WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 03:02 pm BST

PDB ID	:	4K8U
Title	:	Crystal structure of TRAF4 TRAF domain
Authors	:	Park, H.H.; Yoon, J.H.
Deposited on	:	2013-04-18
Resolution	:	2.30 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

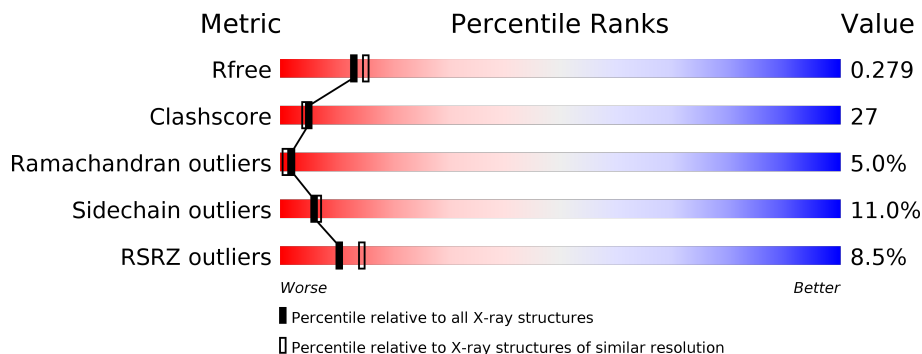|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.279
Clashscore		27
Ramachandran outliers		5.0%
Sidechain outliers		11.0%
RSRZ outliers		8.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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% 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	198	8% · 63% · 20% · 7% · 10%
1	B	198	6% · 53% · 26% · 9% · · · 11%
1	C	198	9% · 47% · 28% · 11% · · · 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4340 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1444	927	256	260	1			
1	B	176	Total	C	N	O	S	0	0	0
			1427	916	254	256	1			
1	C	176	Total	C	N	O	S	0	0	0
			1423	915	253	254	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	LEU	-	expression tag	UNP Q9BUZ4
A	472	GLU	-	expression tag	UNP Q9BUZ4
A	473	HIS	-	expression tag	UNP Q9BUZ4
A	474	HIS	-	expression tag	UNP Q9BUZ4
A	475	HIS	-	expression tag	UNP Q9BUZ4
A	476	HIS	-	expression tag	UNP Q9BUZ4
A	477	HIS	-	expression tag	UNP Q9BUZ4
A	478	HIS	-	expression tag	UNP Q9BUZ4
B	471	LEU	-	expression tag	UNP Q9BUZ4
B	472	GLU	-	expression tag	UNP Q9BUZ4
B	473	HIS	-	expression tag	UNP Q9BUZ4
B	474	HIS	-	expression tag	UNP Q9BUZ4
B	475	HIS	-	expression tag	UNP Q9BUZ4
B	476	HIS	-	expression tag	UNP Q9BUZ4
B	477	HIS	-	expression tag	UNP Q9BUZ4
B	478	HIS	-	expression tag	UNP Q9BUZ4
C	471	LEU	-	expression tag	UNP Q9BUZ4
C	472	GLU	-	expression tag	UNP Q9BUZ4
C	473	HIS	-	expression tag	UNP Q9BUZ4
C	474	HIS	-	expression tag	UNP Q9BUZ4
C	475	HIS	-	expression tag	UNP Q9BUZ4
C	476	HIS	-	expression tag	UNP Q9BUZ4
C	477	HIS	-	expression tag	UNP Q9BUZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	478	HIS	-	expression tag	UNP Q9BUZ4

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total 32	O 32	0	0
2	B	5	Total 5	O 5	0	0
2	C	9	Total 9	O 9	0	0

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 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.
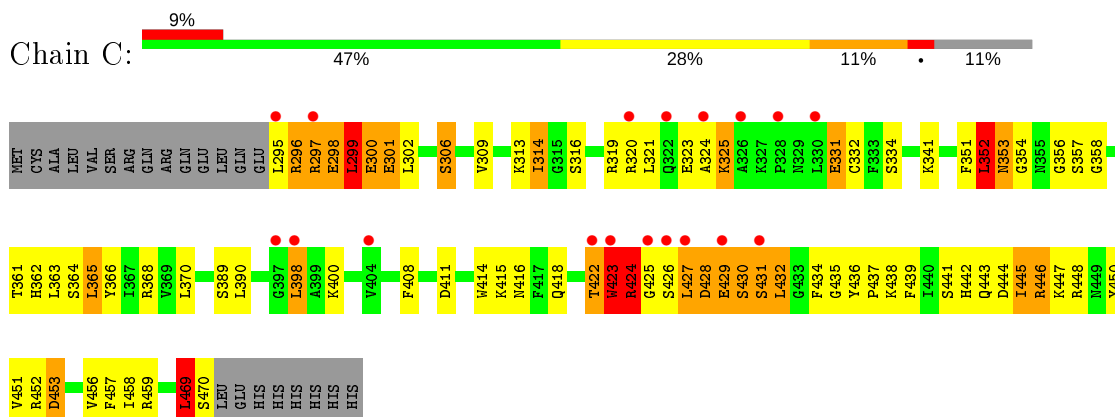
- Molecule 1: TNF receptor-associated factor 4
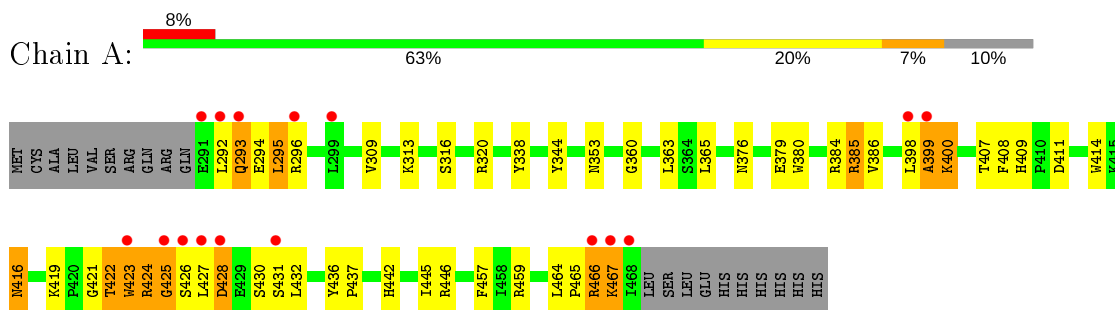
- Molecule 1: TNF receptor-associated factor 4
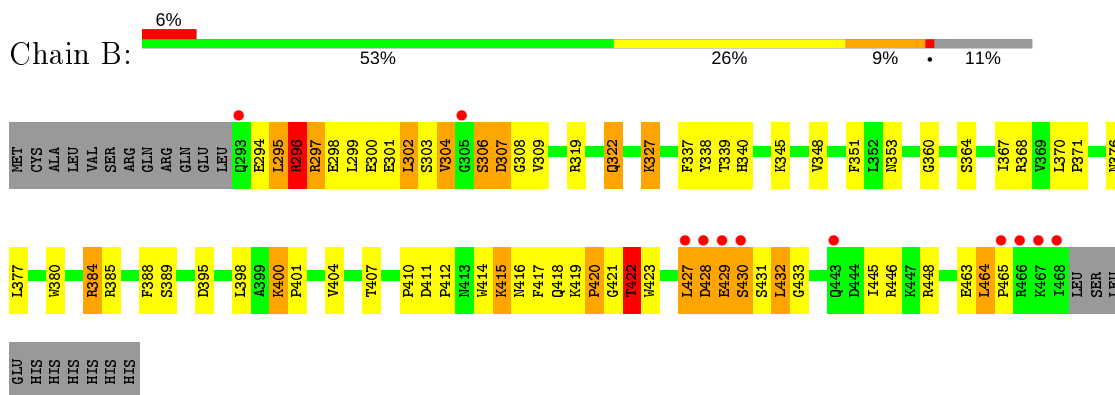
- Molecule 1: TNF receptor-associated factor 4

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.95Å　　87.99Å　　117.36Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	41.59　–　2.30 41.59　–　2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (41.59-2.30) 99.2 (41.59-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.237　,　0.281 0.233　,　0.279	Depositor DCC
R_{free} test set	1383 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4340	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.61	0/1485	0.69	0/2009
1	B	0.48	0/1468	0.63	0/1986
1	C	0.49	0/1464	0.75	1/1981 (0.1%)
All	All	0.53	0/4417	0.69	1/5976 (0.0%)

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	1
1	B	0	1
1	C	0	4
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	353	ASN	N-CA-CB	5.89	121.21	110.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	GLN	Peptide
1	B	420	PRO	Peptide
1	C	299	LEU	Peptide
1	C	306	SER	Peptide
1	C	352	LEU	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	1444	0	1416	45	0
1	B	1427	0	1398	79	1
1	C	1423	0	1401	110	1
2	A	32	0	0	0	0
2	B	5	0	0	0	0
2	C	9	0	0	0	0
All	All	4340	0	4215	230	1

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 230 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:B:415:LYS:NZ	1:B:428:ASP:OD1	1.57	1.36
1:C:352:LEU:N	1:C:353:ASN:OD1	1.77	1.17
1:B:427:LEU:HD13	1:B:427:LEU:N	1.60	1.11
1:B:427:LEU:HA	1:B:429:GLU:OE2	1.51	1.11
1:C:431:SER:HA	1:C:432:LEU:HB2	1.12	1.10

All (1) 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:B:431:SER:OG	1:C:470:SER:OG[3_555]	2.01	0.19

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	176/198 (89%)	157 (89%)	11 (6%)	8 (4%)	2	1
1	B	174/198 (88%)	153 (88%)	15 (9%)	6 (3%)	3	2
1	C	174/198 (88%)	144 (83%)	18 (10%)	12 (7%)	1	0
All	All	524/594 (88%)	454 (87%)	44 (8%)	26 (5%)	2	1

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	ASP
1	B	295	LEU
1	B	307	ASP
1	C	432	LEU
1	C	445	ILE

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	153/172 (89%)	145 (95%)	8 (5%)	23	32
1	B	151/172 (88%)	130 (86%)	21 (14%)	3	3
1	C	151/172 (88%)	130 (86%)	21 (14%)	3	3
All	All	455/516 (88%)	405 (89%)	50 (11%)	6	7

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	422	THR
1	B	445	ILE
1	C	429	GLU
1	B	427	LEU
1	B	429	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	GLN
1	A	442	HIS
1	C	413	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(Å²)	Q<0.9
1	A	178/198 (89%)	0.23	16 (8%)	9	12	28, 43, 104, 116	0
1	B	176/198 (88%)	0.28	11 (6%)	20	25	40, 62, 98, 110	0
1	C	176/198 (88%)	0.63	18 (10%)	6	9	36, 70, 105, 121	0
All	All	530/594 (89%)	0.38	45 (8%)	10	14	28, 58, 104, 121	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	425	GLY	9.3
1	B	429	GLU	6.2
1	A	428	ASP	5.1
1	A	292	LEU	4.9
1	B	293	GLN	4.8

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.