



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 09:56 pm BST

PDB ID : 5XJX
Title : Pre-formed plant receptor ERL1-TMM complex
Authors : Chai, J.; Lin, G.; Zhang, L.; Han, Z.; Yang, X.; Liu, W.; Qi, Y.; Chang, J.;
Li, E.
Deposited on : 2017-05-04
Resolution : 3.06 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

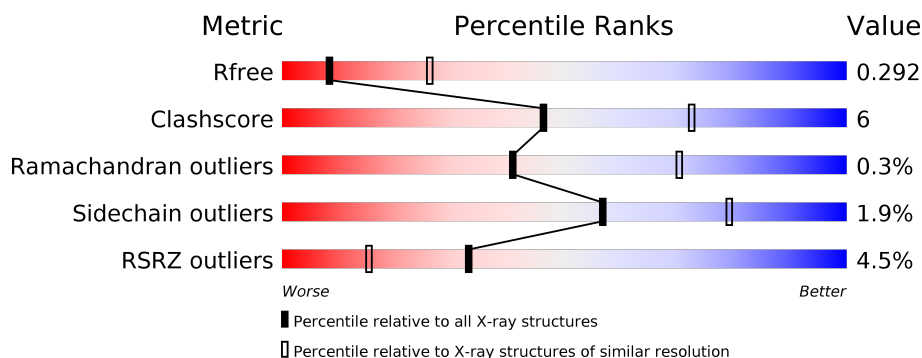
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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>%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>16%</div> </div> </div>
1	D	433	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>14%</div> <div>16%</div> </div> </div>
1	F	433	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>16%</div> </div> </div>
1	H	433	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>15%</div> <div>•</div> <div>16%</div> </div> </div>
1	J	433	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>13%</div> <div>16%</div> </div> </div>
1	L	433	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>15%</div> <div>16%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	A	556	<div><div></div><div>6%</div><div>83%</div><div>14%</div><div>..</div></div>
2	B	556	<div><div></div><div>3%</div><div>83%</div><div>14%</div><div>..</div></div>
2	E	556	<div><div></div><div>4%</div><div>84%</div><div>13%</div><div>..</div></div>
2	G	556	<div><div></div><div>3%</div><div>84%</div><div>13%</div><div>..</div></div>
2	I	556	<div><div></div><div>13%</div><div>83%</div><div>14%</div><div>..</div></div>
2	K	556	<div><div></div><div>7%</div><div>83%</div><div>14%</div><div>..</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41970 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	365	Total	C	N	O	S	0	0	0
			2840	1792	513	524	11			
1	F	365	Total	C	N	O	S	0	0	0
			2840	1792	513	524	11			
1	D	365	Total	C	N	O	S	0	0	0
			2840	1792	513	524	11			
1	L	365	Total	C	N	O	S	0	0	0
			2840	1792	513	524	11			
1	H	365	Total	C	N	O	S	0	0	0
			2840	1792	513	524	11			
1	J	365	Total	C	N	O	S	0	0	0
			2840	1792	513	524	11			

- Molecule 2 is a protein called LRR receptor-like serine/threonine-protein kinase ERL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	544	Total	C	N	O	S	0	0	0
			4155	2641	705	791	18			
2	G	544	Total	C	N	O	S	0	0	0
			4155	2641	705	791	18			
2	A	544	Total	C	N	O	S	0	0	0
			4155	2641	705	791	18			
2	I	544	Total	C	N	O	S	0	0	0
			4155	2641	705	791	18			
2	B	544	Total	C	N	O	S	0	0	0
			4155	2641	705	791	18			
2	E	544	Total	C	N	O	S	0	0	0
			4155	2641	705	791	18			

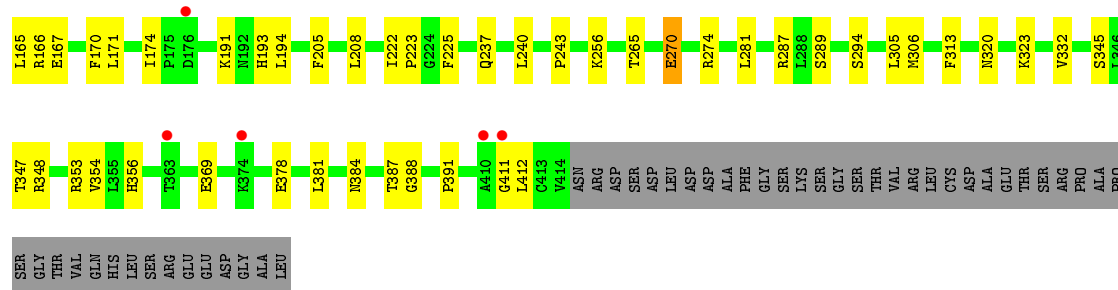
There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	574	HIS	-	expression tag	UNP C0LGW6

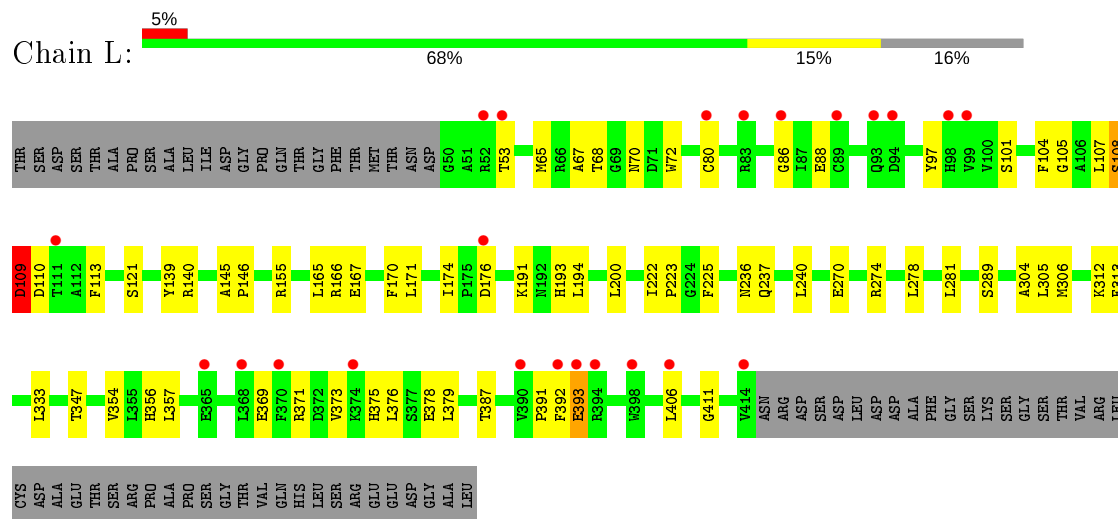
Continued on next page...

Continued from previous page...

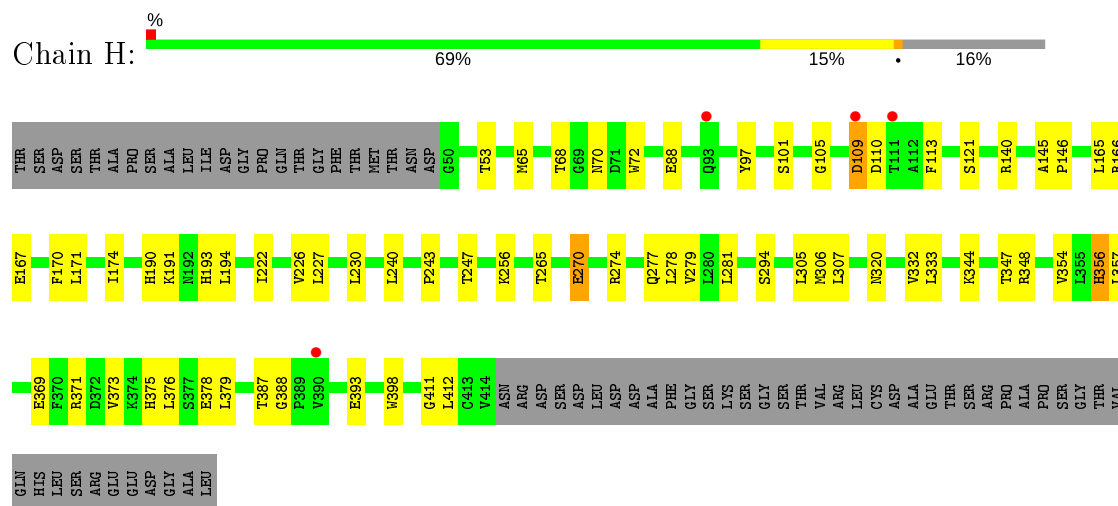
Chain	Residue	Modelled	Actual	Comment	Reference
K	575	HIS	-	expression tag	UNP C0LGW6
K	576	HIS	-	expression tag	UNP C0LGW6
K	577	HIS	-	expression tag	UNP C0LGW6
K	578	HIS	-	expression tag	UNP C0LGW6
K	579	HIS	-	expression tag	UNP C0LGW6
G	574	HIS	-	expression tag	UNP C0LGW6
G	575	HIS	-	expression tag	UNP C0LGW6
G	576	HIS	-	expression tag	UNP C0LGW6
G	577	HIS	-	expression tag	UNP C0LGW6
G	578	HIS	-	expression tag	UNP C0LGW6
G	579	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
A	579	HIS	-	expression tag	UNP C0LGW6
I	574	HIS	-	expression tag	UNP C0LGW6
I	575	HIS	-	expression tag	UNP C0LGW6
I	576	HIS	-	expression tag	UNP C0LGW6
I	577	HIS	-	expression tag	UNP C0LGW6
I	578	HIS	-	expression tag	UNP C0LGW6
I	579	HIS	-	expression tag	UNP C0LGW6
B	574	HIS	-	expression tag	UNP C0LGW6
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
B	579	HIS	-	expression tag	UNP C0LGW6
E	574	HIS	-	expression tag	UNP C0LGW6
E	575	HIS	-	expression tag	UNP C0LGW6
E	576	HIS	-	expression tag	UNP C0LGW6
E	577	HIS	-	expression tag	UNP C0LGW6
E	578	HIS	-	expression tag	UNP C0LGW6
E	579	HIS	-	expression tag	UNP C0LGW6



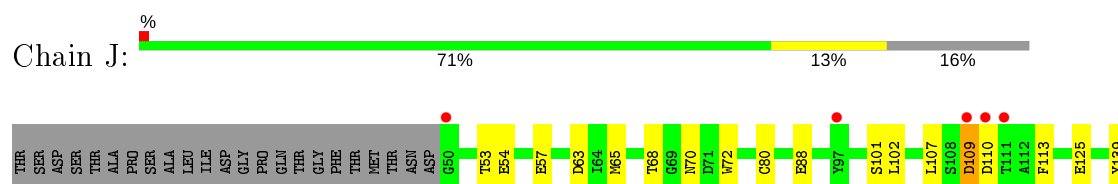
• Molecule 1: Protein TOO MANY MOUTHS

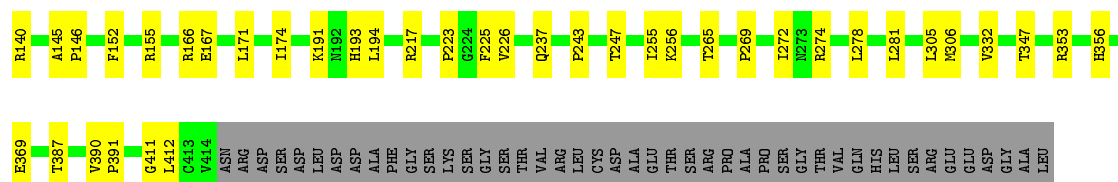


• Molecule 1: Protein TOO MANY MOUTHS

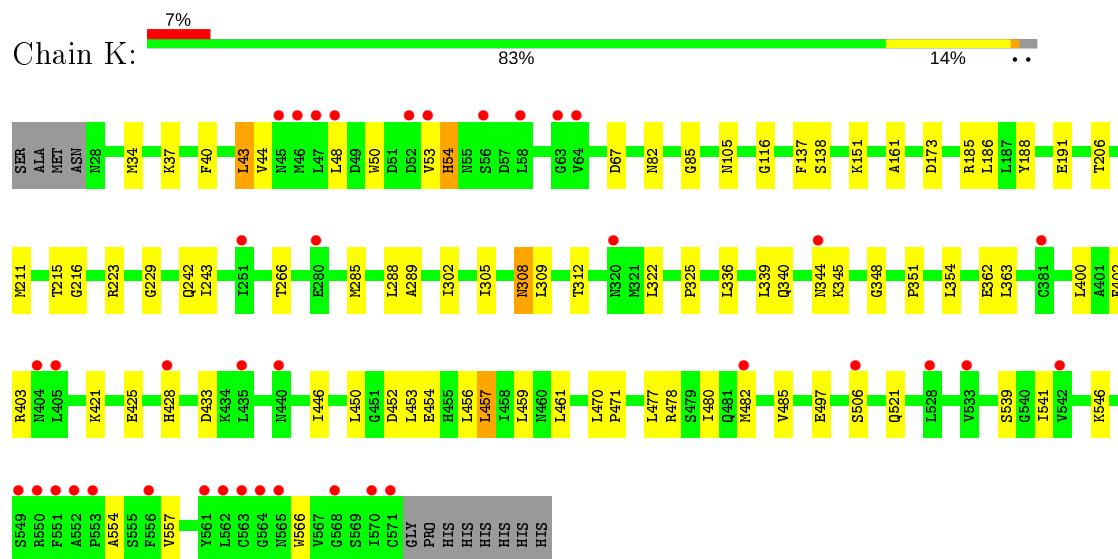


• Molecule 1: Protein TOO MANY MOUTHS

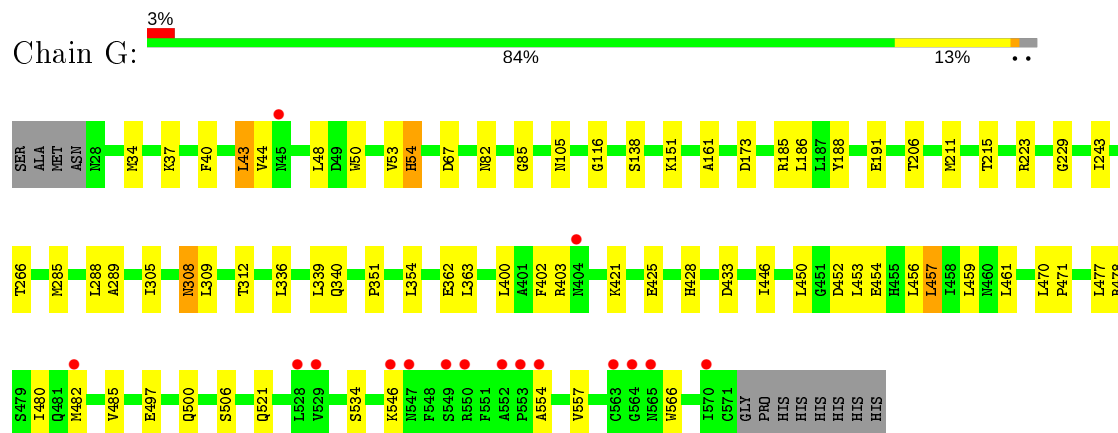




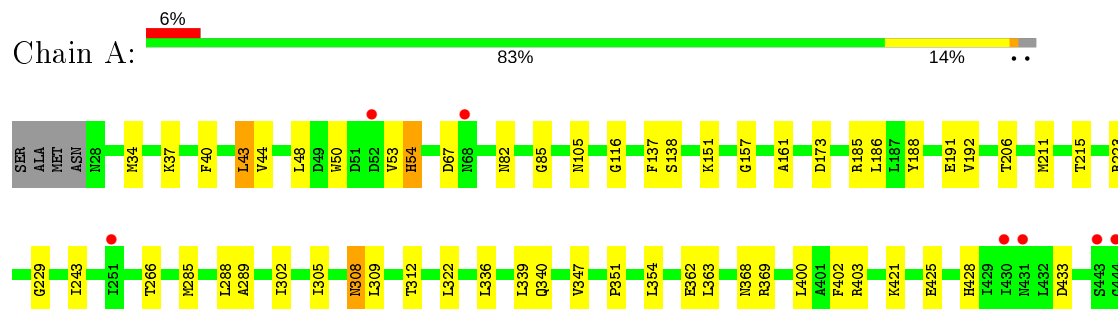
• Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1

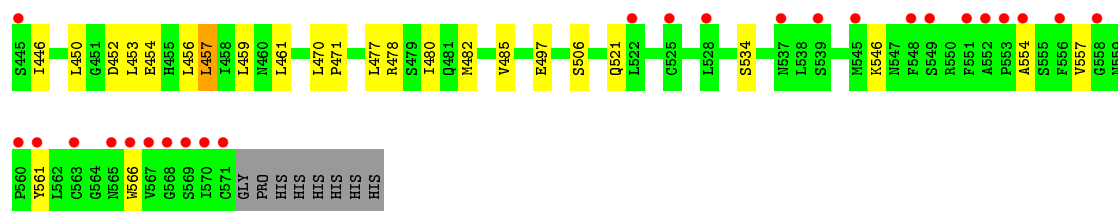


• Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1

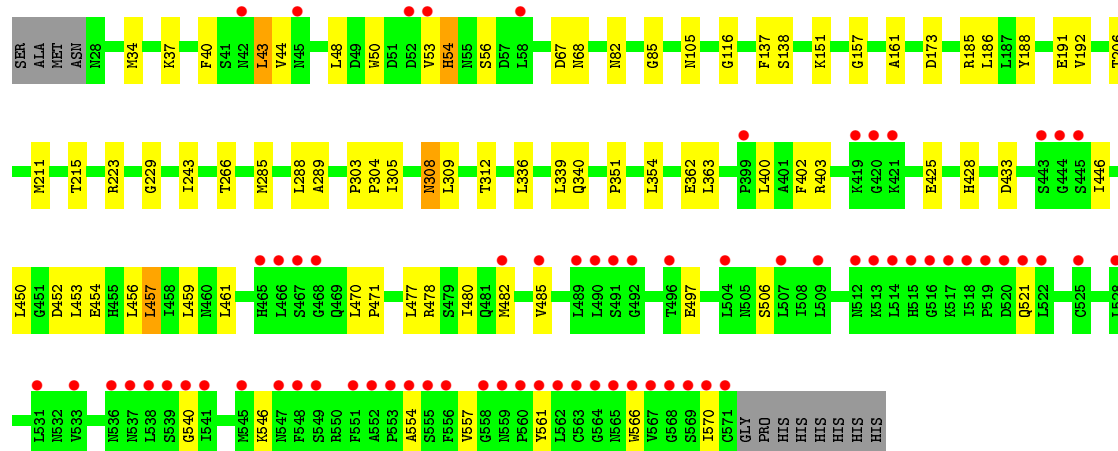
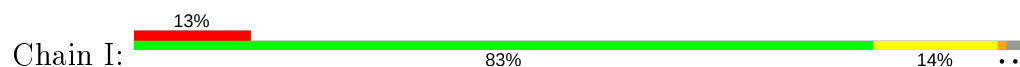


• Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1

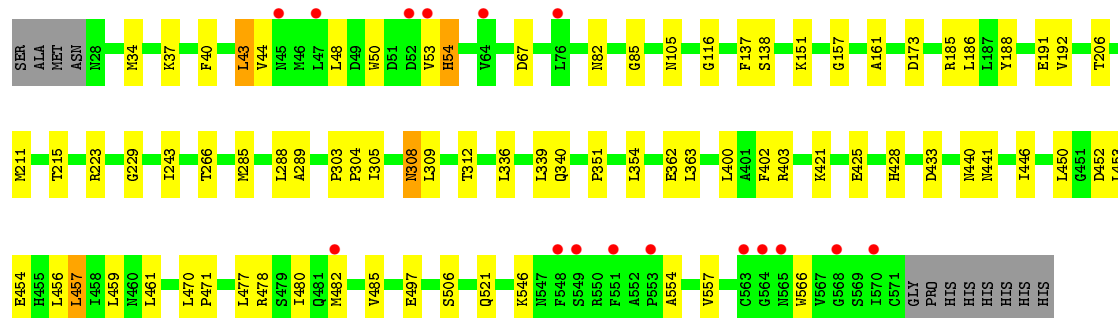
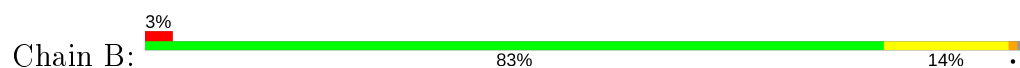




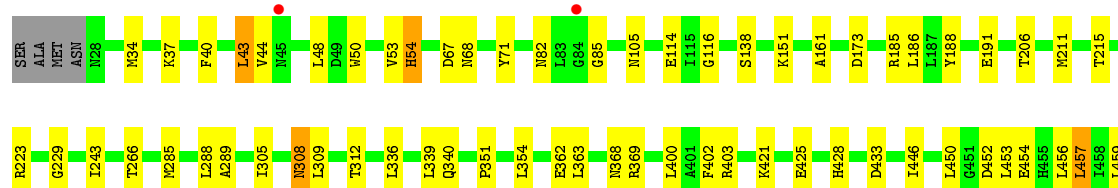
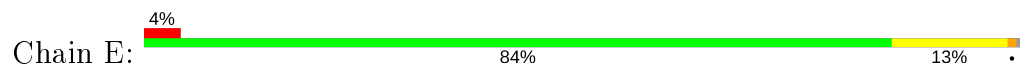
- Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1

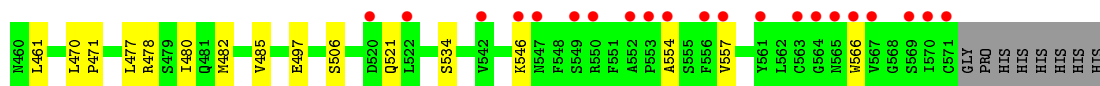


- Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1



- Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	116.17Å 114.39Å 191.95Å 89.57° 90.46° 59.86°	Depositor
Resolution (Å)	43.25 – 3.06 49.87 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.25-3.06) 97.6 (49.87-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.254 , 0.276 0.279 , 0.292	Depositor DCC
R_{free} test set	7889 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 14.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,-h+k,l 0.000 for h-k,h,l 0.011 for -h+k,-h,l 0.011 for -k,h-k,l 0.087 for -h+k,k,-l 0.016 for -k,-h,-l 0.002 for -h,-k,l 0.002 for -h,-h+k,-l 0.031 for h,h-k,-l 0.000 for h-k,-k,-l 0.001 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	41970	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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	C	0.27	0/2896	0.50	0/3933
1	D	0.26	0/2896	0.50	0/3933
1	F	0.26	0/2896	0.50	0/3933
1	H	0.31	0/2896	0.52	0/3933
1	J	0.26	0/2896	0.50	0/3933
1	L	0.34	0/2896	0.54	2/3933 (0.1%)
2	A	0.27	0/4231	0.51	0/5758
2	B	0.27	0/4231	0.51	0/5758
2	E	0.27	0/4231	0.51	0/5758
2	G	0.27	0/4231	0.51	0/5758
2	I	0.27	0/4231	0.51	0/5758
2	K	0.27	0/4231	0.51	0/5758
All	All	0.28	0/42762	0.51	2/58146 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	108	SER	C-N-CA	5.12	134.49	121.70
1	L	109	ASP	N-CA-CB	5.04	119.68	110.60

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	2840	0	2889	39	3
1	D	2840	0	2889	43	0
1	F	2840	0	2889	46	0
1	H	2840	0	2889	43	0
1	J	2840	0	2889	38	1
1	L	2840	0	2889	44	0
2	A	4155	0	4195	56	1
2	B	4155	0	4195	52	0
2	E	4155	0	4195	53	0
2	G	4155	0	4195	51	0
2	I	4155	0	4195	52	3
2	K	4155	0	4195	58	0
All	All	41970	0	42504	534	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 6.

The worst 5 of 534 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:K:242:GLN:HG3	1:L:110:ASP:OD2	1.21	1.29
2:K:242:GLN:CG	1:L:110:ASP:OD2	2.12	0.98
2:A:454:GLU:OE1	2:A:478:ARG:NH1	1.97	0.97
2:G:454:GLU:OE1	2:G:478:ARG:NH1	1.97	0.97
2:E:454:GLU:OE1	2:E:478:ARG:NH1	1.97	0.97

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)
1:C:83:ARG:O	2:I:570:ILE:O[1_546]	1.93	0.27
1:C:113:PHE:O	2:I:561:TYR:OH[1_546]	1.96	0.24
1:C:72:TRP:CB	2:I:540:GLY:CA[1_546]	2.16	0.04
1:J:113:PHE:O	2:A:561:TYR:OH[1_554]	2.19	0.01

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	363/433 (84%)	334 (92%)	27 (7%)	2 (1%)	25	55
1	D	363/433 (84%)	333 (92%)	28 (8%)	2 (1%)	25	55
1	F	363/433 (84%)	333 (92%)	28 (8%)	2 (1%)	25	55
1	H	363/433 (84%)	334 (92%)	28 (8%)	1 (0%)	41	70
1	J	363/433 (84%)	332 (92%)	29 (8%)	2 (1%)	25	55
1	L	363/433 (84%)	334 (92%)	27 (7%)	2 (1%)	25	55
2	A	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
2	B	542/556 (98%)	484 (89%)	57 (10%)	1 (0%)	47	77
2	E	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
2	G	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
2	I	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
2	K	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
All	All	5430/5934 (92%)	4909 (90%)	504 (9%)	17 (0%)	41	70

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	109	ASP
1	F	109	ASP
1	D	109	ASP
1	L	109	ASP
1	H	109	ASP

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	C	322/378 (85%)	318 (99%)	4 (1%)	71	87
1	D	322/378 (85%)	320 (99%)	2 (1%)	86	93
1	F	322/378 (85%)	316 (98%)	6 (2%)	57	79
1	H	322/378 (85%)	318 (99%)	4 (1%)	71	87
1	J	322/378 (85%)	320 (99%)	2 (1%)	86	93
1	L	322/378 (85%)	315 (98%)	7 (2%)	52	76
2	A	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	B	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	E	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	G	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	I	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	K	476/486 (98%)	465 (98%)	11 (2%)	50	75
All	All	4788/5184 (92%)	4697 (98%)	91 (2%)	57	79

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	308	ASN
2	A	67	ASP
2	E	223	ARG
2	G	402	PHE
2	G	566	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	70	ASN
2	G	428	HIS
2	I	428	HIS
1	H	70	ASN
2	A	428	HIS

5.3.3 RNA ⓘ

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 ⓘ

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	365/433 (84%)	-0.24	3 (0%) 86 70	30, 42, 66, 85	0
1	D	365/433 (84%)	-0.08	8 (2%) 62 38	31, 51, 79, 91	0
1	F	365/433 (84%)	-0.01	7 (1%) 66 43	29, 51, 75, 91	0
1	H	365/433 (84%)	-0.02	4 (1%) 80 60	30, 50, 84, 100	0
1	J	365/433 (84%)	-0.17	5 (1%) 75 53	29, 43, 70, 90	0
1	L	365/433 (84%)	0.24	23 (6%) 20 8	30, 61, 99, 112	0
2	A	544/556 (97%)	0.41	32 (5%) 22 9	40, 61, 84, 109	0
2	B	544/556 (97%)	0.17	16 (2%) 51 26	40, 61, 84, 109	0
2	E	544/556 (97%)	0.31	23 (4%) 36 17	40, 61, 84, 109	0
2	G	544/556 (97%)	0.16	16 (2%) 51 26	40, 61, 84, 109	0
2	I	544/556 (97%)	0.84	71 (13%) 3 1	40, 61, 84, 109	0
2	K	544/556 (97%)	0.36	39 (7%) 15 5	40, 61, 84, 109	0
All	All	5454/5934 (91%)	0.21	247 (4%) 33 15	29, 58, 84, 112	0

The worst 5 of 247 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	569	SER	14.0
2	I	563	CYS	12.6
2	I	548	PHE	12.1
2	A	568	GLY	11.5
2	I	568	GLY	11.3

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

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.