



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 27, 2025 – 12:19 PM EST

PDB ID : 9DQ5
Title : Crystal structure of Anti-CTLA-4 Fab (9D9) in complex with mouse CTLA-4
Authors : Lee, P.S.; Diong, S.J.; Robison, B.
Deposited on : 2024-09-23
Resolution : 3.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

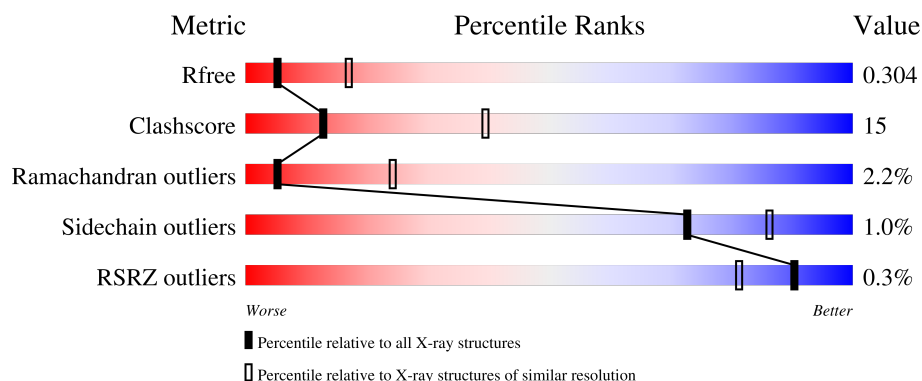
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	228	
1	I	228	
1	J	228	
2	L	219	
2	M	219	

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Mol	Chain	Length	Quality of chain
2	N	219	<div><div></div><div>72%</div><div>26%</div><div></div></div>
3	C	135	<div>%<div><div></div><div>44%</div><div>35%</div><div>20%</div><div></div></div></div>
3	D	135	<div>%<div><div></div><div>41%</div><div>39%</div><div>19%</div><div></div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11258 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 9D9 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	213	Total	C	N	O	S	0	0	0
			1504	950	243	304	7			
1	I	213	Total	C	N	O	S	0	0	0
			1608	1023	261	317	7			
1	J	215	Total	C	N	O	S	0	0	0
			1626	1035	263	321	7			

- Molecule 2 is a protein called 9D9 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	218	Total	C	N	O	S	0	0	0
			1603	1009	264	325	5			
2	M	218	Total	C	N	O	S	0	0	0
			1682	1057	283	337	5			
2	N	218	Total	C	N	O	S	0	0	0
			1682	1057	283	337	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	108	Total	C	N	O	S	0	0	0
			753	477	119	151	6			
3	D	110	Total	C	N	O	S	0	0	0
			800	505	130	159	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP P09793
C	-17	HIS	-	expression tag	UNP P09793
C	-16	HIS	-	expression tag	UNP P09793
C	-15	HIS	-	expression tag	UNP P09793

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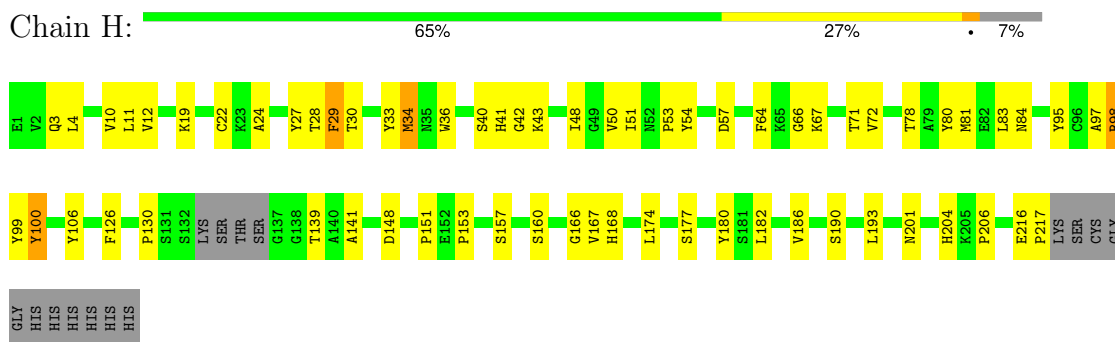
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP P09793
C	-13	HIS	-	expression tag	UNP P09793
C	-12	GLY	-	expression tag	UNP P09793
C	-11	SER	-	expression tag	UNP P09793
C	-10	GLY	-	expression tag	UNP P09793
C	-9	SER	-	expression tag	UNP P09793
C	-8	GLU	-	expression tag	UNP P09793
C	-7	ASN	-	expression tag	UNP P09793
C	-6	LEU	-	expression tag	UNP P09793
C	-5	TYR	-	expression tag	UNP P09793
C	-4	PHE	-	expression tag	UNP P09793
C	-3	GLN	-	expression tag	UNP P09793
D	-18	HIS	-	expression tag	UNP P09793
D	-17	HIS	-	expression tag	UNP P09793
D	-16	HIS	-	expression tag	UNP P09793
D	-15	HIS	-	expression tag	UNP P09793
D	-14	HIS	-	expression tag	UNP P09793
D	-13	HIS	-	expression tag	UNP P09793
D	-12	GLY	-	expression tag	UNP P09793
D	-11	SER	-	expression tag	UNP P09793
D	-10	GLY	-	expression tag	UNP P09793
D	-9	SER	-	expression tag	UNP P09793
D	-8	GLU	-	expression tag	UNP P09793
D	-7	ASN	-	expression tag	UNP P09793
D	-6	LEU	-	expression tag	UNP P09793
D	-5	TYR	-	expression tag	UNP P09793
D	-4	PHE	-	expression tag	UNP P09793
D	-3	GLN	-	expression tag	UNP P09793

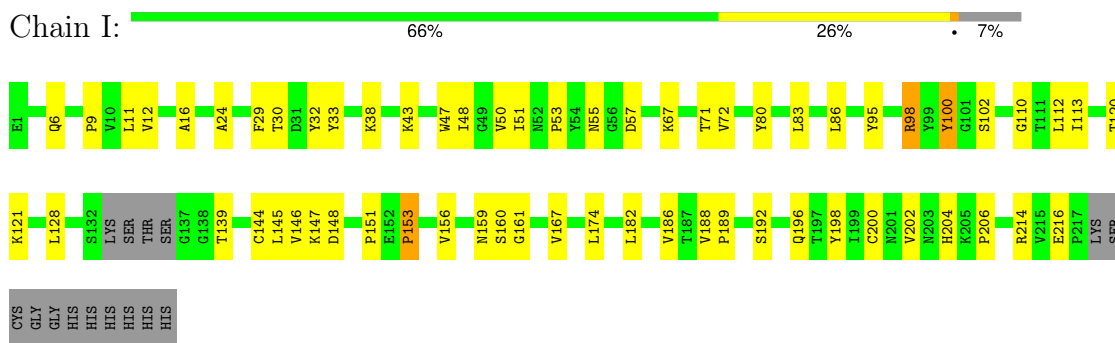
3 Residue-property plots [i](#)

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.

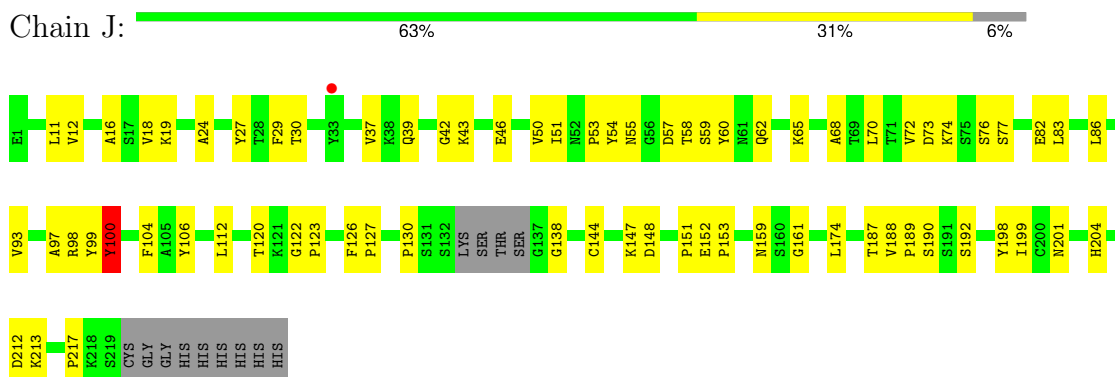
- Molecule 1: 9D9 heavy chain



- Molecule 1: 9D9 heavy chain



- Molecule 1: 9D9 heavy chain



A49		V58		F60		S67		F70		L77		I79		Q80		G81		L82		R83		T87		Y90		L91		C92		R93		V94		E95		L96		R97		Y98		P99		F100		P101		Y102		F103		V104		G105		M106		G107		N108		G109		T110		Q111		I112		Y113		V114		I115		ASP
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.51Å 208.84Å 91.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.48 – 3.10 36.48 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (36.48-3.10) 97.1 (36.48-3.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.13Å)	Xtriage
Refinement program	PHENIX (???)	Depositor
R, R_{free}	0.238 , 0.301 0.238 , 0.304	Depositor DCC
R_{free} test set	2320 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	126.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.8	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	0.93	EDS
Total number of atoms	11258	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

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	H	0.52	0/1546	0.69	1/2130 (0.0%)
1	I	0.49	0/1650	0.69	2/2250 (0.1%)
1	J	0.47	1/1669 (0.1%)	0.65	0/2276
2	L	0.50	0/1640	0.71	1/2242 (0.0%)
2	M	0.47	0/1719	0.69	1/2331 (0.0%)
2	N	0.49	0/1719	0.69	0/2331
3	C	0.47	0/768	0.68	0/1057
3	D	0.40	0/816	0.59	0/1119
All	All	0.48	1/11527 (0.0%)	0.68	5/15736 (0.0%)

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
2	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	144	CYS	CB-SG	-5.10	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	174	LEU	CA-CB-CG	7.58	132.75	115.30
1	H	182	LEU	CA-CB-CG	5.99	129.07	115.30
2	M	11	LEU	CA-CB-CG	5.88	128.83	115.30
2	L	109	LEU	CA-CB-CG	5.64	128.27	115.30
1	I	182	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	113	ARG	Sidechain

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	H	1504	0	1316	38	0
1	I	1608	0	1563	42	0
1	J	1626	0	1577	45	0
2	L	1603	0	1482	44	0
2	M	1682	0	1641	50	0
2	N	1682	0	1641	42	0
3	C	753	0	677	35	0
3	D	800	0	749	40	0
All	All	11258	0	10646	326	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 15.

The worst 5 of 326 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:M:42:LEU:HD12	2:M:91:TYR:CZ	2.01	0.95
3:C:27:HIS:O	3:C:27:HIS:ND1	1.98	0.95
2:L:38:LEU:HD12	2:L:76:PHE:CD2	2.13	0.84
2:L:31:HIS:ND1	2:L:33:ASN:OD1	2.08	0.84
2:M:42:LEU:HD12	2:M:91:TYR:CE2	2.14	0.82

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	H	209/228 (92%)	175 (84%)	25 (12%)	9 (4%)	2	13
1	I	209/228 (92%)	189 (90%)	16 (8%)	4 (2%)	6	27
1	J	211/228 (92%)	185 (88%)	24 (11%)	2 (1%)	14	45
2	L	216/219 (99%)	193 (89%)	21 (10%)	2 (1%)	14	45
2	M	216/219 (99%)	190 (88%)	20 (9%)	6 (3%)	4	20
2	N	216/219 (99%)	198 (92%)	14 (6%)	4 (2%)	6	27
3	C	104/135 (77%)	86 (83%)	14 (14%)	4 (4%)	2	15
3	D	106/135 (78%)	91 (86%)	13 (12%)	2 (2%)	6	27
All	All	1487/1611 (92%)	1307 (88%)	147 (10%)	33 (2%)	5	24

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	204	GLN
2	L	216	ARG
1	I	43	LYS
1	I	160	SER
2	M	56	VAL

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	151/195 (77%)	149 (99%)	2 (1%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	181/195 (93%)	177 (98%)	4 (2%)	47	71
1	J	183/195 (94%)	181 (99%)	2 (1%)	70	84
2	L	174/194 (90%)	173 (99%)	1 (1%)	84	91
2	M	193/194 (100%)	192 (100%)	1 (0%)	86	92
2	N	193/194 (100%)	193 (100%)	0	100	100
3	C	78/120 (65%)	78 (100%)	0	100	100
3	D	88/120 (73%)	85 (97%)	3 (3%)	32	62
All	All	1241/1407 (88%)	1228 (99%)	13 (1%)	73	86

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	95	GLN
3	D	12	SER
1	J	151	PRO
3	D	83	ARG
1	J	100	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	6	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	213/228 (93%)	-0.33	0 100 100	84, 108, 146, 153	0
1	I	213/228 (93%)	-0.42	0 100 100	82, 113, 145, 151	0
1	J	215/228 (94%)	-0.35	1 (0%) 87 75	76, 115, 160, 180	0
2	L	218/219 (99%)	-0.50	1 (0%) 87 75	79, 102, 145, 155	0
2	M	218/219 (99%)	-0.45	0 100 100	86, 106, 137, 172	0
2	N	218/219 (99%)	-0.44	0 100 100	75, 112, 160, 180	0
3	C	108/135 (80%)	-0.07	1 (0%) 81 66	92, 124, 145, 148	0
3	D	110/135 (81%)	0.09	1 (0%) 81 66	114, 156, 177, 186	0
All	All	1513/1611 (93%)	-0.35	4 (0%) 90 81	75, 113, 158, 186	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	115	ILE	3.9
1	J	33	TYR	2.3
2	L	218	GLU	2.3
3	C	113	TYR	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.