



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2024 – 06:05 PM EDT

PDB ID : 1KZY  
Title : Crystal Structure of the 53bp1 BRCT Region Complexed to Tumor Suppressor P53  
Authors : Joo, W.S.; Jeffrey, P.D.; Cantor, S.B.; Finnin, M.S.; Livingston, D.M.; Pavletich, N.P.  
Deposited on : 2002-02-08  
Resolution : 2.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

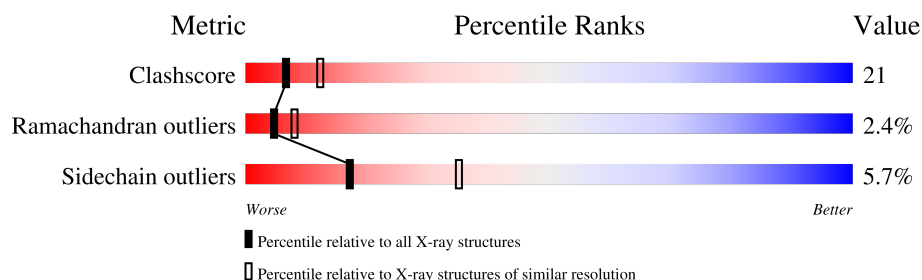
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	195	 67% 31% •
1	B	195	 66% 29% 5%
2	C	259	 56% 30% • 10%
2	D	259	 52% 31% 6% 10%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6986 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 CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1530	942	282	290	16			
1	B	195	Total	C	N	O	S	0	0	0
			1530	942	282	290	16			

- Molecule 2 is a protein called TUMOR SUPPRESSOR P53-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	232	Total	C	N	O	S	0	0	0
			1854	1184	320	339	11			
2	D	232	Total	C	N	O	S	0	0	0
			1854	1184	320	339	11			

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	58	Total	O	0	0
			58	58		
4	C	50	Total	O	0	0
			50	50		
4	D	51	Total	O	0	0
			51	51		

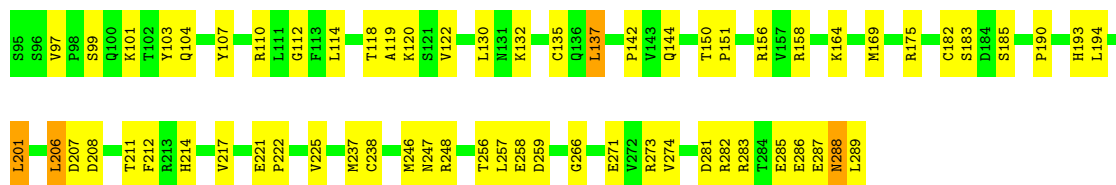
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

Note EDS was not executed.

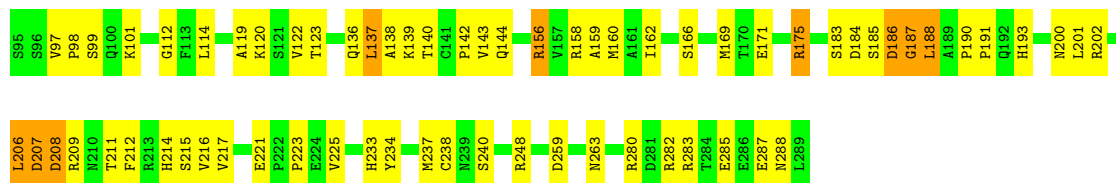
#### • Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A: 



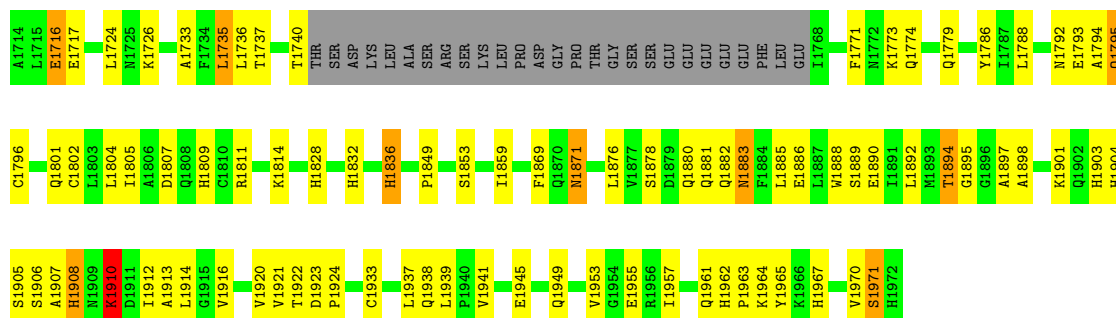
#### • Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B: 



#### • Molecule 2: TUMOR SUPPRESSOR P53-BINDING PROTEIN 1

Chain C: 



#### • Molecule 2: TUMOR SUPPRESSOR P53-BINDING PROTEIN 1

Chain D: 

A1714	L1715	E1716	E1717	Q1718	R1719	G1720	P1721	L1722	P1723	L1724	N1725	G1731	L1736	T1737	T1740	THR	SER	ASP	LYS	LEU	ALA	SER	ARG	SER	LYS	LEU	PRO	ASP	GLY	PRO	THR	GLY	SER	SER	GLU	GLU	GLU	GLU	PHE	LEU	GLU	I1768	P1769	P1770	F1771	N1772	K1773	Q1774	Y1775	T1776	E1777	S1778	Q1779	L1780	R1781
Y1786	I1787	L1788	E1789	M1792	E1793	E1795	C1796	C1802	L1803	L1804	I1805	A1806	D1807	Q1808	H1809	C1810	R1811	K1814	H1828	H1832	C1835	H1836	A1837	N1838	S1853	L1854	E1855	E1856	Q1857	I1858	L1859	R1865	I1867	M1871	V1874	L1875	Q1881	Q1882	N1883	F1884	L1885	E1886	E1890	T1894											
A1898	K1901	Q1902	H1903	H1904	S1905	S1906	A1907	H1908	N1909	K1910	D1911	I1912	A1913	L1914	G1915	V1916	V1919	V1920	V1921	T1922	D1923	P1924	P1927	V1930	L1937	Q1938	V1941	V1942	S1943	Q1949	V1953	G1954	E1955	R1956	I1957	Q1961	H1962	P1963	K1964	Y1965	K1966	H1967	D1968	Y1969	V1970	S1971	H1972								

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.13Å 94.98Å 133.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

## 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

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	0.63	0/1565	0.79	0/2121
1	B	0.61	0/1565	0.81	2/2121 (0.1%)
2	C	0.63	0/1901	0.79	0/2584
2	D	0.65	0/1901	0.81	3/2584 (0.1%)
All	All	0.63	0/6932	0.80	5/9410 (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	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LEU	CA-CB-CG	6.94	131.27	115.30
2	D	1723	PRO	N-CA-C	5.58	126.62	112.10
2	D	1722	LEU	N-CA-C	-5.24	96.84	111.00
2	D	1811	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	282	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	TYR	Sidechain

## 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	1530	0	1485	53	0
1	B	1530	0	1485	62	0
2	C	1854	0	1814	79	0
2	D	1854	0	1814	92	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	57	0	0	4	0
4	B	58	0	0	7	0
4	C	50	0	0	9	0
4	D	51	0	0	10	0
All	All	6986	0	6598	281	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 21.

The worst 5 of 281 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)
2:D:1774:GLN:HA	4:D:51:HOH:O	1.54	1.06
2:D:1890:GLU:O	2:D:1894:THR:HG22	1.58	1.01
2:D:1923:ASP:HB2	2:D:1924:PRO:HD2	1.43	1.00
1:B:171:GLU:HG3	4:B:318:HOH:O	1.60	1.00
2:D:1776:THR:HA	2:D:1779:GLN:HE21	1.25	1.00

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	193/195 (99%)	180 (93%)	11 (6%)	2 (1%)	13	25
1	B	193/195 (99%)	175 (91%)	13 (7%)	5 (3%)	4	7
2	C	228/259 (88%)	206 (90%)	17 (8%)	5 (2%)	5	9
2	D	228/259 (88%)	204 (90%)	16 (7%)	8 (4%)	3	4
All	All	842/908 (93%)	765 (91%)	57 (7%)	20 (2%)	5	8

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASP
1	B	208	ASP
2	C	1905	SER
2	C	1910	LYS
2	C	1971	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	175/175 (100%)	167 (95%)	8 (5%)	23	45
1	B	175/175 (100%)	166 (95%)	9 (5%)	20	40
2	C	203/227 (89%)	190 (94%)	13 (6%)	14	30
2	D	203/227 (89%)	190 (94%)	13 (6%)	14	30
All	All	756/804 (94%)	713 (94%)	43 (6%)	17	35

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1961	GLN
2	D	1881	GLN
2	C	1963	PRO
2	D	1789	GLU

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Mol	Chain	Res	Type
2	D	1908	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	1839	GLN
2	D	1871	ASN
2	D	1961	GLN
1	B	288	ASN
1	B	263	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.