



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2017 – 08:55 PM EDT

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 : unknown
Resolution : 3.92 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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

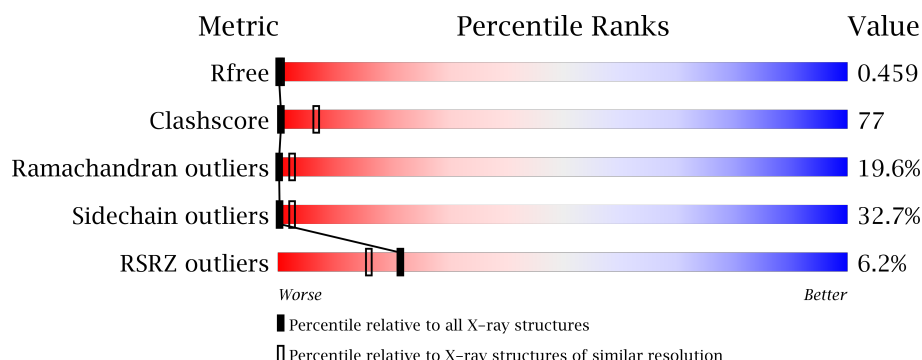
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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.




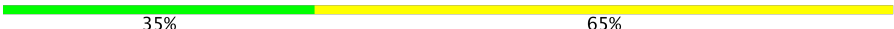

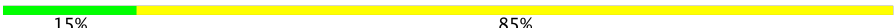
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1012 (4.24-3.60)
Clashscore	112137	1108 (4.24-3.60)
Ramachandran outliers	110173	1067 (4.24-3.60)
Sidechain outliers	110143	1058 (4.24-3.60)
RSRZ outliers	101464	1025 (4.24-3.60)

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 $\leq 5\%$. 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	A	246	<div> <div>4%</div> <div>8% 14% 9% 69%</div> </div>
1	B	246	<div> <div>3%</div> <div>7% 15% 7% 69%</div> </div>
2	C	264	<div> <div>3%</div> <div>16% 39% 27% 8% 10%</div> </div>
3	D	8	<div> <div>38% 63%</div> </div>
4	E	7	<div> <div>71% 29%</div> </div>

Continued on next page...

Continued from previous page...

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

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	C	N	O	S	0	0	0
			648	393	126	125	4			
1	B	76	Total	C	N	O	S	0	0	0
			643	393	122	123	5			

- Molecule 2 is a protein called DNA ligase IV.

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

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

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

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

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

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

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

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

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

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

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

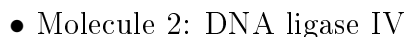
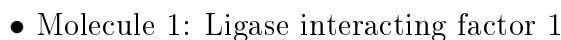
- Molecule 8 is a protein called Ligase interacting factor 1.

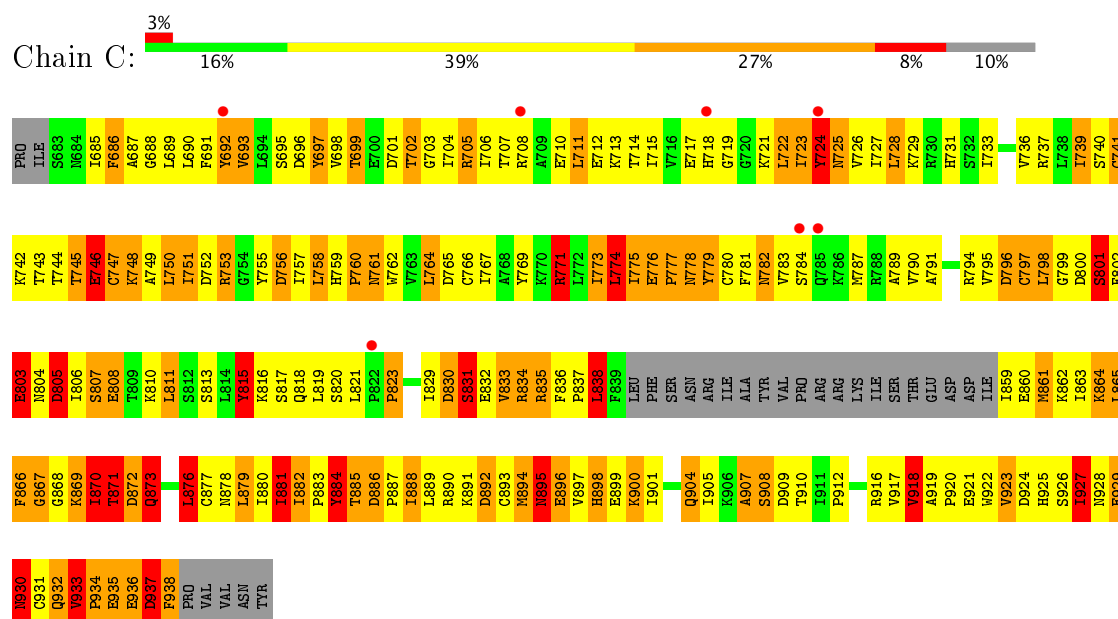
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	20	Total	C	N	O	0	0	0
			118	78	20	20			

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

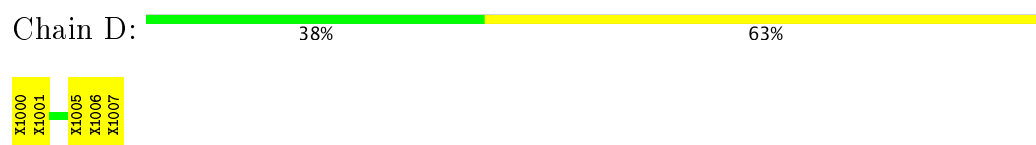
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	13	Total	C	N	O	0	0	0
			76	50	13	13			

- Molecule 1: Ligase interacting factor 1

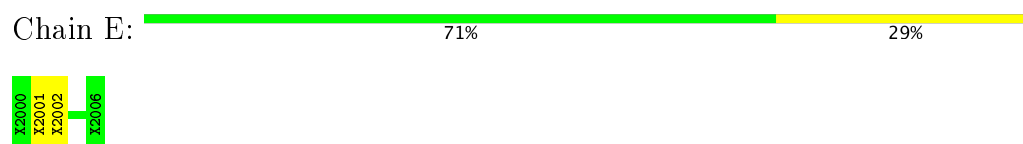




- Molecule 3: Ligase interacting factor 1



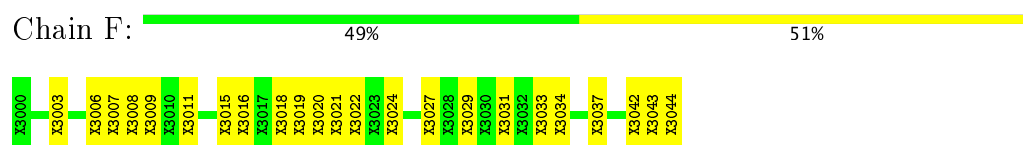
- Molecule 4: Ligase interacting factor 1



- Molecule 4: Ligase interacting factor 1

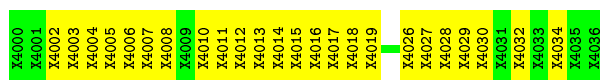


- Molecule 5: Ligase interacting factor 1



- Molecule 6: Ligase interacting factor 1

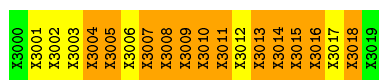




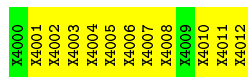
- Molecule 7: Ligase interacting factor 1



- Molecule 8: Ligase interacting factor 1



- Molecule 9: Ligase interacting factor 1



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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	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 ⓘ

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	17
1	B	74/246 (30%)	41 (55%)	21 (28%)	12 (16%)	0	4
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	6

Continued on next page...

Continued from previous page...

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	2

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(Å ²)	Q<0.9
1	A	77/246 (31%)	0.76	10 (12%) 4 4	53, 88, 113, 115	0
1	B	76/246 (30%)	0.44	7 (9%) 10 8	49, 89, 100, 105	0
2	C	237/264 (89%)	0.17	7 (2%) 51 40	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%)	0.34	24 (6%) 21 16	23, 81, 110, 115	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ASN	4.9
1	B	169	VAL	4.2
1	A	175	ASN	4.2
1	B	170	ASN	3.2
1	B	183	ASN	3.2

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.