wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 05:23 am BST

PDB ID	:	1TNF
Title	:	THE STRUCTURE OF TUMOR NECROSIS FACTOR-ALPHA AT 2.6 ANGSTROMS RESOLUTION. IMPLICATIONS FOR RECEPTOR BINDING
Authors	:	Eck, M.J.; Sprang, S.R.
Deposited on	:	1989-08-25
Resolution	:	2.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

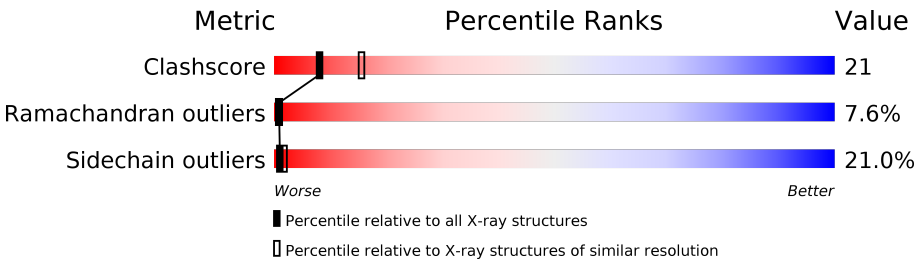
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	157	42% 37% 13% • •
1	B	157	36% 44% 13% • •
1	C	157	31% 44% 15% 6% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3552 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
			Total	C	N	O	S			
1	A	152	1184	757	204	221	2	0	0	0
			Total	C	N	O	S			
1	B	152	1184	757	204	221	2	0	0	0
			Total	C	N	O	S			
1	C	152	1184	757	204	221	2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	ASP	LEU	CONFLICT	UNP P01375
B	45	ASP	LEU	CONFLICT	UNP P01375
C	45	ASP	LEU	CONFLICT	UNP P01375

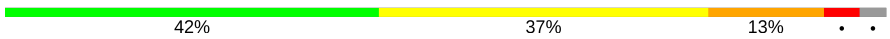
3 Residue-property plots (i)

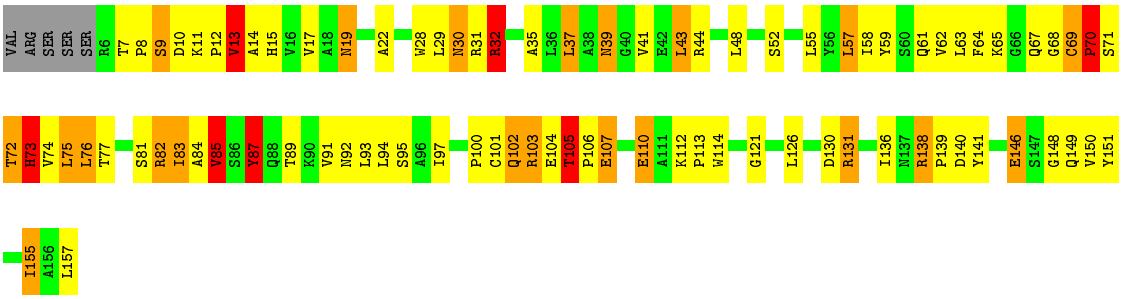
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: TUMOR NECROSIS FACTOR-ALPHA

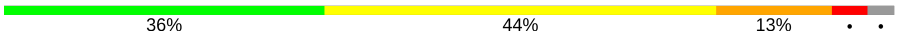
Chain A:

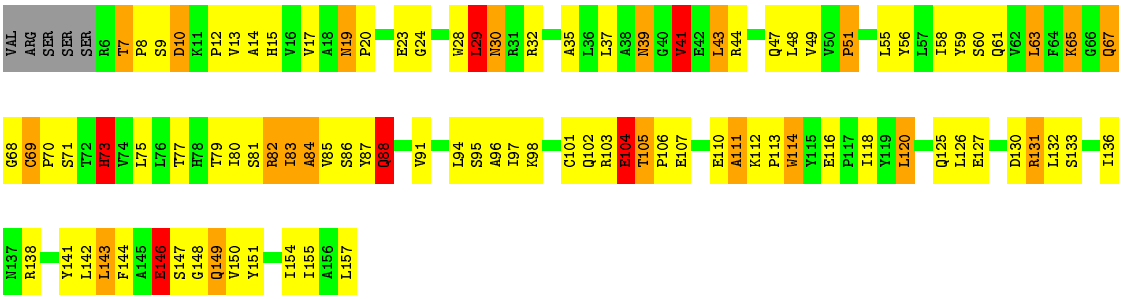




- Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

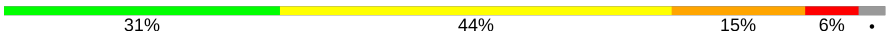
Chain B:

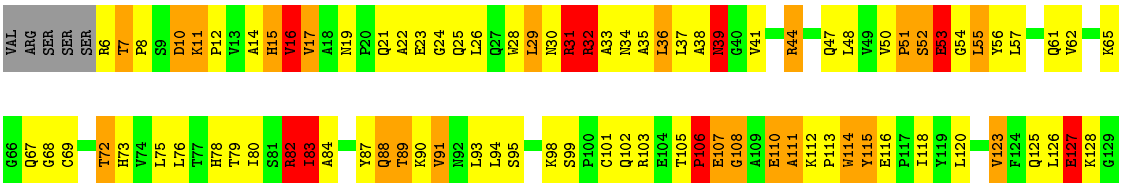




- Molecule 1: TUMOR NECROSIS FACTOR-ALPHA

Chain C:





D130
R131
L132
S133
R138
P139
D140
L143
F144
A145
E146
S147
G148
Q149
F152
G153
I154
L157

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	95.00Å 95.00Å 117.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3552	wwPDB-VP
Average B, all atoms ($Å^2$)	25.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	0.94	0/1211	2.03	43/1649 (2.6%)
1	B	0.96	1/1211 (0.1%)	1.95	30/1649 (1.8%)
1	C	0.97	0/1211	1.95	43/1649 (2.6%)
All	All	0.96	1/3633 (0.0%)	1.98	116/4947 (2.3%)

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	2
1	B	0	2
1	C	0	3
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	VAL	CA-CB	5.03	1.65	1.54

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ARG	NE-CZ-NH2	16.25	128.43	120.30
1	B	138	ARG	NE-CZ-NH2	11.87	126.24	120.30
1	C	32	ARG	NE-CZ-NH2	11.09	125.84	120.30
1	B	131	ARG	NE-CZ-NH2	10.50	125.55	120.30
1	B	88	GLN	CA-CB-CG	10.07	135.56	113.40

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	THR	Peptide
1	A	7	THR	Peptide
1	B	105	THR	Peptide
1	B	7	THR	Peptide
1	C	7	THR	Peptide

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	1184	0	1181	49	0
1	B	1184	0	1181	67	0
1	C	1184	0	1181	56	0
All	All	3552	0	3543	151	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 151 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:8:PRO:HG3	1:C:54:GLY:HA2	1.49	0.93
1:B:94:LEU:HA	1:C:148:GLY:HA3	1.60	0.82
1:B:98:LYS:HD2	1:B:116:GLU:HG3	1.65	0.79
1:A:149:GLN:HG3	1:A:150:VAL:H	1.47	0.79
1:C:53:GLU:HG3	1:C:127:GLU:HG3	1.67	0.76

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	150/157 (96%)	121 (81%)	19 (13%)	10 (7%)	1	1
1	B	150/157 (96%)	115 (77%)	25 (17%)	10 (7%)	1	1
1	C	150/157 (96%)	111 (74%)	25 (17%)	14 (9%)	0	0
All	All	450/471 (96%)	347 (77%)	69 (15%)	34 (8%)	1	1

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	100	PRO
1	A	104	GLU
1	A	107	GLU
1	B	84	ALA

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	127/133 (96%)	104 (82%)	23 (18%)	1	2
1	B	127/133 (96%)	101 (80%)	26 (20%)	1	2
1	C	127/133 (96%)	96 (76%)	31 (24%)	0	1
All	All	381/399 (96%)	301 (79%)	80 (21%)	1	2

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	SER
1	B	110	GLU
1	C	106	PRO
1	B	82	ARG
1	B	86	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	A	102	GLN
1	C	78	HIS
1	B	125	GLN
1	A	61	GLN
1	C	30	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 carbohydrates 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.