



wwPDB X-ray Structure Validation Summary Report ⓘ

May 26, 2020 – 01:53 pm BST

PDB ID : 5XKJ
Title : Crystal structure of plant receptor ERL1-TMM in complexe with EPF2
Authors : Chai, J.; Lin, G.
Deposited on : 2017-05-07
Resolution : 3.48 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 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

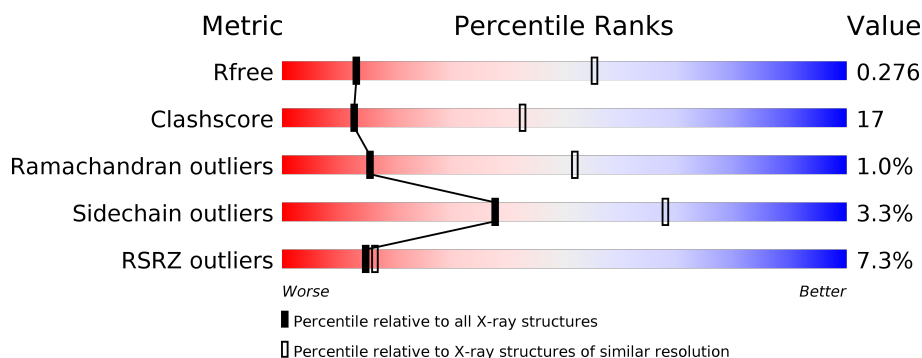
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1379 (3.56-3.40)
Clashscore	141614	1461 (3.56-3.40)
Ramachandran outliers	138981	1424 (3.56-3.40)
Sidechain outliers	138945	1425 (3.56-3.40)
RSRZ outliers	127900	1289 (3.56-3.40)

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 ≥ 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	C	433	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>26%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	433	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>25%</div> <div>•</div> <div>16%</div> </div> </div>
2	E	52	<div> <div>10%</div> <div> <div></div> <div>35%</div> <div>40%</div> <div>6%</div> <div>6%</div> <div>13%</div> </div> </div>
2	F	52	<div> <div>13%</div> <div> <div></div> <div>29%</div> <div>46%</div> <div>6%</div> <div>6%</div> <div>13%</div> </div> </div>
3	A	555	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>26%</div> <div>•</div> <div>8%</div> </div> </div>
3	B	555	<div> <div>9%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>•</div> <div>8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14174 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 Protein TOO MANY MOUTHS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	363	Total	C	N	O	S	0	0	0
			2827	1784	511	522	10			
1	D	363	Total	C	N	O	S	0	0	0
			2827	1784	511	522	10			

- Molecule 2 is a protein called Protein EPIDERMAL PATTERNING FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	45	Total	C	N	O	S	0	0	0
			340	209	63	60	8			
2	F	45	Total	C	N	O	S	0	0	0
			340	209	63	60	8			

- Molecule 3 is a protein called LRR receptor-like serine/threonine-protein kinase ERL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	513	Total	C	N	O	S	0	0	0
			3920	2487	666	752	15			
3	B	513	Total	C	N	O	S	0	0	0
			3920	2487	666	752	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	573	HIS	-	expression tag	UNP C0LGW6
A	574	HIS	-	expression tag	UNP C0LGW6
A	575	HIS	-	expression tag	UNP C0LGW6
A	576	HIS	-	expression tag	UNP C0LGW6
A	577	HIS	-	expression tag	UNP C0LGW6
A	578	HIS	-	expression tag	UNP C0LGW6
B	573	HIS	-	expression tag	UNP C0LGW6
B	574	HIS	-	expression tag	UNP C0LGW6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	575	HIS	-	expression tag	UNP C0LGW6
B	576	HIS	-	expression tag	UNP C0LGW6
B	577	HIS	-	expression tag	UNP C0LGW6
B	578	HIS	-	expression tag	UNP C0LGW6

VAL
ARG
LEU
CYS
ASP
ALA
GLU
THR
SER
SER
ARG
PRO
ALA
PRO
SER
GLY
THR
VAL
GLN
HIS
LEU
SER
SER
ARG
GLU
GLU
ASP
GLY
ALA
LEU

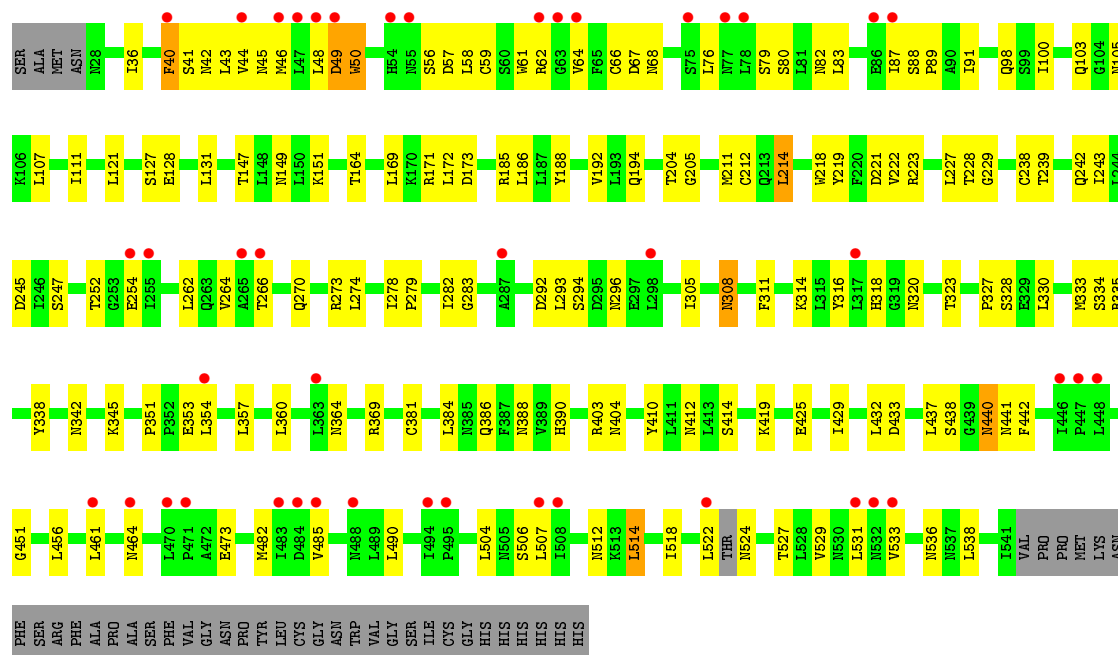
• Molecule 2: Protein EPIDERMAL PATTERNING FACTOR 2



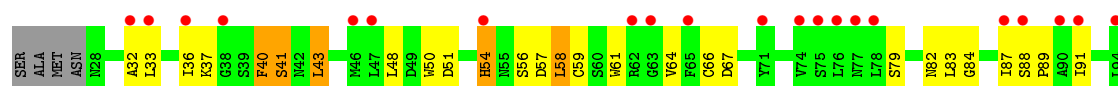
• Molecule 2: Protein EPIDERMAL PATTERNING FACTOR 2



• Molecule 3: LRR receptor-like serine/threonine-protein kinase ERL1



• Molecule 3: LRR receptor-like serine/threonine-protein kinase ERL1



N530	L531	N532	V533	N536	N537	L538	I541	VAL	PRO	PRO	MET	LYS	ASN	PHE	SER	ARG	PHE	ALA	PRO	ALA	SER	PHE	VAL	GLY	ASN	PRO	TYR	LEU	CYS	GLY	ASN	TRP	VAL	GLY	SER	ILE	CYS	GLY	HIS	HIS	HIS	HIS	HIS		
S438	G439	N440	N441	F442	I446	P447	L448	G451	L456	L461	N464	H465	Q469	L470	P471	A472	E473	F474	R478	I479	N480	Q481	M482	V485	N488	L489	P495	L501	L504	N505	S506	L507	I508	N512	K513	L514	I518	L522	THR	N524	C525	F526	T527		
L1315	Y316	L317	H318	G319	N320	T323	P327	L330	N333	S334	R335	Y338	K345	P351	L354	L357	L360	L363	N364	L365	R369	S379	Q386	R390	R403	N404	L405	Y410	L411	N412	L413	S414	E425	L426	L429	N524	C525	F526	T527	L432	D433	L437			
Y219	F220	D221	V222	R223	L227	T228	G229	C238	T239	Q242	L243	L244	D245	I246	S247	E254	I255	L262	D263	V264	A265	T266	L269	Q270	R273	L274	R277	I278	P279	E280	V281	I282	G283	D292	L293	S294	N296	G300	T305	N308	L309	S310	F311	T312	K314
Q98	S99	I100	Q103	G104	N105	K106	L107	A108	G109	L121	E128	Y132	I135	P136	N149	T164	Q165	L169	R170	L171	L172	D173	R185	L186	L187	Y188	H189	N190	E191	V192	L193	Q194	Y195	R199	T204	G205	T206	L207	S208	M211	G212	Q213	L214	L217	W218

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.15Å 65.60Å 142.50Å 102.86° 97.60° 93.58°	Depositor
Resolution (Å)	46.19 – 3.48 47.91 – 3.48	Depositor EDS
% Data completeness (in resolution range)	94.7 (46.19-3.48) 94.8 (47.91-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.254 , 0.277 0.254 , 0.276	Depositor DCC
R_{free} test set	1420 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , -1.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	14174	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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	C	0.31	0/2883	0.54	0/3915
1	D	0.32	0/2883	0.54	0/3915
2	E	0.53	0/347	0.90	2/466 (0.4%)
2	F	0.60	0/347	0.91	1/466 (0.2%)
3	A	0.35	0/3985	0.53	0/5419
3	B	0.34	0/3985	0.55	1/5419 (0.0%)
All	All	0.35	0/14430	0.56	4/19600 (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	F	15	CYS	CA-CB-SG	7.09	126.76	114.00
3	B	214	LEU	N-CA-C	-6.97	92.17	111.00
2	E	15	CYS	CA-CB-SG	6.02	124.84	114.00
2	E	49	PRO	CB-CA-C	-5.00	99.49	112.00

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	C	2827	0	2875	79	1
1	D	2827	0	2875	113	1
2	E	340	0	327	36	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	340	0	327	62	0
3	A	3920	0	3971	124	1
3	B	3920	0	3972	127	2
All	All	14174	0	14347	473	3

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 17.

The worst 5 of 473 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:B:59:CYS:SG	3:B:66:CYS:CB	2.23	1.24
1:D:111:THR:CG2	3:B:194:GLN:OE1	1.89	1.20
1:D:193:HIS:O	1:D:217:ARG:NH1	1.76	1.19
3:A:59:CYS:SG	3:A:66:CYS:SG	1.20	1.16
3:B:41:SER:OG	3:B:83:LEU:O	1.61	1.16

All (3) 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)
1:D:326:LYS:NZ	3:B:404:ASN:O[1_655]	1.86	0.34
1:C:326:LYS:NZ	3:A:404:ASN:O[1_545]	1.89	0.31
2:E:42:ARG:NH1	3:B:54:HIS:NE2[1_565]	2.11	0.09

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	C	361/433 (83%)	316 (88%)	41 (11%)	4 (1%)	14	50
1	D	361/433 (83%)	317 (88%)	41 (11%)	3 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	41/52 (79%)	32 (78%)	5 (12%)	4 (10%)	0	6
2	F	41/52 (79%)	32 (78%)	5 (12%)	4 (10%)	0	6
3	A	509/555 (92%)	439 (86%)	68 (13%)	2 (0%)	34	70
3	B	509/555 (92%)	437 (86%)	71 (14%)	1 (0%)	47	80
All	All	1822/2080 (88%)	1573 (86%)	231 (13%)	18 (1%)	15	52

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	49	PRO
2	F	49	PRO
3	A	50	TRP
3	A	334	SER
3	B	334	SER

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	C	320/378 (85%)	312 (98%)	8 (2%)	47	74
1	D	320/378 (85%)	312 (98%)	8 (2%)	47	74
2	E	39/45 (87%)	33 (85%)	6 (15%)	2	14
2	F	39/45 (87%)	33 (85%)	6 (15%)	2	14
3	A	450/485 (93%)	441 (98%)	9 (2%)	55	79
3	B	450/485 (93%)	434 (96%)	16 (4%)	35	65
All	All	1618/1816 (89%)	1565 (97%)	53 (3%)	38	68

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	52	ARG
1	D	292	PHE

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Mol	Chain	Res	Type
2	F	15	CYS
1	D	78	ASP
1	D	111	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	364	ASN
3	A	536	ASN
1	D	85	HIS
3	B	511	ASN
3	B	536	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 [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	C	363/433 (83%)	0.32	14 (3%) 39 36	41, 56, 75, 85	0
1	D	363/433 (83%)	0.40	17 (4%) 31 30	40, 58, 74, 86	0
2	E	45/52 (86%)	0.78	5 (11%) 5 7	51, 72, 94, 99	0
2	F	45/52 (86%)	0.73	7 (15%) 2 3	51, 74, 96, 103	0
3	A	513/555 (92%)	0.43	44 (8%) 10 12	36, 49, 60, 76	0
3	B	513/555 (92%)	0.53	48 (9%) 8 10	40, 52, 83, 102	0
All	All	1842/2080 (88%)	0.45	135 (7%) 15 16	36, 53, 77, 103	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	143	GLY	6.6
3	B	75	SER	6.0
1	D	144	ARG	5.2
3	B	47	LEU	5.1
3	B	63	GLY	4.9

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 carbohydrates 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.