

# wwPDB X-ray Structure Validation Summary Report (i)

#### Sep 23, 2023 – 07:18 PM EDT

PDB ID : 5TRU

Title : Structure of the first-in-class checkpoint inhibitor Ipilimumab bound to human

CTLA-4

Authors: Ramagopal, U.A.; Liu, W.; Garrett-Thomson, S.C.; Yan, Q.; Srinivasan, M.;

Wong, S.C.; Bell, A.; Mankikar, S.; Rangan, V.S.; Deshpande, S.; Bonanno,

J.B.; Korman, A.J.; Almo, S.C.

Deposited on : 2016-10-27

Resolution : 3.00 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 (i) 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 (1)) were used in the production of this report:

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

EDS : 2.35.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

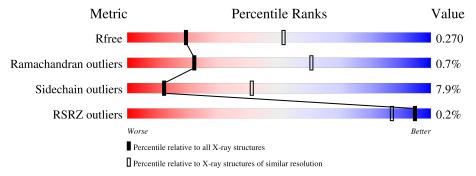
Validation Pipeline (wwPDB-VP) : 2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	Similar resolution
Wiedite	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	L	215	91%	8% •
1	1	215	94%	•••
2	Н	225	91%	
2	h	225	84%	10% 6%
3	С	118	90%	7% •
3	c	118	94%	



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8036 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 Ipilimumab Fab light chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	L	213	Total 1627	C 1023	N 275	O 325	S 4	0	0	0
1	1	212	Total 1579	_	N 271	O 317	S 4	0	0	0

• Molecule 2 is a protein called Ipilimumab Fab heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Н	215	Total	С	N	О	S	0	0	0
	11	210	1619	1030	270	313	6		U	0
2	h	212	Total	С	N	О	S	0	0	0
2	11	212	1589	1011	266	306	6	0	U	0

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

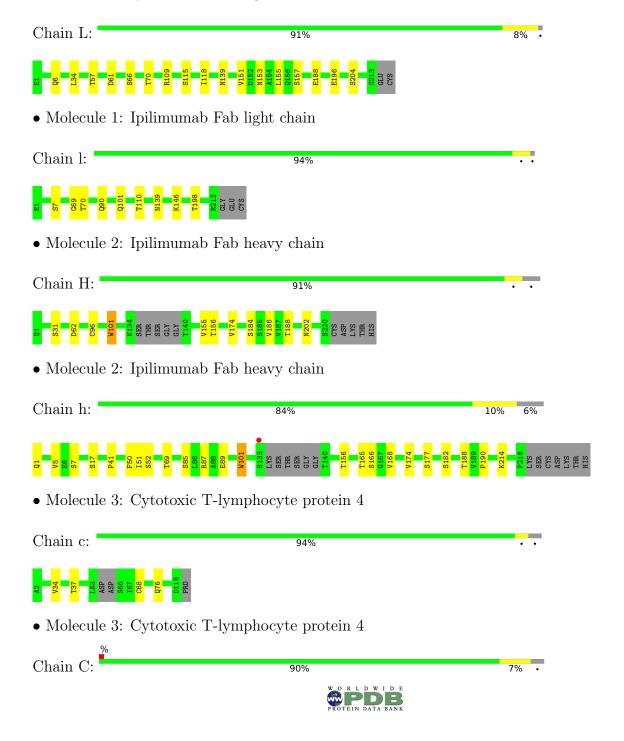
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	С	115	Total 816			O 158		0	0	0
3	С	114	Total 806	_		O 155	S 9	0	0	0



# 3 Residue-property plots (i)

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 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.

• Molecule 1: Ipilimumab Fab light chain







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	95.84Å 197.50Å 148.12Å	Donositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.91 - 3.00	Depositor
Resolution (A)	34.91 - 3.00	EDS
% Data completeness	99.2 (34.91-3.00)	Depositor
(in resolution range)	99.3 (34.91-3.00)	EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.67 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5	Depositor
D D.	0.203 , 0.268	Depositor
$R, R_{free}$	0.206 , $0.270$	DCC
$R_{free}$ test set	1447 reflections $(5.10\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.27 , 13.4	EDS
L-test for twinning <sup>2</sup>	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	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.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	L	0.51	0/1665	0.73	0/2263	
1	1	0.47	0/1616	0.68	0/2200	
2	Н	0.54	0/1661	0.75	0/2268	
2	h	0.53	0/1631	0.70	0/2229	
3	С	0.49	0/819	0.67	0/1118	
3	c	0.47	0/828	0.65	0/1129	
All	All	0.51	0/8220	0.71	0/11207	

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 (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	L	211/215 (98%)	199 (94%)	11 (5%)	1 (0%)	29 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	1	$210/215\ (98\%)$	201 (96%)	7 (3%)	2 (1%)	15	53
2	Н	$211/225\ (94\%)$	196 (93%)	14 (7%)	1 (0%)	29	68
2	h	$208/225\ (92\%)$	196 (94%)	9 (4%)	3 (1%)	11	43
3	$\mathbf{C}$	110/118~(93%)	104 (94%)	6 (6%)	0	100	100
3	c	111/118 (94%)	100 (90%)	11 (10%)	0	100	100
All	All	1061/1116~(95%)	996 (94%)	58 (6%)	7 (1%)	22	60

#### 5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Н	101	TRP
2	h	101	TRP
1	1	139	ASN
2	h	41	PRO
1	L	139	ASN

#### 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	L	180/185 (97%)	164 (91%)	16 (9%)	9 35
1	1	166/185 (90%)	159 (96%)	7 (4%)	30 66
2	Н	174/191 (91%)	163 (94%)	11 (6%)	18 51
2	h	173/191 (91%)	152 (88%)	21 (12%)	5 21
3	С	78/97 (80%)	70 (90%)	8 (10%)	7 28
3	c	82/97 (84%)	78 (95%)	4 (5%)	25 61
All	All	853/946 (90%)	786 (92%)	67 (8%)	12 41

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Mol Chain		Type
3	c	68	CYS

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Mol	Chain	Res	Type
3	С	4	HIS
3	С	87	MET
2	Н	186	VAL
2	Н	184	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	c	4	HIS
3	С	75	ASN
2	Н	204	ASN
1	1	90	GLN
1	1	138	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 (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,  $95^{th}$  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>	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	L	213/215 (99%)	-0.55	0 100 100	45, 59, 73, 81	0
1	1	212/215 (98%)	-0.28	0 100 100	45, 68, 132, 149	0
2	Н	215/225~(95%)	-0.43	0 100 100	48, 63, 91, 109	0
2	h	212/225 (94%)	-0.32	1 (0%) 91 75	46, 65, 108, 125	0
3	С	114/118 (96%)	-0.28	1 (0%) 84 63	60, 84, 108, 126	0
3	c	115/118 (97%)	-0.17	0 100 100	57, 84, 112, 134	0
All	All	1081/1116 (96%)	-0.36	2 (0%) 95 87	45, 66, 115, 149	0

#### All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	h	133	SER	2.9
3	С	23	CYS	2.2

#### 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.

