



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:10 AM GMT

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
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

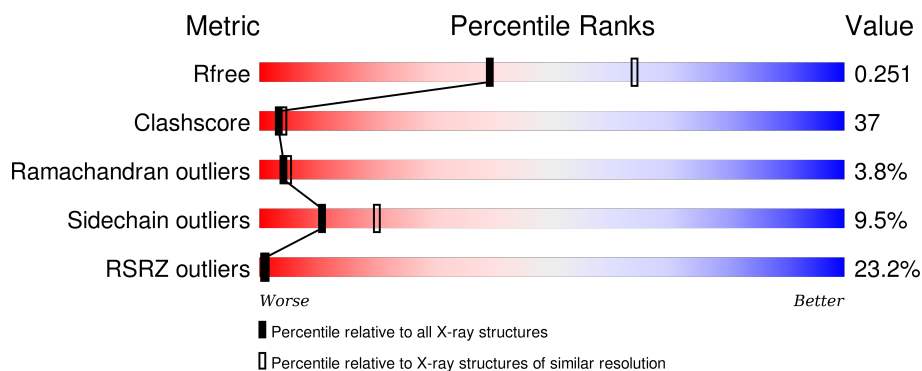
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 ≥ 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	390	<div> <div>19%</div> <div> <div>33%</div> <div>49%</div> <div>8%</div> <div>10%</div> </div> </div>
1	B	390	<div> <div>18%</div> <div> <div>39%</div> <div>42%</div> <div>8%</div> <div>10%</div> </div> </div>
1	C	390	<div> <div>25%</div> <div> <div>33%</div> <div>50%</div> <div>7%</div> <div>10%</div> </div> </div>
1	D	390	<div> <div>22%</div> <div> <div>35%</div> <div>49%</div> <div>6%</div> <div>10%</div> </div> </div>
1	E	390	<div> <div>19%</div> <div> <div>39%</div> <div>44%</div> <div>7%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	390	<div><div></div><div>22%</div><div>35%</div><div>48%</div><div>7%</div><div>10%</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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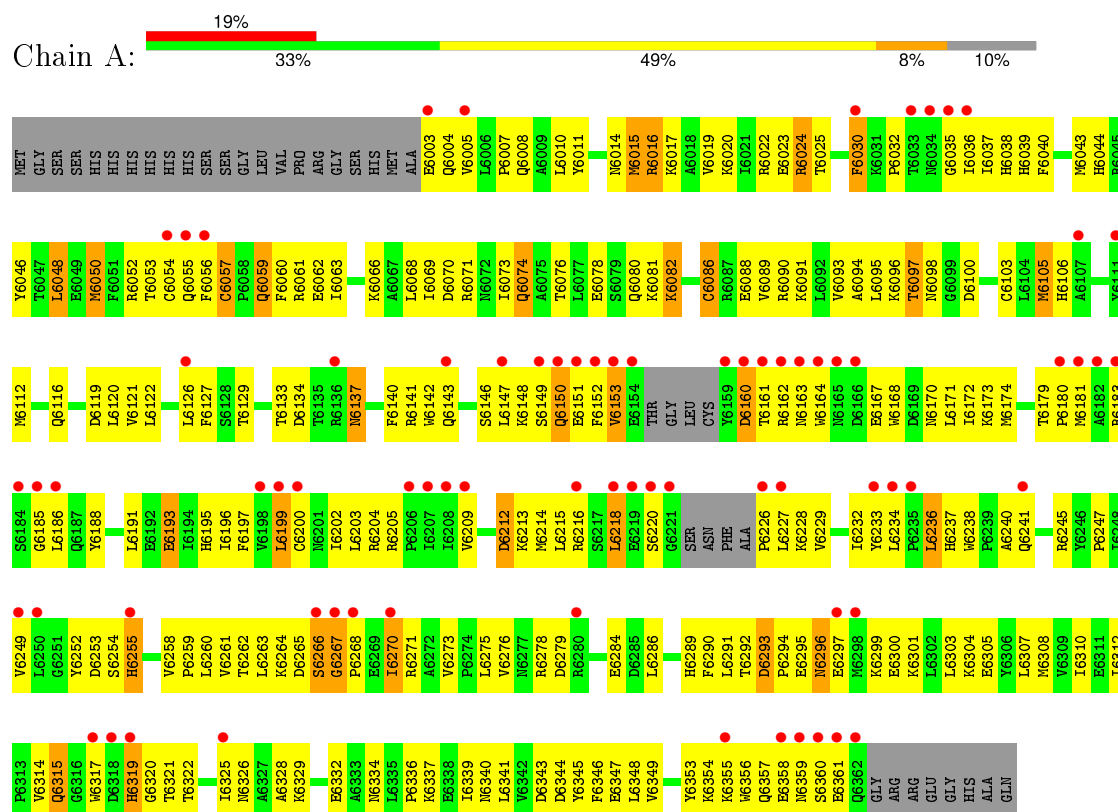
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Chain	Residue	Modelled	Actual	Comment	Reference
F	4982	GLY	-	EXPRESSION TAG	UNP P21580
F	4983	SER	-	EXPRESSION TAG	UNP P21580
F	4984	SER	-	EXPRESSION TAG	UNP P21580
F	4985	HIS	-	EXPRESSION TAG	UNP P21580
F	4986	HIS	-	EXPRESSION TAG	UNP P21580
F	4987	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

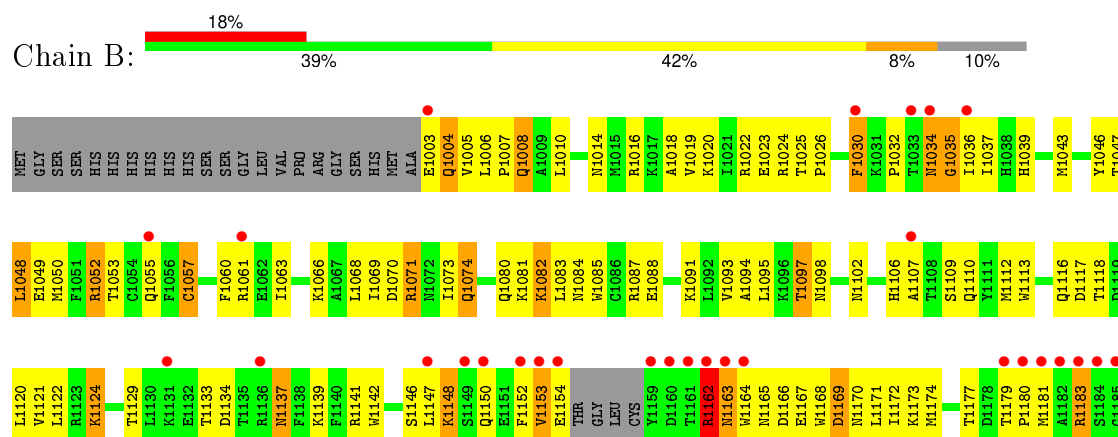
3 Residue-property plots

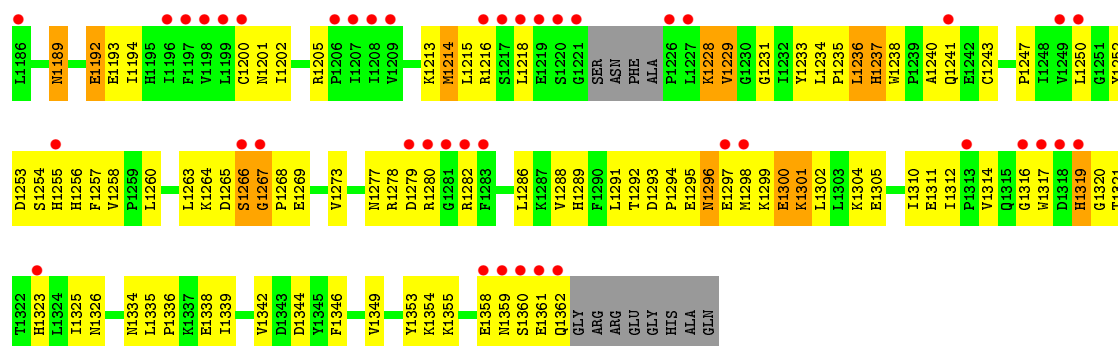
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

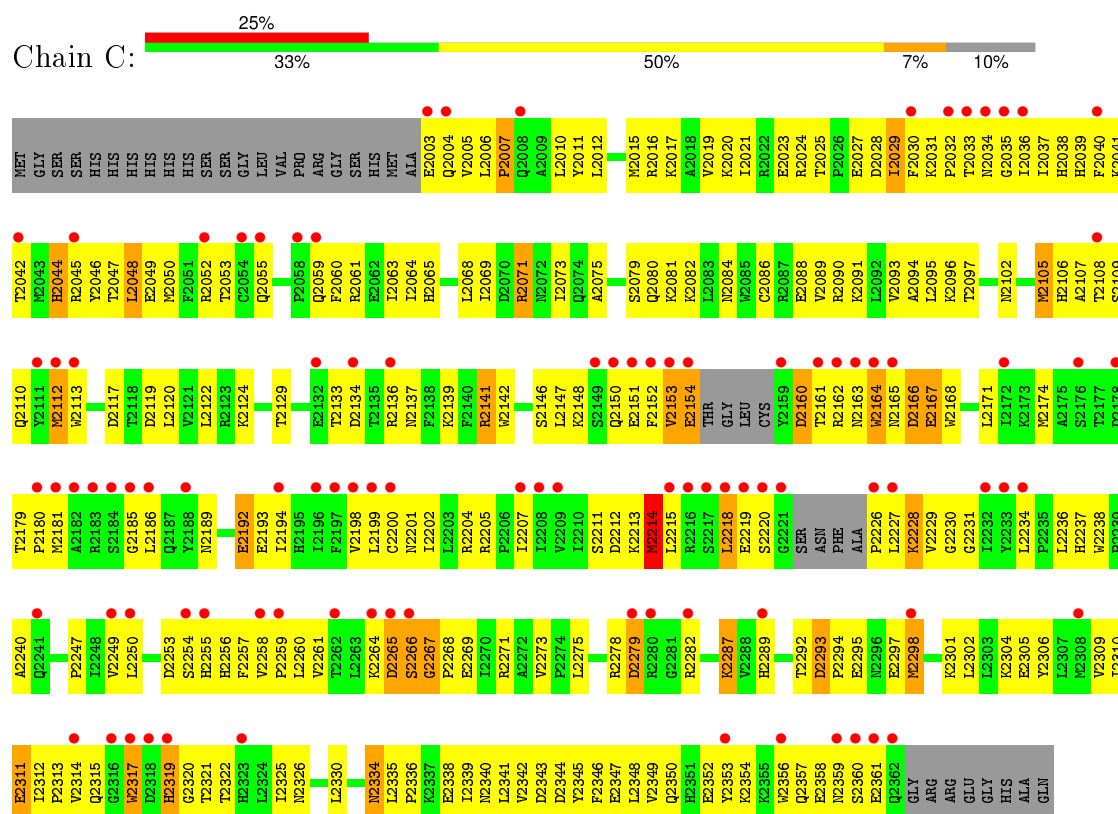


- Molecule 1: Tumor necrosis factor, alpha-induced protein 3

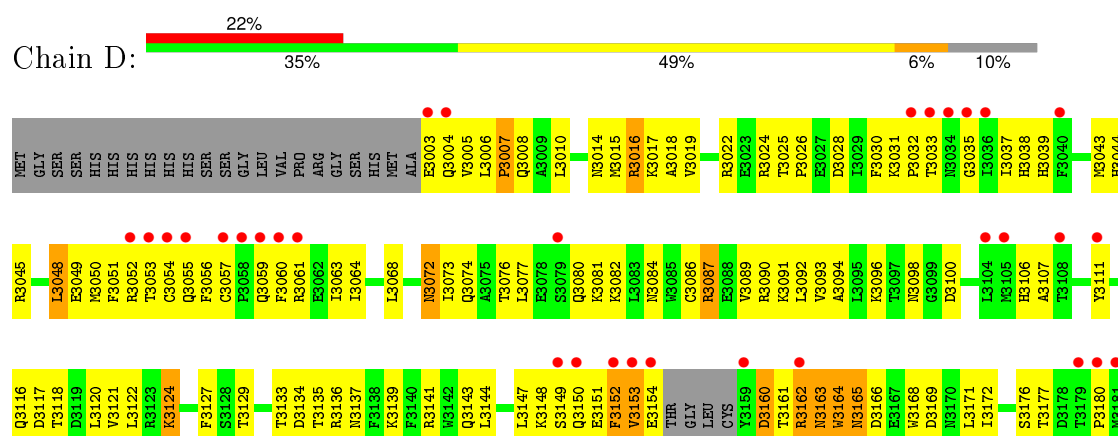


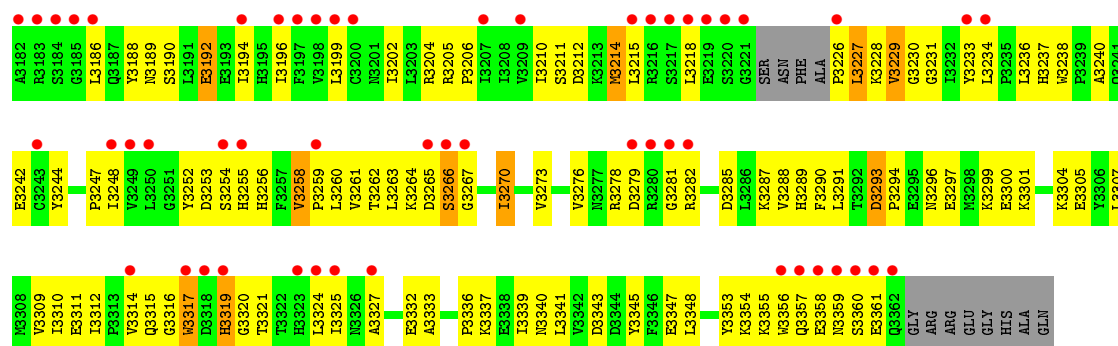


• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

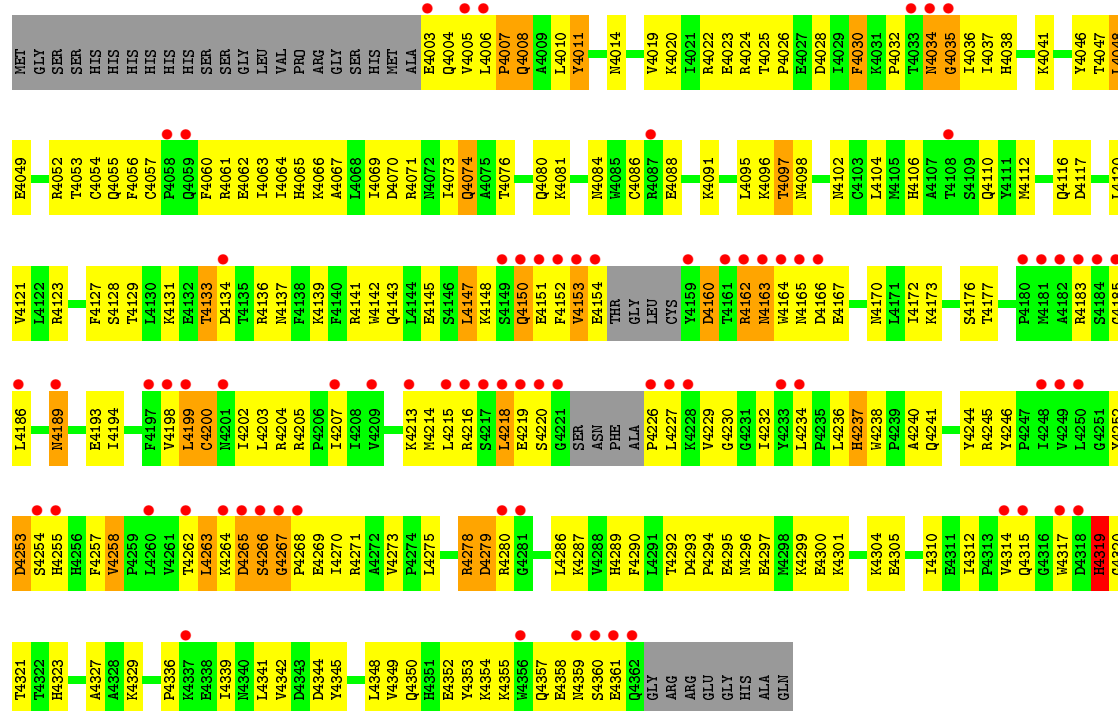
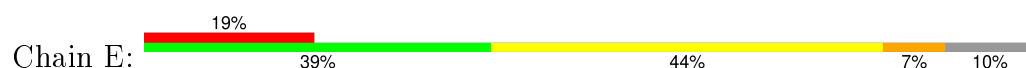


• Molecule 1: Tumor necrosis factor, alpha-induced protein 3

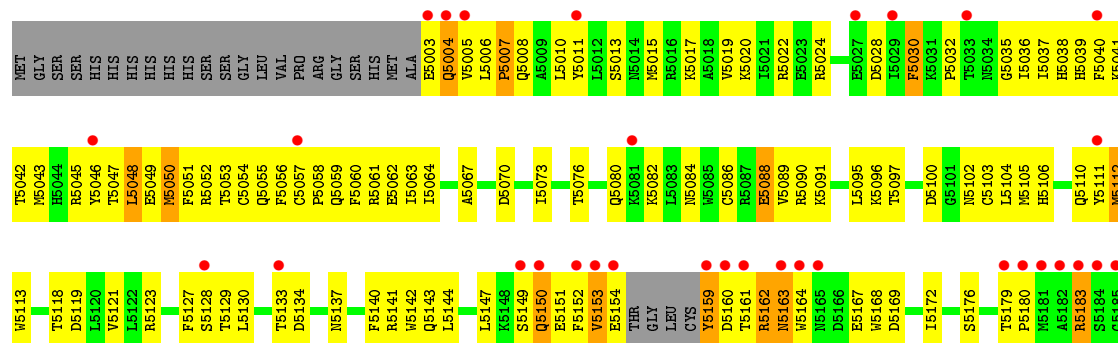


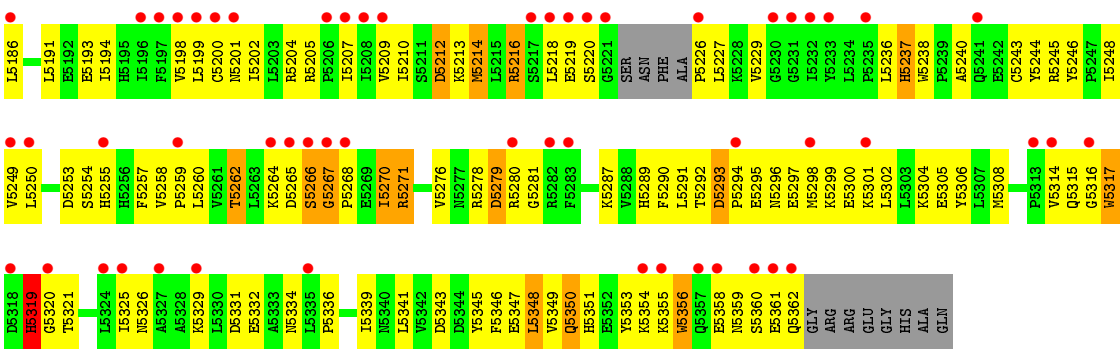


• Molecule 1: Tumor necrosis factor, alpha-induced protein 3



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	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) 95.9 (29.74-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.246 0.206 , 0.251	Depositor DCC
R_{free} test set	7871 reflections (10.75%)	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 78.3	EDS
Estimated twinning fraction	0.038 for -h,-k,l 0.039 for h,-h-k,-l 0.488 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 84471 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17550	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹ Intensities estimated from amplitudes.

² 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](#)

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%)	4	5
1	B	346/390 (89%)	298 (86%)	33 (10%)	15 (4%)	3	4
1	C	346/390 (89%)	294 (85%)	39 (11%)	13 (4%)	4	5
1	D	346/390 (89%)	298 (86%)	34 (10%)	14 (4%)	4	4
1	E	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	4	6
1	F	346/390 (89%)	296 (86%)	38 (11%)	12 (4%)	4	6
All	All	2076/2340 (89%)	1779 (86%)	218 (10%)	79 (4%)	4	5

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%)	8	16
1	B	325/354 (92%)	289 (89%)	36 (11%)	8	14
1	C	325/354 (92%)	296 (91%)	29 (9%)	12	23
1	D	325/354 (92%)	300 (92%)	25 (8%)	16	30
1	E	325/354 (92%)	294 (90%)	31 (10%)	11	20
1	F	325/354 (92%)	294 (90%)	31 (10%)	11	20
All	All	1950/2124 (92%)	1764 (90%)	186 (10%)	11	20

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

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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, 95th 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 ²)	Q<0.9
1	A	352/390 (90%)	1.42	75 (21%) 1 1	20, 62, 150, 195	0
1	B	352/390 (90%)	1.23	71 (20%) 1 1	19, 50, 142, 179	0
1	C	352/390 (90%)	1.75	97 (27%) 1 0	30, 66, 148, 185	0
1	D	352/390 (90%)	1.49	84 (23%) 1 1	23, 59, 145, 188	0
1	E	352/390 (90%)	1.29	75 (21%) 1 1	19, 52, 145, 175	0
1	F	352/390 (90%)	1.54	87 (24%) 1 1	28, 67, 146, 194	0
All	All	2112/2340 (90%)	1.45	489 (23%) 1 1	19, 59, 146, 195	0

The worst 5 of 489 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4153	VAL	22.0
1	C	2318	ASP	20.7
1	A	6153	VAL	16.7
1	F	5153	VAL	16.6
1	A	6159	TYR	15.9

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.