W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID	:	1Z56
Title	:	Co-Crystal Structure of Lif1p-Lig4p
Authors	:	Dore, A.S.; Furnham, N.; Davies, O.R.; Sibanda, B.L.; Chirgadze, D.Y.; Jackson, S.P.; Pellegrini, L.; Blundell, T.L.
Deposited on	:	2005-03-17
Resolution	:	3.92 Å(reported)

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

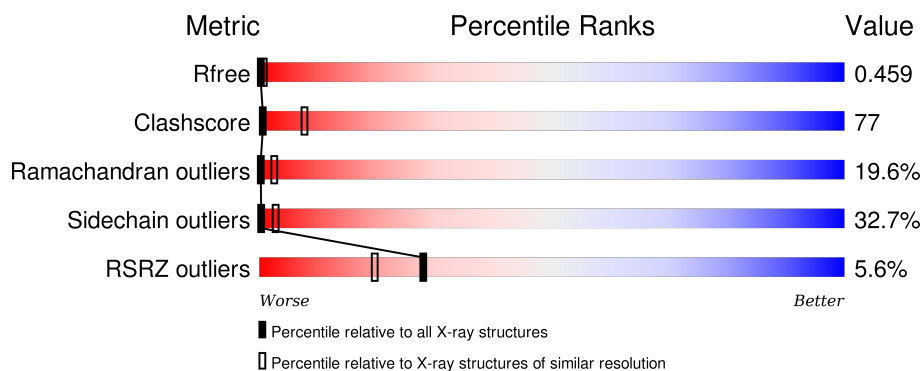|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.92 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.
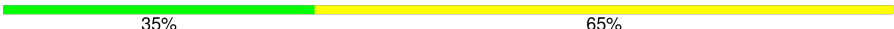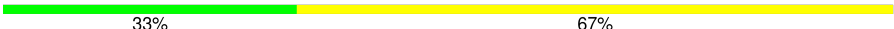
Metric	Percentile Ranks	Value
Rfree		0.459
Clashscore		77
Ramachandran outliers		19.6%
Sidechain outliers		32.7%
RSRZ outliers		5.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
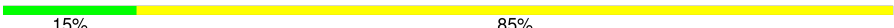
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1047 (4.32-3.52)
Clashscore	102246	1008 (4.26-3.58)
Ramachandran outliers	100387	1044 (4.30-3.54)
Sidechain outliers	100360	1035 (4.30-3.54)
RSRZ outliers	91569	1002 (4.30-3.54)

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	246	4% 8% 14% 9% 69%
1	B	246	2% 7% 15% 7% • 69%
2	C	264	2% 16% 39% 27% 8% 10%
3	D	8	38% 63%
4	E	7	71% 29%

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Mol	Chain	Length	Quality of chain
4	H	7	57% 43%
5	F	45	49% 51%
6	G	37	35% 65%
7	I	30	33% 67%
8	J	20	10% 30% 60%
9	K	13	15% 85%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4164 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 Ligase interacting factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	77	Total 648	C 393	N 126	O 125	S 4	0	0	0
1	B	76	Total 643	C 393	N 122	O 123	S 5	0	0	0

- Molecule 2 is a protein called DNA ligase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	237	Total 1899	C 1209	N 319	O 359	S 12	0	0	0

- Molecule 3 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	8	Total 47	C 31	N 8	O 8	0	0	0

- Molecule 4 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	7	Total 42	C 28	N 7	O 7	0	0	0
4	H	7	Total 42	C 28	N 7	O 7	0	0	0

- Molecule 5 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	45	Total 258	C 168	N 45	O 45	0	0	0

- Molecule 6 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	G	37	218	144	37	37	0	0	0

- Molecule 7 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	I	30	173	113	30	30	0	0	0

- Molecule 8 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	J	20	118	78	20	20	0	0	0

- Molecule 9 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	K	13	76	50	13	13	0	0	0

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 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.
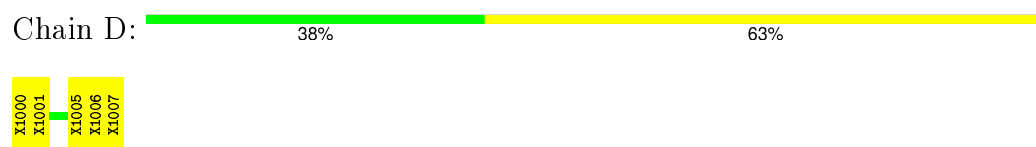
- Molecule 1: Ligase interacting factor 1

- Molecule 1: Ligase interacting factor 1

- Molecule 2: DNA ligase IV

Chain C:
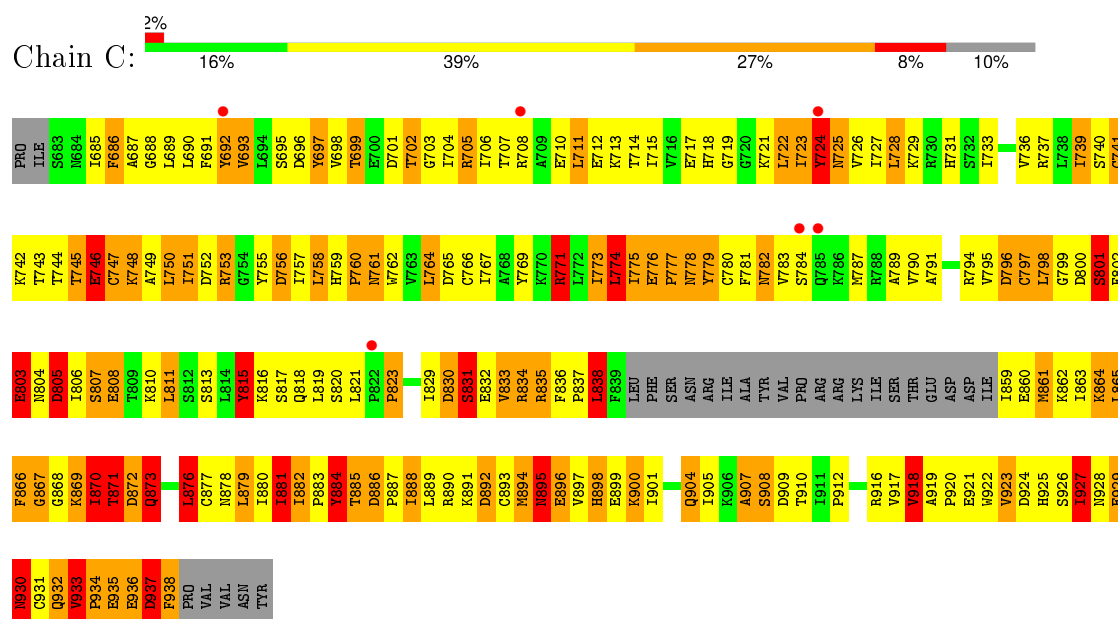
- Molecule 3: Ligase interacting factor 1

Chain D:

- Molecule 4: Ligase interacting factor 1

Chain E:

- Molecule 4: Ligase interacting factor 1

Chain H:
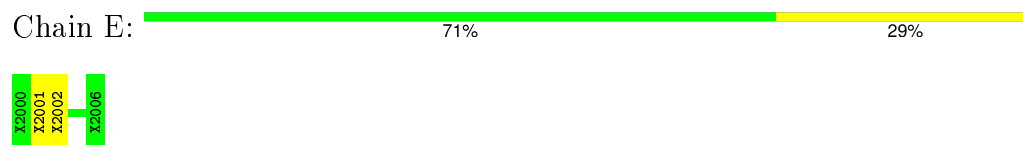
- Molecule 5: Ligase interacting factor 1

Chain F:
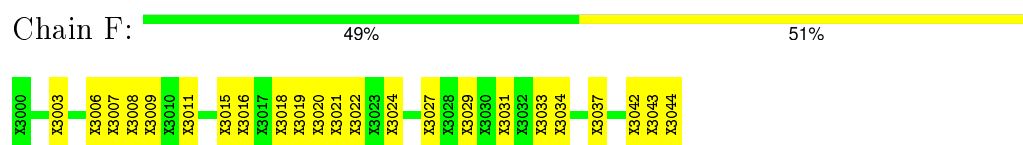
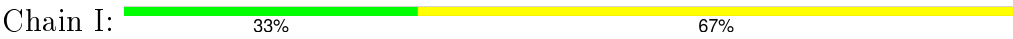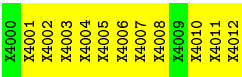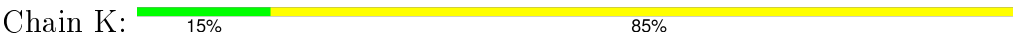- Molecule 6: Ligase interacting factor 1

Chain G:

• Molecule 7: Ligase interacting factor 1

Chain I:

• Molecule 8: Ligase interacting factor 1

Chain J:

• Molecule 9: Ligase interacting factor 1

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	247.62Å 247.62Å 98.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.20 – 3.92 49.20 – 3.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.20-3.92) 99.9 (49.20-3.92)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$<I/\sigma(I)>$ [1]	3.03 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.400 , 0.467 0.398 , 0.459	Depositor DCC
R_{free} test set	829 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	109.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 110.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.32$	Xtriage
Outliers	0 of 16470 reflections	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	4164	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.69	0/650	0.85	0/865
1	B	0.77	0/646	0.90	1/858 (0.1%)
2	C	0.91	2/1931 (0.1%)	1.12	7/2609 (0.3%)
All	All	0.84	2/3227 (0.1%)	1.03	8/4332 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	5
8	J	0	18
All	All	0	23

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	835	ARG	CG-CD	5.18	1.64	1.51
2	C	803	GLU	CG-CD	5.16	1.59	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	835	ARG	NE-CZ-NH1	10.99	125.80	120.30
2	C	876	LEU	CA-CB-CG	7.73	133.09	115.30
1	B	200	LEU	CA-CB-CG	-7.50	98.04	115.30
2	C	758	LEU	CA-CB-CG	5.94	128.96	115.30
2	C	881	ILE	N-CA-C	-5.83	95.25	111.00

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	724	TYR	Peptide
2	C	771	ARG	Peptide
2	C	805	ASP	Peptide
2	C	884	TYR	Peptide
2	C	895	ASN	Peptide

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	648	0	670	69	0
1	B	643	0	663	105	0
2	C	1899	0	1927	342	1
3	D	47	0	49	9	0
4	E	42	0	48	7	0
4	H	42	0	48	4	0
5	F	258	0	233	36	0
6	G	218	0	218	53	0
7	I	173	0	161	42	0
8	J	118	0	122	19	0
9	K	76	0	76	19	0
All	All	4164	0	4215	643	1

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 77.

The worst 5 of 643 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:C:922:TRP:HA	2:C:925:HIS:CE1	1.50	1.43
2:C:883:PRO:O	2:C:889:LEU:HB3	1.34	1.22
2:C:892:ASP:O	2:C:895:ASN:HB2	1.44	1.18
1:B:188:GLU:HA	1:B:192:ARG:HH21	1.08	1.17
2:C:834:ARG:HG2	2:C:869:LYS:CD	1.78	1.13

All (1) 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:C:727:ILE:CG2	2:C:916:ARG:NE[5_555]	1.96	0.24

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	75/246 (30%)	51 (68%)	18 (24%)	6 (8%)	1	18
1	B	74/246 (30%)	41 (55%)	21 (28%)	12 (16%)	0	5
2	C	233/264 (88%)	120 (52%)	56 (24%)	57 (24%)	0	1
All	All	382/756 (50%)	212 (56%)	95 (25%)	75 (20%)	0	2

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	ILE
2	C	693	VAL
2	C	711	LEU
2	C	745	THR
2	C	748	LYS

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	74/229 (32%)	51 (69%)	23 (31%)	0	3
1	B	73/229 (32%)	55 (75%)	18 (25%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	217/244 (89%)	139 (64%)	78 (36%)	0	1
All	All	364/702 (52%)	245 (67%)	119 (33%)	0	3

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	711	LEU
2	C	751	ILE
2	C	909	ASP
2	C	722	LEU
2	C	736	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	217	ASN
2	C	930	ASN
2	C	878	ASN
1	A	189	GLN
2	C	928	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(Å²)	Q<0.9
1	A	77/246 (31%)	0.78	10 (12%)	5	4	53, 88, 113, 115	0
1	B	76/246 (30%)	0.46	6 (7%)	15	11	49, 89, 100, 105	0
2	C	237/264 (89%)	0.19	6 (2%)	61	48	23, 76, 104, 114	0
3	D	0/8	-	-			-	-
4	E	0/7	-	-			-	-
4	H	0/7	-	-			-	-
5	F	0/45	-	-			-	-
6	G	0/37	-	-			-	-
7	I	0/30	-	-			-	-
8	J	0/20	-	-			-	-
9	K	0/13	-	-			-	-
All	All	390/923 (42%)	0.36	22 (5%)	28	20	23, 81, 110, 115	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ASN	4.9
1	A	175	ASN	4.2
1	B	169	VAL	4.2
1	B	170	ASN	3.3
1	B	183	ASN	3.3

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.