



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 06:43 am BST

PDB ID : 5XKN  
Title : Crystal structure of plant receptor ERL2 in complex with EPFL4  
Authors : Chai, J.; Lin, G.  
Deposited on : 2017-05-08  
Resolution : 3.65 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.

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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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

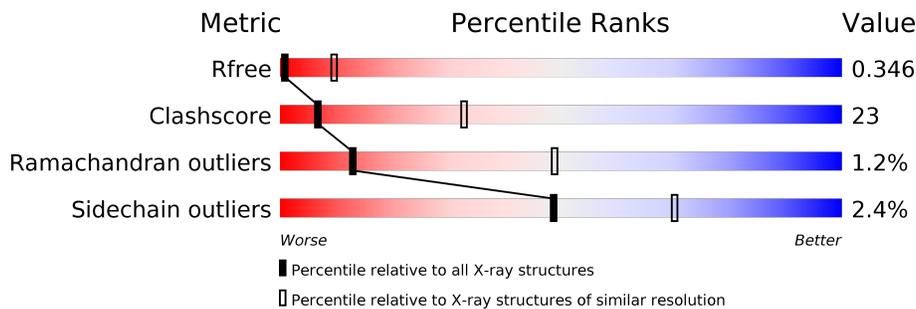
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)

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 on 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	E	51	45% (green), 22% (yellow), 33% (grey)
1	F	51	37% (green), 29% (yellow), 33% (grey)
2	A	552	65% (green), 31% (yellow), .. (grey)
2	B	552	65% (green), 32% (yellow), .. (grey)

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 8824 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 EPIDERMAL PATTERNING FACTOR-like protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	34	269	175	45	45	4	0	0	0
1	F	34	269	175	45	45	4	0	0	0

- Molecule 2 is a protein called LRR receptor-like serine/threonine-protein kinase ERL2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	540	4143	2646	696	785	16	0	0	0
2	B	540	4143	2646	696	785	16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	576	HIS	-	expression tag	UNP Q6XAT2
A	577	HIS	-	expression tag	UNP Q6XAT2
A	578	HIS	-	expression tag	UNP Q6XAT2
A	579	HIS	-	expression tag	UNP Q6XAT2
A	580	HIS	-	expression tag	UNP Q6XAT2
A	581	HIS	-	expression tag	UNP Q6XAT2
B	576	HIS	-	expression tag	UNP Q6XAT2
B	577	HIS	-	expression tag	UNP Q6XAT2
B	578	HIS	-	expression tag	UNP Q6XAT2
B	579	HIS	-	expression tag	UNP Q6XAT2
B	580	HIS	-	expression tag	UNP Q6XAT2
B	581	HIS	-	expression tag	UNP Q6XAT2

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: EPIDERMAL PATTERNING FACTOR-like protein 4

Chain E: 



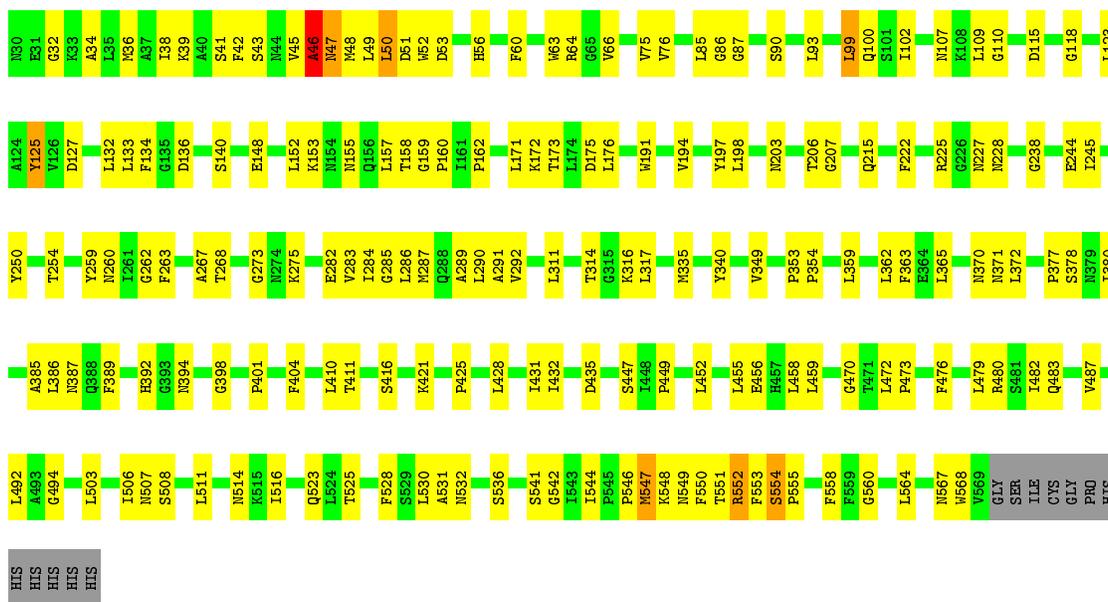
- Molecule 1: EPIDERMAL PATTERNING FACTOR-like protein 4

Chain F: 



- Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL2

Chain A: 



- Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL2

Chain B: 

PRO	V487	N379	N228	N30
HIS	I380	I385	G238	E31
HIS	A385	I386	A124	G32
HIS	I492	N367	Y125	K33
HIS	A493	G388	E244	A34
HIS	G494	F389	I245	I35
HIS	L503	H392	Y250	K36
	I506	G393	T254	A37
	M507	N394	F134	I38
	S508	G398	G135	K39
	L511	P401	D136	S41
	M514	F404	S140	S43
	I516	L410	E148	N44
	Q523	T411	A267	V45
	L524	S416	T268	A46
	T525	K421	G273	N47
	F528	P425	K275	M48
	S529	L428	E282	L49
	L530	I431	V283	L50
	A531	I432	I284	D51
	M532	M493	G285	M52
	S536	L434	L286	D53
	S541	D435	M287	H56
	G542	S447	Q288	D59
	I543	I448	A289	F60
	I544	P449	L290	D61
	P545	L452	A291	S62
	P546	L455	D292	M63
	M547	E456	V292	R64
	K548	H457	L311	G65
	M549	L459	L175	V66
	F550	L469	L176	V75
	T551	G470	L177	V76
	R552	T471	R187	L85
	S554	L472	G315	G86
	P555	P473	K316	G87
	F558	F476	L317	S90
	F559	F476	M335	I93
	G560	L479	Y340	L99
	L564	R480	L359	Q100
	W568	S481	L362	S101
	V569	I482	F363	I102
GLY		S481	E364	M107
SER		R480	L365	K108
ILE		S481	L366	L109
CYS		I482	N370	G110
GLY		Q463	N371	D115
			L372	G118
			P377	
			S378	
			N227	

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.00Å 112.33Å 175.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.30 – 3.65 47.29 – 3.65	Depositor EDS
% Data completeness (in resolution range)	88.7 (47.30-3.65) 88.4 (47.29-3.65)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 3.67Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.282 , 0.312 0.336 , 0.346	Depositor DCC
$R_{free}$ test set	1096 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	93.4	Xtrriage
Anisotropy	0.662	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	8824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<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	E	0.34	0/279	0.59	0/377
1	F	0.34	0/279	0.59	0/377
2	A	0.33	0/4224	0.60	2/5750 (0.0%)
2	B	0.33	0/4224	0.60	2/5750 (0.0%)
All	All	0.33	0/9006	0.60	4/12254 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	46	ALA	CB-CA-C	8.65	123.08	110.10
2	A	46	ALA	CB-CA-C	8.64	123.06	110.10
2	A	51	ASP	N-CA-C	5.60	126.11	111.00
2	B	51	ASP	N-CA-C	5.59	126.10	111.00

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	E	269	0	261	16	0
1	F	269	0	261	21	0
2	A	4143	0	4155	197	4
2	B	4143	0	4158	195	4
All	All	8824	0	8835	413	4

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 23.

The worst 5 of 413 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:525:THR:CB	2:B:550:PHE:HZ	1.33	1.40
2:A:525:THR:CB	2:A:550:PHE:CZ	2.04	1.40
2:A:525:THR:CB	2:A:550:PHE:HZ	1.33	1.38
2:B:525:THR:CB	2:B:550:PHE:CZ	2.04	1.36
2:A:554:SER:HB2	2:A:555:PRO:CD	1.59	1.32

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:349:VAL:CG1	2:B:187:ARG:NE[2_555]	1.63	0.57
2:A:349:VAL:CG1	2:B:187:ARG:CZ[2_555]	1.90	0.30
2:A:567:ASN:O	2:B:48:MET:SD[3_645]	1.95	0.25
2:A:371:ASN:CB	2:B:187:ARG:NH1[2_555]	2.01	0.19

## 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	E	28/51 (55%)	23 (82%)	4 (14%)	1 (4%)	3	29
1	F	28/51 (55%)	23 (82%)	4 (14%)	1 (4%)	3	29
2	A	538/552 (98%)	476 (88%)	56 (10%)	6 (1%)	14	51
2	B	538/552 (98%)	476 (88%)	56 (10%)	6 (1%)	14	51
All	All	1132/1206 (94%)	998 (88%)	120 (11%)	14 (1%)	13	49

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	46	ALA
2	A	546	PRO
2	B	46	ALA
2	B	546	PRO
2	A	432	ILE

### 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	E	31/46 (67%)	31 (100%)	0	100	100
1	F	31/46 (67%)	31 (100%)	0	100	100
2	A	471/481 (98%)	459 (98%)	12 (2%)	47	69
2	B	471/481 (98%)	459 (98%)	12 (2%)	47	69
All	All	1004/1054 (95%)	980 (98%)	24 (2%)	49	70

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	549	ASN
2	B	53	ASP
2	B	549	ASN
2	A	552	ARG
2	B	47	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	549	ASN
2	B	549	ASN
2	B	394	ASN
2	A	394	ASN
2	B	387	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 carbohydrates 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.