



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7UA2 / pdb_00007ua2
Title : Pfs230 D1 domain in complex with 230AL-18
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Deposited on : 2022-03-11
Resolution : 2.19 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

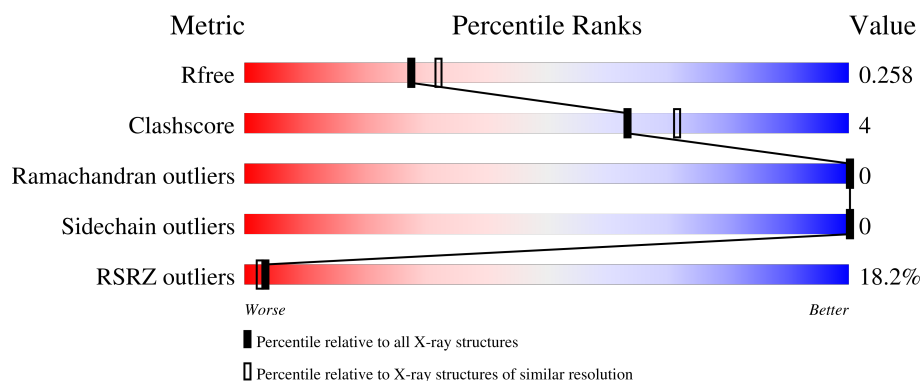
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	191	10% 85% 6% 9%
2	B	261	32% 79% 7% 14%
3	H	260	4% 77% 11% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9755 atoms, of which 4809 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 Gametocyte surface protein P230.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	174	Total	C	H	N	O	S	0	0	0
			2795	891	1404	217	279	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	585	GLN	ASN	engineered mutation	UNP P68874

- Molecule 2 is a protein called LMIV230-01.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	224	Total	C	H	N	O	S	0	0	0
			3413	1091	1692	290	333	7			

- Molecule 3 is a protein called 230AL-18.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	229	Total	C	H	N	O	S	0	0	0
			3478	1110	1713	307	340	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	9	Total	O	0	0
			9	9		
4	H	42	Total	O	0	0
			42	42		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.65Å 77.93Å 58.78Å 90.00° 99.22° 90.00°	Depositor
Resolution (Å)	36.56 – 2.19 36.56 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.1 (36.56-2.19) 97.2 (36.56-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.222 , 0.256 0.222 , 0.258	Depositor DCC
R_{free} test set	1703 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9755	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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

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	0.20	0/1417	0.39	0/1916
2	B	0.18	0/1760	0.35	0/2385
3	H	0.27	0/1805	0.44	0/2446
All	All	0.22	0/4982	0.39	0/6747

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	1391	1404	1403	7	0
2	B	1721	1692	1693	11	0
3	H	1765	1713	1715	22	0
4	A	18	0	0	0	0
4	B	9	0	0	0	0
4	H	42	0	0	0	0
All	All	4946	4809	4811	39	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.

All (39) 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:H:153:LEU:HD11	3:H:161:VAL:HG21	1.73	0.69
3:H:18:LEU:HB2	3:H:83:MET:HE3	1.79	0.65
1:A:568:GLU:O	1:A:722:ILE:HD11	1.97	0.65
3:H:40:ALA:HB3	3:H:43:LYS:HD3	1.82	0.61
2:B:154:LEU:HD22	2:B:156:LEU:HD11	1.83	0.61
3:H:155:LEU:CD1	3:H:161:VAL:HB	2.31	0.59
2:B:164:LEU:HG	2:B:245:THR:HG21	1.86	0.58
3:H:225:PHE:CD1	3:H:248:GLU:HA	2.40	0.57
1:A:663:LEU:HG	1:A:670:LEU:HD22	1.88	0.56
3:H:221:GLU:O	3:H:249:ILE:HD13	2.05	0.56
1:A:670:LEU:HD13	1:A:692:LEU:HD23	1.88	0.56
3:H:179:GLN:HB2	3:H:189:LEU:HD11	1.89	0.55
3:H:224:ASP:HB2	3:H:249:ILE:HD11	1.89	0.54
1:A:670:LEU:HD12	1:A:691:THR:O	2.09	0.53
3:H:224:ASP:HB2	3:H:249:ILE:CD1	2.40	0.51
2:B:174:SER:O	2:B:193:LYS:O	2.28	0.51
3:H:150:PRO:O	3:H:245:THR:HG23	2.11	0.51
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.91	0.51
3:H:155:LEU:HD11	3:H:161:VAL:HB	1.91	0.51
2:B:176:LEU:HD22	2:B:214:PHE:CG	2.45	0.50
3:H:12:VAL:HG11	3:H:86:LEU:CD1	2.43	0.48
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.95	0.48
3:H:12:VAL:HG11	3:H:86:LEU:HD13	1.95	0.47
2:B:176:LEU:HD12	2:B:232:GLN:O	2.15	0.47
2:B:147:MET:HE3	2:B:166:CYS:SG	2.54	0.47
3:H:155:LEU:HD22	3:H:159:GLU:OE1	2.17	0.45
2:B:151:PRO:O	2:B:245:THR:HG23	2.16	0.45
1:A:564:TYR:OH	1:A:642:VAL:HG11	2.18	0.44
3:H:196:ARG:HD3	3:H:204:PHE:O	2.18	0.44
2:B:102:ARG:O	2:B:103:ALA:HB3	2.19	0.43
2:B:176:LEU:O	2:B:193:LYS:O	2.36	0.43
1:A:585:GLN:HG3	3:H:105:ALA:HB2	2.01	0.43
2:B:104:VAL:HG13	2:B:234:TYR:CZ	2.55	0.42
1:A:654:GLU:O	1:A:655:GLU:CG	2.67	0.42
2:B:3:GLN:C	2:B:4:LEU:HD12	2.44	0.42
3:H:68:PHE:HA	3:H:82:GLN:O	2.20	0.42
3:H:225:PHE:HD1	3:H:248:GLU:HA	1.85	0.41
3:H:236:TRP:HB2	3:H:237:PRO:HA	2.01	0.41
3:H:154:SER:HA	3:H:248:GLU:O	2.22	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	172/191 (90%)	168 (98%)	4 (2%)	0	100	100
2	B	220/261 (84%)	212 (96%)	8 (4%)	0	100	100
3	H	225/260 (86%)	217 (96%)	8 (4%)	0	100	100
All	All	617/712 (87%)	597 (97%)	20 (3%)	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	163/177 (92%)	163 (100%)	0	100	100
2	B	185/200 (92%)	185 (100%)	0	100	100
3	H	190/203 (94%)	190 (100%)	0	100	100
All	All	538/580 (93%)	538 (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. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	170	HIS
3	H	184	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 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 [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	174/191 (91%)	1.07	20 (11%) 9 7	42, 62, 99, 120	0
2	B	224/261 (85%)	1.92	84 (37%) 1 0	49, 95, 169, 231	0
3	H	229/260 (88%)	0.53	10 (4%) 39 36	37, 49, 69, 87	0
All	All	627/712 (88%)	1.18	114 (18%) 3 2	37, 61, 133, 231	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	247	LEU	6.1
2	B	194	ALA	6.0
2	B	249	ILE	5.6
2	B	159	GLY	5.3
2	B	227	ALA	5.3
2	B	162	ALA	5.2
2	B	221	LEU	5.1
2	B	158	LEU	4.8
2	B	218	ILE	4.8
2	B	226	PHE	4.4
2	B	220	SER	4.3
2	B	163	THR	4.1
2	B	244	GLY	4.1
2	B	156	LEU	4.1
2	B	175	TRP	4.1
2	B	178	TRP	3.9
2	B	245	THR	3.9
2	B	205	PHE	3.8
2	B	207	GLY	3.7
2	B	172	ILE	3.6
3	H	249	ILE	3.6
2	B	179	TYR	3.6
2	B	191	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	234	TYR	3.6
2	B	223	PRO	3.5
2	B	155	ALA	3.4
3	H	121	SER	3.4
2	B	229	TYR	3.4
2	B	228	THR	3.4
1	A	670	LEU	3.4
2	B	152	ALA	3.3
2	B	201	VAL	3.3
1	A	602	THR	3.3
2	B	195	SER	3.3
2	B	176	LEU	3.3
3	H	225	PHE	3.2
2	B	164	LEU	3.2
2	B	202	PRO	3.2
2	B	56	ASP	3.2
2	B	216	LEU	3.1
2	B	165	TYR	3.0
2	B	198	GLU	3.0
2	B	186	ALA	3.0
2	B	190	LEU	3.0
1	A	732	ASN	3.0
2	B	192	TYR	3.0
2	B	11	VAL	3.0
2	B	68	VAL	2.9
1	A	698	LYS	2.9
2	B	232	GLN	2.9
2	B	199	SER	2.9
2	B	197	LEU	2.8
2	B	241	PHE	2.8
2	B	40	ALA	2.8
2	B	168	ALA	2.8
2	B	166	CYS	2.8
3	H	73	ASP	2.7
2	B	242	GLY	2.7
2	B	246	LYS	2.7
3	H	250	LYS	2.7
1	A	706	CYS	2.7
2	B	118	SER	2.6
1	A	635	LEU	2.6
1	A	559	LYS	2.6
1	A	638	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	214	PHE	2.5
2	B	104	VAL	2.5
2	B	211	GLY	2.5
2	B	144	ASP	2.5
2	B	239	TRP	2.5
1	A	587	THR	2.4
1	A	677	ASN	2.4
1	A	601	PRO	2.4
2	B	189	LEU	2.4
2	B	196	THR	2.4
2	B	231	CYS	2.4
3	H	155	LEU	2.3
2	B	42	GLY	2.3
2	B	63	LYS	2.3
2	B	1	GLN	2.3
2	B	180	GLN	2.3
1	A	715	ASN	2.3
1	A	633	GLU	2.3
1	A	588	ASN	2.3
2	B	177	ALA	2.3
1	A	689	GLU	2.3
2	B	222	GLN	2.3
2	B	187	PRO	2.3
2	B	174	SER	2.2
1	A	560	ILE	2.2
1	A	678	GLU	2.2
3	H	143	GLU	2.2
2	B	153	SER	2.2
2	B	147	MET	2.2
2	B	225	ASP	2.2
2	B	200	GLY	2.2
2	B	243	GLN	2.2
2	B	203	SER	2.2
3	H	56	ARG	2.2
1	A	687	VAL	2.1
2	B	10	GLU	2.1
2	B	69	THR	2.1
3	H	248	GLU	2.1
1	A	603	GLU	2.1
2	B	93	VAL	2.1
1	A	655	GLU	2.0
2	B	224	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	87	ARG	2.0
2	B	215	THR	2.0
2	B	230	TYR	2.0
2	B	206	SER	2.0
3	H	212	ASP	2.0
2	B	212	THR	2.0
2	B	237	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.