wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 09:25 PM EDT

PDB ID	:	1CA4
Title	:	STRUCTURE OF TNF RECEPTOR ASSOCIATED FACTOR 2 (TRAF2)
Authors	:	Park, Y.C.; Burkitt, V.; Villa, A.R.; Tong, L.; Wu, H.
Deposited on	:	1999-02-23
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

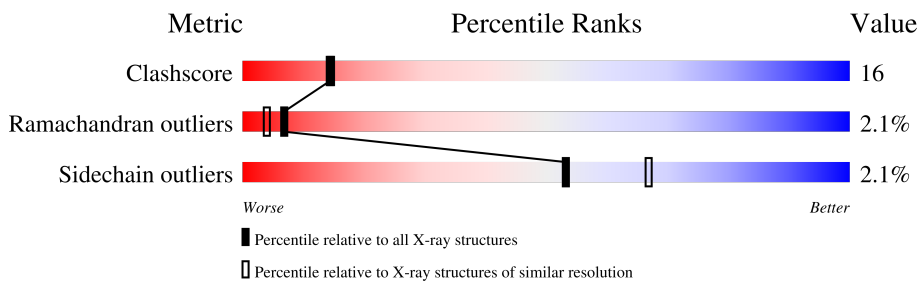|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.20 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
Clashscore		16
Ramachandran outliers		2.1%
Sidechain outliers		2.1%

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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 of 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	168	71% 26% •
1	B	168	77% 21% •
1	C	168	74% 24% •
1	D	168	67% 30% •
1	E	168	69% 29% •
1	F	168	76% 21% •

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2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8435 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 PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	B	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	C	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	D	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	E	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	F	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			

- Molecule 2 is water.

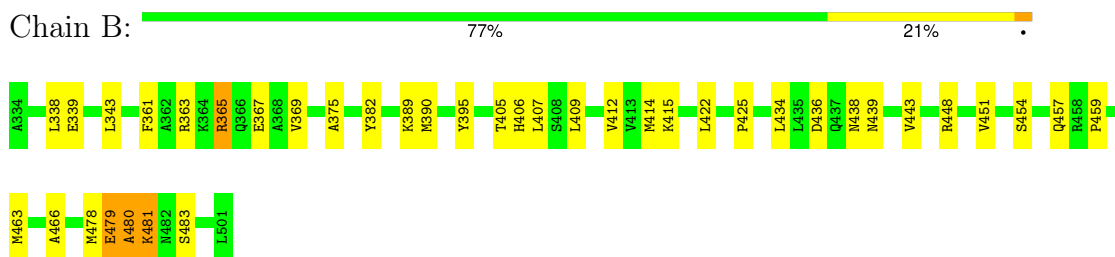| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	118	Total	O	0	0
			118	118		
2	B	136	Total	O	0	0
			136	136		
2	C	138	Total	O	0	0
			138	138		
2	D	90	Total	O	0	0
			90	90		
2	E	94	Total	O	0	0
			94	94		
2	F	167	Total	O	0	0
			167	167		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
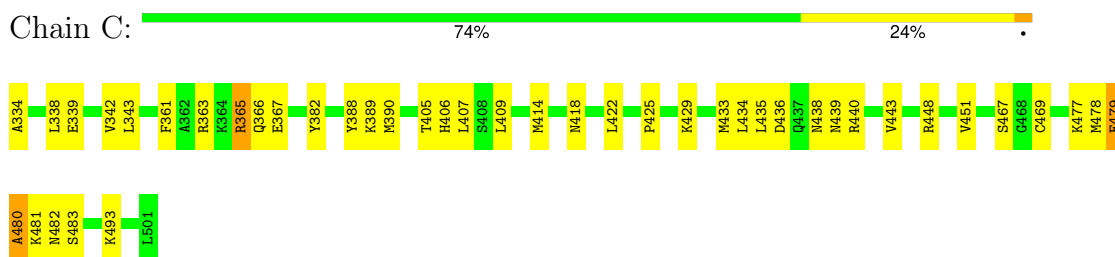
Note EDS was not executed.

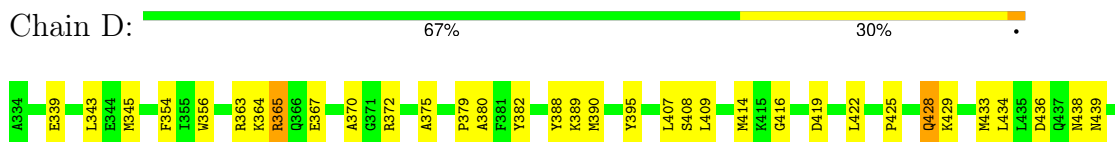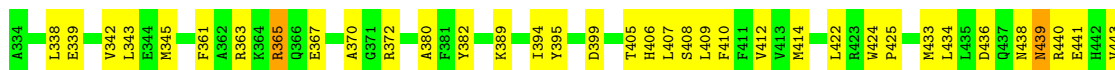• Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

Chain A:

• Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

Chain B:

• Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

Chain C:

• Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

Chain D:

V443 R448 V451 S454 Q457 M463 F472 C473 P474 V475 S476 K477 M478 E479 A480 K481 N482 S483 R486 F491 I492 K493 D497 L501

• Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

Chain E:

69%   29%   •

A334 L338 E339 V342 L343 E344 M345 F361 A362 R363 K364 R365 Q366 E367 A370 G371 R372 A380 F381 Y382 K389 I394 Y395 D399 T405 H406 L407 S408 L409 F410 F411 V412 V413 M414 L422 R423 W424 P425 M433 L434 L435 D436 Q437 N438 N439 R440 E441 H442 V443

P449 D450 V451 S455 F456 P459 N464 I465 A466 C473 P474 V475 M478 E479 A480 K481 N482 S483 R486 L501

• Molecule 1: PROTEIN (TNF RECEPTOR ASSOCIATED FACTOR 2)

Chain F:

76%   21%   •

A334 K341 M345 F361 R365 A380 F381 Y382 K389 M390 I394 Y395 D399 T405 H406 L407 S408 L409 M414 N418 L421 L422 P425 L434 L435 D436 N439 V443 R448 P449 D450 V451 S454 S455 F456 Q457 P474 K477 M478 E479

A480 K481 N482 S483 R486 L501

4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	134.92Å 84.96Å 124.07Å 90.00° 118.60° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	92.7 (20.00-2.20)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.209 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8435	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.37	0/1312	0.67	0/1781
1	B	0.37	0/1312	0.67	0/1781
1	C	0.37	0/1312	0.68	0/1781
1	D	0.35	0/1312	0.65	0/1781
1	E	0.36	0/1312	0.66	0/1781
1	F	0.39	0/1312	0.68	1/1781 (0.1%)
All	All	0.37	0/7872	0.67	1/10686 (0.0%)

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	F	434	LEU	N-CA-C	-5.18	97.02	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1282	0	1242	39	0
1	B	1282	0	1242	36	0
1	C	1282	0	1242	39	0
1	D	1282	0	1242	45	0
1	E	1282	0	1242	43	0
1	F	1282	0	1242	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	118	0	0	0	0
2	B	136	0	0	3	0
2	C	138	0	0	4	0
2	D	90	0	0	0	0
2	E	94	0	0	3	0
2	F	167	0	0	5	0
All	All	8435	0	7452	235	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 16.

The worst 5 of 235 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:425:PRO:HG3	1:A:451:VAL:HG13	1.33	1.03
1:C:425:PRO:HG3	1:C:451:VAL:HG13	1.44	0.99
1:E:425:PRO:HG3	1:E:451:VAL:HG13	1.45	0.98
1:F:394:ILE:HD11	1:F:407:LEU:HD21	1.45	0.96
1:F:425:PRO:HG3	1:F:451:VAL:HG13	1.51	0.92

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	166/168 (99%)	155 (93%)	7 (4%)	4 (2%)	6	3
1	B	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	8	5
1	C	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	8	5
1	D	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	8	5
1	E	166/168 (99%)	154 (93%)	7 (4%)	5 (3%)	4	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	166/168 (99%)	155 (93%)	8 (5%)	3 (2%)	8	5
All	All	996/1008 (99%)	929 (93%)	46 (5%)	21 (2%)	7	4

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	479	GLU
1	A	481	LYS
1	B	479	GLU
1	B	480	ALA
1	B	481	LYS

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	132/144 (92%)	129 (98%)	3 (2%)	50	63
1	B	132/144 (92%)	129 (98%)	3 (2%)	50	63
1	C	132/144 (92%)	130 (98%)	2 (2%)	65	78
1	D	132/144 (92%)	129 (98%)	3 (2%)	50	63
1	E	132/144 (92%)	129 (98%)	3 (2%)	50	63
1	F	132/144 (92%)	129 (98%)	3 (2%)	50	63
All	All	792/864 (92%)	775 (98%)	17 (2%)	53	67

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	365	ARG
1	F	422	LEU
1	C	409	LEU
1	D	365	ARG
1	D	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	366	GLN
1	F	439	ASN
1	C	439	ASN
1	C	461	ASN
1	D	406	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.