



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:32 AM GMT

PDB ID : 2V0V  
Title : CRYSTAL STRUCTURE OF REV-ERB BETA  
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Deposited on : 2007-05-19  
Resolution : 2.40 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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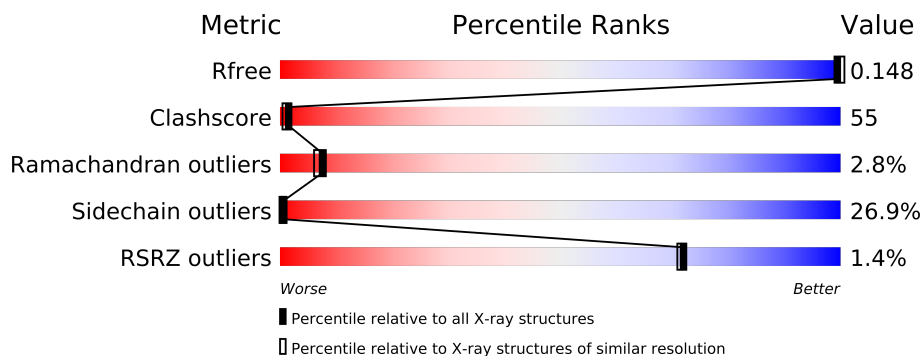
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	194	
1	B	194	
1	C	194	
1	D	194	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5810 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 NR1D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1436	915	241	273	7			
1	B	181	Total	C	N	O	S	0	0	0
			1436	915	241	273	7			
1	C	179	Total	C	N	O	S	0	0	0
			1421	906	238	270	7			
1	D	179	Total	C	N	O	S	0	0	0
			1421	906	238	270	7			

- Molecule 2 is water.

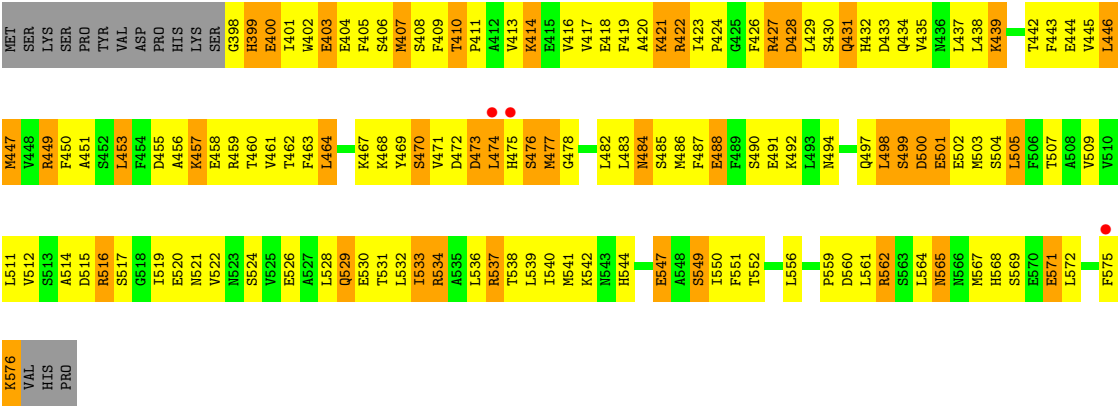
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	26	Total	O	0	0
			26	26		
2	C	22	Total	O	0	0
			22	22		
2	D	25	Total	O	0	0
			25	25		



VAL  
HIS  
PRO

● Molecule 1: ORPHAN NUCLEAR RECEPTOR NR1D2

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.46Å 102.46Å 143.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.40 29.54 – 2.29	Depositor EDS
% Data completeness (in resolution range)	93.6 (99.00-2.40) 90.8 (29.54-2.29)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 2.29Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.138 , 0.220 0.155 , 0.148	Depositor DCC
$R_{free}$ test set	1484 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 54.3	EDS
Estimated twinning fraction	0.096 for -1/2*h+1/2*k-1/2*l, 1/2*h-1/2*k-1/2*l, -h-k 0.096 for -1/2*h+1/2*k+1/2*l, 1/2*h-1/2*k+1/2*l, h+k 0.097 for -1/2*h-1/2*k+1/2*l, -1/2*h-1/2*k-1/2*l, h-k 0.096 for -1/2*h-1/2*k-1/2*l, -1/2*h-1/2*k+1/2*l, -h+k 0.487 for -h, k, -l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 30088 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5810	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0/1460	0.97	3/1965 (0.2%)
1	B	0.39	0/1460	0.87	0/1965
1	C	0.33	0/1445	0.90	0/1946
1	D	0.38	0/1445	0.91	1/1946 (0.1%)
All	All	0.36	0/5810	0.91	4/7822 (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	3
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	SER	CB-CA-C	10.55	130.14	110.10
1	A	409	PHE	N-CA-CB	-5.99	99.82	110.60
1	A	409	PHE	N-CA-C	5.95	127.07	111.00
1	D	562	ARG	NE-CZ-NH1	5.46	123.03	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	MET	Peptide

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Mol	Chain	Res	Type	Group
1	A	410	THR	Peptide
1	A	475	HIS	Peptide
1	B	476	SER	Peptide
1	B	547	GLU	Peptide

## 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	1436	0	1446	147	0
1	B	1436	0	1446	172	0
1	C	1421	0	1428	163	0
1	D	1421	0	1428	166	0
2	A	23	0	0	3	0
2	B	26	0	0	5	0
2	C	22	0	0	7	0
2	D	25	0	0	10	0
All	All	5810	0	5748	633	0

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 55.

The worst 5 of 633 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:473:ASP:C	1:B:477:MET:HG2	1.47	1.33
1:B:473:ASP:O	1:B:477:MET:CG	1.80	1.28
1:A:470:SER:HB3	1:A:473:ASP:OD1	1.17	1.24
1:A:474:LEU:O	1:A:476:SER:O	1.67	1.13
1:B:473:ASP:O	1:B:476:SER:OG	1.66	1.13

There are no symmetry-related clashes.



## 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	179/194 (92%)	146 (82%)	28 (16%)	5 (3%)	8	6
1	B	179/194 (92%)	154 (86%)	21 (12%)	4 (2%)	10	11
1	C	177/194 (91%)	142 (80%)	26 (15%)	9 (5%)	3	1
1	D	177/194 (91%)	146 (82%)	29 (16%)	2 (1%)	21	29
All	All	712/776 (92%)	588 (83%)	104 (15%)	20 (3%)	8	6

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	GLY
1	A	408	SER
1	A	409	PHE
1	B	470	SER
1	A	470	SER

### 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	161/174 (92%)	115 (71%)	46 (29%)	0	0
1	B	161/174 (92%)	119 (74%)	42 (26%)	1	0
1	C	159/174 (91%)	120 (76%)	39 (24%)	1	1
1	D	159/174 (91%)	114 (72%)	45 (28%)	0	0
All	All	640/696 (92%)	468 (73%)	172 (27%)	1	0

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	531	THR
1	C	410	THR
1	D	516	ARG
1	B	537	ARG
1	B	573	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	565	ASN
1	C	399	HIS
1	C	565	ASN
1	B	546	ASN
1	D	432	HIS

### 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 ⓘ

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 ⓘ

### 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, 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	181/194 (93%)	-0.83	2 (1%) 77 77	9, 28, 89, 135	0
1	B	181/194 (93%)	-0.80	2 (1%) 77 77	8, 30, 97, 129	0
1	C	179/194 (92%)	-0.77	3 (1%) 67 65	5, 29, 81, 122	0
1	D	179/194 (92%)	-0.70	3 (1%) 67 65	7, 35, 115, 138	0
All	All	720/776 (92%)	-0.77	10 (1%) 72 71	5, 31, 94, 138	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	474	LEU	12.0
1	D	475	HIS	4.2
1	D	474	LEU	3.4
1	D	575	PHE	3.3
1	C	475	HIS	3.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.