



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 08:12 PM EDT

PDB ID : 6SRU  
Title : Structure of Ig-like V-type domain of mouse Programmed cell death 1 ligand 1 (PD-L1)  
Authors : Magiera-Mularz, K.; Sala, D.; Grudnik, P.; Holak, T.A.  
Deposited on : 2019-09-06  
Resolution : 2.53 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](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 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)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

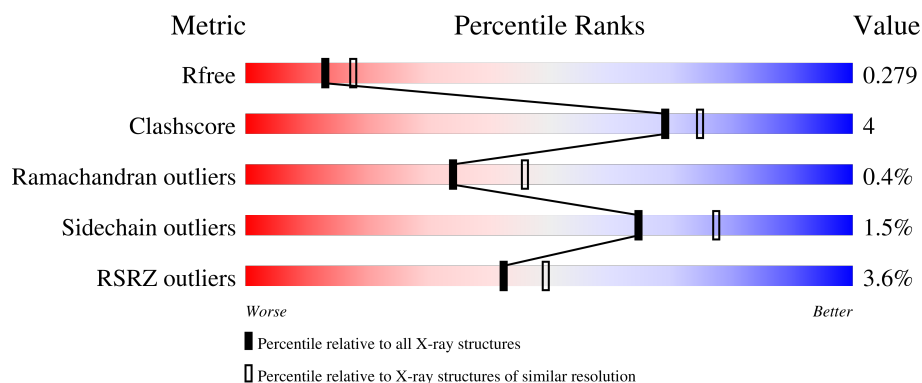
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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.



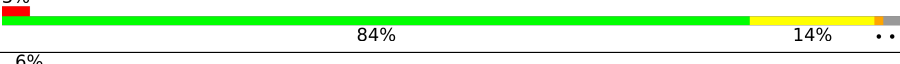

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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  $\geq 3$ , 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	118	
1	B	118	
1	C	118	
1	D	118	
1	E	118	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	118	
1	G	118	
1	H	118	
1	I	118	
1	J	118	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16851 atoms, of which 8175 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
1	A	116	Total	C	H	N	O	S	0	0	0
			1727	569	844	141	169	4			
1	B	116	Total	C	H	N	O	S	0	0	0
			1745	575	855	140	171	4			
1	C	115	Total	C	H	N	O	S	0	0	0
			1698	558	830	138	168	4			
1	D	114	Total	C	H	N	O	S	0	0	0
			1639	546	790	134	165	4			
1	E	115	Total	C	H	N	O	S	0	0	0
			1660	551	805	138	162	4			
1	F	116	Total	C	H	N	O	S	0	0	0
			1747	574	856	141	172	4			
1	G	114	Total	C	H	N	O	S	0	0	0
			1642	548	793	137	160	4			
1	H	116	Total	C	H	N	O	S	0	0	0
			1724	566	844	142	168	4			
1	I	111	Total	C	H	N	O	S	0	0	0
			1604	533	774	131	162	4			
1	J	113	Total	C	H	N	O	S	0	0	0
			1624	541	784	132	163	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP Q9EP73
A	18	GLY	-	expression tag	UNP Q9EP73
B	17	MET	-	initiating methionine	UNP Q9EP73
B	18	GLY	-	expression tag	UNP Q9EP73
C	17	MET	-	initiating methionine	UNP Q9EP73
C	18	GLY	-	expression tag	UNP Q9EP73
D	17	MET	-	initiating methionine	UNP Q9EP73
D	18	GLY	-	expression tag	UNP Q9EP73
E	17	MET	-	initiating methionine	UNP Q9EP73

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	18	GLY	-	expression tag	UNP Q9EP73
F	17	MET	-	initiating methionine	UNP Q9EP73
F	18	GLY	-	expression tag	UNP Q9EP73
G	17	MET	-	initiating methionine	UNP Q9EP73
G	18	GLY	-	expression tag	UNP Q9EP73
H	17	MET	-	initiating methionine	UNP Q9EP73
H	18	GLY	-	expression tag	UNP Q9EP73
I	17	MET	-	initiating methionine	UNP Q9EP73
I	18	GLY	-	expression tag	UNP Q9EP73
J	17	MET	-	initiating methionine	UNP Q9EP73
J	18	GLY	-	expression tag	UNP Q9EP73

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total O 4 4	0	0
2	B	10	Total O 10 10	0	0
2	C	4	Total O 4 4	0	0
2	D	5	Total O 5 5	0	0
2	E	4	Total O 5 5	0	1
2	F	4	Total O 4 4	0	0
2	G	4	Total O 5 5	0	1
2	H	2	Total O 2 2	0	0
2	I	1	Total O 1 1	0	0
2	J	1	Total O 1 1	0	0

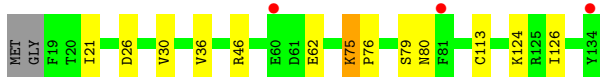
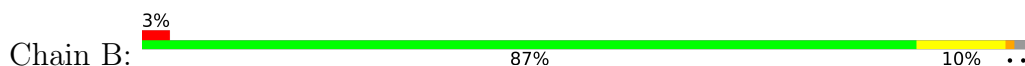
### 3 Residue-property plots [i](#)

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.

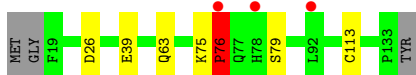
- Molecule 1: Programmed cell death 1 ligand 1



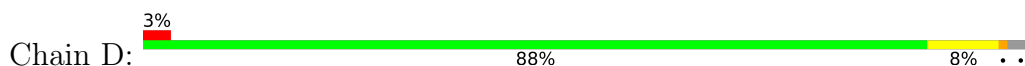
- Molecule 1: Programmed cell death 1 ligand 1



- Molecule 1: Programmed cell death 1 ligand 1



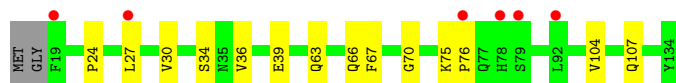
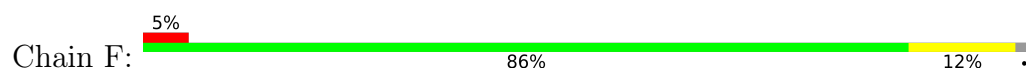
- Molecule 1: Programmed cell death 1 ligand 1



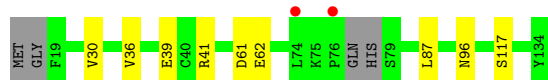
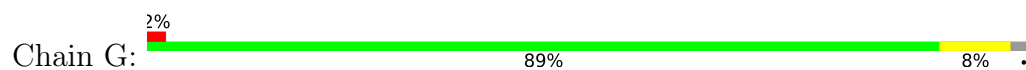
- Molecule 1: Programmed cell death 1 ligand 1



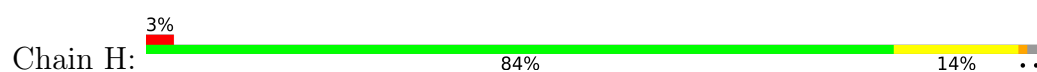
- Molecule 1: Programmed cell death 1 ligand 1



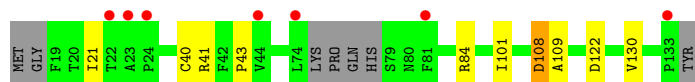
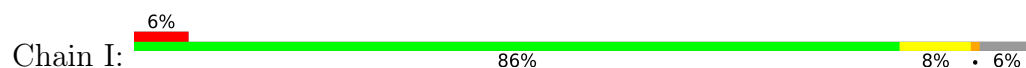
- Molecule 1: Programmed cell death 1 ligand 1



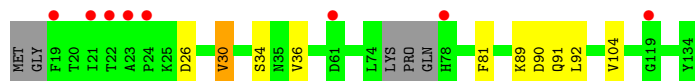
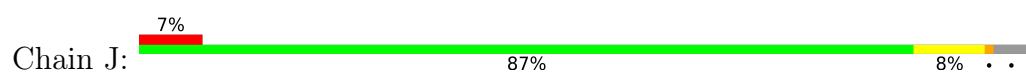
- Molecule 1: Programmed cell death 1 ligand 1



- Molecule 1: Programmed cell death 1 ligand 1



- Molecule 1: Programmed cell death 1 ligand 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.92Å 107.72Å 79.53Å 90.00° 99.15° 90.00°	Depositor
Resolution (Å)	49.66 – 2.53 49.66 – 2.53	Depositor EDS
% Data completeness (in resolution range)	93.7 (49.66-2.53) 93.8 (49.66-2.53)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.228 , 0.279 0.228 , 0.279	Depositor DCC
$R_{free}$ test set	1906 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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

### 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	A	0.33	0/900	0.56	0/1225
1	B	0.39	0/907	0.60	0/1235
1	C	0.37	0/884	0.71	2/1206 (0.2%)
1	D	0.32	0/863	0.53	0/1175
1	E	0.45	0/869	0.61	0/1182
1	F	0.35	0/908	0.53	0/1236
1	G	0.49	1/863 (0.1%)	0.57	0/1171
1	H	0.35	0/896	0.54	0/1220
1	I	0.35	0/844	0.57	0/1150
1	J	0.34	0/854	0.56	0/1165
All	All	0.38	1/8788 (0.0%)	0.58	2/11965 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	87	LEU	C-N	9.49	1.52	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	PRO	CA-N-CD	-11.84	94.92	111.50
1	C	76	PRO	N-CA-CB	-5.35	96.71	102.60

There are no chirality outliers.

There are no planarity outliers.

### 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	A	883	844	844	4	0
1	B	890	855	853	9	0
1	C	868	830	830	4	0
1	D	849	790	783	8	0
1	E	855	805	802	2	0
1	F	891	856	854	8	0
1	G	849	793	790	6	0
1	H	880	844	844	10	0
1	I	830	774	770	7	0
1	J	840	784	782	7	0
2	A	4	0	0	0	0
2	B	10	0	0	2	0
2	C	4	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	3	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
All	All	8676	8175	8152	62	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 4.

The worst 5 of 62 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)
1:B:76:PRO:HG2	1:B:79:SER:HB2	1.39	1.01
1:J:30:VAL:HG21	1:J:36:VAL:HG22	1.53	0.90
1:B:75:LYS:CB	2:B:207:HOH:O	2.25	0.83
1:F:30:VAL:HG11	1:F:36:VAL:HG22	1.62	0.82
1:D:30:VAL:HG11	1:D:36:VAL:HG22	1.64	0.78

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	114/118 (97%)	106 (93%)	8 (7%)	0	100	100
1	B	114/118 (97%)	105 (92%)	8 (7%)	1 (1%)	17	24
1	C	113/118 (96%)	106 (94%)	6 (5%)	1 (1%)	17	24
1	D	110/118 (93%)	104 (94%)	6 (6%)	0	100	100
1	E	111/118 (94%)	105 (95%)	5 (4%)	1 (1%)	17	24
1	F	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
1	G	110/118 (93%)	104 (94%)	6 (6%)	0	100	100
1	H	114/118 (97%)	108 (95%)	5 (4%)	1 (1%)	17	24
1	I	107/118 (91%)	104 (97%)	3 (3%)	0	100	100
1	J	109/118 (92%)	105 (96%)	4 (4%)	0	100	100
All	All	1116/1180 (95%)	1055 (94%)	57 (5%)	4 (0%)	34	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	76	PRO
1	H	75	LYS
1	E	47	GLU
1	B	75	LYS

### 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	A	89/101 (88%)	88 (99%)	1 (1%)	73	83
1	B	91/101 (90%)	91 (100%)	0	100	100
1	C	89/101 (88%)	87 (98%)	2 (2%)	52	66
1	D	81/101 (80%)	80 (99%)	1 (1%)	71	81
1	E	82/101 (81%)	81 (99%)	1 (1%)	71	81
1	F	91/101 (90%)	90 (99%)	1 (1%)	73	83
1	G	78/101 (77%)	77 (99%)	1 (1%)	69	80
1	H	89/101 (88%)	85 (96%)	4 (4%)	27	37
1	I	81/101 (80%)	80 (99%)	1 (1%)	71	81
1	J	82/101 (81%)	81 (99%)	1 (1%)	71	81
All	All	853/1010 (84%)	840 (98%)	13 (2%)	65	77

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

Mol	Chain	Res	Type
1	H	30	VAL
1	H	46	ARG
1	J	30	VAL
1	H	105	LYS
1	I	108	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 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<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	116/118 (98%)	0.17	3 (2%) 56 62	40, 56, 76, 84	0
1	B	116/118 (98%)	0.25	3 (2%) 56 62	36, 58, 82, 98	0
1	C	115/118 (97%)	0.31	3 (2%) 56 62	38, 55, 82, 103	0
1	D	114/118 (96%)	0.36	4 (3%) 44 51	43, 66, 87, 105	0
1	E	115/118 (97%)	0.25	2 (1%) 70 76	41, 58, 85, 105	0
1	F	116/118 (98%)	0.22	6 (5%) 27 32	37, 57, 78, 105	0
1	G	114/118 (96%)	0.21	2 (1%) 68 74	40, 64, 84, 113	0
1	H	116/118 (98%)	0.40	3 (2%) 56 62	46, 66, 85, 106	0
1	I	111/118 (94%)	0.40	7 (6%) 20 23	47, 66, 82, 91	0
1	J	113/118 (95%)	0.46	8 (7%) 16 19	42, 68, 86, 92	0
All	All	1146/1180 (97%)	0.30	41 (3%) 42 49	36, 62, 84, 113	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	24	PRO	6.7
1	D	78	HIS	5.8
1	H	134	TYR	5.6
1	D	24	PRO	5.5
1	I	23	ALA	5.1

### 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.