



wwPDB X-ray Structure Validation Summary Report

Oct 23, 2021 – 02:42 PM EDT

PDB ID : 1FLL
Title : MOLECULAR BASIS FOR CD40 SIGNALING MEDIATED BY TRAF3
Authors : Ni, C.-Z.; Welsh, K.; Leo, E.; Chiou, C.-K.; Wu, H.; Reed, J.C.; Ely, K.R.
Deposited on : 2000-08-14
Resolution : 3.50 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

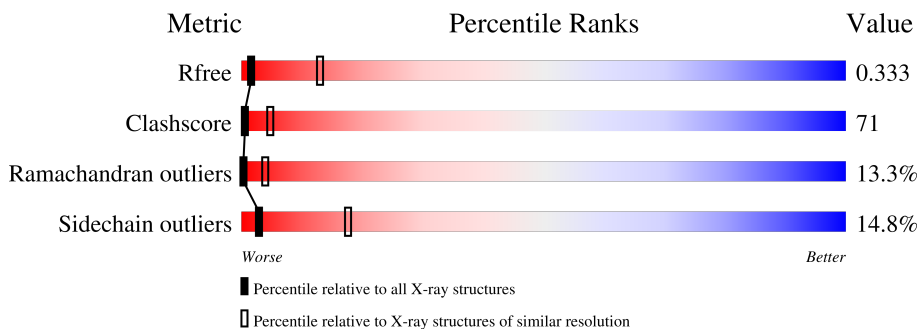
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	228	21% (green), 55% (yellow), 13% (orange), 10% (red), 1% (grey)
1	B	228	19% (green), 55% (yellow), 16% (orange), 10% (red), 1% (grey)
2	X	21	19% (green), 52% (yellow), 24% (orange), 5% (red), 1% (grey)
2	Y	21	19% (green), 62% (yellow), 10% (orange), 10% (red), 1% (grey)

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3558 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	205	1626	1035	277	303	11	0	0	0
1	B	205	1626	1035	277	303	11	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	X	21	153	92	27	34	0	0	0
2	Y	21	153	92	27	34	0	0	0

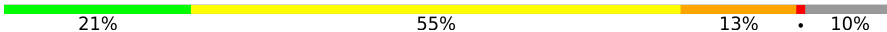
There are 4 discrepancies between the modelled and reference sequences:

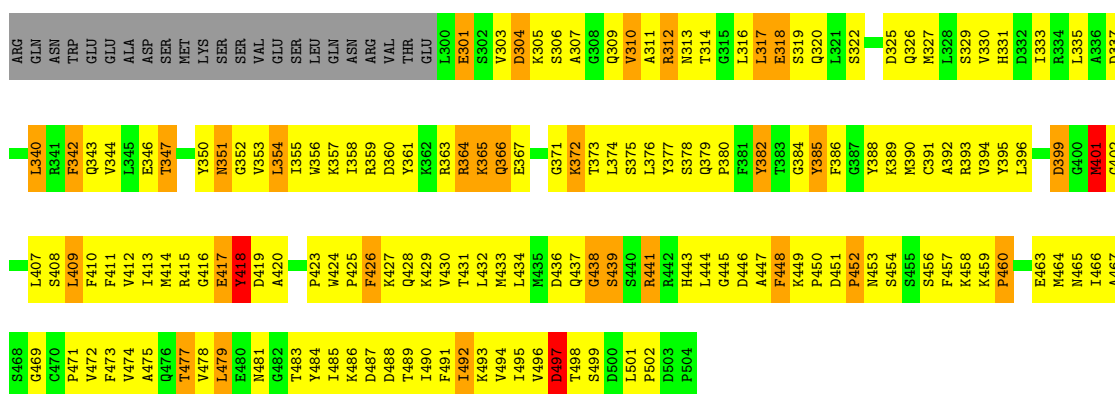
Chain	Residue	Modelled	Actual	Comment	Reference
X	246	LYS	ASN	engineered mutation	UNP P25942
X	258	SER	CYS	engineered mutation	UNP P25942
Y	246	LYS	ASN	engineered mutation	UNP P25942
Y	258	SER	CYS	engineered mutation	UNP P25942

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.

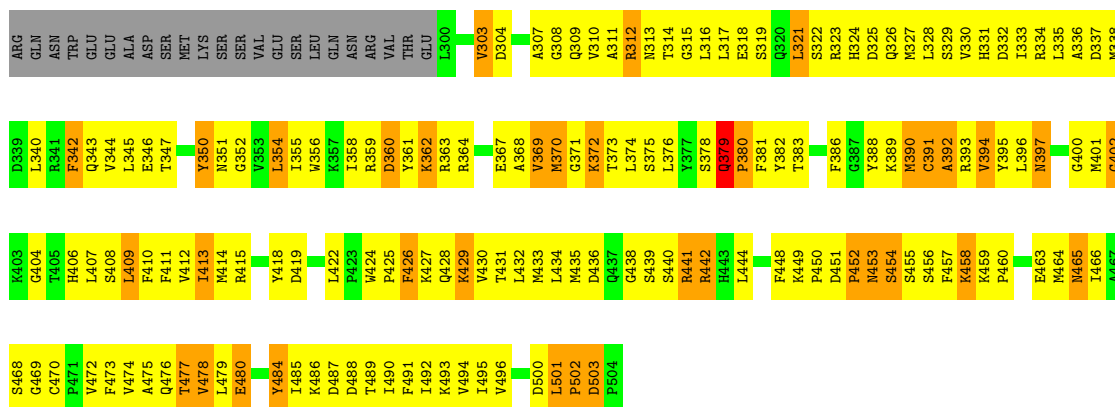
- Molecule 1: TNF RECEPTOR ASSOCIATED FACTOR 3

Chain A: 




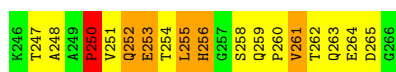
- Molecule 1: TNF RECEPTOR ASSOCIATED FACTOR 3

Chain B: 

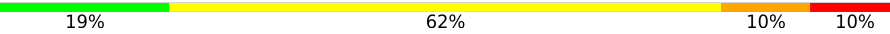


- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain X: 



- Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain Y:  19% 62% 10% 10%

K246	T247	A248	A249	P250	Y251	Q252	E253	T254	L255	H256	G257	S258	Q259	P260	V261	T262	Q263	E264	I265	G266
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4 Data and refinement statistics i

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.76Å 83.76Å 212.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.50 41.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	72.6 (8.00-3.50) 81.9 (41.88-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 3.48Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.312 0.228 , 0.333	Depositor DCC
R_{free} test set	432 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtrriage
Anisotropy	0.980	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.398 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3558	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.39	0/1661	0.72	0/2239
1	B	0.42	0/1661	0.71	0/2239
2	X	0.52	0/155	0.78	0/211
2	Y	0.67	0/155	0.81	0/211
All	All	0.42	0/3632	0.72	0/4900

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
2	X	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	388	TYR	Sidechain
2	X	264	GLU	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	1626	0	1622	237	0
1	B	1626	0	1622	234	0
2	X	153	0	144	25	0
2	Y	153	0	144	26	0
All	All	3558	0	3532	504	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 71.

The worst 5 of 504 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)
2:X:254:THR:OG1	2:X:265:ASP:HB2	1.40	1.19
1:A:466:ILE:HG23	2:X:253:GLU:HB2	1.37	1.07
1:B:312:ARG:HE	1:B:312:ARG:HA	1.24	1.02
2:X:252:GLN:HE21	2:X:252:GLN:N	1.59	1.00
1:B:410:PHE:HA	1:B:469:GLY:HA3	1.45	0.96

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	203/228 (89%)	144 (71%)	36 (18%)	23 (11%)	0	6
1	B	203/228 (89%)	139 (68%)	38 (19%)	26 (13%)	0	4
2	X	19/21 (90%)	9 (47%)	4 (21%)	6 (32%)	0	0
2	Y	19/21 (90%)	7 (37%)	8 (42%)	4 (21%)	0	1
All	All	444/498 (89%)	299 (67%)	86 (19%)	59 (13%)	0	4

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	GLU
1	A	318	GLU
1	A	319	SER
1	A	371	GLY
1	A	417	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	179/201 (89%)	151 (84%)	28 (16%)	2	16
1	B	179/201 (89%)	157 (88%)	22 (12%)	4	23
2	X	17/17 (100%)	12 (71%)	5 (29%)	0	2
2	Y	17/17 (100%)	14 (82%)	3 (18%)	2	10
All	All	392/436 (90%)	334 (85%)	58 (15%)	3	17

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	250	PRO
2	Y	250	PRO
1	B	327	MET
1	B	480	GLU
1	B	441	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	309	GLN
1	B	324	HIS
1	B	476	GLN
1	B	428	GLN
1	B	465	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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.