



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2021 – 04:09 PM JST

PDB ID : 7ELX
Title : The crystal structure of CTLA-4 and Fab
Authors : Yu, X.J.; Wang, L.; Yu, C.F.
Deposited on : 2021-04-12
Resolution : 2.14 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

<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	:	2.20
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)	:	2.20

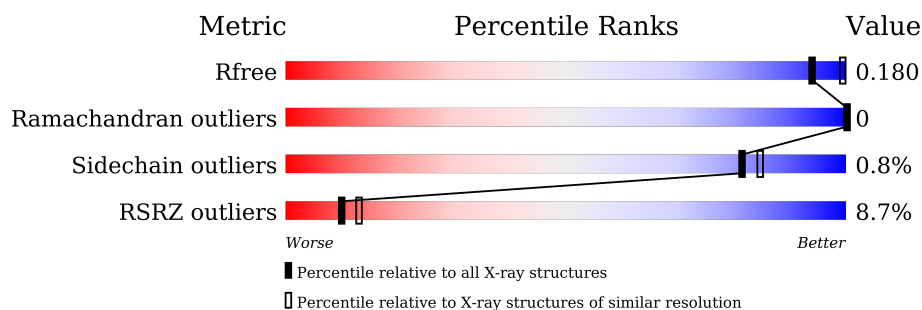
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	2523 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 $\leq 5\%$. 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	H	467	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>55%</div> </div> </div>
1	h	467	<div> <div>4%</div> <div> <div></div> <div>44%</div> <div>•</div> <div>55%</div> </div> </div>
2	L	235	<div> <div></div> <div> <div></div> <div>89%</div> <div>•</div> <div>10%</div> </div> </div>
2	l	235	<div> <div>12%</div> <div> <div></div> <div>87%</div> <div>••</div> <div>10%</div> </div> </div>
3	C	126	<div> <div>17%</div> <div> <div></div> <div>91%</div> <div></div> <div>9%</div> </div> </div>
3	c	126	<div> <div>12%</div> <div> <div></div> <div>90%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8836 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 heavy chain of Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	211	Total	C	N	O	S	2	0	0
			1608	1021	272	309	6			
1	h	212	Total	C	N	O	S	2	0	0
			1614	1024	273	311	6			

- Molecule 2 is a protein called light chain of Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	1	0	0
			1633	1026	276	327	4			
2	l	212	Total	C	N	O	S	1	0	0
			1633	1026	276	327	4			

- Molecule 3 is a protein called Cytotoxic T-lymphocyte protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	c	115	Total	C	N	O	S	1	0	0
			858	541	142	166	9			
3	C	115	Total	C	N	O	S	0	0	0
			858	541	142	166	9			

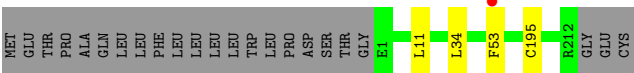
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	141	Total	O	0	0
			141	141		
4	L	178	Total	O	0	0
			178	178		
4	h	105	Total	O	0	0
			105	105		
4	l	133	Total	O	0	0
			133	133		

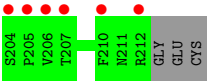
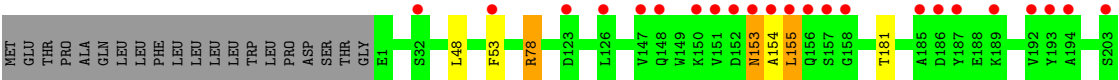
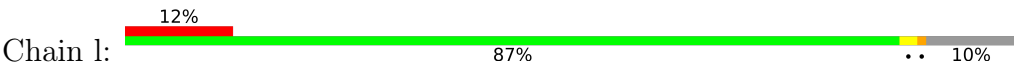
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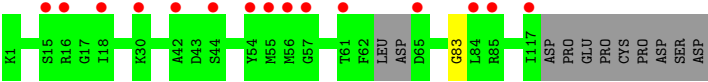
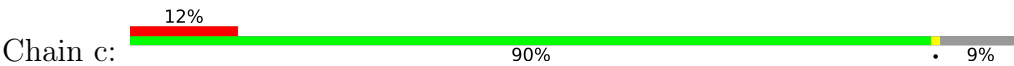
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	c	40	Total	O	0	0
			40	40		
4	C	35	Total	O	0	0
			35	35		



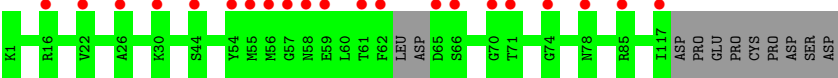
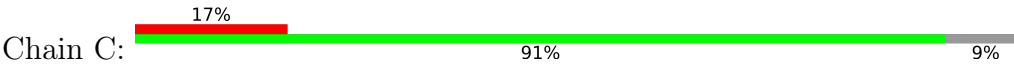
● Molecule 2: light chain of Fab



● Molecule 3: Cytotoxic T-lymphocyte protein 4



● Molecule 3: Cytotoxic T-lymphocyte protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.92Å 196.92Å 148.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.20 – 2.14 45.64 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.20-2.14) 99.8 (45.64-2.14)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.177 , 0.217 0.178 , 0.180	Depositor DCC
R_{free} test set	3853 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8836	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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	H	0.64	1/1650 (0.1%)	0.75	4/2250 (0.2%)
1	h	0.63	2/1656 (0.1%)	0.79	4/2258 (0.2%)
2	L	0.63	1/1671 (0.1%)	0.74	2/2270 (0.1%)
2	l	0.55	0/1671	1.01	8/2270 (0.4%)
3	C	0.48	0/871	0.73	0/1183
3	c	0.47	0/871	0.70	0/1183
All	All	0.59	4/8390 (0.0%)	0.81	18/11414 (0.2%)

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	h	0	1
3	c	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	206	LYS	CD-CE	8.43	1.72	1.51
1	h	211	LYS	CD-CE	6.73	1.68	1.51
1	h	211	LYS	CE-NZ	6.61	1.65	1.49
2	L	195	CYS	CB-SG	-6.56	1.71	1.82

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	78	ARG	NE-CZ-NH1	-24.18	108.21	120.30
2	l	78	ARG	NE-CZ-NH2	19.05	129.83	120.30
1	h	214	LYS	N-CA-CB	9.35	127.43	110.60
1	h	214	LYS	CA-CB-CG	7.61	130.14	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	155	LEU	CA-CB-CG	7.21	131.88	115.30
1	H	206	LYS	CG-CD-CE	-6.73	91.71	111.90
1	H	19	ARG	CG-CD-NE	6.54	125.54	111.80
2	l	181	THR	OG1-CB-CG2	6.15	124.14	110.00
1	H	206	LYS	CA-CB-CG	-6.05	100.08	113.40
2	L	11	LEU	CA-CB-CG	5.86	128.78	115.30
2	l	154	ALA	C-N-CA	-5.63	107.63	121.70
2	l	153	ASN	CB-CA-C	-5.60	99.19	110.40
2	l	155	LEU	CB-CG-CD2	5.53	120.40	111.00
1	h	16	ARG	NE-CZ-NH1	-5.36	117.62	120.30
2	l	48	LEU	CA-CB-CG	5.34	127.59	115.30
2	L	34	LEU	CA-CB-CG	-5.08	103.62	115.30
1	h	38	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	H	183	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	c	83	GLY	Peptide
1	h	131	PRO	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	H	207/467 (44%)	207 (100%)	0	0	100	100
1	h	208/467 (44%)	204 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	210/235 (89%)	206 (98%)	4 (2%)	0	100	100
2	l	210/235 (89%)	205 (98%)	5 (2%)	0	100	100
3	C	111/126 (88%)	104 (94%)	7 (6%)	0	100	100
3	c	111/126 (88%)	107 (96%)	4 (4%)	0	100	100
All	All	1057/1656 (64%)	1033 (98%)	24 (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	H	179/413 (43%)	178 (99%)	1 (1%)	86	89
1	h	180/413 (44%)	179 (99%)	1 (1%)	86	89
2	L	183/203 (90%)	182 (100%)	1 (0%)	88	91
2	l	183/203 (90%)	179 (98%)	4 (2%)	52	53
3	C	94/105 (90%)	94 (100%)	0	100	100
3	c	94/105 (90%)	94 (100%)	0	100	100
All	All	913/1442 (63%)	906 (99%)	7 (1%)	81	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	206	LYS
2	L	53	PHE
1	h	182	SER
2	l	53	PHE
2	l	78	ARG
2	l	153	ASN
2	l	155	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	H	110	GLN
2	l	159	ASN
2	l	190	HIS
3	C	41	GLN
3	C	75	ASN
3	C	76	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	H	211/467 (45%)	0.18	9 (4%)	35	43	28, 40, 64, 83	1 (0%)
1	h	212/467 (45%)	0.41	19 (8%)	9	12	30, 45, 83, 110	1 (0%)
2	L	212/235 (90%)	0.06	1 (0%)	91	93	24, 35, 52, 71	2 (0%)
2	l	212/235 (90%)	0.62	29 (13%)	3	3	26, 46, 96, 112	2 (0%)
3	C	115/126 (91%)	0.96	21 (18%)	1	1	33, 56, 105, 133	0
3	c	115/126 (91%)	0.69	15 (13%)	3	4	35, 55, 94, 104	1 (0%)
All	All	1077/1656 (65%)	0.43	94 (8%)	10	13	24, 44, 87, 133	7 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	57	GLY	9.1
3	c	84	LEU	9.0
1	h	195	GLY	8.2
1	h	132	SER	7.9
2	l	155	LEU	7.8
2	l	192	VAL	6.5
3	C	56	MET	6.4
1	h	194	LEU	6.1
2	l	185	ALA	5.8
2	l	151	VAL	5.8
2	L	53	PHE	5.6
3	c	117	ILE	5.2
1	h	197	GLN	5.1
3	C	65	ASP	5.1
3	C	61	THR	5.0
1	H	197	GLN	4.9
3	c	56	MET	4.8
1	h	133	SER	4.7
3	C	58	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	h	191	SER	4.6
1	H	195	GLY	4.6
3	C	117	ILE	4.5
2	l	193	TYR	4.5
2	l	194	ALA	4.4
3	C	44	SER	4.4
3	c	44	SER	4.3
3	C	66	SER	4.3
3	c	57	GLY	4.0
2	l	153	ASN	3.9
2	l	205	PRO	3.9
1	h	198	THR	3.8
1	h	192	SER	3.8
2	l	53	PHE	3.8
2	l	148	GLN	3.7
1	H	196	THR	3.6
2	l	32	SER	3.6
3	c	61	THR	3.6
1	h	200	ILE	3.6
2	l	203	SER	3.5
2	l	210	PHE	3.5
2	l	206	VAL	3.5
3	C	26	ALA	3.4
3	c	16	ARG	3.3
3	c	65	ASP	3.2
1	H	192	SER	3.2
2	l	154	ALA	3.2
2	l	123	ASP	3.2
3	C	59	GLU	3.1
2	l	186	ASP	3.1
1	H	198	THR	3.1
2	l	150	LYS	3.0
1	H	194	LEU	3.0
1	h	196	THR	2.9
3	C	71	THR	2.9
3	C	54	TYR	2.9
2	l	204	SER	2.9
1	h	190	PRO	2.8
2	l	212	ARG	2.8
2	l	187	TYR	2.8
3	C	16	ARG	2.8
3	c	85	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	h	161	SER	2.8
3	C	70	GLY	2.7
1	H	1	GLN	2.7
3	c	54	TYR	2.5
2	l	152	ASP	2.5
2	l	158	GLY	2.5
2	l	189	LYS	2.5
1	h	218	PRO	2.5
3	c	18	ILE	2.5
3	C	22	VAL	2.5
3	C	30	LYS	2.4
3	c	42	ALA	2.4
1	h	75	SER	2.3
1	H	193	SER	2.3
1	h	215	ARG	2.3
1	H	206	LYS	2.3
2	l	207	THR	2.2
3	C	78	ASN	2.2
1	h	214	LYS	2.2
3	c	55	MET	2.2
3	C	55	MET	2.2
2	l	126	LEU	2.2
1	h	140	THR	2.2
2	l	147	VAL	2.2
3	C	85	ARG	2.2
1	h	199	TYR	2.1
3	c	30	LYS	2.1
2	l	156	GLN	2.1
3	c	15	SER	2.1
3	C	62	PHE	2.1
2	l	157	SER	2.0
1	h	163	ALA	2.0
3	C	74	GLY	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.