Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:03 PM GMT

PDB ID	:	4H22
Title	:	Crystal structure of the dimeric coiled-coil domain of the cytosolic nucleic acid sensor LRRFIP1
Authors	:	Nguyen, J.B.; Modis, Y.
Deposited on	:	2012-09-11
Resolution	:	2.89 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

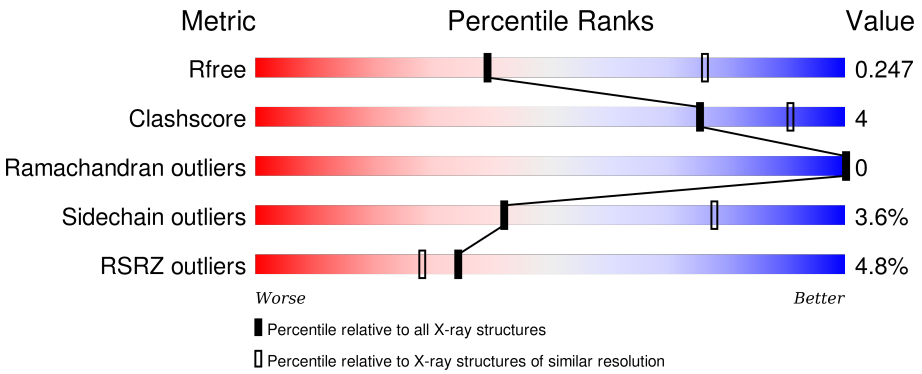
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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 <=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	103	2%, 65%, 12%, •, 21%
1	B	103	4%, 73%, 7%, •, 19%
1	C	103	7%, 65%, 7%, 28%
1	D	103	2%, 63%, 9%, 28%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2656 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 Leucine-rich repeat flightless-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	81	684	427	117	136	4	0	0	0
1	B	83	700	437	119	140	4	0	0	0
1	C	74	621	389	106	123	3	0	0	0
1	D	74	625	392	107	123	3	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	MET	-	EXPRESSION TAG	UNP Q32MZ4
A	250	PRO	-	EXPRESSION TAG	UNP Q32MZ4
A	251	LYS	-	EXPRESSION TAG	UNP Q32MZ4
A	252	LEU	-	EXPRESSION TAG	UNP Q32MZ4
A	253	ALA	-	EXPRESSION TAG	UNP Q32MZ4
A	254	ALA	-	EXPRESSION TAG	UNP Q32MZ4
A	255	ALA	-	EXPRESSION TAG	UNP Q32MZ4
A	256	LEU	-	EXPRESSION TAG	UNP Q32MZ4
A	257	GLU	-	EXPRESSION TAG	UNP Q32MZ4
A	258	HIS	-	EXPRESSION TAG	UNP Q32MZ4
A	259	HIS	-	EXPRESSION TAG	UNP Q32MZ4
A	260	HIS	-	EXPRESSION TAG	UNP Q32MZ4
A	261	HIS	-	EXPRESSION TAG	UNP Q32MZ4
A	262	HIS	-	EXPRESSION TAG	UNP Q32MZ4
A	263	HIS	-	EXPRESSION TAG	UNP Q32MZ4
B	161	MET	-	EXPRESSION TAG	UNP Q32MZ4
B	250	PRO	-	EXPRESSION TAG	UNP Q32MZ4
B	251	LYS	-	EXPRESSION TAG	UNP Q32MZ4
B	252	LEU	-	EXPRESSION TAG	UNP Q32MZ4
B	253	ALA	-	EXPRESSION TAG	UNP Q32MZ4
B	254	ALA	-	EXPRESSION TAG	UNP Q32MZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	255	ALA	-	EXPRESSION TAG	UNP Q32MZ4
B	256	LEU	-	EXPRESSION TAG	UNP Q32MZ4
B	257	GLU	-	EXPRESSION TAG	UNP Q32MZ4
B	258	HIS	-	EXPRESSION TAG	UNP Q32MZ4
B	259	HIS	-	EXPRESSION TAG	UNP Q32MZ4
B	260	HIS	-	EXPRESSION TAG	UNP Q32MZ4
B	261	HIS	-	EXPRESSION TAG	UNP Q32MZ4
B	262	HIS	-	EXPRESSION TAG	UNP Q32MZ4
B	263	HIS	-	EXPRESSION TAG	UNP Q32MZ4
C	161	MET	-	EXPRESSION TAG	UNP Q32MZ4
C	250	PRO	-	EXPRESSION TAG	UNP Q32MZ4
C	251	LYS	-	EXPRESSION TAG	UNP Q32MZ4
C	252	LEU	-	EXPRESSION TAG	UNP Q32MZ4
C	253	ALA	-	EXPRESSION TAG	UNP Q32MZ4
C	254	ALA	-	EXPRESSION TAG	UNP Q32MZ4
C	255	ALA	-	EXPRESSION TAG	UNP Q32MZ4
C	256	LEU	-	EXPRESSION TAG	UNP Q32MZ4
C	257	GLU	-	EXPRESSION TAG	UNP Q32MZ4
C	258	HIS	-	EXPRESSION TAG	UNP Q32MZ4
C	259	HIS	-	EXPRESSION TAG	UNP Q32MZ4
C	260	HIS	-	EXPRESSION TAG	UNP Q32MZ4
C	261	HIS	-	EXPRESSION TAG	UNP Q32MZ4
C	262	HIS	-	EXPRESSION TAG	UNP Q32MZ4
C	263	HIS	-	EXPRESSION TAG	UNP Q32MZ4
D	161	MET	-	EXPRESSION TAG	UNP Q32MZ4
D	250	PRO	-	EXPRESSION TAG	UNP Q32MZ4
D	251	LYS	-	EXPRESSION TAG	UNP Q32MZ4
D	252	LEU	-	EXPRESSION TAG	UNP Q32MZ4
D	253	ALA	-	EXPRESSION TAG	UNP Q32MZ4
D	254	ALA	-	EXPRESSION TAG	UNP Q32MZ4
D	255	ALA	-	EXPRESSION TAG	UNP Q32MZ4
D	256	LEU	-	EXPRESSION TAG	UNP Q32MZ4
D	257	GLU	-	EXPRESSION TAG	UNP Q32MZ4
D	258	HIS	-	EXPRESSION TAG	UNP Q32MZ4
D	259	HIS	-	EXPRESSION TAG	UNP Q32MZ4
D	260	HIS	-	EXPRESSION TAG	UNP Q32MZ4
D	261	HIS	-	EXPRESSION TAG	UNP Q32MZ4
D	262	HIS	-	EXPRESSION TAG	UNP Q32MZ4
D	263	HIS	-	EXPRESSION TAG	UNP Q32MZ4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	8	8	8	0	0
			Total	O		
2	B	6	6	6	0	0
			Total	O		
2	C	4	4	4	0	0
			Total	O		
2	D	8	8	8	0	0

3 Residue-property plots (i)

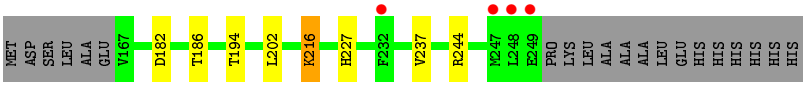
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Leucine-rich repeat flightless-interacting protein 1

Chain A:

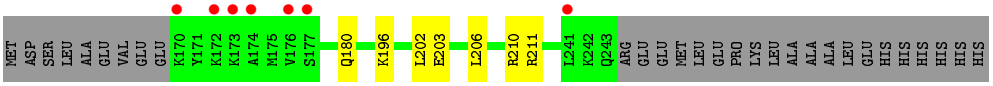
- Molecule 1: Leucine-rich repeat flightless-interacting protein 1

Chain B:



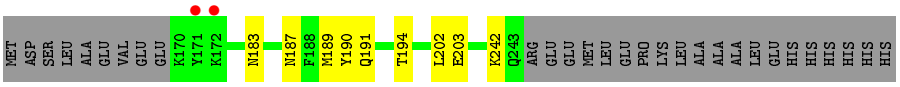
- Molecule 1: Leucine-rich repeat flightless-interacting protein 1

Chain C:



- Molecule 1: Leucine-rich repeat flightless-interacting protein 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.36Å 71.45Å 68.03Å 90.00° 110.10° 90.00°	Depositor
Resolution (Å)	50.00 – 2.89 49.12 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.89) 99.1 (49.12-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.235 , 0.248 0.235 , 0.247	Depositor DCC
R_{free} test set	776 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	59.7	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 15501 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	2656	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.38	0/692	0.46	0/921
1	B	0.51	0/708	0.49	0/943
1	C	0.44	0/629	0.48	0/839
1	D	0.39	0/633	0.46	0/843
All	All	0.43	0/2662	0.48	0/3546

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	A	684	0	663	10	0
1	B	700	0	678	8	0
1	C	621	0	599	7	0
1	D	625	0	610	7	0
2	A	8	0	0	0	0
2	B	6	0	0	0	0
2	C	4	0	0	0	0
2	D	8	0	0	0	0
All	All	2656	0	2550	20	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 (20) 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)
1:A:217:ASN:HD22	1:B:216:LYS:HE3	1.56	0.69
1:C:202:LEU:HD23	1:D:202:LEU:HB3	1.74	0.69
1:C:206:LEU:HD21	1:C:210:ARG:HH21	1.59	0.66
1:A:217:ASN:HD22	1:B:216:LYS:CE	2.11	0.64
1:A:190:TYR:O	1:A:194:THR:HG23	2.06	0.56
1:C:196:LYS:NZ	1:D:191:GLN:HE22	2.07	0.52
1:C:202:LEU:HD21	1:D:203:GLU:HG3	1.93	0.51
1:D:183:ASN:O	1:D:187:ASN:HB2	2.13	0.48
1:B:182:ASP:O	1:B:186:THR:HG23	2.14	0.48
1:A:185:LYS:HE2	1:A:189:MET:HE1	1.95	0.47
1:D:190:TYR:O	1:D:194:THR:HG23	2.14	0.47
1:B:216:LYS:HA	1:B:216:LYS:HD3	1.78	0.45
1:A:230:LEU:HD12	1:B:227:HIS:CE1	2.54	0.43
1:D:189:MET:HE2	1:D:189:MET:HB2	1.81	0.43
1:A:237:VAL:HG12	1:B:237:VAL:HG12	2.02	0.42
1:A:202:LEU:HD23	1:B:202:LEU:CB	2.50	0.42
1:A:191:GLN:HG2	1:C:203:GLU:OE2	2.21	0.40
1:A:241:LEU:HD22	1:B:237:VAL:HG13	2.02	0.40
1:A:187:ASN:ND2	1:C:211:ARG:HH11	2.19	0.40
1:C:202:LEU:HB3	1:D:202:LEU:HD23	2.03	0.40

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	A	79/103 (77%)	79 (100%)	0	0	100	100
1	B	81/103 (79%)	78 (96%)	3 (4%)	0	100	100
1	C	72/103 (70%)	70 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	72/103 (70%)	72 (100%)	0	0	100	100
All	All	304/412 (74%)	299 (98%)	5 (2%)	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	A	73/93 (78%)	68 (93%)	5 (7%)	20	49
1	B	75/93 (81%)	72 (96%)	3 (4%)	38	74
1	C	66/93 (71%)	65 (98%)	1 (2%)	72	92
1	D	67/93 (72%)	66 (98%)	1 (2%)	72	92
All	All	281/372 (76%)	271 (96%)	10 (4%)	42	78

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	194	THR
1	A	203	GLU
1	A	222	ARG
1	A	230	LEU
1	B	194	THR
1	B	216	LYS
1	B	244	ARG
1	C	180	GLN
1	D	242	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN

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Mol	Chain	Res	Type
1	A	217	ASN
1	B	227	HIS
1	D	191	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 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	A	81/103 (78%)	0.27	2 (2%)	61	55	63, 88, 168, 180	0
1	B	83/103 (80%)	0.41	4 (4%)	34	28	57, 96, 154, 212	0
1	C	74/103 (71%)	0.47	7 (9%)	10	6	62, 87, 155, 173	0
1	D	74/103 (71%)	0.28	2 (2%)	58	52	65, 91, 171, 194	0
All	All	312/412 (75%)	0.36	15 (4%)	34	28	57, 91, 167, 212	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	TYR	4.2
1	B	247	MET	3.9
1	B	248	LEU	3.9
1	C	174	ALA	3.8
1	B	232	PHE	3.6
1	C	176	VAL	3.6
1	C	170	LYS	3.4
1	A	248	LEU	2.8
1	A	245	GLU	2.7
1	B	249	GLU	2.3
1	D	172	LYS	2.3
1	C	241	LEU	2.3
1	C	173	LYS	2.1
1	C	177	SER	2.0
1	C	172	LYS	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 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.