



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 7UFW / pdb_00007ufw
Title : Pfs230 D1D2 in complex with LMIV230-01
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Deposited on : 2022-03-23
Resolution : 2.10 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 ⓘ 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

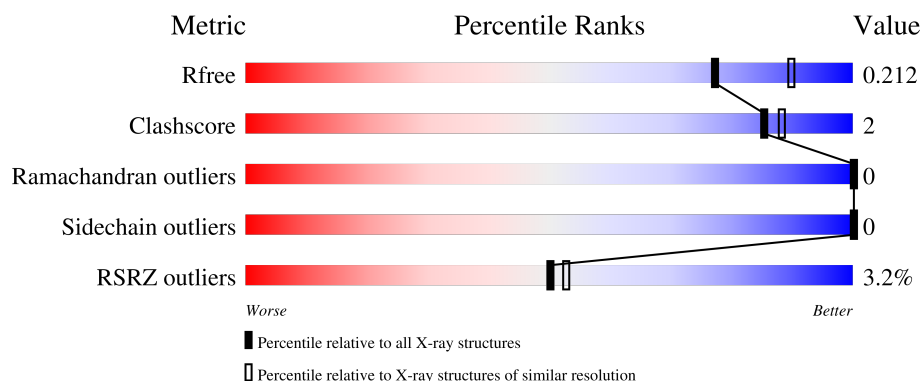
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	H	261	2% 80% 8% 12%
1	I	261	% 82% 6% 13%
2	A	355	4% 84% 5% 12%
2	B	355	4% 86% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17571 atoms, of which 8579 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 LMIV230-01.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	229	Total	C	H	N	O	S	0	0	0
			3483	1110	1728	299	339	7			
1	I	228	Total	C	H	N	O	S	0	0	0
			3476	1108	1725	298	338	7			

- Molecule 2 is a protein called Gametocyte surface protein P230.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	314	Total	C	H	N	O	S	0	0	0
			5082	1633	2545	396	496	12			
2	B	320	Total	C	H	N	O	S	0	0	0
			5164	1659	2581	405	507	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	540	THR	-	expression tag	UNP P68874
A	541	GLY	-	expression tag	UNP P68874
A	887	GLY	-	expression tag	UNP P68874
A	888	THR	-	expression tag	UNP P68874
A	889	HIS	-	expression tag	UNP P68874
A	890	HIS	-	expression tag	UNP P68874
A	891	HIS	-	expression tag	UNP P68874
A	892	HIS	-	expression tag	UNP P68874
A	893	HIS	-	expression tag	UNP P68874
A	894	HIS	-	expression tag	UNP P68874
B	540	THR	-	expression tag	UNP P68874
B	541	GLY	-	expression tag	UNP P68874
B	887	GLY	-	expression tag	UNP P68874
B	888	THR	-	expression tag	UNP P68874
B	889	HIS	-	expression tag	UNP P68874
B	890	HIS	-	expression tag	UNP P68874

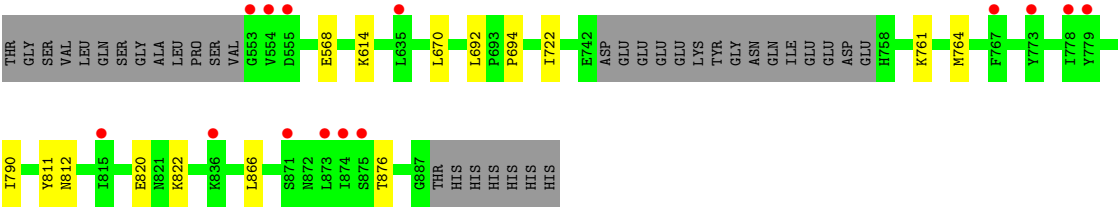
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Chain	Residue	Modelled	Actual	Comment	Reference
B	891	HIS	-	expression tag	UNP P68874
B	892	HIS	-	expression tag	UNP P68874
B	893	HIS	-	expression tag	UNP P68874
B	894	HIS	-	expression tag	UNP P68874

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	111	Total 111	O 111	0	0
3	I	85	Total 85	O 85	0	0
3	A	99	Total 99	O 99	0	0
3	B	71	Total 71	O 71	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.44Å 151.37Å 99.04Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	19.92 – 2.10 19.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.92-2.10) 99.5 (19.92-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.09Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.190 , 0.213 0.190 , 0.212	Depositor DCC
R_{free} test set	3783 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.094 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17571	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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 [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	H	0.14	0/1794	0.35	0/2428
1	I	0.13	0/1790	0.34	0/2423
2	A	0.14	0/2587	0.38	0/3493
2	B	0.14	0/2634	0.39	0/3557
All	All	0.14	0/8805	0.37	0/11901

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 [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	H	1755	1728	1730	10	0
1	I	1751	1725	1727	8	0
2	A	2537	2545	2545	10	0
2	B	2583	2581	2580	9	0
3	A	99	0	0	1	0
3	B	71	0	0	1	0
3	H	111	0	0	0	0
3	I	85	0	0	1	0
All	All	8992	8579	8582	37	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 2.

The worst 5 of 37 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)
2:B:866:LEU:HD12	2:B:876:THR:HB	1.60	0.83
1:I:221:LEU:HD21	1:I:247:LEU:HD21	1.74	0.69
2:A:844:ASN:ND2	3:A:901:HOH:O	2.26	0.68
1:H:176:LEU:HD22	1:H:214:PHE:CG	2.29	0.67
1:H:46:GLU:OE2	1:H:63:LYS:NZ	2.31	0.59

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	H	225/261 (86%)	220 (98%)	5 (2%)	0	100	100
1	I	224/261 (86%)	218 (97%)	6 (3%)	0	100	100
2	A	310/355 (87%)	296 (96%)	14 (4%)	0	100	100
2	B	316/355 (89%)	300 (95%)	16 (5%)	0	100	100
All	All	1075/1232 (87%)	1034 (96%)	41 (4%)	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	H	188/200 (94%)	188 (100%)	0	100	100
1	I	188/200 (94%)	188 (100%)	0	100	100
2	A	295/331 (89%)	295 (100%)	0	100	100
2	B	300/331 (91%)	300 (100%)	0	100	100
All	All	971/1062 (91%)	971 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	776	ASN
2	B	735	ASN
2	A	844	ASN
2	A	586	ASN
2	A	859	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 oligosaccharides 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 ⓘ

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, 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	H	229/261 (87%)	-0.17	4 (1%) 69 71	37, 48, 77, 127	0
1	I	228/261 (87%)	-0.12	3 (1%) 75 77	37, 51, 83, 156	0
2	A	314/355 (88%)	0.20	14 (4%) 38 40	38, 60, 117, 187	0
2	B	320/355 (90%)	0.28	14 (4%) 39 41	40, 63, 133, 161	0
All	All	1091/1232 (88%)	0.08	35 (3%) 50 53	37, 55, 111, 187	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	873	LEU	4.5
2	B	779	TYR	3.7
2	B	553	GLY	3.7
2	A	873	LEU	3.7
2	A	875	SER	3.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.