



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:34 PM GMT

PDB ID : 1XU1  
Title : The crystal structure of APRIL bound to TACI  
Authors : Hymowitz, S.G.; Patel, D.R.; Wallweber, H.J.A.; Runyon, S.; Yan, M.; Yin, J.; Shriver, S.K.; Gordon, N.C.; Pan, B.; Skelton, N.J.; Kelley, R.F.; Starovasnik, M.A.  
Deposited on : 2004-10-25  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

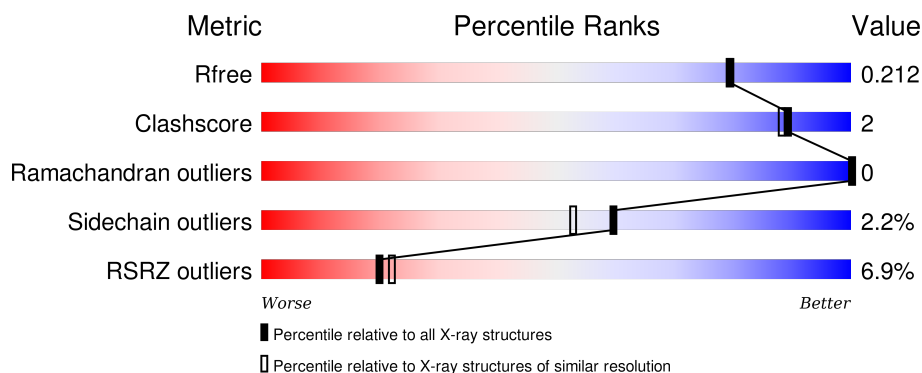
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	138	<div> <div>4%</div> <div>92%</div> <div>7%</div> </div>
1	B	138	<div> <div>5%</div> <div>85%</div> <div>14%</div> </div>
1	D	138	<div> <div>8%</div> <div>88%</div> <div>12%</div> </div>
2	R	42	<div> <div>10%</div> <div>83%</div> <div>7%</div> <div>10%</div> </div>
2	S	42	<div> <div>10%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	T	42	 A horizontal bar chart showing the quality of chain T. The bar is divided into four segments: a red segment at the beginning labeled '10%', a large green segment labeled '88%', a small yellow segment labeled '5%', and a grey segment at the end labeled '7%'.

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4280 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 ligand superfamily member 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1086	689	198	194	5			
1	B	137	Total	C	N	O	S	0	0	0
			1086	689	198	194	5			
1	D	137	Total	C	N	O	S	0	0	0
			1080	686	195	194	5			

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 13B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	38	Total	C	N	O	S	0	0	0
			301	186	54	55	6			
2	S	36	Total	C	N	O	S	6	0	0
			289	178	53	52	6			
2	T	39	Total	C	N	O	S	0	0	0
			307	191	56	54	6			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	35	Total	O	0	0
			35	35		
4	D	40	Total	O	0	0
			40	40		

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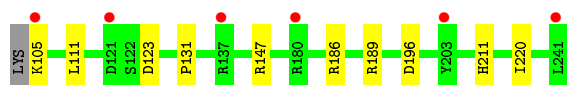
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	8	Total 8	O 8	0	0
4	S	8	Total 8	O 8	0	0
4	T	7	Total 7	O 7	0	0

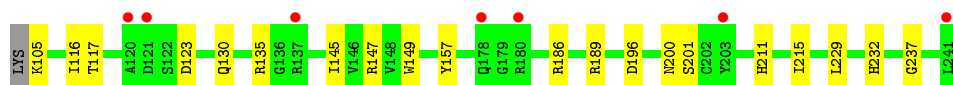
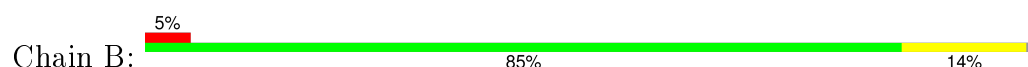
### 3 Residue-property plots [i](#)

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.

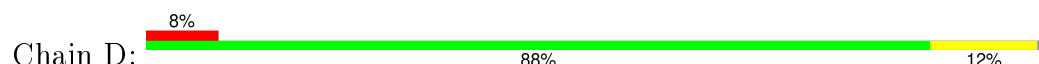
- Molecule 1: Tumor necrosis factor ligand superfamily member 13



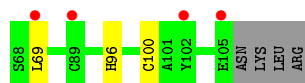
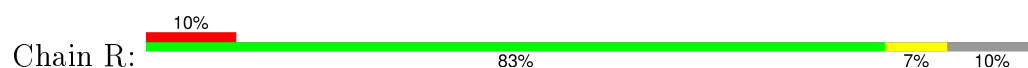
- Molecule 1: Tumor necrosis factor ligand superfamily member 13



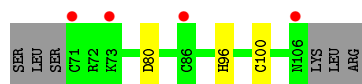
- Molecule 1: Tumor necrosis factor ligand superfamily member 13



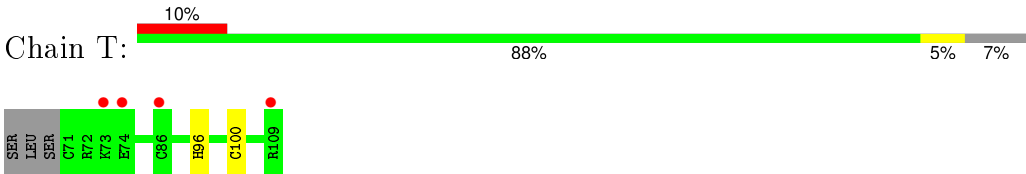
- Molecule 2: Tumor necrosis factor receptor superfamily member 13B



- Molecule 2: Tumor necrosis factor receptor superfamily member 13B



- Molecule 2: Tumor necrosis factor receptor superfamily member 13B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.34Å 91.84Å 102.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 35.69 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-1.90) 99.6 (35.69-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.99 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.167 , 0.203 0.181 , 0.212	Depositor DCC
$R_{free}$ test set	4449 reflections (11.10%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44519 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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

### 5.1 Standard geometry

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

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	0/1111	0.77	2/1504 (0.1%)
1	B	0.45	0/1111	0.81	4/1504 (0.3%)
1	D	0.41	0/1105	0.74	3/1497 (0.2%)
2	R	0.41	0/307	0.65	0/409
2	S	0.41	0/295	0.64	1/393 (0.3%)
2	T	0.38	0/313	0.62	0/417
All	All	0.42	0/4242	0.75	10/5724 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	186	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	196	ASP	CB-CG-OD2	5.72	123.44	118.30
1	D	196	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	123	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	196	ASP	CB-CG-OD2	5.42	123.18	118.30
2	S	80	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	150	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	194	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	123	ASP	CB-CG-OD2	5.06	122.85	118.30

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	1086	0	1087	5	0
1	B	1086	0	1087	9	0
1	D	1080	0	1076	6	0
2	R	301	0	280	1	0
2	S	289	0	265	1	0
2	T	307	0	285	1	0
3	A	1	0	0	0	0
4	A	32	0	0	0	0
4	B	35	0	0	1	0
4	D	40	0	0	0	0
4	R	8	0	0	0	0
4	S	8	0	0	0	0
4	T	7	0	0	0	0
All	All	4280	0	4080	20	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 2.

All (20) 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:186:ARG:HE	1:B:232:HIS:HD2	1.25	0.84
1:D:145:ILE:HG22	1:D:217:THR:HG22	1.87	0.56
1:D:175:ARG:HD2	1:D:214:ASP:OD2	2.08	0.54
1:A:186:ARG:NE	1:B:232:HIS:HD2	2.02	0.54
1:B:147:ARG:HG2	1:B:149:TRP:CZ2	2.43	0.53
1:D:157:TYR:CZ	1:D:237:GLY:HA3	2.45	0.52
1:A:189:ARG:NH2	1:B:201:SER:O	2.34	0.52
1:A:220:ILE:N	1:A:220:ILE:HD12	2.26	0.50
1:B:116:ILE:HG23	1:B:229:LEU:HD21	1.95	0.48
1:B:211:HIS:HE1	4:B:252:HOH:O	1.97	0.47
2:R:96:HIS:HB2	2:R:100:CYS:HB2	1.99	0.45
2:T:96:HIS:HB2	2:T:100:CYS:HB2	1.98	0.44
1:B:157:TYR:CZ	1:B:237:GLY:HA3	2.52	0.44
1:D:163:HIS:HE1	1:D:195:PRO:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:96:HIS:HB2	2:S:100:CYS:HB2	2.00	0.43
1:A:111:LEU:HD23	1:A:131:PRO:HA	2.02	0.42
1:D:108:VAL:HG22	1:D:135:ARG:HB3	2.02	0.41
1:B:189:ARG:HG2	1:B:200:ASN:HB3	2.02	0.41
1:B:145:ILE:HD13	1:B:215:ILE:HD12	2.03	0.41
1:D:220:ILE:HD12	1:D:220:ILE:N	2.36	0.40

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	135/138 (98%)	134 (99%)	1 (1%)	0	100	100
1	B	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
1	D	135/138 (98%)	134 (99%)	1 (1%)	0	100	100
2	R	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
2	S	34/42 (81%)	34 (100%)	0	0	100	100
2	T	37/42 (88%)	36 (97%)	1 (3%)	0	100	100
All	All	512/540 (95%)	504 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	120/121 (99%)	117 (98%)	3 (2%)	55	47
1	B	120/121 (99%)	116 (97%)	4 (3%)	45	34
1	D	119/121 (98%)	117 (98%)	2 (2%)	68	64
2	R	34/38 (90%)	33 (97%)	1 (3%)	50	40
2	S	32/38 (84%)	32 (100%)	0	100	100
2	T	33/38 (87%)	33 (100%)	0	100	100
All	All	458/477 (96%)	448 (98%)	10 (2%)	60	53

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LYS
1	A	147	ARG
1	A	211	HIS
1	B	105	LYS
1	B	117	THR
1	B	130	GLN
1	B	135	ARG
1	D	115	ASN
1	D	181	ARG
2	R	69	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	B	130	GLN
1	B	142	GLN
1	B	211	HIS
1	B	212	GLN
1	B	232	HIS
1	D	115	ASN
1	D	163	HIS
1	D	178	GLN
1	D	209	HIS

### 5.3.3 RNA ⓘ

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

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	137/138 (99%)	0.20	6 (4%) 38 41	12, 17, 30, 42	0
1	B	137/138 (99%)	0.35	7 (5%) 32 35	11, 17, 33, 40	0
1	D	137/138 (99%)	0.41	11 (8%) 15 17	10, 17, 33, 40	0
2	R	38/42 (90%)	0.68	4 (10%) 8 9	7, 17, 28, 36	0
2	S	36/42 (85%)	0.76	4 (11%) 7 8	10, 17, 32, 33	1 (2%)
2	T	39/42 (92%)	0.32	4 (10%) 9 9	9, 15, 35, 35	0
All	All	524/540 (97%)	0.38	36 (6%) 20 22	7, 17, 33, 42	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	102	TYR	5.7
1	A	137	ARG	4.9
2	T	74	GLU	4.7
2	R	69	LEU	4.7
1	D	121	ASP	4.5
1	B	120	ALA	4.2
1	D	178	GLN	4.1
1	D	120	ALA	3.9
1	D	179	GLY	3.9
1	D	181	ARG	3.9
1	D	137	ARG	3.7
2	T	73	LYS	3.3
1	B	180	ARG	3.3
1	A	121	ASP	3.1
2	S	73	LYS	3.1
1	A	105	LYS	2.8
1	A	180	ARG	2.8
2	S	86	CYS	2.8
1	B	178	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	S	106	ASN	2.7
1	B	203	TYR	2.7
1	D	105	LYS	2.6
1	D	177	GLY	2.5
2	R	105	GLU	2.4
2	S	71	CYS	2.3
2	R	89	CYS	2.3
1	B	241	LEU	2.3
1	B	137	ARG	2.3
1	B	121	ASP	2.3
1	A	203	TYR	2.3
2	T	86	CYS	2.3
2	T	109	ARG	2.2
1	D	203	TYR	2.1
1	D	122	SER	2.1
1	A	241	LEU	2.1
1	D	241	LEU	2.1

## 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NI	A	101	1/1	1.00	0.04	-	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.