



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 01:57 PM EDT

PDB ID : 1LB6
Title : TRAF6-CD40 Complex
Authors : Ye, H.; Arron, J.R.; Lamothe, B.; Cirilli, M.; Kobayashi, T.; Shevde, N.K.; Segal, D.; Dzivenu, O.; Vologodskaja, M.; Yim, M.; Du, K.; Singh, S.; Pike, J.W.; Darnay, B.G.; Choi, Y.; Wu, H.
Deposited on : unknown
Resolution : 1.80 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

A user guide is available at

<http://wwpdb.org/validation/2016/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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

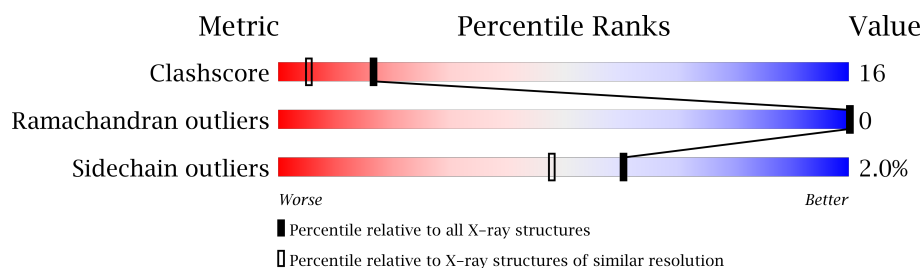
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	160	 73% 24% . .
2	B	9	 89% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1462 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 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1260	808	221	221	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	505	LEU	-	CLONING ARTIFACT	UNP Q9Y4K3
A	506	GLU	-	CLONING ARTIFACT	UNP Q9Y4K3

- Molecule 2 is a protein called CD40 antigen.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			80	50	12	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	608	ASP	ASN	CONFLICT	UNP P25942

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	112	Total	O	0	0
			112	112		
3	B	10	Total	O	0	0
			10	10		

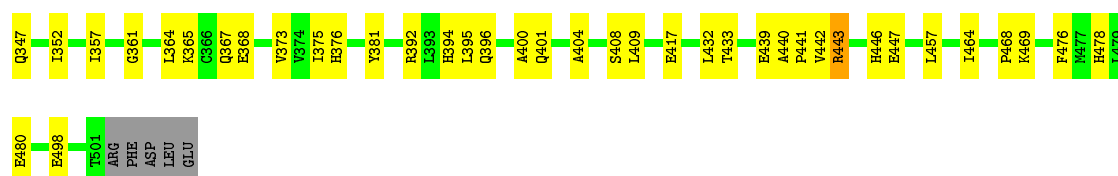
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.


Note EDS was not executed.

- Molecule 1: TNF receptor-associated factor 6

Chain A: 



- Molecule 2: CD40 antigen

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.88 Å 43.81 Å 101.44 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.16 – 1.80	Depositor
% Data completeness (in resolution range)	6.0 (33.16-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.203 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1462	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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	0.36	0/1295	0.69	0/1754
2	B	0.41	0/81	0.53	0/106
All	All	0.36	0/1376	0.69	0/1860

There are no bond length outliers.

There are no bond angle outliers.

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	1260	0	1247	42	0
2	B	80	0	71	1	0
3	A	112	0	0	5	0
3	B	10	0	0	0	0
All	All	1462	0	1318	42	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.

All (42) 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:478:HIS:HD2	1:A:480:GLU:H	1.20	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ARG:CZ	1:A:394:HIS:HE1	1.92	0.83
1:A:440:ALA:N	1:A:441:PRO:HD2	1.94	0.81
1:A:439:GLU:C	1:A:441:PRO:HD2	2.08	0.74
1:A:478:HIS:CD2	1:A:480:GLU:H	2.07	0.70
1:A:392:ARG:NH2	1:A:394:HIS:HE1	1.94	0.66
1:A:401:GLN:HA	1:A:401:GLN:OE1	1.94	0.66
1:A:394:HIS:HB2	1:A:408:SER:HB2	1.77	0.65
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.14	0.62
1:A:392:ARG:HG3	1:A:392:ARG:HH11	1.64	0.62
1:A:376:HIS:CE1	1:A:392:ARG:HH11	2.17	0.62
1:A:440:ALA:N	1:A:441:PRO:CD	2.61	0.62
1:A:361:GLY:O	1:A:365:LYS:HG2	2.01	0.60
1:A:376:HIS:CE1	1:A:392:ARG:NH1	2.71	0.58
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.72	0.54
1:A:392:ARG:NH1	3:A:729:HOH:O	2.40	0.53
1:A:392:ARG:HG3	1:A:392:ARG:NH1	2.24	0.52
1:A:396:GLN:NE2	3:A:707:HOH:O	2.42	0.52
1:A:443:ARG:CG	1:A:443:ARG:HH11	2.22	0.52
1:A:392:ARG:NH2	1:A:394:HIS:CE1	2.77	0.51
1:A:464:ILE:HD11	1:A:468:PRO:HG3	1.93	0.50
1:A:400:ALA:O	1:A:404:ALA:HB2	2.12	0.50
1:A:457:LEU:HD12	1:A:457:LEU:N	2.27	0.50
1:A:446:HIS:HE1	1:A:476:PHE:O	1.94	0.49
1:A:392:ARG:CZ	1:A:394:HIS:CE1	2.84	0.49
1:A:439:GLU:CB	1:A:441:PRO:HD2	2.44	0.47
1:A:439:GLU:HB3	1:A:441:PRO:HD2	1.97	0.47
1:A:347:GLN:N	3:A:764:HOH:O	2.49	0.46
1:A:364:LEU:O	1:A:368:GLU:HG3	2.17	0.45
1:A:469:LYS:NZ	2:B:608:ASP:OD2	2.44	0.45
1:A:433:THR:HG23	1:A:447:GLU:HB3	2.00	0.44
1:A:440:ALA:O	1:A:441:PRO:C	2.55	0.44
1:A:478:HIS:CD2	1:A:480:GLU:HB2	2.52	0.44
1:A:392:ARG:NH2	3:A:808:HOH:O	2.52	0.43
1:A:373:VAL:HB	1:A:395:LEU:HB2	2.02	0.42
1:A:352:ILE:HG12	1:A:498:GLU:HG3	2.02	0.42
1:A:400:ALA:O	1:A:404:ALA:N	2.53	0.42
1:A:432:LEU:O	1:A:447:GLU:HB2	2.20	0.42
1:A:357:ILE:HD13	1:A:375:ILE:HD11	2.02	0.41
1:A:441:PRO:O	1:A:442:VAL:HG23	2.21	0.41
1:A:376:HIS:HE1	3:A:729:HOH:O	2.03	0.40
1:A:381:TYR:OH	1:A:417:GLU:HG2	2.20	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	153/160 (96%)	147 (96%)	6 (4%)	0	100	100
2	B	7/9 (78%)	7 (100%)	0	0	100	100
All	All	160/169 (95%)	154 (96%)	6 (4%)	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	138/144 (96%)	135 (98%)	3 (2%)	57	44
2	B	9/9 (100%)	9 (100%)	0	100	100
All	All	147/153 (96%)	144 (98%)	3 (2%)	60	48

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	GLN
1	A	409	LEU
1	A	443	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	367	GLN
1	A	376	HIS
1	A	394	HIS
1	A	396	GLN
1	A	405	ASN
1	A	446	HIS
1	A	478	HIS

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

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.