



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:13 PM GMT

PDB ID : 4BV2  
Title : CRYSTAL STRUCTURE OF SIR2 IN COMPLEX WITH THE INHIBITOR  
EX-527, 2'-O-ACETYL-ADP-RIBOSE AND DEACETYLATED P53-  
PEPTIDE  
Authors : Gertz, M.; Weyand, M.; Steegborn, C.  
Deposited on : 2013-06-24  
Resolution : 3.30 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.

---

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

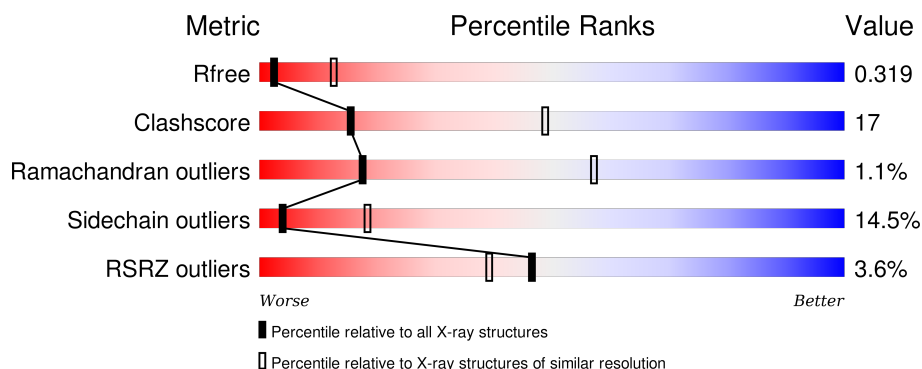
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 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	246	<div> <div>4%</div> <div>59%</div> <div>27%</div> <div>7%</div> <div>• •</div> </div>
1	B	246	<div> <div>3%</div> <div>62%</div> <div>25%</div> <div>5%</div> <div>• 7%</div> </div>
2	E	13	<div> <div>8%</div> <div>15%</div> <div>23%</div> <div>62%</div> </div>
2	H	13	<div> <div>15%</div> <div>8%</div> <div>15%</div> <div>62%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3853 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 NAD-DEPENDENT PROTEIN DEACETYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1846	1184	305	348	9			
1	B	230	Total	C	N	O	S	0	0	0
			1805	1159	299	338	9			

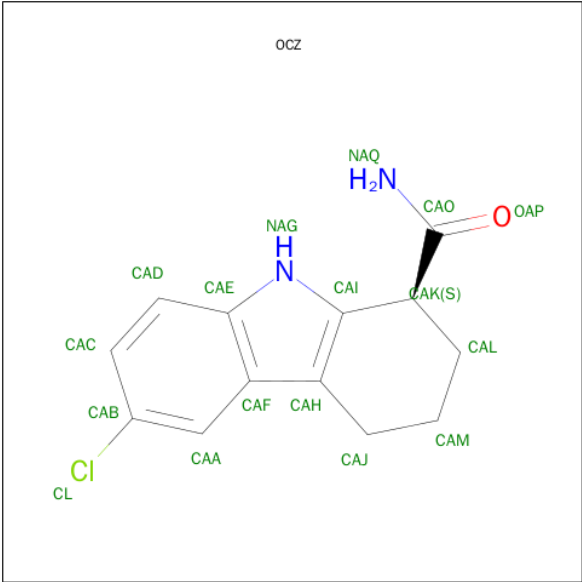
- Molecule 2 is a protein called CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	S	0	0	0
			44	29	9	5	1			
2	H	5	Total	C	N	O	S	0	0	0
			44	29	9	5	1			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

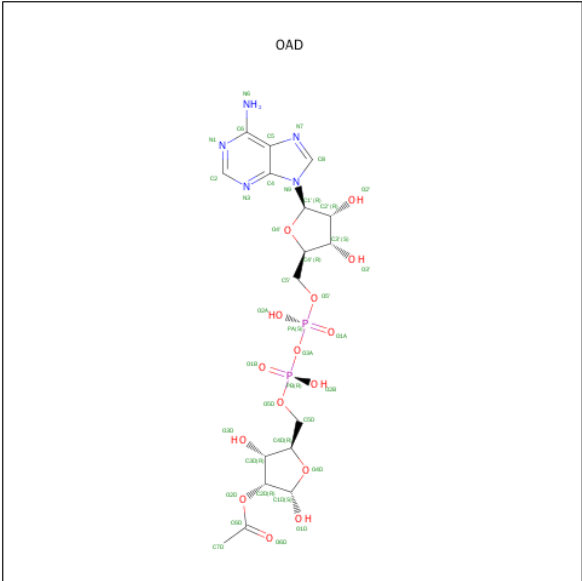
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (1S)-6-CHLORO-2,3,4,9-TETRAHYDRO-1H-CARBAZOLE-1- CARBOX-AMIDE (three-letter code: OCZ) (formula: C<sub>13</sub>H<sub>13</sub>ClN<sub>2</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		
4	B	1	Total	C	Cl	N	O	0	0
			17	13	1	2	1		

- Molecule 5 is 2'-O-ACETYL ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: OAD) (formula: C<sub>17</sub>H<sub>25</sub>N<sub>5</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			39	17	5	15	2		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			39	17	5	15	2		



SER	THR	SER	ARG	H1	K2	K3	L4	M5	PHE	LYS	THR	GLU
-----	-----	-----	-----	----	----	----	----	----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.95Å 45.95Å 241.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.47 – 3.30 60.47 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (60.47-3.30) 99.7 (60.47-3.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.245 , 0.318 0.244 , 0.319	Depositor DCC
$R_{free}$ test set	374 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.8	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 78.8	EDS
Estimated twinning fraction	0.297 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 7476 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OAD, OCZ

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	0.53	0/1879	0.91	10/2540 (0.4%)
1	B	0.50	0/1836	0.96	7/2481 (0.3%)
2	E	0.61	0/44	0.85	0/55
2	H	0.58	0/44	0.88	0/55
All	All	0.52	0/3803	0.93	17/5131 (0.3%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	TYR	C-N-CD	-20.44	75.62	120.60
1	A	194	TYR	C-N-CD	-15.56	86.36	120.60
1	B	194	TYR	C-N-CA	13.29	177.80	122.00
1	A	156	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	A	45	GLN	N-CA-C	7.15	130.30	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	TYR	Peptide
1	B	194	TYR	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	1846	0	1862	73	2
1	B	1805	0	1825	55	0
2	E	44	0	55	5	0
2	H	44	0	55	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	17	0	13	1	0
4	B	17	0	13	2	0
5	A	39	0	23	10	0
5	B	39	0	23	5	0
All	All	3853	0	3869	133	2

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 17.

The worst 5 of 133 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:168:GLN:NE2	1:A:168:GLN:H	1.49	1.09
1:A:180:ARG:HH11	1:A:180:ARG:HG3	1.14	1.07
1:B:168:GLN:H	1:B:168:GLN:NE2	1.51	1.07
1:B:180:ARG:HH11	1:B:180:ARG:HG3	1.23	1.03
1:B:214:ASN:HD22	1:B:215:LEU:N	1.63	0.95

All (2) 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:A:59:GLU:OE2	1:A:87:GLU:O[1_565]	1.88	0.32

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASN:OD1	1:A:45:GLN:NE2[1_545]	2.10	0.10

## 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	231/246 (94%)	226 (98%)	3 (1%)	2 (1%)	21	60
1	B	224/246 (91%)	221 (99%)	2 (1%)	1 (0%)	39	76
2	E	3/13 (23%)	2 (67%)	1 (33%)	0	100	100
2	H	3/13 (23%)	1 (33%)	0	2 (67%)	0	0
All	All	461/518 (89%)	450 (98%)	6 (1%)	5 (1%)	17	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	PRO
1	B	195	PRO
2	H	4	LEU
1	A	45	GLN
2	H	3	LYS

### 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	205/215 (95%)	174 (85%)	31 (15%)	3	16
1	B	200/215 (93%)	172 (86%)	28 (14%)	4	20
2	E	5/13 (38%)	4 (80%)	1 (20%)	1	6
2	H	5/13 (38%)	5 (100%)	0	100	100
All	All	415/456 (91%)	355 (86%)	60 (14%)	4	18

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	THR
1	B	46	ASN
1	B	225	THR
1	A	237	ARG
1	B	55	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	HIS
1	B	214	ASN
1	B	118	ASN
1	A	168	GLN
1	B	168	GLN

### 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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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$
4	OCZ	A	1247	-	18,19,19	3.41	8 (44%)	18,28,28	1.78	5 (27%)
5	OAD	A	1248	-	34,42,42	1.66	5 (14%)	42,64,64	2.60	11 (26%)
4	OCZ	B	1247	-	18,19,19	3.28	7 (38%)	18,28,28	1.27	3 (16%)
5	OAD	B	1248	-	34,42,42	1.66	6 (17%)	42,64,64	3.26	11 (26%)

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
4	OCZ	A	1247	-	-	0/3/14/14	0/3/3/3
5	OAD	A	1248	-	-	0/22/58/58	0/4/4/4
4	OCZ	B	1247	-	-	0/3/14/14	0/3/3/3
5	OAD	B	1248	-	-	0/22/58/58	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1247	OCZ	CAK-CAO	-10.48	1.42	1.53
4	B	1247	OCZ	CAK-CAO	-9.42	1.43	1.53
4	A	1247	OCZ	CAJ-CAH	-6.39	1.39	1.51
4	B	1247	OCZ	CAJ-CAH	-5.47	1.40	1.51
4	B	1247	OCZ	CAD-CAE	-4.39	1.33	1.41

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1248	OAD	N3-C2-N1	-16.60	116.19	128.89
5	A	1248	OAD	N3-C2-N1	-9.60	121.54	128.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1248	OAD	C4'-O4'-C1'	-8.00	100.93	109.72
5	A	1248	OAD	C2D-O2D-C6D	-7.30	106.38	117.70
5	A	1248	OAD	C4'-O4'-C1'	-4.81	104.44	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1247	OCZ	1	0
5	A	1248	OAD	10	0
4	B	1247	OCZ	2	0
5	B	1248	OAD	5	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	235/246 (95%)	0.29	9 (3%) 44 37	72, 111, 151, 173	0
1	B	230/246 (93%)	0.20	7 (3%) 54 47	75, 114, 158, 181	0
2	E	5/13 (38%)	0.83	1 (20%) 1 1	85, 89, 94, 109	0
2	H	5/13 (38%)	0.59	0 100 100	92, 100, 114, 129	0
All	All	475/518 (91%)	0.26	17 (3%) 46 39	72, 112, 155, 181	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	168	GLN	3.5
1	A	15	LEU	3.3
1	B	126	ARG	3.2
1	B	195	PRO	3.1
1	A	91	LEU	2.8

### 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
4	OCZ	B	1247	17/17	0.96	0.30	0.33	89,102,124,132	0
4	OCZ	A	1247	17/17	0.93	0.27	-0.15	81,97,126,160	0
5	OAD	A	1248	39/39	0.96	0.17	-0.77	90,105,156,159	0
5	OAD	B	1248	39/39	0.92	0.18	-0.85	109,116,142,148	0
3	ZN	A	1246	1/1	0.98	0.06	-1.59	122,122,122,122	0
3	ZN	B	1249	1/1	0.99	0.07	-1.64	131,131,131,131	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.