

# wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 22, 2023 – 11:23 AM JST

PDB ID : 7VG7

Title : Plexin B1 extracellular fragment in complex with lasso-grafted PB1m6A9 pep-

tide

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J.

Deposited on : 2021-09-14

Resolution : 2.50 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

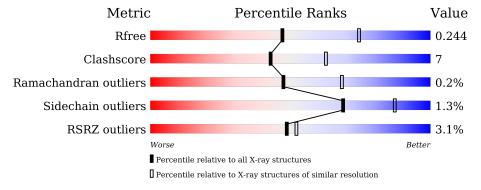
Validation Pipeline (wwPDB-VP) : 2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.50 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	525	79%	14% • 6%
2	В	160	69%	22% • 9%



## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5047 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 Plexin-B1.

$\mathbf{Mol}$	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	496	Total 3763	C 2365	N 656	O 720	S 22	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	THR	engineered mutation	UNP O43157
A	536	THR	-	expression tag	UNP O43157
A	537	ARG	-	expression tag	UNP O43157
A	538	GLU	-	expression tag	UNP O43157
A	539	ASN	-	expression tag	UNP O43157
A	540	LEU	-	expression tag	UNP O43157
A	541	TYR	-	expression tag	UNP O43157
A	542	PHE	-	expression tag	UNP O43157
A	543	GLN	-	expression tag	UNP O43157

• Molecule 2 is a protein called Uteroglobin, PB1m6A9 peptide, Uteroglobin.

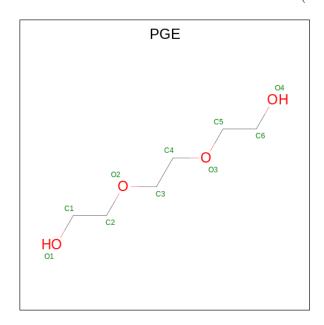
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	146	Total 1160	C 734	N 195	O 221	S 10	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	21	SER	ALA	engineered mutation	UNP P11684
В	175	HIS	-	expression tag	UNP P11684
В	176	HIS	-	expression tag	UNP P11684
В	177	HIS	-	expression tag	UNP P11684
В	178	HIS	-	expression tag	UNP P11684
В	179	HIS	-	expression tag	UNP P11684
В	180	HIS	-	expression tag	UNP P11684

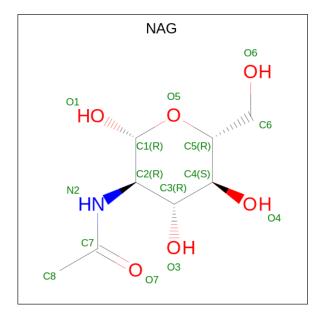


• Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total C 10 6	O 4	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 8	N 1	O 5	0	0



#### • Molecule 5 is water.

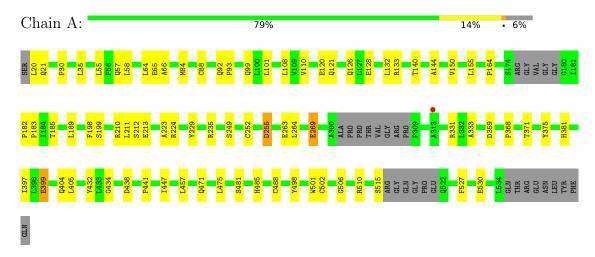
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	92	Total O 92 92	0	0
5	В	8	Total O 8 8	0	0



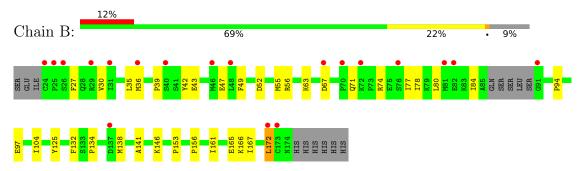
# 3 Residue-property plots (i)

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: Plexin-B1



• Molecule 2: Uteroglobin, PB1m6A9 peptide, Uteroglobin





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	69.19Å 62.49Å 82.60Å	Donogitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $111.92^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.78 - 2.50	Depositor
Resolution (A)	48.43 - 2.50	EDS
% Data completeness	100.0 (44.78-2.50)	Depositor
(in resolution range)	94.4 (48.43-2.50)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
D.D.	0.180 , 0.243	Depositor
$R, R_{free}$	0.181 , $0.244$	DCC
$R_{free}$ test set	1123 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.663	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 49.5	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5047	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $<L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, NAG

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		nd lengths	Bond angles		
IVIOI		RMSZ	# Z  > 5	RMSZ	# Z >5	
1	A	0.55	$4/3857 \ (0.1\%)$	0.68	3/5268 (0.1%)	
2	В	0.44	0/1180	0.68	2/1590 (0.1%)	
All	All	0.53	4/5037 (0.1%)	0.68	5/6858 (0.1%)	

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
1	A	399	GLU	CG-CD	8.07	1.64	1.51
1	A	269	GLU	CB-CG	7.05	1.65	1.52
1	A	399	GLU	CB-CG	6.92	1.65	1.52
1	A	269	GLU	CG-CD	5.93	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
2	В	172	LEU	CB-CG-CD2	-13.30	88.39	111.00
1	A	399	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	A	132	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	457	LEU	CA-CB-CG	5.14	127.13	115.30
2	В	172	LEU	CA-CB-CG	5.05	126.91	115.30

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3763	0	3613	44	0
2	В	1160	0	1183	23	0
3	A	10	0	14	1	0
4	A	14	0	13	1	0
5	A	92	0	0	1	0
5	В	8	0	0	0	0
All	A11	5047	0	4823	66	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 66 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:99:GLN:HG2	1:A:144:ALA:HB1	1.63	0.78
1:A:404:GLN:NE2	1:A:405:LEU:O	2.21	0.73
1:A:30:PRO:HG3	1:A:35:LEU:HD21	1.70	0.73
1:A:331:ARG:HG3	4:A:602:NAG:H81	1.74	0.69
1:A:210:ARG:HB3	1:A:213:GLU:HG3	1.74	0.69

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	Perce	ntiles
1	A	488/525 (93%)	470 (96%)	17 (4%)	1 (0%)	47	68
2	В	142/160 (89%)	136 (96%)	6 (4%)	0	100	100
All	All	$630/685 \; (92\%)$	606 (96%)	23 (4%)	1 (0%)	47	68

All (1) Ramachandran outliers are listed below:



Mol	Chain	$\operatorname{Res}$	Type
1	A	255	ASP

#### 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	Rotameric Outliers	
1	A	402/424~(95%)	397 (99%)	5 (1%)	71 88
2	В	131/145 (90%)	129 (98%)	2 (2%)	65 85
All	All	533/569 (94%)	526 (99%)	7 (1%)	69 87

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	SER
1	A	527	PHE
2	В	166	LYS
2	В	71	GLN
1	A	471	GLN

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	21	GLN
1	A	158	GLN
1	A	256	GLN
1	A	449	GLN
2	В	136	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PGE	A	601	-	9,9,9	0.42	0	8,8,8	0.39	0
4	NAG	A	602	1	14,14,15	0.37	0	17,19,21	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	A	601	-	-	4/7/7/7	-
4	NAG	A	602	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	NAG	O5-C5-C6-O6
4	A	602	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	601	PGE	O1-C1-C2-O2
3	A	601	PGE	C4-C3-O2-C2
3	A	601	PGE	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	PGE	1	0
4	A	602	NAG	1	0

### 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,  $95^{th}$  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	$\begin{array}{c cccc} \textbf{Analysed} & <& \textbf{RSRZ}> & \#\textbf{RSRZ}> \textbf{2} \end{array}$		$OWAB(A^2)$	Q < 0.9
1	A	$496/525 \ (94\%)$	-0.21	1 (0%) 95 95	11, 22, 46, 58	0
2	В	146/160 (91%)	0.72	19 (13%) 3 3	13, 53, 74, 92	0
All	All	642/685 (93%)	0.00	20 (3%) 49 52	11, 26, 63, 92	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	173	CYS	4.5
2	В	70	PRO	3.7
2	В	46	MET	3.5
2	В	31	ILE	3.3
2	В	25	PRO	3.2

### 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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	NAG	A	602	14/15	0.90	0.18	32,39,47,48	0
3	PGE	A	601	10/10	0.91	0.24	25,33,40,40	0

# 6.5 Other polymers (i)

There are no such residues in this entry.

