



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID : 3M06  
Title : Crystal Structure of TRAF2  
Authors : Kabaleeswaran, V.; Wu, H.  
Deposited on : 2010-03-02  
Resolution : 2.67 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  
<http://wwpdb.org/validation/2016/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  
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

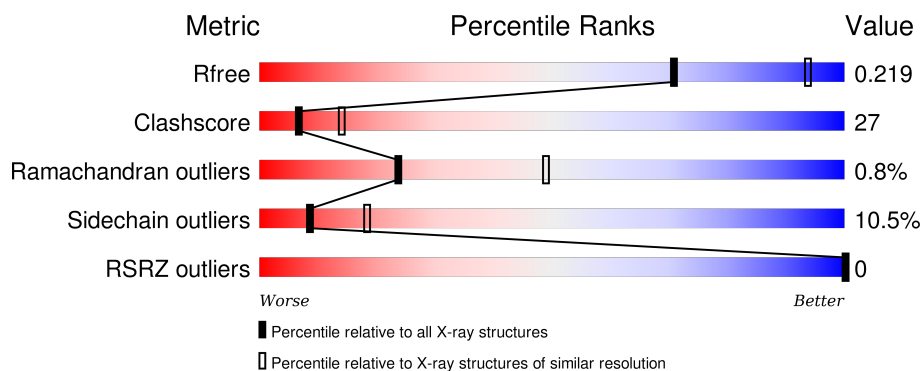
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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. 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	72	<div> <div>49%</div> <div>35%</div> <div>•</div> <div>14%</div> </div>
1	B	72	<div> <div>51%</div> <div>33%</div> <div>•</div> <div>14%</div> </div>
1	C	72	<div> <div>60%</div> <div>22%</div> <div>•</div> <div>14%</div> </div>
1	D	72	<div> <div>51%</div> <div>31%</div> <div>•</div> <div>14%</div> </div>
1	E	72	<div> <div>46%</div> <div>35%</div> <div>6%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	72	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (43%), yellow (33%), orange (10%), and grey (14%).

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2686 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 TNF receptor-associated factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	62	Total	C	N	O	S	0	0	0
			447	273	81	90	3			
1	B	62	Total	C	N	O	S	0	0	0
			449	273	83	89	4			
1	C	62	Total	C	N	O	S	0	0	0
			414	253	75	83	3			
1	D	62	Total	C	N	O	S	0	0	0
			453	279	82	88	4			
1	E	62	Total	C	N	O	S	0	0	0
			443	271	78	90	4			
1	F	62	Total	C	N	O	S	0	0	0
			419	257	75	84	3			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	LEU	-	EXPRESSION TAG	UNP Q12933
A	331	GLU	-	EXPRESSION TAG	UNP Q12933
A	332	HIS	-	EXPRESSION TAG	UNP Q12933
A	333	HIS	-	EXPRESSION TAG	UNP Q12933
A	334	HIS	-	EXPRESSION TAG	UNP Q12933
A	335	HIS	-	EXPRESSION TAG	UNP Q12933
A	336	HIS	-	EXPRESSION TAG	UNP Q12933
A	337	HIS	-	EXPRESSION TAG	UNP Q12933
B	330	LEU	-	EXPRESSION TAG	UNP Q12933
B	331	GLU	-	EXPRESSION TAG	UNP Q12933
B	332	HIS	-	EXPRESSION TAG	UNP Q12933
B	333	HIS	-	EXPRESSION TAG	UNP Q12933
B	334	HIS	-	EXPRESSION TAG	UNP Q12933
B	335	HIS	-	EXPRESSION TAG	UNP Q12933
B	336	HIS	-	EXPRESSION TAG	UNP Q12933
B	337	HIS	-	EXPRESSION TAG	UNP Q12933
C	330	LEU	-	EXPRESSION TAG	UNP Q12933

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Chain	Residue	Modelled	Actual	Comment	Reference
C	331	GLU	-	EXPRESSION TAG	UNP Q12933
C	332	HIS	-	EXPRESSION TAG	UNP Q12933
C	333	HIS	-	EXPRESSION TAG	UNP Q12933
C	334	HIS	-	EXPRESSION TAG	UNP Q12933
C	335	HIS	-	EXPRESSION TAG	UNP Q12933
C	336	HIS	-	EXPRESSION TAG	UNP Q12933
C	337	HIS	-	EXPRESSION TAG	UNP Q12933
D	330	LEU	-	EXPRESSION TAG	UNP Q12933
D	331	GLU	-	EXPRESSION TAG	UNP Q12933
D	332	HIS	-	EXPRESSION TAG	UNP Q12933
D	333	HIS	-	EXPRESSION TAG	UNP Q12933
D	334	HIS	-	EXPRESSION TAG	UNP Q12933
D	335	HIS	-	EXPRESSION TAG	UNP Q12933
D	336	HIS	-	EXPRESSION TAG	UNP Q12933
D	337	HIS	-	EXPRESSION TAG	UNP Q12933
E	330	LEU	-	EXPRESSION TAG	UNP Q12933
E	331	GLU	-	EXPRESSION TAG	UNP Q12933
E	332	HIS	-	EXPRESSION TAG	UNP Q12933
E	333	HIS	-	EXPRESSION TAG	UNP Q12933
E	334	HIS	-	EXPRESSION TAG	UNP Q12933
E	335	HIS	-	EXPRESSION TAG	UNP Q12933
E	336	HIS	-	EXPRESSION TAG	UNP Q12933
E	337	HIS	-	EXPRESSION TAG	UNP Q12933
F	330	LEU	-	EXPRESSION TAG	UNP Q12933
F	331	GLU	-	EXPRESSION TAG	UNP Q12933
F	332	HIS	-	EXPRESSION TAG	UNP Q12933
F	333	HIS	-	EXPRESSION TAG	UNP Q12933
F	334	HIS	-	EXPRESSION TAG	UNP Q12933
F	335	HIS	-	EXPRESSION TAG	UNP Q12933
F	336	HIS	-	EXPRESSION TAG	UNP Q12933
F	337	HIS	-	EXPRESSION TAG	UNP Q12933

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	8	Total O 8 8	0	0
2	C	9	Total O 9 9	0	0
2	D	10	Total O 10 10	0	0

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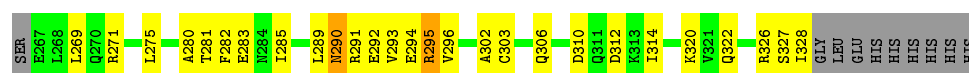
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	10	Total	O	0	0
			10	10		
2	F	11	Total	O	0	0
			11	11		

### 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 ( $RSRZ > 2$ ). 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: TNF receptor-associated factor 2

Chain A: 



- Molecule 1: TNF receptor-associated factor 2

Chain B: 



- Molecule 1: TNF receptor-associated factor 2

Chain C: 



- Molecule 1: TNF receptor-associated factor 2

Chain D: 



- Molecule 1: TNF receptor-associated factor 2

Chain E: 



- Molecule 1: TNF receptor-associated factor 2

Chain F: 

SER	E267	L268	L269	Q270	R271	C272	E276	T279	A280	T281	F282	E283	I284	L285	V286	C287	V288	L289	I290	R291	R295	V296	A297	E301	A302	C303	S304	R305	Q306	H307	R308	L309	R313	T314	E315	S318	R319	R320	L324	I328	GLY	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.71 Å   150.71 Å   86.73 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	36.13 – 2.67 36.12 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (36.13-2.67) 99.8 (36.12-2.67)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.68 Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.192 , 0.233 0.225 , 0.219	Depositor DCC
$R_{free}$ test set	1067 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.6	EDS
Estimated twinning fraction	0.525 for H, K, L 0.475 for K, H, -L 0.466 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.525 for H, K, L 0.475 for K, H, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 20823 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2686	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 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	0.50	0/448	0.66	0/607
1	B	0.48	0/450	0.62	0/609
1	C	0.66	1/415 (0.2%)	0.59	0/566
1	D	0.54	0/454	0.59	0/613
1	E	0.56	0/444	0.63	0/601
1	F	0.74	0/420	0.66	0/571
All	All	0.58	1/2631 (0.0%)	0.62	0/3567

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	272	CYS	CB-SG	-6.30	1.71	1.82

There are no bond angle outliers.

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	447	0	418	26	0
1	B	449	0	420	22	0
1	C	414	0	361	19	0
1	D	453	0	441	31	0
1	E	443	0	408	35	0
1	F	419	0	372	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	0	0	0
2	B	8	0	0	0	0
2	C	9	0	0	1	0
2	D	10	0	0	1	0
2	E	10	0	0	0	0
2	F	11	0	0	3	0
All	All	2686	0	2420	136	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 27.

The worst 5 of 136 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:D:286:VAL:HG22	1:F:286:VAL:HG21	1.48	0.95
1:A:295:ARG:HH22	1:F:291:ARG:HH21	1.19	0.87
1:A:275:LEU:HD23	1:B:275:LEU:HD13	1.57	0.86
1:D:275:LEU:HD21	1:F:276:GLU:HB3	1.59	0.84
1:E:304:SER:HA	1:F:303:CYS:HB2	1.62	0.78

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	60/72 (83%)	56 (93%)	4 (7%)	0	100	100
1	B	60/72 (83%)	58 (97%)	2 (3%)	0	100	100
1	C	60/72 (83%)	56 (93%)	4 (7%)	0	100	100
1	D	60/72 (83%)	55 (92%)	5 (8%)	0	100	100
1	E	60/72 (83%)	57 (95%)	2 (3%)	1 (2%)	11	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	60/72 (83%)	53 (88%)	5 (8%)	2 (3%)	5	10
All	All	360/432 (83%)	335 (93%)	22 (6%)	3 (1%)	24	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	269	LEU
1	F	269	LEU
1	F	276	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	45/66 (68%)	40 (89%)	5 (11%)	8	16
1	B	45/66 (68%)	42 (93%)	3 (7%)	20	42
1	C	37/66 (56%)	34 (92%)	3 (8%)	15	31
1	D	47/66 (71%)	43 (92%)	4 (8%)	13	28
1	E	44/66 (67%)	38 (86%)	6 (14%)	5	10
1	F	38/66 (58%)	32 (84%)	6 (16%)	3	7
All	All	256/396 (65%)	229 (90%)	27 (10%)	8	18

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	270	GLN
1	E	268	LEU
1	F	290	ASN
1	D	292	GLU
1	A	322	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	290	ASN
1	E	306	GLN
1	D	270	GLN
1	B	306	GLN
1	C	307	HIS

### 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	62/72 (86%)	-0.49	0 100 100	27, 49, 64, 65	0
1	B	62/72 (86%)	-0.48	0 100 100	30, 47, 68, 69	0
1	C	62/72 (86%)	-0.63	0 100 100	28, 47, 68, 69	0
1	D	62/72 (86%)	-0.43	0 100 100	29, 57, 70, 75	0
1	E	62/72 (86%)	-0.49	0 100 100	21, 51, 73, 75	0
1	F	62/72 (86%)	-0.61	0 100 100	32, 55, 73, 78	0
All	All	372/432 (86%)	-0.52	0 100 100	21, 52, 71, 78	0

There are no RSRZ outliers to report.

### 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.