



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:17 PM UTC

PDB ID : 5XXY / pdb_00005xxy
Title : Crystal structure of PD-L1 complexed with atezolizumab fab at 2.9A
Authors : Zhou, A.; Zhang, F.
Deposited on : 2017-07-05
Resolution : 2.90 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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

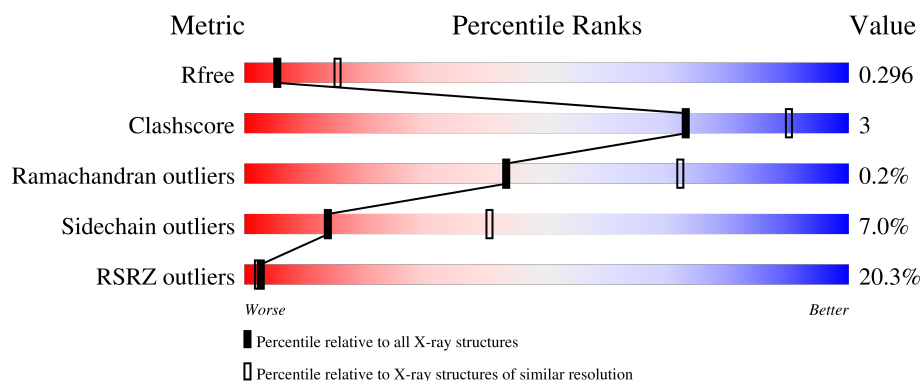
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	240	12% 75% 11% • 13%
2	L	214	20% 86% 12% ••
3	A	124	26% 70% 10% 20%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7868 atoms, of which 3889 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 atezolizumab fab.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	208	Total	C	H	N	O	S	0	0	0
			3087	1001	1517	263	301	5			

- Molecule 2 is a protein called light chain of atezolizumab fab.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	211	Total	C	H	N	O	S	0	0	0
			3207	1022	1582	270	328	5			

- Molecule 3 is a protein called Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	99	Total	C	H	N	O	S	0	0	0
			1572	503	790	129	145	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	GLY	-	expression tag	UNP Q9NZQ7
A	135	SER	-	expression tag	UNP Q9NZQ7
A	136	HIS	-	expression tag	UNP Q9NZQ7
A	137	HIS	-	expression tag	UNP Q9NZQ7
A	138	HIS	-	expression tag	UNP Q9NZQ7
A	139	HIS	-	expression tag	UNP Q9NZQ7
A	140	HIS	-	expression tag	UNP Q9NZQ7
A	141	HIS	-	expression tag	UNP Q9NZQ7

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		

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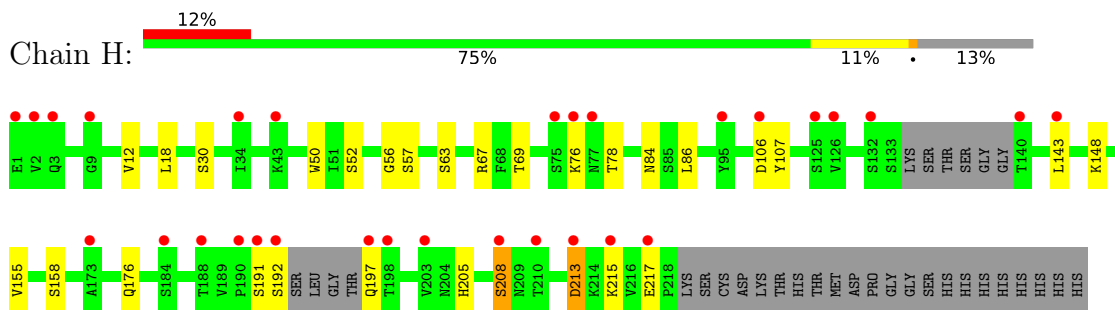
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	1	Total	O	0	0
			1	1		

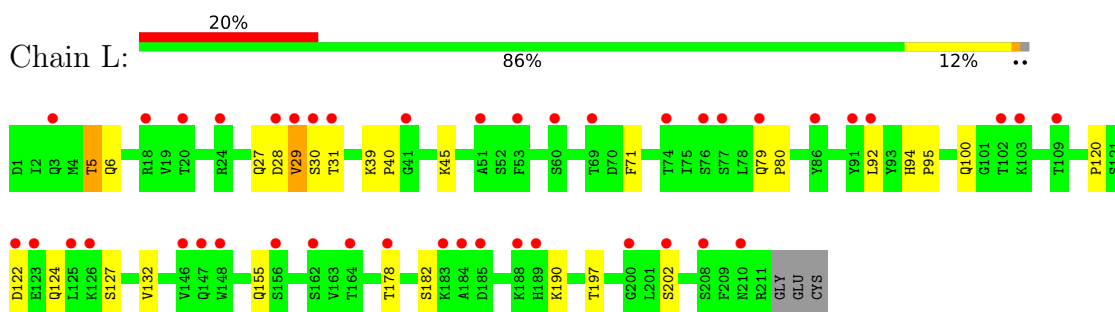
3 Residue-property plots [i](#)

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.

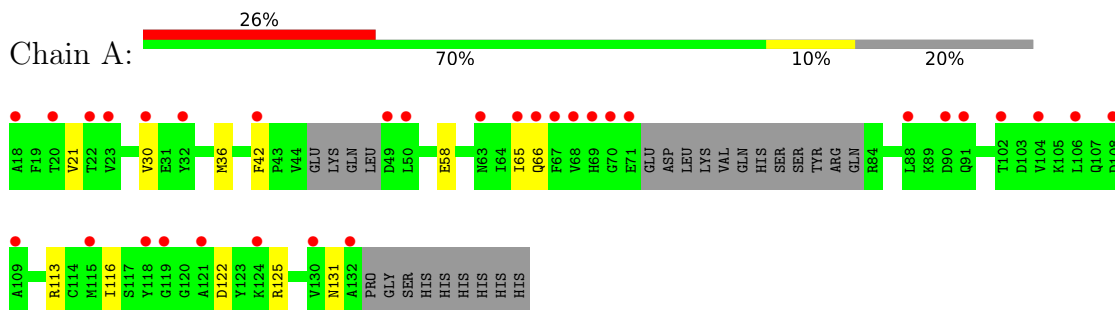
- Molecule 1: heavy chain of atezolizumab fab



- Molecule 2: light chain of atezolizumab fab



- Molecule 3: Programmed cell death 1 ligand 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.22Å 72.71Å 63.80Å 90.00° 104.44° 90.00°	Depositor
Resolution (Å)	61.60 – 2.90 61.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.9 (61.60-2.90) 93.0 (61.60-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.236 , 0.295 0.238 , 0.296	Depositor DCC
R_{free} test set	547 reflections (4.29%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	1.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7868	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.25% 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	0.30	0/1615	0.62	0/2206
2	L	0.32	0/1662	0.64	0/2259
3	A	0.27	0/793	0.60	0/1070
All	All	0.30	0/4070	0.62	0/5535

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](#)

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	1570	1517	1513	10	0
2	L	1625	1582	1579	10	0
3	A	782	790	789	5	0
4	H	1	0	0	0	0
4	L	1	0	0	1	0
All	All	3979	3889	3881	25	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 3.

All (25) 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)
3:A:21:VAL:HG23	3:A:122:ASP:HB3	1.71	0.72
1:H:67:ARG:O	1:H:84:ASN:ND2	2.23	0.71
2:L:190:LYS:NZ	4:L:301:HOH:O	2.26	0.68
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.77	0.65
1:H:148:LYS:NZ	1:H:176:GLN:OE1	2.31	0.63
3:A:21:VAL:HG22	3:A:116:ILE:HD11	1.85	0.58
1:H:106:ASP:OD1	1:H:107:TYR:N	2.40	0.54
2:L:29:VAL:HG12	2:L:30:SER:N	2.24	0.52
2:L:5:THR:O	2:L:5:THR:OG1	2.27	0.51
2:L:124:GLN:O	2:L:127:SER:OG	2.29	0.49
2:L:94:HIS:HA	2:L:95:PRO:C	2.38	0.48
3:A:58:GLU:OE2	3:A:113:ARG:NH1	2.47	0.48
2:L:29:VAL:HG12	2:L:30:SER:H	1.80	0.47
1:H:12:VAL:HG11	1:H:86:LEU:HD12	1.97	0.46
1:H:205:HIS:ND1	1:H:208:SER:OG	2.49	0.46
2:L:6:GLN:O	2:L:100:GLN:NE2	2.48	0.46
2:L:39:LYS:HB2	2:L:40:PRO:HD2	1.96	0.46
2:L:79:GLN:HG3	2:L:80:PRO:HD2	1.97	0.45
1:H:52:SER:O	1:H:56:GLY:N	2.47	0.45
1:H:213:ASP:OD1	1:H:213:ASP:N	2.46	0.45
3:A:42:PHE:HB3	3:A:116:ILE:CD1	2.49	0.43
1:H:217:GLU:OE1	1:H:217:GLU:N	2.47	0.42
3:A:30:VAL:HG11	3:A:36:MET:HB3	2.02	0.42
1:H:50:TRP:CD1	1:H:50:TRP:C	2.99	0.41
1:H:76:LYS:HZ3	1:H:78:THR:HG21	1.86	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	H	202/240 (84%)	192 (95%)	10 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	209/214 (98%)	197 (94%)	11 (5%)	1 (0%)	24	54
3	A	93/124 (75%)	88 (95%)	5 (5%)	0	100	100
All	All	504/578 (87%)	477 (95%)	26 (5%)	1 (0%)	43	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	29	VAL

5.3.2 Protein sidechains ⓘ

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	171/198 (86%)	157 (92%)	14 (8%)	10	32
2	L	185/187 (99%)	172 (93%)	13 (7%)	14	40
3	A	84/108 (78%)	80 (95%)	4 (5%)	23	55
All	All	440/493 (89%)	409 (93%)	31 (7%)	14	40

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	18	LEU
1	H	30	SER
1	H	57	SER
1	H	63	SER
1	H	69	THR
1	H	143	LEU
1	H	155	VAL
1	H	158	SER
1	H	191	SER
1	H	192	SER
1	H	197	GLN
1	H	208	SER
1	H	213	ASP

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Mol	Chain	Res	Type
1	H	215	LYS
2	L	5	THR
2	L	27	GLN
2	L	28	ASP
2	L	31	THR
2	L	45	LYS
2	L	71	PHE
2	L	92	LEU
2	L	122	ASP
2	L	155	GLN
2	L	178	THR
2	L	182	SER
2	L	197	THR
2	L	202	SER
3	A	65	ILE
3	A	66	GLN
3	A	125	ARG
3	A	131	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	84	ASN
1	H	169	HIS
3	A	35	ASN
3	A	66	GLN
3	A	69	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	208/240 (86%)	1.18	30 (14%) 6 5	30, 46, 67, 79	0
2	L	211/214 (98%)	1.38	43 (20%) 3 2	31, 50, 68, 88	0
3	A	99/124 (79%)	1.57	32 (32%) 1 1	31, 53, 73, 84	0
All	All	518/578 (89%)	1.34	105 (20%) 3 2	30, 48, 69, 88	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	41	GLY	5.0
2	L	30	SER	4.6
3	A	18	ALA	4.4
2	L	122	ASP	4.1
1	H	140	THR	4.0
1	H	210	THR	4.0
2	L	20	THR	3.7
1	H	192	SER	3.7
2	L	92	LEU	3.7
2	L	125	LEU	3.6
1	H	190	PRO	3.5
2	L	164	THR	3.4
2	L	60	SER	3.4
3	A	68	VAL	3.4
3	A	69	HIS	3.3
2	L	210	ASN	3.3
1	H	132	SER	3.3
3	A	22	THR	3.1
2	L	147	GLN	3.1
3	A	104	VAL	3.0
2	L	28	ASP	3.0
3	A	119	GLY	3.0
1	H	188	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	43	LYS	2.9
2	L	208	SER	2.9
3	A	118	TYR	2.9
1	H	213	ASP	2.9
2	L	123	GLU	2.8
3	A	65	ILE	2.8
3	A	32	TYR	2.8
2	L	74	THR	2.8
1	H	1	GLU	2.7
2	L	126	LYS	2.7
3	A	70	GLY	2.7
3	A	88	LEU	2.7
2	L	162	SER	2.7
2	L	188	LYS	2.6
1	H	125	SER	2.6
1	H	184	SER	2.6
3	A	67	PHE	2.6
2	L	3	GLN	2.6
3	A	109	ALA	2.6
2	L	185	ASP	2.6
2	L	148	TRP	2.5
3	A	132	ALA	2.5
3	A	91	GLN	2.5
3	A	121	ALA	2.5
3	A	23	VAL	2.5
3	A	102	THR	2.5
2	L	29	VAL	2.4
2	L	91	TYR	2.4
3	A	124	LYS	2.4
2	L	102	THR	2.4
2	L	24	ARG	2.4
1	H	106	ASP	2.4
3	A	30	VAL	2.4
1	H	208	SER	2.4
2	L	86	TYR	2.4
2	L	103	LYS	2.3
3	A	49	ASP	2.3
3	A	71	GLU	2.3
2	L	79	GLN	2.3
3	A	130	VAL	2.3
3	A	63	ASN	2.3
3	A	108	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	143	LEU	2.3
2	L	77	SER	2.3
2	L	189	HIS	2.3
2	L	146	VAL	2.3
2	L	31	THR	2.3
3	A	20	THR	2.3
2	L	51	ALA	2.3
2	L	183	LYS	2.3
3	A	115	MET	2.2
3	A	66	GLN	2.2
2	L	18	ARG	2.2
2	L	178	THR	2.2
1	H	2	VAL	2.2
1	H	77	ASN	2.2
1	H	215	LYS	2.2
2	L	69	THR	2.2
1	H	95	TYR	2.2
2	L	53	PHE	2.2
3	A	50	LEU	2.2
1	H	34	ILE	2.2
1	H	9	GLY	2.2
2	L	184	ALA	2.2
2	L	109	THR	2.1
2	L	202	SER	2.1
1	H	3	GLN	2.1
1	H	191	SER	2.1
1	H	217	GLU	2.1
1	H	173	ALA	2.1
1	H	197	GLN	2.1
1	H	76	LYS	2.1
3	A	106	LEU	2.1
2	L	200	GLY	2.1
3	A	42	PHE	2.1
3	A	90	ASP	2.1
2	L	76	SER	2.0
2	L	156	SER	2.0
1	H	203	VAL	2.0
1	H	75	SER	2.0
1	H	198	THR	2.0
1	H	126	VAL	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 oligosaccharides 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.