	1:B:155:MET:HA	1.93	0.50
1:A:228:PRO:HD3	1:B:221:SER:HB3	1.94	0.50
1:A:281:PHE:CZ	1:A:323:MET:HE1	2.45	0.48
1:A:202:VAL:HG11	1:A:417:ILE:HD11	1.96	0.48
1:A:381:ARG:HB3	1:A:386:HIS:CD2	2.49	0.48
1:B:422:THR:OG1	1:B:425:MET:HG3	2.16	0.46
1:A:211:VAL:HG21	1:A:306:TYR:HB3	1.97	0.45
1:A:277:LYS:HD2	1:A:450:HIS:NE2	2.31	0.45
1:A:405:ALA:O	1:A:409:GLN:HG2	2.17	0.45
1:B:350:SER:HB3	1:B:401:ARG:HH22	1.83	0.44
1:B:254:ILE:HD12	1:B:283:LEU:HB3	2.00	0.43
1:A:259:LYS:HD3	1:A:457:LEU:HA	2.00	0.43
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.83	0.43
1:B:278:GLY:HA3	1:B:353:ARG:HD2	2.01	0.43
1:A:210:LYS:HA	1:A:210:LYS:HD2	1.78	0.41
1:B:342:LEU:HD13	1:B:373:LEU:HA	2.02	0.41
1:B:352:ASP:OD1	1:B:401:ARG:NH2	2.54	0.41

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	282/351 (80%)	276 (98%)	6 (2%)	0	100	100
1	B	283/351 (81%)	279 (99%)	4 (1%)	0	100	100
All	All	565/702 (80%)	555 (98%)	10 (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	240/310 (77%)	235 (98%)	5 (2%)	47	63
1	B	246/310 (79%)	241 (98%)	5 (2%)	48	64
All	All	486/620 (78%)	476 (98%)	10 (2%)	47	63

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	A	206	LEU
1	A	260	VAL
1	A	383	GLN
1	A	453	LEU
1	B	155	MET
1	B	209	LEU
1	B	320	LEU
1	B	323	MET
1	B	411	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	201	GLN
1	A	383	GLN
1	A	386	HIS
1	B	201	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

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	287/351 (81%)	0.59	31 (10%) 11 8	24, 68, 110, 134	3 (1%)
1	B	289/351 (82%)	0.51	22 (7%) 20 17	25, 69, 110, 148	2 (0%)
All	All	576/702 (82%)	0.55	53 (9%) 14 12	24, 68, 110, 148	5 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	GLU	4.3
1	A	178	LEU	4.3
1	A	309	GLU	4.0
1	B	385	ALA	4.0
1	A	192	SER	3.9
1	A	382	PRO	3.6
1	B	384	PRO	3.5
1	A	229	ALA	3.5
1	B	310	ASP	3.4
1	A	232	GLY	3.4
1	A	177	VAL	3.3
1	A	316	GLN	3.2
1	A	193	ARG	3.0
1	B	207	CYS	3.0
1	A	318	LEU	3.0
1	B	197	ALA	3.0
1	B	314	GLY	3.0
1	A	207	CYS	2.9
1	A	235	GLU	2.9
1	A	319	LEU	2.9
1	B	431	ILE	2.9
1	A	317	GLN	2.8
1	B	318	LEU	2.8
1	A	445	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	202	VAL	2.8
1	A	195	GLU	2.7
1	A	236	ILE	2.6
1	B	315	PHE	2.6
1	B	196	ALA	2.6
1	A	199	TRP	2.6
1	B	316	GLN	2.5
1	B	383	GLN	2.5
1	A	303	ARG	2.5
1	A	209	LEU	2.4
1	A	352	ASP	2.4
1	B	178	LEU	2.4
1	B	200	SER	2.4
1	A	320	LEU	2.4
1	A	432	THR	2.3
1	A	233	GLY	2.2
1	B	317	GLN	2.2
1	A	323	MET	2.2
1	B	199	TRP	2.2
1	B	150[A]	MET	2.2
1	A	197	ALA	2.2
1	B	461	SER	2.2
1	A	194	GLU	2.1
1	A	407	HIS	2.1
1	A	269	ILE	2.1
1	B	205	ASP	2.1
1	B	215	LEU	2.0
1	A	251	PHE	2.0
1	A	379	CYS	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.