



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:56 AM UTC

PDB ID : 7UVS / pdb_00007uvs
Title : Pfs230 domain 1 bound by LMIV230-02 Fab
Authors : Ivanochko, D.; Julien, J.P.
Deposited on : 2022-05-02
Resolution : 2.06 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

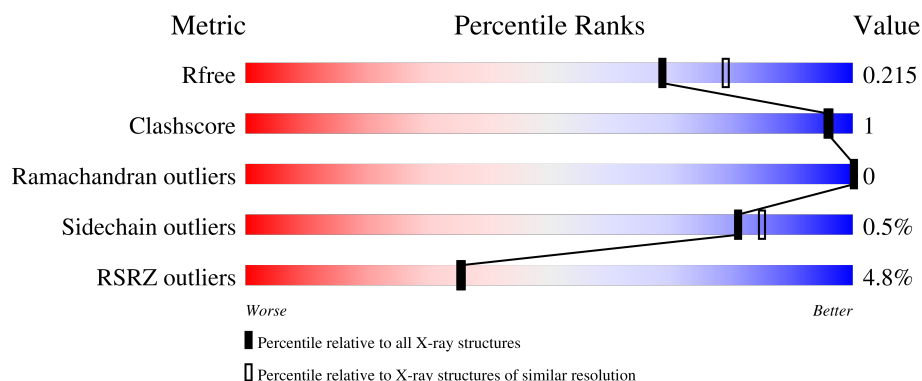
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	A	226	5% 94% 6%
1	D	226	7% 95% • •
2	B	221	97% •
2	E	221	98% •
3	C	199	3% 88% • 10%

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Mol	Chain	Length	Quality of chain
3	F	199	12% 83% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10235 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 LMIV230-02 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1662	1045	275	336	6			
1	D	223	Total	C	N	O	S	0	0	0
			1640	1034	271	330	5			

- Molecule 2 is a protein called LMIV230-02 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1710	1071	289	344	6			
2	E	220	Total	C	N	O	S	0	0	0
			1704	1068	288	343	5			

- Molecule 3 is a protein called Gametocyte surface protein P230.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	180	Total	C	N	O	S	0	0	0
			1431	915	222	290	4			
3	F	172	Total	C	N	O	S	0	0	0
			1374	881	213	276	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	585	GLN	ASN	conflict	UNP P68874
C	732	GLY	-	expression tag	UNP P68874
C	733	SER	-	expression tag	UNP P68874
C	734	LEU	-	expression tag	UNP P68874
C	735	LYS	-	expression tag	UNP P68874
C	736	GLU	-	expression tag	UNP P68874
C	737	ASN	-	expression tag	UNP P68874
C	738	LEU	-	expression tag	UNP P68874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	739	TYR	-	expression tag	UNP P68874
C	740	PHE	-	expression tag	UNP P68874
C	741	GLN	-	expression tag	UNP P68874
C	742	GLY	-	expression tag	UNP P68874
C	743	TRP	-	expression tag	UNP P68874
C	744	SER	-	expression tag	UNP P68874
C	745	HIS	-	expression tag	UNP P68874
C	746	PRO	-	expression tag	UNP P68874
C	747	GLN	-	expression tag	UNP P68874
C	748	PHE	-	expression tag	UNP P68874
C	749	GLU	-	expression tag	UNP P68874
C	750	LYS	-	expression tag	UNP P68874
F	585	GLN	ASN	conflict	UNP P68874
F	732	GLY	-	expression tag	UNP P68874
F	733	SER	-	expression tag	UNP P68874
F	734	LEU	-	expression tag	UNP P68874
F	735	LYS	-	expression tag	UNP P68874
F	736	GLU	-	expression tag	UNP P68874
F	737	ASN	-	expression tag	UNP P68874
F	738	LEU	-	expression tag	UNP P68874
F	739	TYR	-	expression tag	UNP P68874
F	740	PHE	-	expression tag	UNP P68874
F	741	GLN	-	expression tag	UNP P68874
F	742	GLY	-	expression tag	UNP P68874
F	743	TRP	-	expression tag	UNP P68874
F	744	SER	-	expression tag	UNP P68874
F	745	HIS	-	expression tag	UNP P68874
F	746	PRO	-	expression tag	UNP P68874
F	747	GLN	-	expression tag	UNP P68874
F	748	PHE	-	expression tag	UNP P68874
F	749	GLU	-	expression tag	UNP P68874
F	750	LYS	-	expression tag	UNP P68874

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Na 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	147	Total 147	O 147	0	0
5	B	140	Total 140	O 140	0	0
5	C	123	Total 123	O 123	0	0
5	D	122	Total 122	O 122	0	0
5	E	166	Total 166	O 166	0	0
5	F	15	Total 15	O 15	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: LMIV230-02 Fab heavy chain



- Molecule 1: LMIV230-02 Fab heavy chain



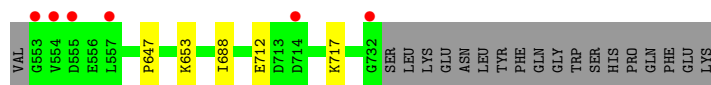
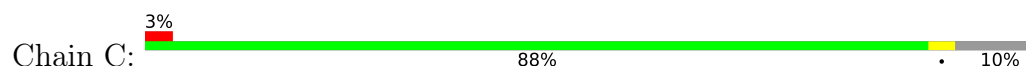
- Molecule 2: LMIV230-02 Fab light chain



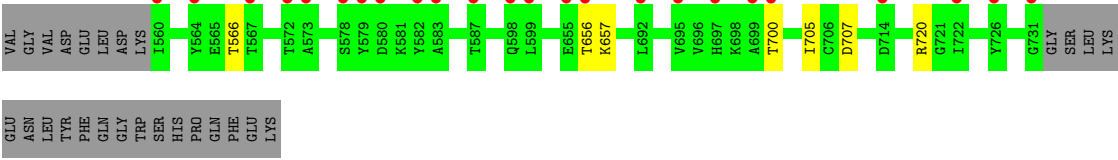
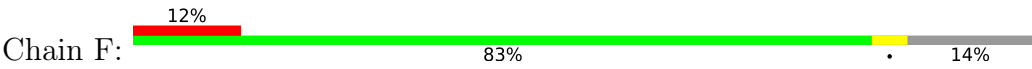
- Molecule 2: LMIV230-02 Fab light chain



- Molecule 3: Gametocyte surface protein P230



- Molecule 3: Gametocyte surface protein P230



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.36Å 132.47Å 125.07Å 90.00° 102.35° 90.00°	Depositor
Resolution (Å)	29.85 – 2.06 29.85 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.85-2.06) 99.1 (29.85-2.06)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.06Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.174 , 0.215 0.175 , 0.215	Depositor DCC
R_{free} test set	2020 reflections (2.25%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10235	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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

5.1 Standard geometry

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

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	0.40	0/1703	0.60	0/2320
1	D	0.32	0/1681	0.54	0/2292
2	B	0.34	0/1748	0.58	0/2373
2	E	0.35	0/1742	0.58	0/2365
3	C	0.39	0/1457	0.66	0/1970
3	F	0.27	0/1400	0.64	0/1894
All	All	0.35	0/9731	0.60	0/13214

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

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	1662	0	1616	6	0
1	D	1640	0	1596	4	0
2	B	1710	0	1660	2	0
2	E	1704	0	1656	2	0
3	C	1431	0	1437	3	0
3	F	1374	0	1384	3	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	147	0	0	0	0
5	B	140	0	0	0	0
5	C	123	0	0	0	0
5	D	122	0	0	0	0
5	E	166	0	0	0	0
5	F	15	0	0	0	0
All	All	10235	0	9349	20	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 1.

All (20) 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:D:67:VAL:HG22	1:D:82:VAL:HG22	1.85	0.59
2:B:78:LEU:HD11	2:B:104:LEU:HD21	1.90	0.53
1:A:30:ASN:O	1:A:53:SER:OG	2.28	0.52
2:E:54:ARG:NH1	2:E:62:PHE:O	2.44	0.49
1:A:67:VAL:HG22	1:A:82:VAL:HG22	1.94	0.48
3:C:712:GLU:HG2	3:C:717:LYS:HG2	1.96	0.47
3:C:647:PRO:HB3	3:C:688:ILE:HD12	1.96	0.47
3:F:707:ASP:OD2	3:F:720:ARG:NH1	2.49	0.46
1:A:83:ARG:NH1	1:A:85:GLU:OE1	2.49	0.45
3:C:653:LYS:HE2	3:C:653:LYS:HB3	1.75	0.44
3:F:656:THR:HB	3:F:657:LYS:HE2	1.99	0.44
1:D:60:ALA:HB3	1:D:63:PHE:HD2	1.84	0.43
1:A:12:LYS:HE2	1:A:18:VAL:HG23	2.01	0.42
1:D:12:LYS:HG3	1:D:18:VAL:HB	2.02	0.42
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.03	0.41
1:A:128:SER:N	1:A:216:CYS:OXT	2.54	0.41
2:B:40:PRO:HG2	2:B:166:GLU:HG3	2.02	0.41
2:E:27(D):TYR:CZ	2:E:27(F):SER:HB2	2.56	0.40
1:D:145:TYR:CE2	1:D:150:VAL:HG13	2.56	0.40
3:F:705:ILE:HD13	3:F:720:ARG:NH2	2.36	0.40

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	224/226 (99%)	222 (99%)	2 (1%)	0	100	100
1	D	221/226 (98%)	219 (99%)	2 (1%)	0	100	100
2	B	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
2	E	218/221 (99%)	212 (97%)	6 (3%)	0	100	100
3	C	178/199 (89%)	173 (97%)	5 (3%)	0	100	100
3	F	170/199 (85%)	163 (96%)	7 (4%)	0	100	100
All	All	1230/1292 (95%)	1202 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	187/187 (100%)	186 (100%)	1 (0%)	81	85
1	D	184/187 (98%)	184 (100%)	0	100	100
2	B	194/194 (100%)	192 (99%)	2 (1%)	68	71
2	E	193/194 (100%)	193 (100%)	0	100	100
3	C	167/185 (90%)	167 (100%)	0	100	100
3	F	161/185 (87%)	159 (99%)	2 (1%)	63	65
All	All	1086/1132 (96%)	1081 (100%)	5 (0%)	81	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	PHE
2	B	60	ASP
2	B	215	CYS
3	F	566	THR
3	F	700	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	D	192	GLN
1	D	199	ASN
2	E	37	GLN
2	E	138	ASN
2	E	190	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 [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	A	226/226 (100%)	-0.03	11 (4%) 35 35	24, 36, 81, 151	0
1	D	223/226 (98%)	0.16	16 (7%) 21 21	24, 43, 95, 130	0
2	B	221/221 (100%)	-0.28	1 (0%) 87 89	24, 36, 58, 125	0
2	E	220/221 (99%)	-0.25	1 (0%) 87 89	23, 37, 61, 82	0
3	C	180/199 (90%)	-0.21	6 (3%) 49 49	23, 35, 71, 99	0
3	F	172/199 (86%)	1.19	24 (13%) 6 6	58, 88, 126, 160	0
All	All	1242/1292 (96%)	0.07	59 (4%) 35 35	23, 41, 102, 160	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	130	SER	6.8
1	A	29	PHE	4.9
1	D	133	GLY	4.9
3	F	656	THR	4.2
3	F	560	ILE	4.1
3	F	731	GLY	4.0
2	B	215	CYS	3.7
1	A	27	GLY	3.5
1	D	131	THR	3.4
1	D	128	SER	3.3
1	D	29	PHE	3.3
3	F	579	TYR	3.2
1	A	26	GLY	3.1
1	A	216	CYS	3.0
1	A	28	THR	3.0
1	A	132	SER	2.9
3	C	555	ASP	2.8
1	D	129	LYS	2.8
1	A	30	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	27	GLY	2.6
1	A	128	SER	2.6
3	C	732	GLY	2.6
3	F	567	THR	2.5
3	F	598	GLN	2.5
1	D	214	LYS	2.5
2	E	1	GLU	2.5
3	F	578	SER	2.4
3	F	564	TYR	2.4
3	F	699	ALA	2.4
1	A	2	VAL	2.3
3	C	557	LEU	2.3
1	D	25	SER	2.3
1	A	131	THR	2.3
3	F	572	THR	2.3
3	F	599	LEU	2.3
3	F	655	GLU	2.3
1	D	2	VAL	2.3
3	F	573	ALA	2.3
3	F	580	ASP	2.3
1	D	65	GLY	2.3
3	C	554	VAL	2.2
3	F	582	TYR	2.2
3	F	587	THR	2.2
3	C	553	GLY	2.2
1	D	73	THR	2.2
3	F	692	LEU	2.1
1	D	132	SER	2.1
3	F	714	ASP	2.1
1	D	64	GLN	2.1
3	F	722	ILE	2.1
1	A	133	GLY	2.1
3	F	695	VAL	2.1
3	F	700	THR	2.1
3	C	714	ASP	2.1
3	F	726	TYR	2.1
3	F	583	ALA	2.1
3	F	697	HIS	2.0
1	D	71	THR	2.0
1	D	127	SER	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](#)

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, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	C	801	1/1	0.97	0.08	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.