



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:01 AM UTC

PDB ID : 1D00 / pdb_00001d00
Title : STRUCTURE OF TNF RECEPTOR ASSOCIATED FACTOR 2 IN COM-
PLEX WITH A 5-RESIDUE CD40 PEPTIDE
Authors : Ye, H.; Park, Y.C.; Kreishman, M.; Kieff, E.; Wu, H.
Deposited on : 1999-09-07
Resolution : 2.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

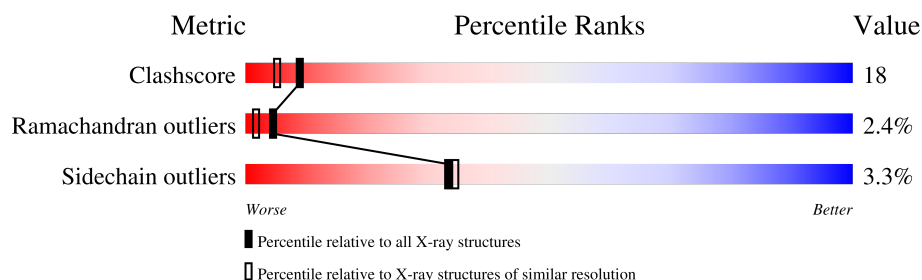
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	69% 26% 5%
1	B	168	64% 30% 6%
1	C	168	66% 29% 5%
1	D	168	65% 30% . .
1	E	168	70% 25% 5% .
1	F	168	67% 29% .
1	G	168	66% 30% .
1	H	168	64% 32% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	7	57% 29% 14%
2	J	7	29% 57% 14%
2	K	7	43% 43% 14%
2	L	7	57% 43%
2	M	7	57% 29% 14%
2	N	7	57% 43%
2	O	7	57% 29% 14%
2	P	7	43% 43% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10670 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 RECEPTOR ASSOCIATED PROTEIN 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			
1	G	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	H	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ALA	PRO	conflict	GB 1363002
A	365	ARG	LEU	conflict	GB 1363002
B	362	ALA	PRO	conflict	GB 1363002
B	365	ARG	LEU	conflict	GB 1363002
C	362	ALA	PRO	conflict	GB 1363002
C	365	ARG	LEU	conflict	GB 1363002
D	362	ALA	PRO	conflict	GB 1363002
D	365	ARG	LEU	conflict	GB 1363002
E	362	ALA	PRO	conflict	GB 1363002
E	365	ARG	LEU	conflict	GB 1363002
F	362	ALA	PRO	conflict	GB 1363002
F	365	ARG	LEU	conflict	GB 1363002

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	362	ALA	PRO	conflict	GB 1363002
G	365	ARG	LEU	conflict	GB 1363002
H	362	ALA	PRO	conflict	GB 1363002
H	365	ARG	LEU	conflict	GB 1363002

- Molecule 2 is a protein called B-CELL SURFACE ANTIGEN CD40.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	J	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	K	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	L	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	M	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	N	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	O	7	Total	C	N	O	0	0	1
			43	26	7	10			
2	P	7	Total	C	N	O	0	0	1
			43	26	7	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	3	Total	O	0	0
			3	3		
3	C	11	Total	O	0	0
			11	11		
3	D	7	Total	O	0	0
			7	7		
3	E	5	Total	O	0	0
			5	5		
3	F	9	Total	O	0	0
			9	9		
3	G	8	Total	O	0	0
			8	8		

Continued on next page...

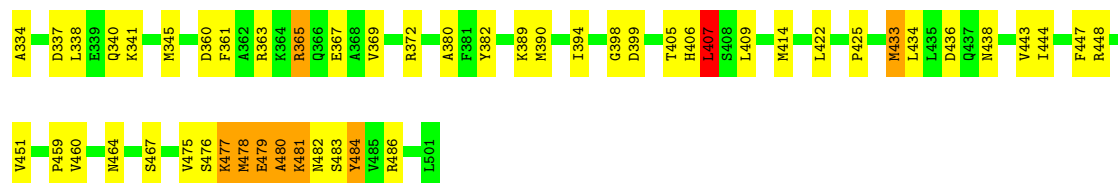
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	13	Total 13	O 13	0	0
3	K	1	Total 1	O 1	0	0
3	L	1	Total 1	O 1	0	0



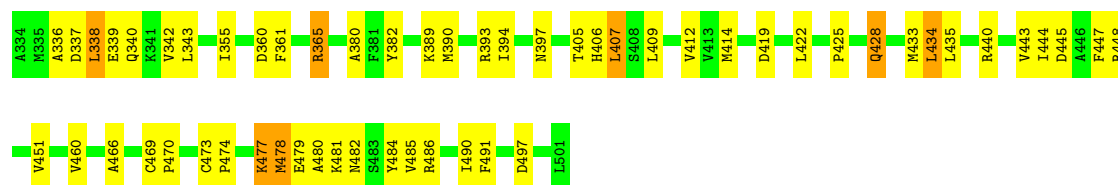
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain E: 70% 25% 5% •



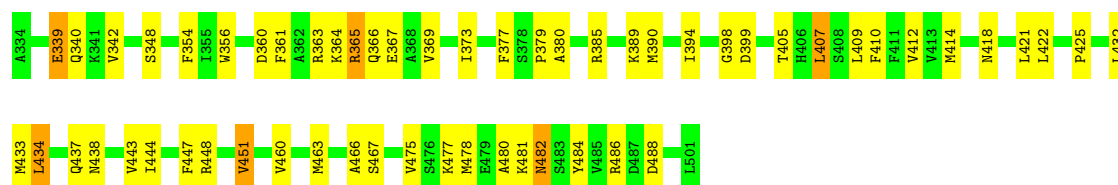
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain F: 67% 29% •



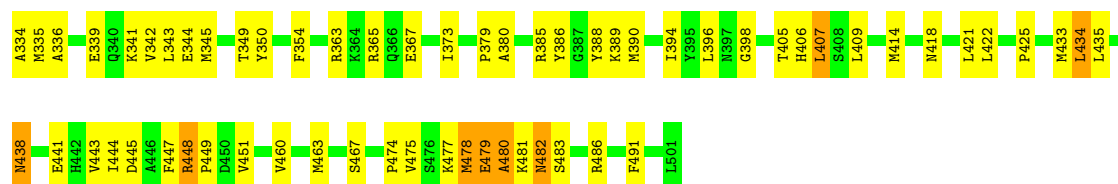
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain G: 66% 30% •



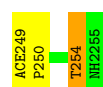
- Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain H: 64% 32% 5% •

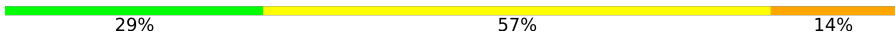


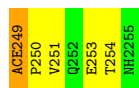
- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain I: 57% 29% 14% •

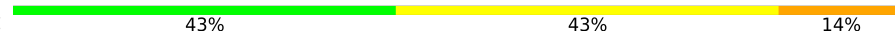


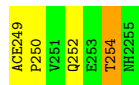
- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain J:  29% 57% 14%



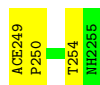
- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain K:  43% 43% 14%



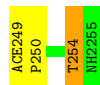
- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain L:  57% 43%



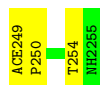
- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain M:  57% 29% 14%



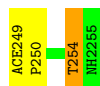
- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain N:  57% 43%

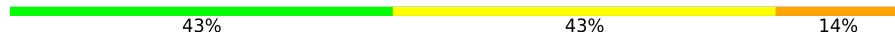


- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain O:  57% 29% 14%



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain P:  43% 43% 14%



4 Data and refinement statistics

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

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, α , β , γ	111.40Å 111.40Å 111.40Å 103.70° 103.70° 103.70°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10670	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2

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	0/1312	1.08	7/1781 (0.4%)
1	B	0.49	0/1312	1.07	9/1781 (0.5%)
1	C	0.48	0/1312	1.11	13/1781 (0.7%)
1	D	0.48	0/1312	1.08	10/1781 (0.6%)
1	E	0.51	0/1312	1.06	6/1781 (0.3%)
1	F	0.48	0/1312	1.06	8/1781 (0.4%)
1	G	0.49	0/1312	1.04	10/1781 (0.6%)
1	H	0.47	0/1312	1.04	9/1781 (0.5%)
2	I	1.49	1/40 (2.5%)	0.86	0/55
2	J	1.47	1/40 (2.5%)	0.87	0/55
2	K	1.51	1/40 (2.5%)	0.88	0/55
2	L	1.44	1/40 (2.5%)	1.04	0/55
2	M	1.54	1/40 (2.5%)	0.87	0/55
2	N	1.50	1/40 (2.5%)	0.87	0/55
2	O	1.45	1/40 (2.5%)	0.90	0/55
2	P	1.49	1/40 (2.5%)	0.91	0/55
All	All	0.55	8/10816 (0.1%)	1.06	72/14688 (0.5%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	249	ACE	C-N	-9.34	1.34	1.43
2	K	249	ACE	C-N	-9.06	1.34	1.43
2	N	249	ACE	C-N	-9.05	1.34	1.43
2	P	249	ACE	C-N	-8.98	1.34	1.43
2	I	249	ACE	C-N	-8.93	1.34	1.43

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	MET	N-CA-C	-10.20	100.96	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	GLY	N-CA-C	8.29	122.51	112.48
1	F	460	VAL	N-CA-C	-8.27	104.69	112.96
1	B	335	MET	N-CA-C	-8.14	103.10	112.87
1	B	460	VAL	N-CA-C	-8.12	104.84	112.96

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	41	0
1	B	1282	0	1242	52	0
1	C	1282	0	1242	44	0
1	D	1282	0	1242	51	0
1	E	1282	0	1242	46	0
1	F	1282	0	1242	47	0
1	G	1282	0	1242	52	0
1	H	1282	0	1242	57	0
2	I	43	0	40	3	0
2	J	43	0	40	8	0
2	K	43	0	40	6	0
2	L	43	0	40	1	0
2	M	43	0	40	3	0
2	N	43	0	40	1	0
2	O	43	0	40	4	0
2	P	43	0	40	9	0
3	A	12	0	0	1	0
3	B	3	0	0	0	0
3	C	11	0	0	0	0
3	D	7	0	0	3	0
3	E	5	0	0	1	0
3	F	9	0	0	4	0
3	G	8	0	0	0	0
3	H	13	0	0	5	0
3	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
All	All	10670	0	10256	385	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 18.

The worst 5 of 385 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:G:389:LYS:HG2	1:G:414:MET:HE3	1.29	1.09
1:A:389:LYS:HG2	1:A:414:MET:HE3	1.36	1.06
1:F:389:LYS:HG2	1:F:414:MET:HE3	1.37	1.06
1:D:389:LYS:HG2	1:D:414:MET:HE3	1.32	1.06
1:C:389:LYS:HG2	1:C:414:MET:HE3	1.40	1.02

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	166/168 (99%)	156 (94%)	6 (4%)	4 (2%)	4	2
1	B	166/168 (99%)	156 (94%)	6 (4%)	4 (2%)	4	2
1	C	166/168 (99%)	154 (93%)	7 (4%)	5 (3%)	3	1
1	D	166/168 (99%)	156 (94%)	7 (4%)	3 (2%)	6	3
1	E	166/168 (99%)	155 (93%)	5 (3%)	6 (4%)	2	1
1	F	166/168 (99%)	158 (95%)	5 (3%)	3 (2%)	6	3
1	G	166/168 (99%)	155 (93%)	9 (5%)	2 (1%)	10	6
1	H	166/168 (99%)	152 (92%)	8 (5%)	6 (4%)	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	5/7 (71%)	5 (100%)	0	0	100	100
2	J	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
2	K	5/7 (71%)	5 (100%)	0	0	100	100
2	L	5/7 (71%)	5 (100%)	0	0	100	100
2	M	5/7 (71%)	5 (100%)	0	0	100	100
2	N	5/7 (71%)	5 (100%)	0	0	100	100
2	O	5/7 (71%)	5 (100%)	0	0	100	100
2	P	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1368/1400 (98%)	1281 (94%)	54 (4%)	33 (2%)	4	2

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	LYS
1	A	480	ALA
1	B	477	LYS
1	B	480	ALA
1	C	477	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%)	128 (97%)	4 (3%)	36	38
1	B	132/144 (92%)	127 (96%)	5 (4%)	29	29
1	C	132/144 (92%)	129 (98%)	3 (2%)	44	49
1	D	132/144 (92%)	128 (97%)	4 (3%)	36	38
1	E	132/144 (92%)	128 (97%)	4 (3%)	36	38
1	F	132/144 (92%)	127 (96%)	5 (4%)	29	29
1	G	132/144 (92%)	129 (98%)	3 (2%)	44	49
1	H	132/144 (92%)	131 (99%)	1 (1%)	73	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	J	5/5 (100%)	5 (100%)	0	100	100
2	K	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	L	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	M	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	N	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	O	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	P	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	1096/1192 (92%)	1060 (97%)	36 (3%)	33	34

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	409	LEU
2	P	254	THR
2	I	254	THR
2	M	254	THR
1	D	365	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	252	GLN
2	K	252	GLN
2	O	252	GLN
1	D	439	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 [i](#)

There are no oligosaccharides 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

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.