



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 25, 2023 – 04:04 pm BST

PDB ID : 8GY5  
Title : High-resolution structure of the cemiplimab Fab in complex with PD-1  
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Deposited on : 2022-09-21  
Resolution : 1.98 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>.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

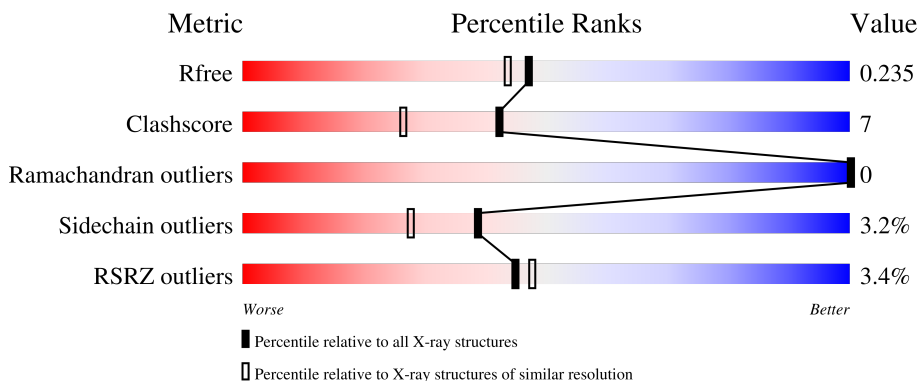
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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.



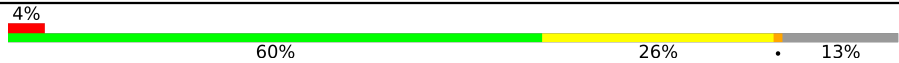
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	229	 3% 80% 12% 7%
1	H	229	 4% 79% 12% 8%
2	B	214	 88% 10% 2%
2	L	214	 2% 87% 12% 1%
3	P	125	 8% 74% 18% 6%

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Mol	Chain	Length	Quality of chain
3	Q	125	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (4%), a large green segment (60%), a yellow segment (26%), and a small grey segment (13%).</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8854 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	Total 1590	C 1012	N 264	O 308	S 6	0	0	0
1	H	211	Total 1581	C 1006	N 262	O 307	S 6	0	0	0

- Molecule 2 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	Total 1621	C 1015	N 273	O 328	S 5	0	0	0
2	L	212	Total 1621	C 1015	N 273	O 328	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	Q	109	Total 862	C 540	N 156	O 162	S 4	0	0	0
3	P	118	Total 935	C 580	N 173	O 178	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	93	SER	CYS	conflict	UNP Q15116
P	93	SER	CYS	conflict	UNP Q15116

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total 142	O 142	0	0

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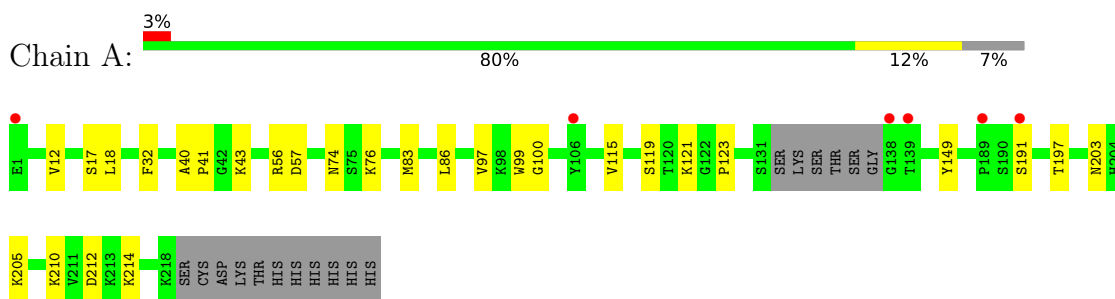
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	139	Total 139	O 139	0	0
4	Q	54	Total 54	O 54	0	0
4	H	132	Total 132	O 132	0	0
4	L	140	Total 140	O 140	0	0
4	P	37	Total 37	O 37	0	0

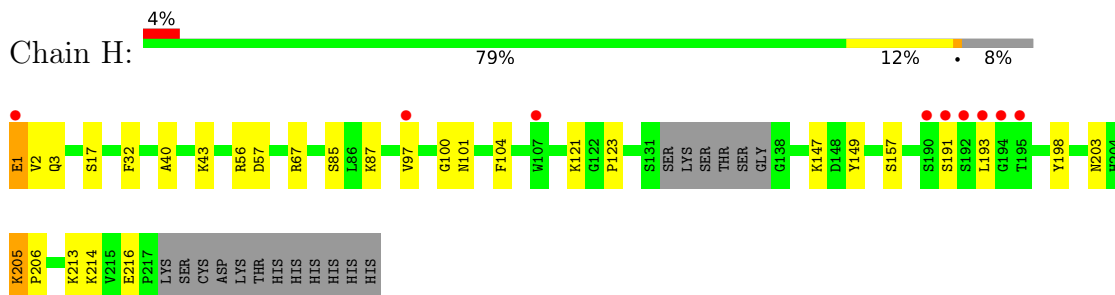
### 3 Residue-property plots [i](#)

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.

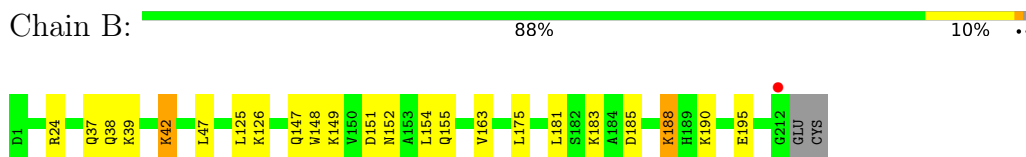
- Molecule 1: heavy chain



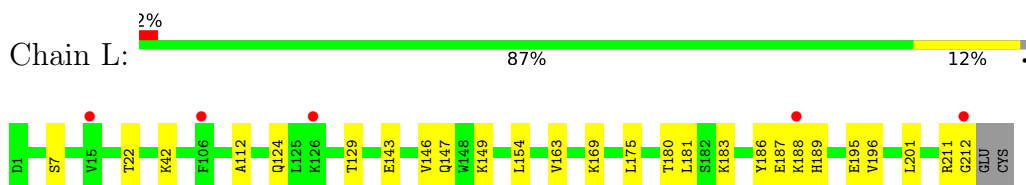
- Molecule 1: heavy chain



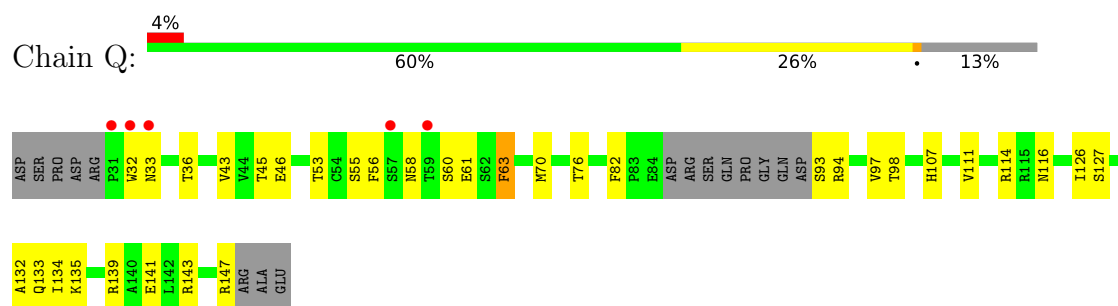
- Molecule 2: light chain



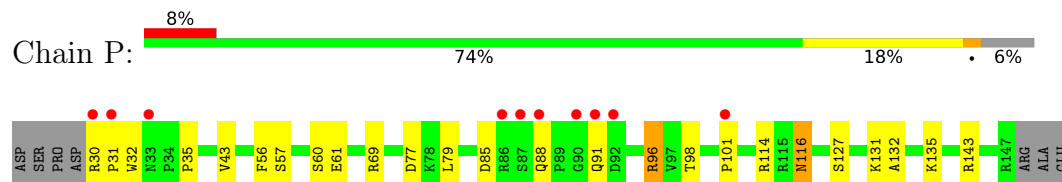
- Molecule 2: light chain



- Molecule 3: Programmed cell death protein 1



- Molecule 3: Programmed cell death protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.06Å 62.96Å 81.29Å 105.73° 98.00° 92.44°	Depositor
Resolution (Å)	29.61 – 1.98 29.61 – 1.92	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.61-1.98) 94.5 (29.61-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.92Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.187 , 0.235 0.188 , 0.235	Depositor DCC
$R_{free}$ test set	3745 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtrriage
Anisotropy	0.199	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2121e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.41	0/1629	0.63	1/2216 (0.0%)
1	H	0.44	0/1620	0.64	0/2205
2	B	0.44	0/1658	0.66	0/2256
2	L	0.43	0/1658	0.67	0/2256
3	P	0.42	0/957	0.75	1/1299 (0.1%)
3	Q	0.40	0/882	0.68	0/1196
All	All	0.43	0/8404	0.67	2/11428 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	101	PRO	N-CD-CG	-5.93	94.31	103.20
1	A	99	TRP	C-N-CA	-5.31	111.14	122.30

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	A	1590	0	1559	21	0
1	H	1581	0	1546	22	0
2	B	1621	0	1567	17	0
2	L	1621	0	1567	16	0
3	P	935	0	905	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	862	0	840	25	0
4	A	142	0	0	3	0
4	B	139	0	0	2	0
4	H	132	0	0	7	0
4	L	140	0	0	7	0
4	P	37	0	0	3	0
4	Q	54	0	0	4	0
All	All	8854	0	7984	112	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 7.

The worst 5 of 112 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:P:116:ASN:ND2	4:P:201:HOH:O	1.91	1.03
3:Q:139:ARG:NH2	4:Q:201:HOH:O	2.09	0.84
3:P:114:ARG:NH2	4:P:202:HOH:O	2.10	0.84
2:B:39:LYS:H	2:B:42:LYS:HE3	1.42	0.83
1:H:205:LYS:HD2	1:H:206:PRO:HD3	1.61	0.81

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	208/229 (91%)	205 (99%)	3 (1%)	0	100 100
1	H	207/229 (90%)	203 (98%)	4 (2%)	0	100 100
2	B	210/214 (98%)	203 (97%)	7 (3%)	0	100 100
2	L	210/214 (98%)	206 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	116/125 (93%)	112 (97%)	4 (3%)	0	100	100
3	Q	105/125 (84%)	102 (97%)	3 (3%)	0	100	100
All	All	1056/1136 (93%)	1031 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	177/193 (92%)	172 (97%)	5 (3%)	43	32
1	H	176/193 (91%)	169 (96%)	7 (4%)	31	19
2	B	186/188 (99%)	181 (97%)	5 (3%)	44	35
2	L	186/188 (99%)	183 (98%)	3 (2%)	62	56
3	P	104/110 (94%)	99 (95%)	5 (5%)	25	13
3	Q	96/110 (87%)	91 (95%)	5 (5%)	23	11
All	All	925/982 (94%)	895 (97%)	30 (3%)	39	28

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Q	98	THR
3	P	96	ARG
1	H	85	SER
3	P	131	LYS
2	L	181	LEU

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

Mol	Chain	Res	Type
1	A	74	ASN
1	A	203	ASN

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Mol	Chain	Res	Type
2	B	93	ASN
3	Q	133	GLN
3	P	116	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<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	212/229 (92%)	0.03	6 (2%) 53 55	24, 34, 54, 64	0
1	H	211/229 (92%)	0.10	9 (4%) 35 37	24, 37, 52, 64	0
2	B	212/214 (99%)	-0.08	1 (0%) 91 91	23, 33, 50, 61	0
2	L	212/214 (99%)	0.05	5 (2%) 59 61	24, 34, 50, 68	0
3	P	118/125 (94%)	0.35	10 (8%) 10 12	30, 44, 80, 99	0
3	Q	109/125 (87%)	0.06	5 (4%) 32 34	29, 41, 62, 84	0
All	All	1074/1136 (94%)	0.06	36 (3%) 45 48	23, 36, 55, 99	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	88	GLN	6.8
3	P	91	GLN	5.4
3	P	92	ASP	5.2
3	P	86	ARG	4.8
3	P	87	SER	4.4

### 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.