



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 08:24 am BST

PDB ID : 3DKB  
Title : Crystal Structure of A20, 2.5 angstrom  
Authors : Lin, S.-C.; Chung, J.Y.; Lo, Y.-C.; Wu, H.  
Deposited on : 2008-06-24  
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.

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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)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

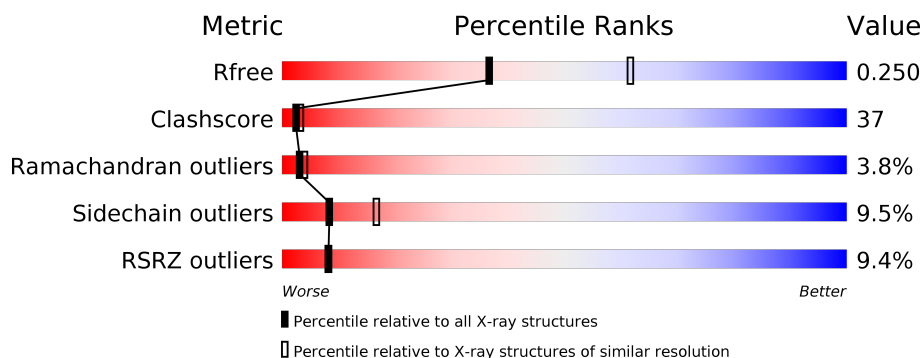
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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  $\leq 5\%$ . 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	390	<div> <div>7%</div> <div> <div></div> <div>33%</div> <div>49%</div> <div>8%</div> <div>10%</div> </div> </div>
1	B	390	<div> <div>8%</div> <div> <div></div> <div>39%</div> <div>42%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	390	<div> <div>11%</div> <div> <div></div> <div>33%</div> <div>50%</div> <div>7%</div> <div>10%</div> </div> </div>
1	D	390	<div> <div>8%</div> <div> <div></div> <div>35%</div> <div>49%</div> <div>6%</div> <div>10%</div> </div> </div>
1	E	390	<div> <div>9%</div> <div> <div></div> <div>39%</div> <div>44%</div> <div>7%</div> <div>10%</div> </div> </div>
1	F	390	<div> <div>8%</div> <div> <div></div> <div>35%</div> <div>48%</div> <div>7%</div> <div>10%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17550 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-induced protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	B	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	C	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	D	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	E	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			
1	F	352	Total	C	N	O	S	0	0	0
			2925	1868	511	530	16			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5981	MET	-	EXPRESSION TAG	UNP P21580
A	5982	GLY	-	EXPRESSION TAG	UNP P21580
A	5983	SER	-	EXPRESSION TAG	UNP P21580
A	5984	SER	-	EXPRESSION TAG	UNP P21580
A	5985	HIS	-	EXPRESSION TAG	UNP P21580
A	5986	HIS	-	EXPRESSION TAG	UNP P21580
A	5987	HIS	-	EXPRESSION TAG	UNP P21580
A	5988	HIS	-	EXPRESSION TAG	UNP P21580
A	5989	HIS	-	EXPRESSION TAG	UNP P21580
A	5990	HIS	-	EXPRESSION TAG	UNP P21580
A	5991	SER	-	EXPRESSION TAG	UNP P21580
A	5992	SER	-	EXPRESSION TAG	UNP P21580
A	5993	GLY	-	EXPRESSION TAG	UNP P21580
A	5994	LEU	-	EXPRESSION TAG	UNP P21580
A	5995	VAL	-	EXPRESSION TAG	UNP P21580
A	5996	PRO	-	EXPRESSION TAG	UNP P21580
A	5997	ARG	-	EXPRESSION TAG	UNP P21580

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Chain	Residue	Modelled	Actual	Comment	Reference
A	5998	GLY	-	EXPRESSION TAG	UNP P21580
A	5999	SER	-	EXPRESSION TAG	UNP P21580
A	6000	HIS	-	EXPRESSION TAG	UNP P21580
B	981	MET	-	EXPRESSION TAG	UNP P21580
B	982	GLY	-	EXPRESSION TAG	UNP P21580
B	983	SER	-	EXPRESSION TAG	UNP P21580
B	984	SER	-	EXPRESSION TAG	UNP P21580
B	985	HIS	-	EXPRESSION TAG	UNP P21580
B	986	HIS	-	EXPRESSION TAG	UNP P21580
B	987	HIS	-	EXPRESSION TAG	UNP P21580
B	988	HIS	-	EXPRESSION TAG	UNP P21580
B	989	HIS	-	EXPRESSION TAG	UNP P21580
B	990	HIS	-	EXPRESSION TAG	UNP P21580
B	991	SER	-	EXPRESSION TAG	UNP P21580
B	992	SER	-	EXPRESSION TAG	UNP P21580
B	993	GLY	-	EXPRESSION TAG	UNP P21580
B	994	LEU	-	EXPRESSION TAG	UNP P21580
B	995	VAL	-	EXPRESSION TAG	UNP P21580
B	996	PRO	-	EXPRESSION TAG	UNP P21580
B	997	ARG	-	EXPRESSION TAG	UNP P21580
B	998	GLY	-	EXPRESSION TAG	UNP P21580
B	999	SER	-	EXPRESSION TAG	UNP P21580
B	1000	HIS	-	EXPRESSION TAG	UNP P21580
C	1981	MET	-	EXPRESSION TAG	UNP P21580
C	1982	GLY	-	EXPRESSION TAG	UNP P21580
C	1983	SER	-	EXPRESSION TAG	UNP P21580
C	1984	SER	-	EXPRESSION TAG	UNP P21580
C	1985	HIS	-	EXPRESSION TAG	UNP P21580
C	1986	HIS	-	EXPRESSION TAG	UNP P21580
C	1987	HIS	-	EXPRESSION TAG	UNP P21580
C	1988	HIS	-	EXPRESSION TAG	UNP P21580
C	1989	HIS	-	EXPRESSION TAG	UNP P21580
C	1990	HIS	-	EXPRESSION TAG	UNP P21580
C	1991	SER	-	EXPRESSION TAG	UNP P21580
C	1992	SER	-	EXPRESSION TAG	UNP P21580
C	1993	GLY	-	EXPRESSION TAG	UNP P21580
C	1994	LEU	-	EXPRESSION TAG	UNP P21580
C	1995	VAL	-	EXPRESSION TAG	UNP P21580
C	1996	PRO	-	EXPRESSION TAG	UNP P21580
C	1997	ARG	-	EXPRESSION TAG	UNP P21580
C	1998	GLY	-	EXPRESSION TAG	UNP P21580
C	1999	SER	-	EXPRESSION TAG	UNP P21580

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2000	HIS	-	EXPRESSION TAG	UNP P21580
D	2981	MET	-	EXPRESSION TAG	UNP P21580
D	2982	GLY	-	EXPRESSION TAG	UNP P21580
D	2983	SER	-	EXPRESSION TAG	UNP P21580
D	2984	SER	-	EXPRESSION TAG	UNP P21580
D	2985	HIS	-	EXPRESSION TAG	UNP P21580
D	2986	HIS	-	EXPRESSION TAG	UNP P21580
D	2987	HIS	-	EXPRESSION TAG	UNP P21580
D	2988	HIS	-	EXPRESSION TAG	UNP P21580
D	2989	HIS	-	EXPRESSION TAG	UNP P21580
D	2990	HIS	-	EXPRESSION TAG	UNP P21580
D	2991	SER	-	EXPRESSION TAG	UNP P21580
D	2992	SER	-	EXPRESSION TAG	UNP P21580
D	2993	GLY	-	EXPRESSION TAG	UNP P21580
D	2994	LEU	-	EXPRESSION TAG	UNP P21580
D	2995	VAL	-	EXPRESSION TAG	UNP P21580
D	2996	PRO	-	EXPRESSION TAG	UNP P21580
D	2997	ARG	-	EXPRESSION TAG	UNP P21580
D	2998	GLY	-	EXPRESSION TAG	UNP P21580
D	2999	SER	-	EXPRESSION TAG	UNP P21580
D	3000	HIS	-	EXPRESSION TAG	UNP P21580
E	3981	MET	-	EXPRESSION TAG	UNP P21580
E	3982	GLY	-	EXPRESSION TAG	UNP P21580
E	3983	SER	-	EXPRESSION TAG	UNP P21580
E	3984	SER	-	EXPRESSION TAG	UNP P21580
E	3985	HIS	-	EXPRESSION TAG	UNP P21580
E	3986	HIS	-	EXPRESSION TAG	UNP P21580
E	3987	HIS	-	EXPRESSION TAG	UNP P21580
E	3988	HIS	-	EXPRESSION TAG	UNP P21580
E	3989	HIS	-	EXPRESSION TAG	UNP P21580
E	3990	HIS	-	EXPRESSION TAG	UNP P21580
E	3991	SER	-	EXPRESSION TAG	UNP P21580
E	3992	SER	-	EXPRESSION TAG	UNP P21580
E	3993	GLY	-	EXPRESSION TAG	UNP P21580
E	3994	LEU	-	EXPRESSION TAG	UNP P21580
E	3995	VAL	-	EXPRESSION TAG	UNP P21580
E	3996	PRO	-	EXPRESSION TAG	UNP P21580
E	3997	ARG	-	EXPRESSION TAG	UNP P21580
E	3998	GLY	-	EXPRESSION TAG	UNP P21580
E	3999	SER	-	EXPRESSION TAG	UNP P21580
E	4000	HIS	-	EXPRESSION TAG	UNP P21580
F	4981	MET	-	EXPRESSION TAG	UNP P21580

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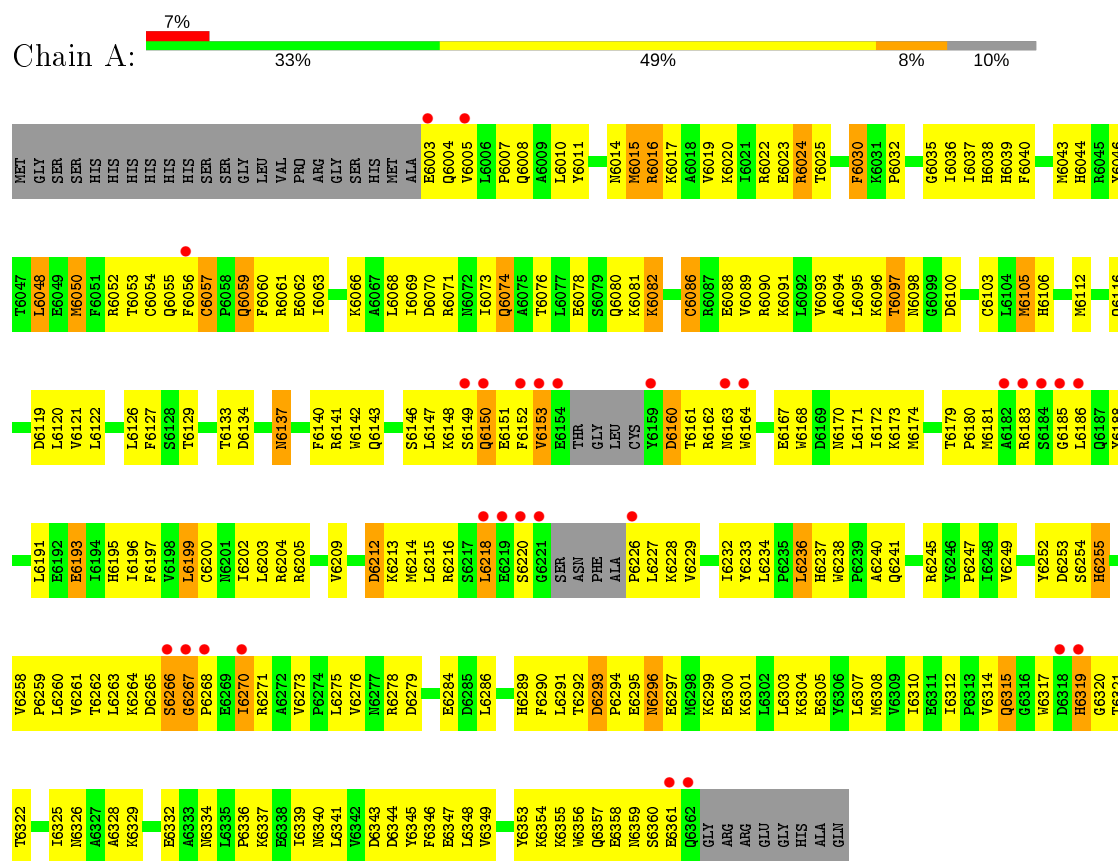
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Chain	Residue	Modelled	Actual	Comment	Reference
F	4982	GLY	-	EXPRESSION TAG	UNP P21580
F	4983	SER	-	EXPRESSION TAG	UNP P21580
F	4984	SER	-	EXPRESSION TAG	UNP P21580
F	4985	HIS	-	EXPRESSION TAG	UNP P21580
F	4986	HIS	-	EXPRESSION TAG	UNP P21580
F	4987	HIS	-	EXPRESSION TAG	UNP P21580
F	4988	HIS	-	EXPRESSION TAG	UNP P21580
F	4989	HIS	-	EXPRESSION TAG	UNP P21580
F	4990	HIS	-	EXPRESSION TAG	UNP P21580
F	4991	SER	-	EXPRESSION TAG	UNP P21580
F	4992	SER	-	EXPRESSION TAG	UNP P21580
F	4993	GLY	-	EXPRESSION TAG	UNP P21580
F	4994	LEU	-	EXPRESSION TAG	UNP P21580
F	4995	VAL	-	EXPRESSION TAG	UNP P21580
F	4996	PRO	-	EXPRESSION TAG	UNP P21580
F	4997	ARG	-	EXPRESSION TAG	UNP P21580
F	4998	GLY	-	EXPRESSION TAG	UNP P21580
F	4999	SER	-	EXPRESSION TAG	UNP P21580
F	5000	HIS	-	EXPRESSION TAG	UNP P21580

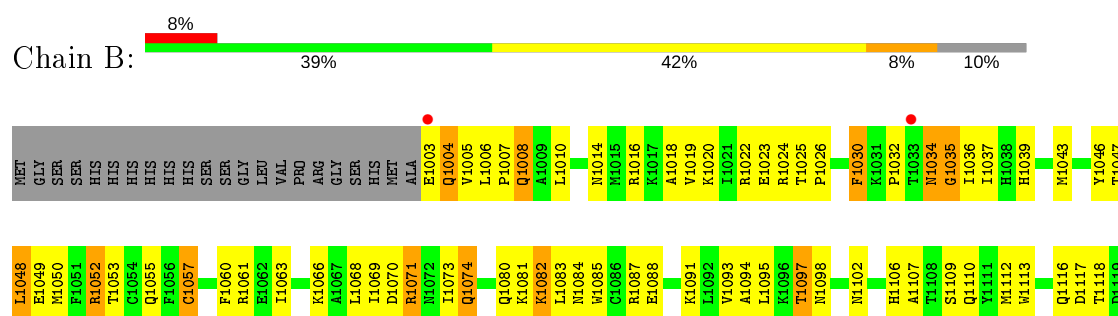
### 3 Residue-property plots [i](#)

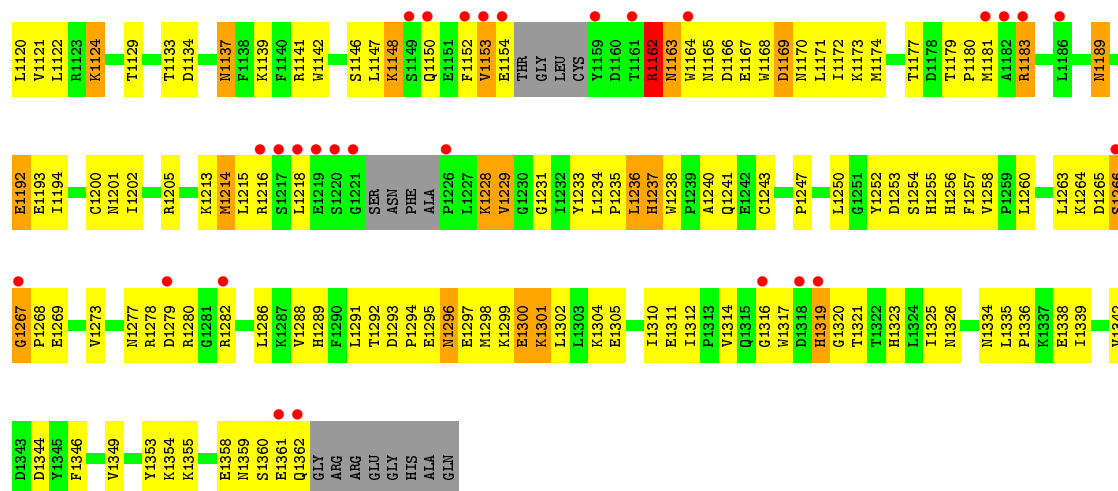
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Tumor necrosis factor, alpha-induced protein 3

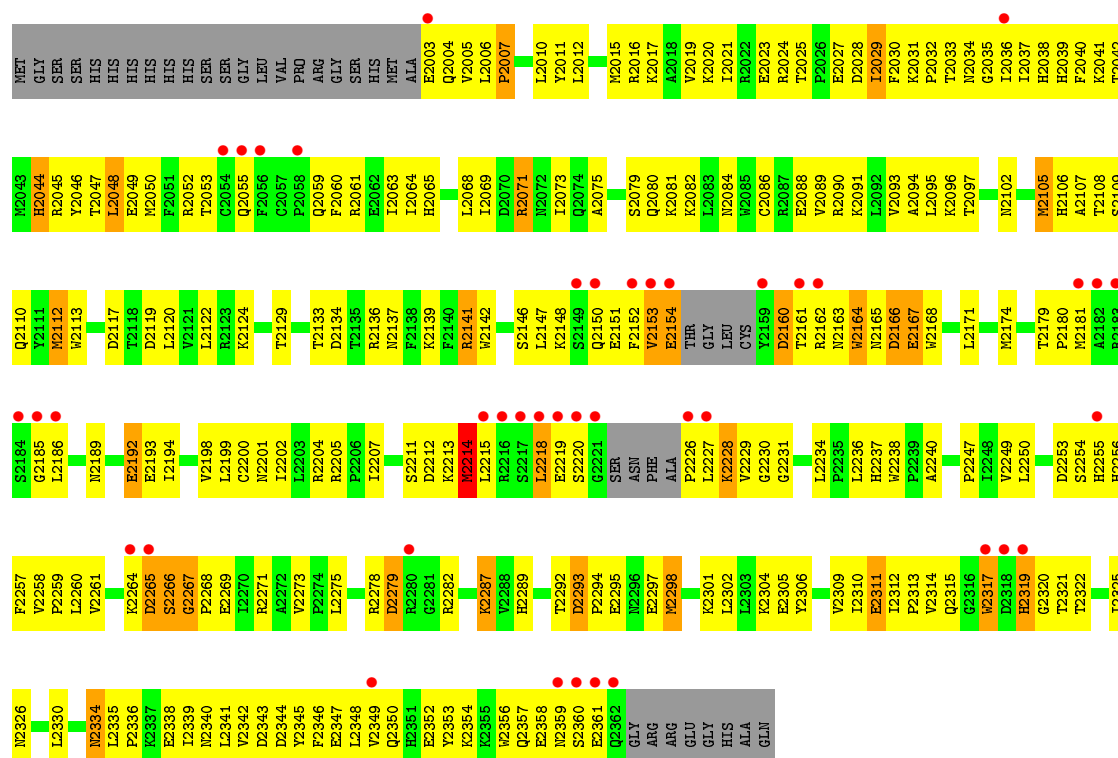


- Molecule 1: Tumor necrosis factor, alpha-induced protein 3

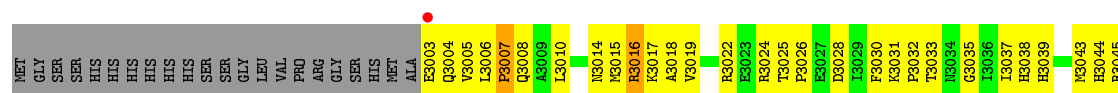


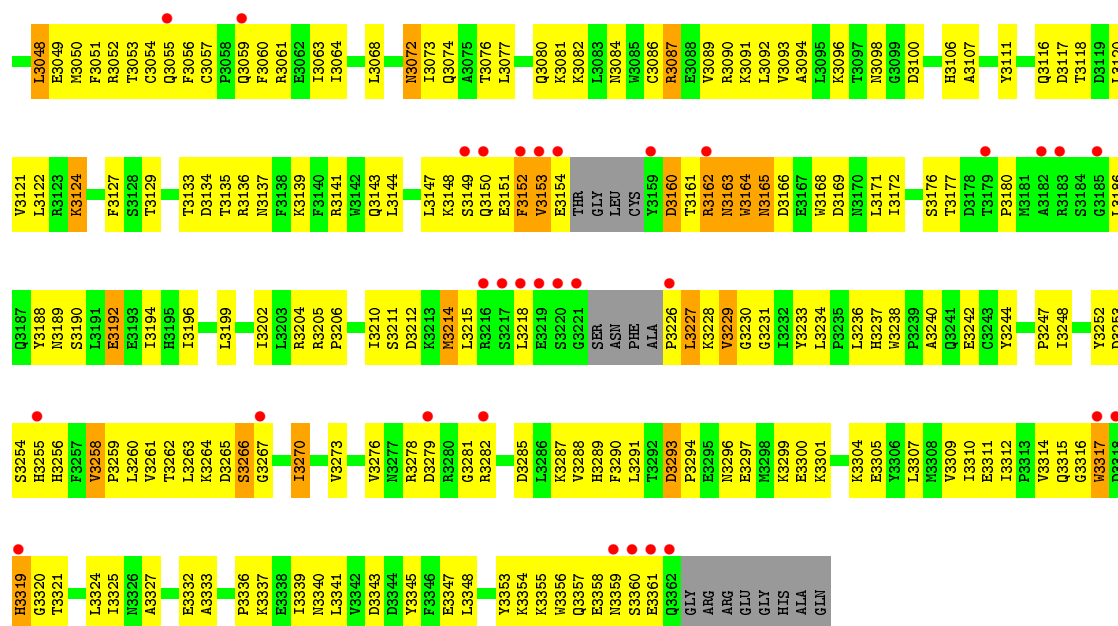


• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

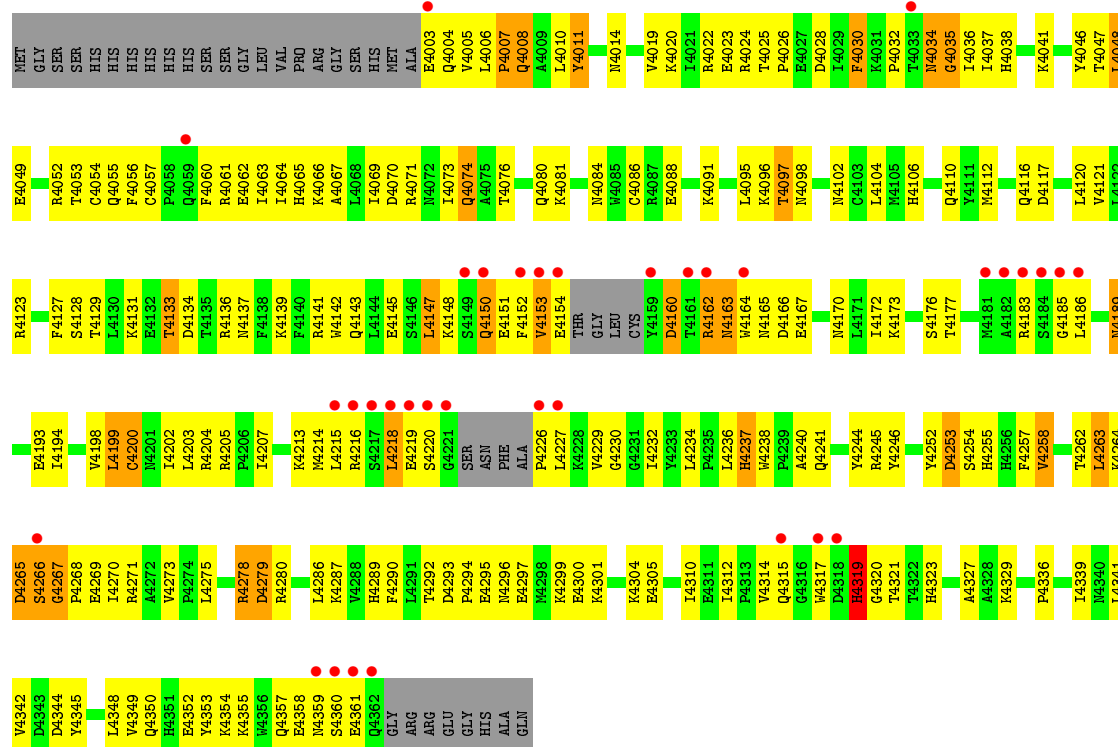


• Molecule 1: Tumor necrosis factor, alpha-induced protein 3





• Molecule 1: Tumor necrosis factor, alpha-induced protein 3



• Molecule 1: Tumor necrosis factor, alpha-induced protein 3



L5335	P5336	I5339	N5340	L5341	N5342	D5343	I5344	Y5345	F5346	F5347	L5348	F5349	Q5350	H5351	E5352	Y5353	K5354	K5355	N5356	Q5357	N5358	N5359	S5360	E5361	Q5362	GLY	ARG	ARG	GLU	GLY	HIS	ALA	GLN																											
V5261	T5262	L5263	K5264	D5265	S5266	G5267	P5268	E5269	L5270	R5271	V5276	N5277	R5278	D5279	R5280	Q5281	K5287	F5288	H5289	F5290	L5291	T5292	D5293	P5294	E5295	N5296	E5297	N5298	K5299	E5300	K5301	L5302	L5303	K5304	E5305	F5306	L5307	N5308																						
E5192	E5193	L5194	V5198	L5199	C5200	N5201	L5202	L5203	R5204	R5205	P5206	L5207	T5208	V5209	L5210	S5211	D5212	K5213	N5214	L5215	R5216	S5217	L5218	E5219	S5220	G5221	SER	ASN	PHE	ALA	P5226	L5227	K5228	V5229	L5236	H5237	N5238	P5239	A5240	G5243	Y5244	R5245	Y5246	P5247	L5248	V5249	L5250	D5253	S5254	H5255	H5256	F5257	V5258	P5259	L5260					
T5118	D5119	L5120	V5121	L5122	R5123	F5127	S5128	T5129	L5130	T5133	D5134	N5137	F5140	R5141	W5142	Q5143	L5144	L5147	K5148	S5149	Q5150	E5151	F5152	V5153	E5154	THR	GLY	LEU	CYS	Y5159	D5160	T5161	N5162	N5163	W5164	E5167	W5168	D5169	I5172	S5176	T5179	P5180	N5181	A5182	R5183	S5184	G5185	L5186	L5191											
H5044	R5045	Y5046	T5047	L5048	E5049	N5050	F5051	R5052	T5053	C5054	Q5055	F5056	C5057	P5058	Q5059	F5060	R5061	E5062	I5063	I5064	A5067	D5070	T5073	T5076	Q5080	K5081	K5082	L5083	N5084	W5085	C5086	R5087	E5088	V5089	R5090	K5091	L5095	K5096	T5097	D5100	G5101	N5102	C5103	L5104	N5105	H5106	Q5110	Y5111	N5112	W5113		G5035	I5036	I5037	H5038	H5039	F5040	K5041	T5042	N5043

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.64Å 123.64Å 143.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 29.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (25.00-2.50) 95.8 (29.74-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.246 0.207 , 0.250	Depositor DCC
$R_{free}$ test set	8218 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.039 for h,-h-k,-l 0.488 for -k,-h,-l	Xtriage
Reported twinning fraction	0.476 for h+k,-k,-l	Depositor
Outliers	0 of 84471 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5482e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	0.43	0/2993	0.65	0/4045
1	B	0.47	0/2993	0.69	1/4045 (0.0%)
1	C	0.40	0/2993	0.65	0/4045
1	D	0.44	0/2993	0.66	0/4045
1	E	0.48	0/2993	0.68	0/4045
1	F	0.42	0/2993	0.66	1/4045 (0.0%)
All	All	0.44	0/17958	0.67	2/24270 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5348	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	1264	LYS	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	2925	0	2915	216	0
1	B	2925	0	2915	208	0
1	C	2925	0	2915	227	0
1	D	2925	0	2915	230	0
1	E	2925	0	2915	207	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2925	0	2915	245	0
All	All	17550	0	17490	1309	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 37.

The worst 5 of 1309 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:6336:PRO:HD2	1:A:6339:ILE:HD11	1.19	1.17
1:B:1228:LYS:HD2	1:B:1228:LYS:H	1.14	1.11
1:C:2105:MET:HG3	1:C:2122:LEU:HB3	1.29	1.09
1:B:1189:ASN:ND2	1:B:1189:ASN:H	1.43	1.09
1:F:5336:PRO:HD2	1:F:5339:ILE:HD11	1.38	1.06

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	346/390 (89%)	297 (86%)	36 (10%)	13 (4%)	3	4
1	B	346/390 (89%)	298 (86%)	33 (10%)	15 (4%)	2	3
1	C	346/390 (89%)	294 (85%)	39 (11%)	13 (4%)	3	4
1	D	346/390 (89%)	298 (86%)	34 (10%)	14 (4%)	3	3
1	E	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	3	4
1	F	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	3	4
All	All	2076/2340 (89%)	1779 (86%)	218 (10%)	79 (4%)	3	4

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6004	GLN
1	A	6266	SER
1	A	6279	ASP
1	B	1004	GLN
1	B	1163	ASN

### 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	325/354 (92%)	291 (90%)	34 (10%)	7	13
1	B	325/354 (92%)	289 (89%)	36 (11%)	6	11
1	C	325/354 (92%)	296 (91%)	29 (9%)	9	19
1	D	325/354 (92%)	300 (92%)	25 (8%)	13	25
1	E	325/354 (92%)	294 (90%)	31 (10%)	8	17
1	F	325/354 (92%)	294 (90%)	31 (10%)	8	17
All	All	1950/2124 (92%)	1764 (90%)	186 (10%)	8	17

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2199	LEU
1	D	3087	ARG
1	F	5193	GLU
1	C	2218	LEU
1	C	2317	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2289	HIS
1	D	3004	GLN
1	F	5165	ASN
1	C	2296	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
1	C	2334	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](#)

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	352/390 (90%)	0.32	29 (8%)	11 11	20, 62, 150, 195	0
1	B	352/390 (90%)	0.21	30 (8%)	10 10	19, 50, 142, 179	0
1	C	352/390 (90%)	0.52	41 (11%)	4 4	30, 66, 148, 185	0
1	D	352/390 (90%)	0.29	32 (9%)	9 9	23, 59, 145, 188	0
1	E	352/390 (90%)	0.24	35 (9%)	7 7	19, 52, 145, 175	0
1	F	352/390 (90%)	0.40	31 (8%)	10 10	28, 67, 146, 194	0
All	All	2112/2340 (90%)	0.33	198 (9%)	8 8	19, 59, 146, 195	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	5153	VAL	22.8
1	C	2318	ASP	19.4
1	E	4153	VAL	18.3
1	D	3153	VAL	16.5
1	A	6150	GLN	15.2

### 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.