



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:14 PM GMT

PDB ID : 1SR7  
Title : Progesterone Receptor Hormone Binding Domain with Bound Mometasone Furoate  
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Deposited on : 2004-03-22  
Resolution : 1.46 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

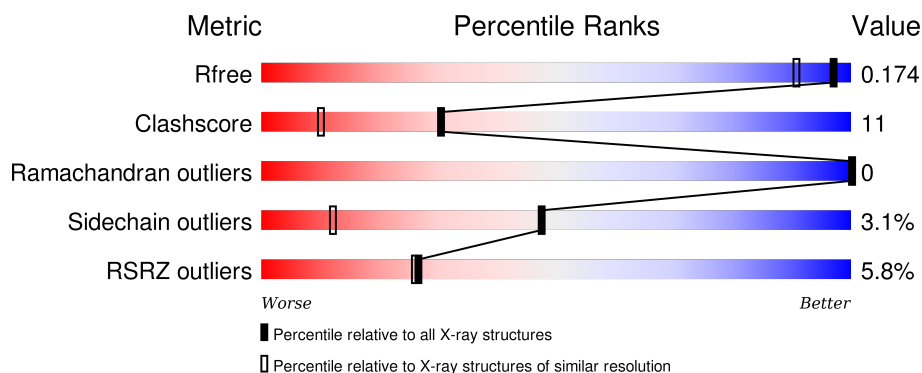
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.46 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))
$R_{free}$	91344	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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. 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	259	 7% 72% 19% 5% .
1	B	259	 4% 69% 23% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	402	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4374 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 Progesterone receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	1	0
			2000	1298	329	359	14			
1	B	249	Total	C	N	O	S	0	1	0
			2007	1301	332	360	14			

There are 2 discrepancies between the modelled and reference sequences:

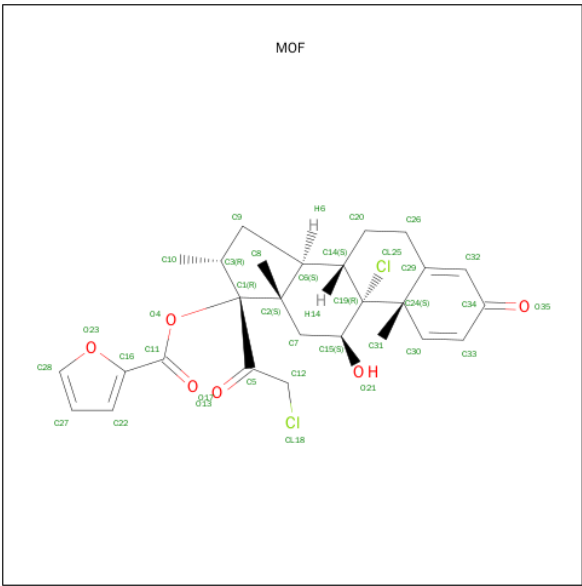
Chain	Residue	Modelled	Actual	Comment	Reference
A	675	GLY	-	CLONING ARTIFACT	UNP P06401
B	675	GLY	-	CLONING ARTIFACT	UNP P06401

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MOMETASONE FUROATE (three-letter code: MOF) (formula: C<sub>27</sub>H<sub>30</sub>Cl<sub>2</sub>O<sub>6</sub>).



- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total 124	O 124	0	0
5	B	162	Total 162	O 162	0	0

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 ( $\text{RSRZ} > 2$ ). 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.

Chain A:

7% 72% 19% 5%

GLY 1 SER 2 PRO 3 GLY 4 GLN 5 ASP 6 ILE 7 Q682 8 L683 9 I684 10 P685 11 M689 12 L690 13 L691 14 M692 15 E695 16 P696 17 D697 18 H703 19 D704 20 H705 21 THR 22 LYS 23 P708 24 D709 25 T710 26 S717 27 E723 28 L727 29 S728 30 K731 31 F739 32 I744 33 D745 34 D746 35 Y753 36 S754 37 W755 38 M756 39 W765 40 R766 41 S767 42 Y768 43 K769 44 H770 45 V771 46 S772 47 V775 48 P780 49 D781 50 E786 51 Q787 52 K790 53 E791 54 K801 55 V802 56 V809 57 K810 58 Q815 59 K822 60 L825 61 A855 62 Q860 63 K861 64 S862 65 V863 66 V864 67 S865 68 S866 69 S867 70 Q868 71 R869 72 F870 73 T874 74 D878 75 H881 76 K885 77 Y890 78 N893 79 Q897 80 S898 81 R899 82 A900 83 L901 84 S902 85 P906 86 Y909 87 Q916 88

Chain B:

Residue Type	Count
GLY	1
SER	1
PRO	1
GLY	1
GLN	1
ASP	1
ILE	1
GLN	1
L683	1
L690	1
E695	1
F696	1
D697	1
Y698	1
G702	1
H703	1
D704	1
N705	1
T706	1
K707	1
F708	1
D709	1
T710	1
S711	1
S712	1
S713	1
L714	1
L715	1
L718	1
N719	1
Q720	1
E723	1
L726	1
L727	1
S728	1
V729	1
V730	1
K731	1
F737	1
S738	1
F739	1
D746	1
V753	1
K759	1
V760	1
F761	1
S767	1
V768	1
V780	1
M775	1
D781	1
L784	1
N785	1
R788	1
S792	1
S793	1
F794	1
V795	1
S796	1
L797	1
H801	1
F808	1
Q812	1
E816	1
E817	1
F818	1
K822	1
L825	1
L835	1
R836	1
R845	1
Y848	1
E851	1
A855	1
I856	1
Q860	1
K861	1
V864	1
S865	1
S866	1
F870	1
Y871	1
K872	1
L873	1
D878	1
N879	1
L880	1
H881	1
K885	1
Y890	1
S898	1
E904	1
F905	1
P906	1
E907	1
N908	1
M924	1
L928	1
H931	1
LYS	1
LYS	1

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.11Å 64.26Å 70.09Å 90.00° 96.88° 90.00°	Depositor
Resolution (Å)	19.96 – 1.46 19.97 – 1.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.96-1.46) 90.5 (19.97-1.46)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.174 , 0.211 0.180 , 0.174	Depositor DCC
$R_{free}$ test set	5561 reflections (7.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.4	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 79930 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, MOF

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	1.71	23/2047 (1.1%)	1.47	16/2770 (0.6%)
1	B	1.85	38/2055 (1.8%)	1.62	38/2782 (1.4%)
All	All	1.78	61/4102 (1.5%)	1.55	54/5552 (1.0%)

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

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	822	LYS	CE-NZ	12.62	1.80	1.49
1	B	775	MET	SD-CE	-10.63	1.18	1.77
1	B	801	MET	SD-CE	-9.94	1.22	1.77
1	A	801	MET	SD-CE	-9.63	1.24	1.77
1	A	756	MET	CB-CG	9.05	1.80	1.51

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	727	LEU	CB-CG-CD1	12.78	132.73	111.00
1	B	845	ARG	NE-CZ-NH2	-12.68	113.96	120.30
1	A	753	TYR	CB-CG-CD2	-10.72	114.57	121.00
1	A	825	LEU	CB-CG-CD2	9.59	127.30	111.00
1	A	697	ASP	CB-CG-OD2	9.40	126.76	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	768	TYR	Sidechain

## 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	2000	0	2035	40	2
1	B	2007	0	2049	45	5
2	B	5	0	0	0	3
3	A	35	0	29	2	0
3	B	35	0	29	5	0
4	B	6	0	8	1	0
5	A	124	0	0	16	8
5	B	162	0	0	11	3
All	All	4374	0	4150	91	11

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 11.

The worst 5 of 91 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:B:822:LYS:CD	1:B:822:LYS:CG	1.79	1.53
1:A:756:MET:CG	1:A:756:MET:CB	1.80	1.53
1:B:908:MET:CE	1:B:908:MET:SD	2.04	1.45
1:A:775:MET:CE	1:A:775:MET:SD	2.02	1.45
1:B:822:LYS:CE	1:B:822:LYS:NZ	1.80	1.41

The worst 5 of 11 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:759:MET:CG	5:A:259:HOH:O[2_555]	1.18	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:SO4:S	5:A:173:HOH:O[1_554]	1.54	0.66
1:B:812:GLN:CG	5:B:253:HOH:O[2_655]	1.59	0.61
2:B:402:SO4:O3	5:A:173:HOH:O[1_554]	1.69	0.51
1:A:775:MET:CG	5:A:225:HOH:O[2_546]	1.74	0.46

## 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	246/259 (95%)	239 (97%)	7 (3%)	0	100	100
1	B	248/259 (96%)	242 (98%)	6 (2%)	0	100	100
All	All	494/518 (95%)	481 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	227/240 (95%)	216 (95%)	11 (5%)	31	4
1	B	229/240 (95%)	226 (99%)	3 (1%)	76	45
All	All	456/480 (95%)	442 (97%)	14 (3%)	47	12

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	867	SER
1	A	897	GLN
1	B	697	ASP
1	A	865	SER
1	A	919	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	897	GLN
1	B	689	ASN
1	B	747	GLN
1	A	812	GLN
1	A	881	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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
3	MOF	A	301	-	31,39,39	2.35	9 (29%)	45,64,64	2.64	20 (44%)
3	MOF	B	302	-	31,39,39	2.40	9 (29%)	45,64,64	3.33	23 (51%)
2	SO4	B	402	-	4,4,4	0.58	0	6,6,6	2.87	2 (33%)
4	GOL	B	501	-	5,5,5	0.41	0	5,5,5	1.91	1 (20%)

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
3	MOF	A	301	-	-	0/15/93/93	0/4/5/5
3	MOF	B	302	-	-	0/15/93/93	0/4/5/5
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0
4	GOL	B	501	-	-	0/4/4/4	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	MOF	C1-C5	-3.64	1.45	1.52
3	A	301	MOF	C7-C15	-3.24	1.48	1.54
3	A	301	MOF	C9-C3	-3.09	1.48	1.54
3	A	301	MOF	C1-C3	-2.98	1.53	1.57
3	B	302	MOF	C6-C14	-2.82	1.48	1.54

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	MOF	C29-C32-C34	-8.22	114.77	122.76
3	B	302	MOF	C30-C33-C34	-8.21	113.71	121.44
3	A	301	MOF	C30-C33-C34	-5.59	116.18	121.44
3	B	302	MOF	O35-C34-C33	-4.63	114.20	121.51
3	B	302	MOF	O4-C11-O17	-4.11	118.35	124.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	MOF	2	0
3	B	302	MOF	5	0
2	B	402	SO4	0	3
4	B	501	GOL	1	0

## 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, 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	249/259 (96%)	0.10	18 (7%)	18 18	12, 19, 41, 52	4 (1%)
1	B	249/259 (96%)	-0.02	11 (4%)	38 38	10, 17, 31, 43	2 (0%)
All	All	498/518 (96%)	0.04	29 (5%)	26 26	10, 18, 37, 52	6 (1%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	683	LEU	7.1
1	A	864	VAL	6.9
1	A	708	PRO	5.0
1	A	901	LEU	4.9
1	A	863	VAL	4.8

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MOF	B	302	35/35	0.91	0.10	0.80	15,18,26,44	0
3	MOF	A	301	35/35	0.93	0.08	0.65	13,18,23,36	0
4	GOL	B	501	6/6	0.96	0.07	-0.70	21,22,26,28	0
2	SO4	B	402	5/5	0.99	0.06	-0.75	20,20,26,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.