



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 09:40 am BST

PDB ID : 4S0S  
Title : STRUCTURE OF HUMAN PREGNANE X RECEPTOR LIGAND BINDING DOMAIN with ADNECTIN-1  
Authors : Khan, J.A.  
Deposited on : 2015-01-05  
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

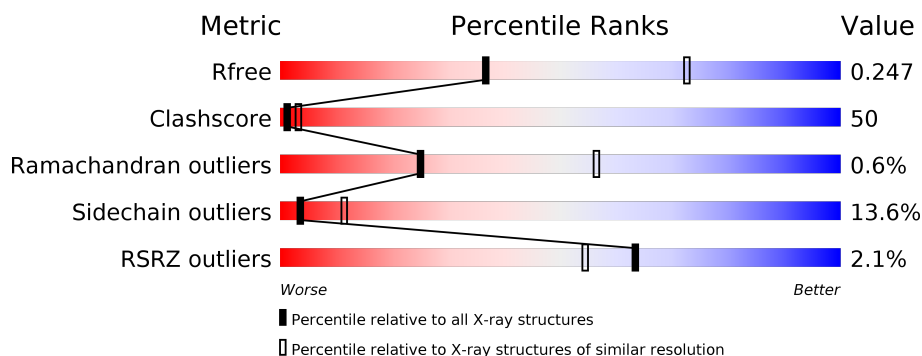
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	315	<div> <div>%</div> <div> <div></div> <div>42%</div> <div>37%</div> <div>7%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	315	<div> <div>%</div> <div> <div></div> <div>45%</div> <div>36%</div> <div>5%</div> <div>•</div> <div>13%</div> </div> </div>
2	D	120	<div> <div>3%</div> <div> <div></div> <div>27%</div> <div>29%</div> <div>13%</div> <div>7%</div> <div>25%</div> </div> </div>
2	E	120	<div> <div>5%</div> <div> <div></div> <div>18%</div> <div>38%</div> <div>16%</div> <div>•</div> <div>25%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5622 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 Nuclear receptor subfamily 1 group I member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2130	1371	354	388	17			
1	B	273	Total	C	N	O	S	0	1	0
			2123	1371	350	384	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	EXPRESSION TAG	UNP O75469
A	121	LYS	-	EXPRESSION TAG	UNP O75469
A	122	LYS	-	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
B	120	MET	-	EXPRESSION TAG	UNP O75469
B	121	LYS	-	EXPRESSION TAG	UNP O75469
B	122	LYS	-	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

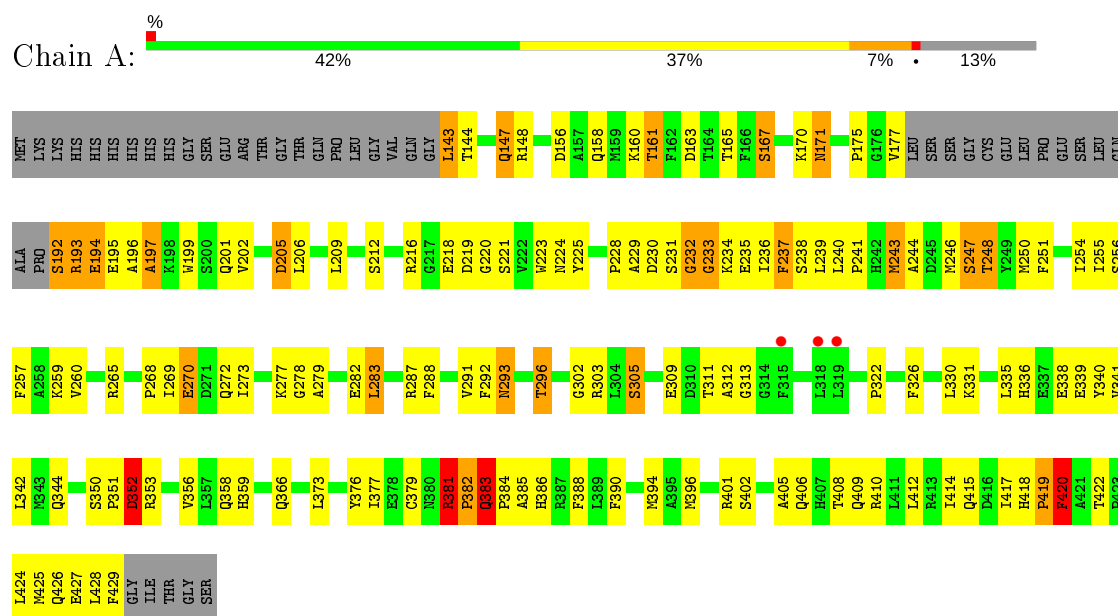
- Molecule 2 is a protein called Adnectin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	90	Total 684	C 448	N 98	O 136	S 2	0	0	0
2	E	90	Total 685	C 448	N 98	O 137	S 2	0	0	0

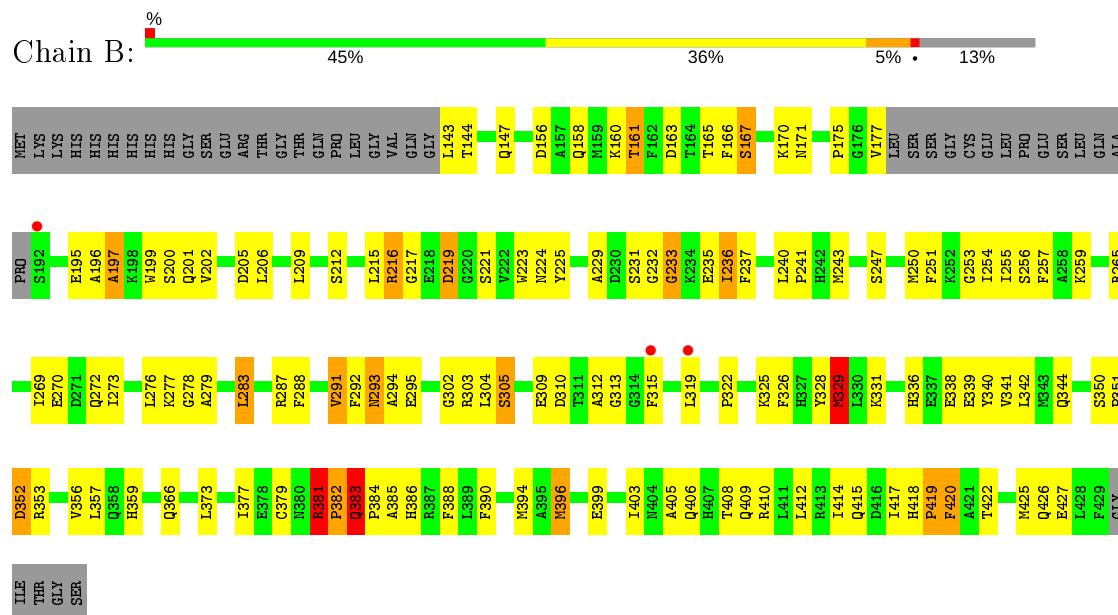
### 3 Residue-property plots

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

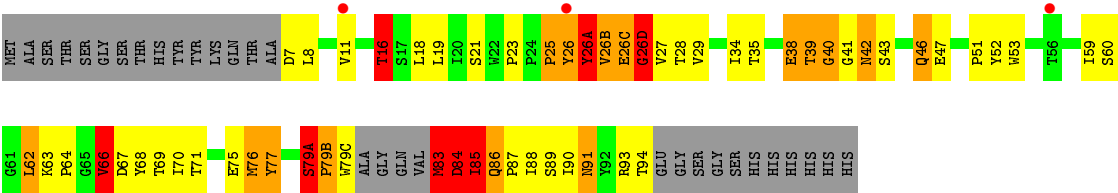
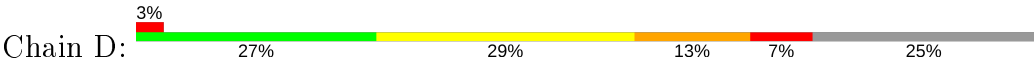
- Molecule 1: Nuclear receptor subfamily 1 group I member 2



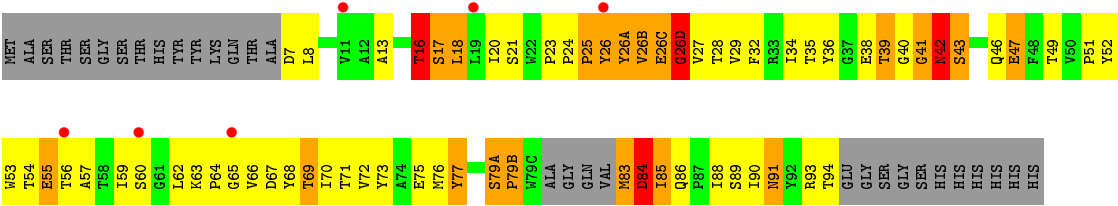
- Molecule 1: Nuclear receptor subfamily 1 group I member 2



● Molecule 2: Adnectin-1



● Molecule 2: Adnectin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.23Å 119.23Å 83.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 – 2.80 48.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.91-2.80) 99.9 (48.56-2.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.6, BUSTER	Depositor
R, $R_{free}$	0.216 , 0.229 0.249 , 0.247	Depositor DCC
$R_{free}$ test set	1479 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.9	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 70.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.33	0/2180	0.39	0/2953
1	B	0.37	2/2176 (0.1%)	1.39	3/2948 (0.1%)
2	D	0.45	1/706 (0.1%)	0.89	3/978 (0.3%)
2	E	0.30	0/707	0.44	0/979
All	All	0.36	3/5769 (0.1%)	0.95	6/7858 (0.1%)

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	18
1	B	0	12
2	D	0	16
2	E	0	12
All	All	0	58

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	66	VAL	C-N	8.88	1.54	1.34
1	B	329[A]	MET	CA-C	5.56	1.67	1.52
1	B	329[B]	MET	CA-C	5.56	1.67	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329[A]	MET	CA-C-O	-49.89	15.33	120.10
1	B	329[B]	MET	CA-C-O	-49.89	15.33	120.10
2	D	66	VAL	O-C-N	16.35	148.85	122.70
2	D	66	VAL	CA-C-N	-16.23	81.48	117.20
1	B	328	TYR	C-N-CA	14.40	157.71	121.70



There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	SER	Peptide
1	A	193	ARG	Peptide
1	A	194	GLU	Peptide
1	A	195	GLU	Peptide
1	A	197	ALA	Peptide

## 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	2130	0	2018	189	0
1	B	2123	0	1998	164	0
2	D	684	0	639	117	0
2	E	685	0	640	101	0
All	All	5622	0	5295	547	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 50.

The worst 5 of 547 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:352:ASP:CB	1:A:401:ARG:HH22	1.10	1.50
1:A:161:THR:HG21	1:A:257:PHE:CB	1.53	1.38
1:B:161:THR:HG21	1:B:257:PHE:CB	1.54	1.37
1:A:161:THR:HG21	1:A:257:PHE:CA	1.58	1.32
1:A:192:SER:N	1:A:193:ARG:O	1.59	1.32

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	269/315 (85%)	263 (98%)	5 (2%)	1 (0%)	34	66
1	B	270/315 (86%)	262 (97%)	7 (3%)	1 (0%)	34	66
2	D	86/120 (72%)	83 (96%)	2 (2%)	1 (1%)	13	39
2	E	86/120 (72%)	81 (94%)	4 (5%)	1 (1%)	13	39
All	All	711/870 (82%)	689 (97%)	18 (2%)	4 (1%)	25	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	26(D)	GLY
2	E	26(D)	GLY
1	A	419	PRO
1	B	419	PRO

### 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	218/279 (78%)	197 (90%)	21 (10%)	8	24
1	B	214/279 (77%)	192 (90%)	22 (10%)	7	21
2	D	75/102 (74%)	57 (76%)	18 (24%)	0	2
2	E	75/102 (74%)	56 (75%)	19 (25%)	0	1
All	All	582/762 (76%)	502 (86%)	80 (14%)	3	11

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	329[A]	MET
2	D	18	LEU
2	E	69	THR
1	B	329[B]	MET
1	B	383	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	406	GLN
1	B	272	GLN
1	B	418	HIS
1	A	409	GLN
1	B	171	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 carbohydrates 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/315 (86%)	-0.06	3 (1%) 80 75	57, 85, 125, 160	0
1	B	273/315 (86%)	0.02	3 (1%) 80 75	58, 85, 125, 161	0
2	D	90/120 (75%)	0.22	3 (3%) 46 36	25, 105, 144, 180	0
2	E	90/120 (75%)	0.41	6 (6%) 17 10	25, 106, 144, 180	0
All	All	726/870 (83%)	0.06	15 (2%) 63 54	25, 90, 131, 180	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	SER	4.2
2	E	65	GLY	3.6
2	E	56	THR	3.4
1	A	318	LEU	3.3
1	A	315	PHE	3.3

### 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 carbohydrates 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.