



# Full wwPDB X-ray Structure Validation Report

May 16, 2020 – 12:39 am BST

PDB ID : 5GGT  
Title : PD-L1 in complex with BMS-936559 Fab  
Authors : Heo, Y.S.  
Deposited on : 2016-06-16  
Resolution : 2.80 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](mailto: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 : 2.11  
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) : 2.11

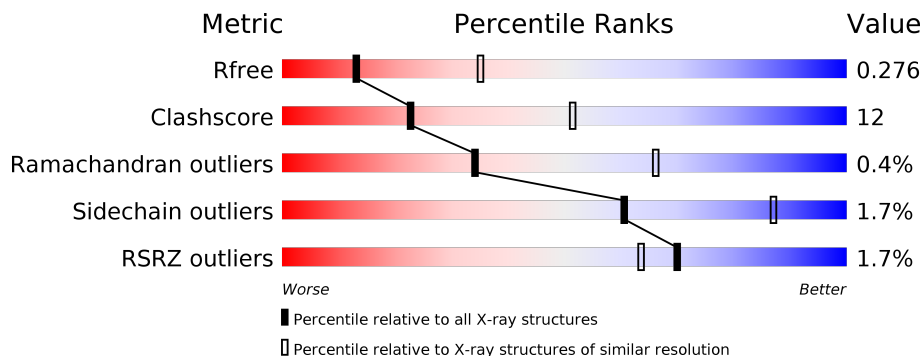
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

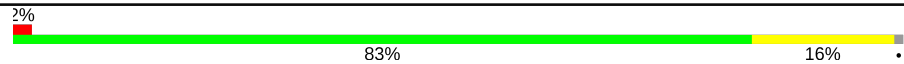
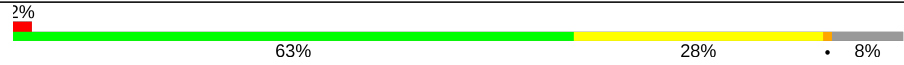

The reported resolution of this entry is 2.80 Å.

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	A	117	 2% 83% 16%
2	H	235	 2% 63% 28% 8%
3	L	213	 % 69% 29%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4155 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 Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	116	928	593	156	174	5	0	0	0

- Molecule 2 is a protein called IgG H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	216	1607	1021	266	313	7	0	0	0

- Molecule 3 is a protein called IGK@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	210	1620	1014	276	326	4	0	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.20Å 91.56Å 164.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.16 – 2.80 29.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.16-2.80) 97.3 (29.16-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.51 (at 2.80Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.211 , 0.269 0.218 , 0.276	Depositor DCC
$R_{free}$ test set	712 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtrriage
Anisotropy	0.698	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4155	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	A	0.35	0/944	0.58	0/1276
2	H	0.31	0/1647	0.54	0/2242
3	L	0.29	0/1656	0.51	0/2252
All	All	0.31	0/4247	0.54	0/5770

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	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	87	ARG	Peptide

### 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	A	928	0	936	13	0
2	H	1607	0	1584	47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1620	0	1581	47	0
All	All	4155	0	4101	95	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 12.

All (95) 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:L:122:GLU:HG2	3:L:123:GLN:N	1.94	0.82
2:H:133:PRO:HD3	2:H:219:LYS:HE2	1.67	0.75
2:H:132:PHE:CD1	3:L:122:GLU:HG3	2.23	0.73
1:A:59:MET:HG2	1:A:60:GLU:HG3	1.71	0.72
3:L:119:PRO:HD3	3:L:131:VAL:HG22	1.72	0.72
3:L:122:GLU:HG2	3:L:123:GLN:H	1.54	0.71
2:H:173:VAL:HG22	2:H:192:VAL:HB	1.74	0.70
1:A:88:LEU:HD11	1:A:100:GLN:HB2	1.75	0.69
2:H:132:PHE:HB3	3:L:122:GLU:OE2	1.93	0.68
3:L:144:LYS:HB3	3:L:196:THR:HB	1.76	0.67
2:H:111:ASP:OD1	3:L:91:ARG:NH2	2.26	0.67
2:H:97:ALA:HB3	2:H:110:MET:HG2	1.76	0.66
2:H:103:VAL:HG13	3:L:49:TYR:HB2	1.78	0.65
2:H:67:ARG:CZ	2:H:87:ARG:HH12	2.11	0.62
2:H:7:SER:HB3	2:H:21:SER:HB3	1.82	0.62
3:L:21:LEU:HD23	3:L:101:THR:HB	1.82	0.61
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.37	0.60
2:H:134:LEU:HB3	3:L:117:PHE:CD1	2.37	0.59
1:A:56:TYR:OH	2:H:59:HIS:NE2	2.34	0.59
2:H:30:SER:HB3	2:H:54:ILE:HG23	1.84	0.58
1:A:107:GLN:OE1	1:A:107:GLN:N	2.37	0.58
3:L:120:SER:HB2	3:L:122:GLU:CD	2.25	0.57
2:H:164:TRP:CZ3	2:H:206:CYS:HB2	2.41	0.56
2:H:33:ALA:HB2	2:H:52:ILE:HG12	1.87	0.56
2:H:22:CYS:HG	2:H:96:CYS:HG	1.54	0.55
3:L:120:SER:HB2	3:L:122:GLU:OE2	2.07	0.55
3:L:153:LEU:HD12	3:L:153:LEU:H	1.72	0.55
2:H:210:HIS:CD2	2:H:212:PRO:HD2	2.41	0.55
3:L:165:GLN:HG3	3:L:172:TYR:CZ	2.42	0.55
2:H:106:SER:H	3:L:91:ARG:HB3	1.72	0.54
2:H:67:ARG:HD3	2:H:87:ARG:HH22	1.74	0.53
2:H:209:ASN:HD21	2:H:211:LYS:HE3	1.74	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:38:GLN:HG3	3:L:44:PRO:HG3	1.92	0.50
2:H:209:ASN:OD1	2:H:216:LYS:HG2	2.10	0.50
3:L:133:CYS:HG	3:L:193:CYS:HG	1.57	0.50
2:H:194:VAL:HG11	2:H:204:TYR:CE1	2.46	0.50
2:H:30:SER:HA	2:H:53:PRO:HB2	1.93	0.50
3:L:157:ASN:ND2	3:L:178:LEU:HD11	2.27	0.49
1:A:121:ALA:H	2:H:31:THR:HG23	1.77	0.49
2:H:13:LYS:HD3	2:H:122:SER:O	2.13	0.49
2:H:64:PHE:HB3	2:H:68:VAL:HG21	1.94	0.49
3:L:85:VAL:HG12	3:L:102:LYS:HB2	1.96	0.48
2:H:2:VAL:HA	2:H:26:GLY:HA3	1.95	0.48
2:H:48:MET:HA	2:H:64:PHE:CD2	2.49	0.48
3:L:119:PRO:HG3	3:L:129:ALA:HB1	1.96	0.48
1:A:109:ALA:HB2	1:A:130:VAL:HG23	1.95	0.47
2:H:163:SER:O	2:H:207:ASN:HB2	2.14	0.47
2:H:64:PHE:HB3	2:H:68:VAL:CG2	2.44	0.47
3:L:33:LEU:HD22	3:L:71:PHE:CG	2.49	0.47
2:H:133:PRO:HD2	3:L:122:GLU:CD	2.36	0.46
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.98	0.46
3:L:63:SER:O	3:L:73:LEU:HD12	2.16	0.46
3:L:6:GLN:HB3	3:L:6:GLN:HE21	1.65	0.45
1:A:68:VAL:HG12	1:A:69:HIS:ND1	2.32	0.45
3:L:122:GLU:CG	3:L:123:GLN:N	2.74	0.45
3:L:125:LYS:HB2	3:L:125:LYS:HE3	1.66	0.45
2:H:132:PHE:HD1	3:L:122:GLU:HG3	1.78	0.45
3:L:195:VAL:HB	3:L:204:VAL:HG13	1.99	0.45
1:A:67:PHE:CZ	1:A:70:GLY:HA2	2.51	0.45
3:L:61:ARG:NE	3:L:82:ASP:OD2	2.47	0.44
2:H:175:THR:HG23	2:H:188:LEU:HD21	2.00	0.44
3:L:120:SER:HB2	3:L:122:GLU:OE1	2.17	0.44
3:L:11:LEU:HD23	3:L:103:VAL:HG13	1.99	0.43
2:H:133:PRO:CD	2:H:219:LYS:HE2	2.40	0.43
1:A:99:LEU:HD21	1:A:101:ILE:HD11	2.00	0.43
3:L:123:GLN:HE22	3:L:130:SER:CB	2.31	0.43
3:L:33:LEU:HD22	3:L:71:PHE:CD2	2.54	0.43
1:A:121:ALA:H	2:H:31:THR:CG2	2.32	0.43
2:H:133:PRO:CB	2:H:221:VAL:HG13	2.49	0.42
3:L:163:THR:HG22	3:L:173:SER:H	1.84	0.42
3:L:189:LYS:HG2	3:L:209:ASN:OD1	2.19	0.42
3:L:94:TRP:HA	3:L:95:PRO:HD3	1.86	0.42
2:H:12:LYS:O	2:H:121:VAL:HA	2.20	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:CD2	2:H:81:MET:HB2	2.54	0.42
3:L:2:ILE:HG12	3:L:27:GLN:NE2	2.34	0.42
1:A:30:VAL:O	1:A:130:VAL:HA	2.20	0.42
3:L:135:LEU:HB2	3:L:174:LEU:HB3	2.01	0.42
1:A:85:ALA:HB1	1:A:99:LEU:HD11	2.02	0.42
2:H:165:ASN:ND2	2:H:169:LEU:HD12	2.34	0.42
2:H:99:LYS:HG2	2:H:100:PHE:O	2.20	0.42
2:H:219:LYS:HD2	2:H:219:LYS:HA	1.73	0.42
2:H:129:PRO:HB3	2:H:155:TYR:HB3	2.02	0.41
2:H:191:VAL:HG11	3:L:134:LEU:HD22	2.02	0.41
3:L:78:LEU:HA	3:L:78:LEU:HD23	1.87	0.41
3:L:13:LEU:O	3:L:106:LYS:N	2.39	0.41
1:A:83:GLN:O	1:A:83:GLN:HG3	2.20	0.41
2:H:11:VAL:HG21	2:H:157:PRO:HG3	2.02	0.41
2:H:3:GLN:HG2	2:H:4:LEU:N	2.36	0.41
3:L:112:PRO:HD3	3:L:197:HIS:ND1	2.36	0.41
3:L:119:PRO:HG2	3:L:124:LEU:HD11	2.01	0.41
3:L:202:SER:HA	3:L:203:PRO:HD3	1.95	0.41
3:L:83:PHE:CG	3:L:105:ILE:HG12	2.55	0.41
3:L:34:ALA:HA	3:L:48:ILE:O	2.21	0.40
2:H:135:ALA:HA	2:H:136:PRO:HD3	1.91	0.40
3:L:139:TYR:CG	3:L:140:PRO:HA	2.56	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	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
2	H	212/235 (90%)	199 (94%)	11 (5%)	2 (1%)	17	46
3	L	208/213 (98%)	200 (96%)	8 (4%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	534/565 (94%)	506 (95%)	26 (5%)	2 (0%)	34 66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	27	ASP
2	H	166	SER

### 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	101/102 (99%)	100 (99%)	1 (1%)	76 93
2	H	181/199 (91%)	177 (98%)	4 (2%)	52 83
3	L	183/185 (99%)	180 (98%)	3 (2%)	62 88
All	All	465/486 (96%)	457 (98%)	8 (2%)	60 87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
2	H	22	CYS
2	H	34	ILE
2	H	89	GLU
2	H	191	VAL
3	L	23	CYS
3	L	38	GLN
3	L	125	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	27	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	L	89	GLN
3	L	136	ASN
3	L	154	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 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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	116/117 (99%)	0.00	2 (1%) 70 63	31, 43, 72, 90	0
2	H	216/235 (91%)	0.16	4 (1%) 66 59	26, 43, 75, 85	0
3	L	210/213 (98%)	0.20	3 (1%) 75 70	26, 48, 71, 84	0
All	All	542/565 (95%)	0.14	9 (1%) 70 63	26, 46, 73, 90	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	26	GLY	3.6
1	A	31	GLU	2.9
2	H	88	SER	2.8
2	H	171	SER	2.4
3	L	10	THR	2.3
3	L	209	ASN	2.2
3	L	169	ASP	2.1
2	H	135	ALA	2.1
1	A	133	PRO	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.