



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 02:09 AM EDT

PDB ID : 2TUN  
Title : CONFORMATIONAL CHANGES IN THE (ALA-84-VAL) MUTANT OF  
TUMOR NECROSIS FACTOR  
Authors : Saludjian, P.; Prange, T.  
Deposited on : 1993-10-06  
Resolution : 3.10 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	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

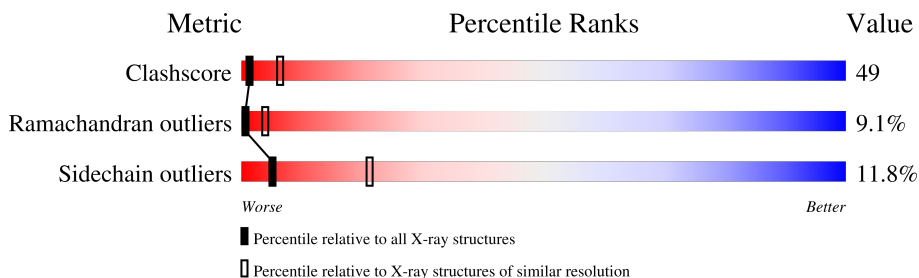
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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	157	
1	B	157	
1	C	157	
1	D	157	
1	E	157	
1	F	157	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7086 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 TUMOR NECROSIS FACTOR-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	B	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	C	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	D	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	E	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			
1	F	151	Total	C	N	O	S	0	0	0
			1181	756	203	220	2			

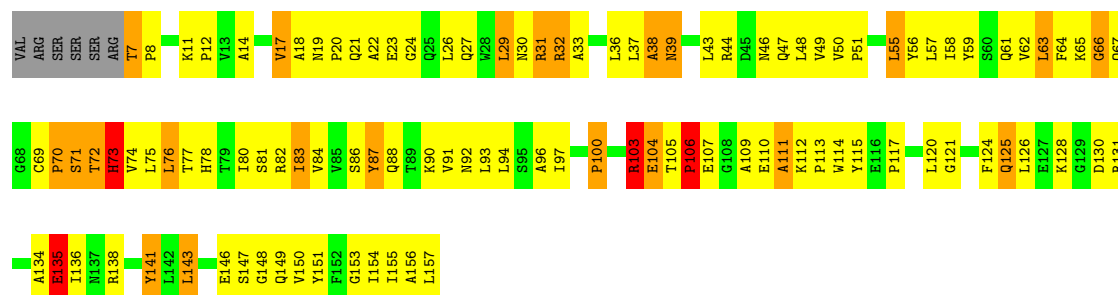
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	VAL	ALA	ENGINEERED MUTATION	UNP P01375
A	143	LEU	ASP	CONFLICT	UNP P01375
B	84	VAL	ALA	ENGINEERED MUTATION	UNP P01375
B	143	LEU	ASP	CONFLICT	UNP P01375
C	84	VAL	ALA	ENGINEERED MUTATION	UNP P01375
C	143	LEU	ASP	CONFLICT	UNP P01375
D	84	VAL	ALA	ENGINEERED MUTATION	UNP P01375
D	143	LEU	ASP	CONFLICT	UNP P01375
E	84	VAL	ALA	ENGINEERED MUTATION	UNP P01375
E	143	LEU	ASP	CONFLICT	UNP P01375
F	84	VAL	ALA	ENGINEERED MUTATION	UNP P01375
F	143	LEU	ASP	CONFLICT	UNP P01375



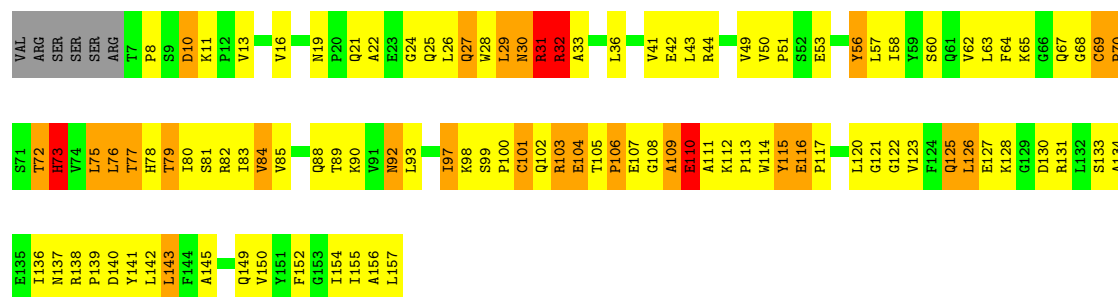
- Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

Chain D:  27% 52% 14%



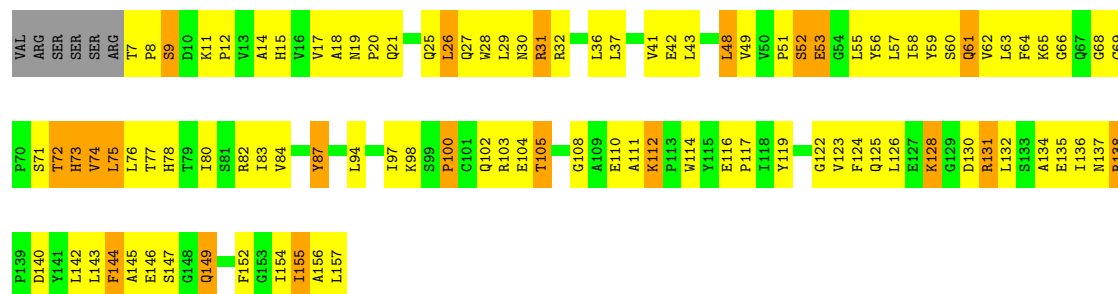
- Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

Chain E:  29% 49% 16%



- Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

Chain F:  32% 50% 13%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.00 Å   166.00 Å   93.70 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	9.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.198 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

## 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	0.75	0/1208	1.47	9/1645 (0.5%)
1	B	0.80	1/1208 (0.1%)	1.58	15/1645 (0.9%)
1	C	0.87	1/1208 (0.1%)	1.81	23/1645 (1.4%)
1	D	0.80	1/1208 (0.1%)	1.68	21/1645 (1.3%)
1	E	0.79	1/1208 (0.1%)	1.55	11/1645 (0.7%)
1	F	0.74	0/1208	1.39	3/1645 (0.2%)
All	All	0.79	4/7248 (0.1%)	1.59	82/9870 (0.8%)

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	C	0	1
1	D	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	8	PRO	N-CD	11.16	1.63	1.47
1	D	7	THR	C-O	8.71	1.40	1.23
1	B	8	PRO	N-CD	7.55	1.58	1.47
1	E	101	CYS	CB-SG	5.33	1.91	1.82

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	8	PRO	CA-N-CD	-17.69	86.73	111.50
1	D	7	THR	CA-C-O	-17.18	84.01	120.10
1	D	7	THR	CA-C-N	16.55	163.43	117.10
1	C	7	THR	O-C-N	16.21	151.90	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	PRO	CA-N-CD	-16.18	88.85	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	7	THR	Peptide
1	D	7	THR	Mainchain,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	1181	0	1183	137	2
1	B	1181	0	1183	120	0
1	C	1181	0	1183	135	0
1	D	1181	0	1183	119	2
1	E	1181	0	1183	126	0
1	F	1181	0	1183	119	0
All	All	7086	0	7098	696	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 49.

The worst 5 of 696 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:C:98:LYS:HD3	1:C:118:ILE:HG12	1.31	1.06
1:A:19:ASN:HB2	1:A:29:LEU:HD23	1.37	1.04
1:C:14:ALA:HB2	1:C:41:VAL:HG21	1.38	1.03
1:F:42:GLU:HB3	1:F:49:VAL:HB	1.39	1.00
1:D:19:ASN:HB2	1:D:29:LEU:HD13	1.44	1.00

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:42:GLU:OE2	1:D:86:SER:C[6_765]	2.03	0.17
1:A:42:GLU:OE2	1:D:86:SER:O[6_765]	2.04	0.16

### 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	149/157 (95%)	108 (72%)	28 (19%)	13 (9%)	1	4
1	B	149/157 (95%)	108 (72%)	30 (20%)	11 (7%)	1	6
1	C	149/157 (95%)	108 (72%)	25 (17%)	16 (11%)	0	2
1	D	149/157 (95%)	106 (71%)	27 (18%)	16 (11%)	0	2
1	E	149/157 (95%)	106 (71%)	30 (20%)	13 (9%)	1	4
1	F	149/157 (95%)	108 (72%)	29 (20%)	12 (8%)	1	5
All	All	894/942 (95%)	644 (72%)	169 (19%)	81 (9%)	1	4

5 of 81 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	B	39	ASN
1	B	104	GLU
1	C	8	PRO
1	C	53	GLU

#### 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	128/134 (96%)	114 (89%)	14 (11%)	6	25
1	B	128/134 (96%)	115 (90%)	13 (10%)	7	27
1	C	128/134 (96%)	108 (84%)	20 (16%)	2	11
1	D	128/134 (96%)	116 (91%)	12 (9%)	8	32
1	E	128/134 (96%)	108 (84%)	20 (16%)	2	11
1	F	128/134 (96%)	116 (91%)	12 (9%)	8	32
All	All	768/804 (96%)	677 (88%)	91 (12%)	5	21

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	143	LEU
1	E	101	CYS
1	E	10	ASP
1	E	73	HIS
1	E	125	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	92	ASN
1	E	39	ASN
1	F	102	GLN
1	E	34	ASN
1	E	73	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.