



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3U0V / pdb_00003u0v
Title : Crystal Structure Analysis of human LYPLAL1
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Deposited on : 2011-09-29
Resolution : 1.72 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

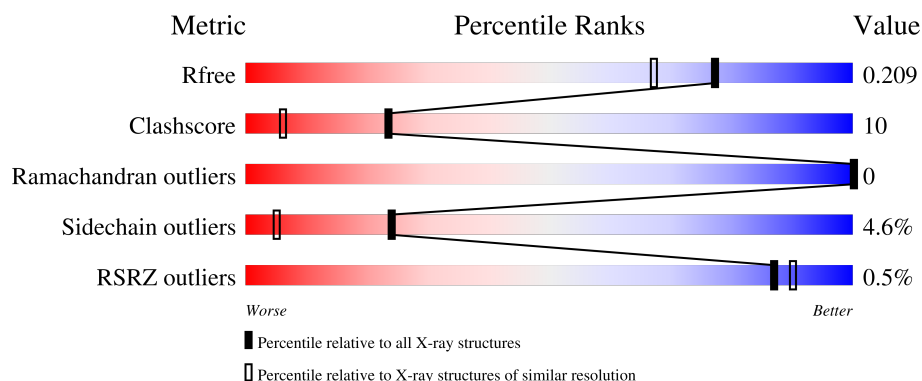
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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 of 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	A	239	 63% 26% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1941 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 Lysophospholipase-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	9	0
			1797	1159	304	322	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q5VWZ2
A	0	PRO	-	expression tag	UNP Q5VWZ2
A	131	MET	ILE	SEE REMARK 999	UNP Q5VWZ2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	144	Total	O	0	0
			144	144		

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- Molecule 1: Lysophospholipase-like protein 1

Glycine	B219	E107	L9	GLY	
	I220	E108	Q10		
	W224	V109	R11		
		I225	K110	V14	
	P230	T113	T118	M129	R19
		GLY	K114	L119	A134
		GLU	K115	T120	H138
		MET		G121	F145
	GLU			A146	
	LYS			S155	
GLN			A160		
LYS			V167		
Alanine		L168	L37	H53	
		P169	M39	R55	
		E170	G34	I56	
		L171	Q35	I57	
		F172	G36	V58	
		Q173	L38	P59	
		C174	R38	T67	
		H175	G32	P68	
		GLU	G31	M69	
		L177	D32	S74	
Serine	V182	L183	L24	P88	
	L184	H184	I25	E89	
	E188		G29	H90	
	E189		S30	L91	
	T190		G31	E92	
	K195		D32	S93	
	V199		S33	V96	
	T200		G34	N97	
	T201		Q35	C98	
	F206		G36	L104	
Valine			L24		
			I25		
			G29		
			S30		
			G31		
			D32		
			S33		
			G34		
			Q35		
			G36		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.78Å 60.78Å 76.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.73 – 1.72 33.73 – 1.72	Depositor EDS
% Data completeness (in resolution range)	98.4 (33.73-1.72) 98.4 (33.73-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.173 , 0.212 0.172 , 0.209	Depositor DCC
R_{free} test set	1216 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1941	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% 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	1.76	27/1868 (1.4%)	1.48	16/2529 (0.6%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	PRO	C-O	8.69	1.34	1.23
1	A	56	ILE	CA-CB	7.91	1.63	1.54
1	A	182	VAL	CA-CB	7.00	1.62	1.53
1	A	155	SER	N-CA	6.61	1.54	1.46
1	A	67	THR	N-CA	6.56	1.53	1.46
1	A	195	LYS	N-CA	6.54	1.54	1.46
1	A	25	ILE	N-CA	6.20	1.54	1.46
1	A	32	ASP	CA-C	6.13	1.61	1.53
1	A	74	SER	N-CA	6.08	1.53	1.45
1	A	138	HIS	CA-CB	6.04	1.57	1.53
1	A	160	ALA	CA-CB	6.02	1.62	1.53
1	A	54	ILE	CA-CB	5.98	1.61	1.54
1	A	176	GLY	N-CA	5.72	1.53	1.45
1	A	30	SER	C-O	-5.61	1.17	1.23
1	A	199	VAL	CA-CB	5.50	1.61	1.54
1	A	200	THR	CA-CB	5.50	1.61	1.53
1	A	168	LEU	N-CA	5.49	1.51	1.45
1	A	134	ALA	CA-CB	-5.47	1.44	1.53
1	A	88	PRO	C-O	5.44	1.30	1.23
1	A	40	TRP	C-O	5.39	1.30	1.24
1	A	160	ALA	C-O	5.39	1.30	1.24
1	A	14	VAL	N-CA	5.36	1.52	1.46
1	A	36	GLY	C-O	-5.28	1.17	1.23
1	A	29	GLY	C-O	5.26	1.29	1.23
1	A	96	VAL	CA-C	5.24	1.59	1.52
1	A	183	LEU	CA-C	5.18	1.59	1.52
1	A	19	ARG	C-O	5.16	1.29	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ILE	N-CA-C	-7.30	97.33	107.99
1	A	33	SER	CA-C-N	-6.64	112.70	120.00
1	A	33	SER	C-N-CA	-6.64	112.70	120.00
1	A	98	CYS	N-CA-C	-6.45	104.25	111.28
1	A	129	MET	N-CA-C	-6.13	104.51	111.07
1	A	190	THR	N-CA-C	-6.04	104.62	111.14
1	A	67	THR	CA-C-N	-5.79	113.85	119.87
1	A	67	THR	C-N-CA	-5.79	113.85	119.87
1	A	25	ILE	CG1-CB-CG2	-5.46	94.33	110.70
1	A	200	THR	CB-CA-C	5.31	118.49	109.84
1	A	119	LEU	N-CA-C	-5.26	100.82	109.40
1	A	57	ILE	N-CA-CB	-5.25	104.84	111.46
1	A	88	PRO	CB-CA-C	-5.18	104.19	110.98
1	A	69	MET	CG-SD-CE	-5.13	89.61	100.90
1	A	167	VAL	CB-CA-C	-5.07	104.63	111.63
1	A	195	LYS	N-CA-CB	5.06	117.55	110.12

There are no chirality outliers.

There are no planarity outliers.

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	1797	0	1826	37	1
2	A	144	0	0	3	1
All	All	1941	0	1826	37	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 10.

All (37) 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:92[A]:GLU:OE1	2:A:290:HOH:O	1.80	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:C	1:A:120[A]:ILE:HD13	1.90	0.96
1:A:120[B]:ILE:HD11	1:A:134:ALA:HB2	1.58	0.84
1:A:216:THR:O	1:A:220[A]:ILE:HG12	1.79	0.82
1:A:35:GLN:OE1	1:A:38:ARG:HD2	1.85	0.76
1:A:104:LEU:O	1:A:107:GLU:HG2	1.90	0.72
1:A:19:ARG:O	1:A:53:HIS:HD2	1.77	0.67
1:A:184[B]:HIS:HD2	1:A:188:GLU:OE2	1.79	0.66
1:A:118:ILE:HG22	1:A:120[A]:ILE:CD1	2.32	0.59
1:A:170:GLU:OE2	1:A:224[A]:TRP:HZ3	1.85	0.59
1:A:90:HIS:HD2	1:A:93:SER:H	1.51	0.57
1:A:115:LYS:NZ	2:A:328:HOH:O	2.42	0.52
1:A:90:HIS:CD2	1:A:93:SER:H	2.28	0.51
1:A:11:ARG:NH1	1:A:107:GLU:OE2	2.40	0.51
1:A:19:ARG:O	1:A:53:HIS:CD2	2.62	0.49
1:A:224[A]:TRP:CD1	1:A:225:ILE:N	2.81	0.49
1:A:146:ALA:O	1:A:173:GLN:HA	2.16	0.46
1:A:170:GLU:CD	1:A:224[A]:TRP:HZ3	2.23	0.46
1:A:172:PHE:CE2	1:A:174:CYS:SG	3.09	0.45
1:A:11:ARG:HH12	1:A:107:GLU:CD	2.24	0.45
1:A:118:ILE:HG22	1:A:120[A]:ILE:HD11	1.98	0.45
1:A:109:VAL:HA	1:A:113:ILE:O	2.16	0.44
1:A:177[A]:THR:HA	1:A:184[A]:HIS:CD2	2.52	0.44
1:A:121:GLY:HA3	1:A:145:PHE:CD2	2.52	0.44
1:A:24:LEU:HD11	1:A:145:PHE:HE2	1.83	0.43
1:A:69:MET:HE3	1:A:69:MET:HB2	1.57	0.42
1:A:24:LEU:HD11	1:A:145:PHE:CE2	2.54	0.42
1:A:171:LEU:HB3	1:A:201[A]:THR:HB	2.02	0.42
1:A:145:PHE:HA	1:A:172:PHE:O	2.20	0.42
1:A:90:HIS:CD2	1:A:93:SER:OG	2.74	0.41
1:A:121:GLY:HA3	1:A:145:PHE:CE2	2.55	0.41
1:A:215:LYS:HD2	2:A:360:HOH:O	2.21	0.41
1:A:177[B]:THR:HG23	1:A:206:PHE:C	2.46	0.40

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)
1:A:110:LYS:NZ	2:A:330:HOH:O[4_456]	2.12	0.08

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	229/239 (96%)	220 (96%)	9 (4%)	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	203/205 (99%)	191 (94%)	12 (6%)	18	3

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	92[A]	GLU
1	A	92[B]	GLU
1	A	114	LYS
1	A	120[A]	ILE
1	A	120[B]	ILE
1	A	167	VAL
1	A	200	THR
1	A	215	LYS
1	A	218	LEU
1	A	224[A]	TRP
1	A	224[B]	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	90	HIS

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 oligosaccharides 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	222/239 (92%)	-0.22	1 (0%) 87 90	8, 17, 32, 40	9 (4%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	VAL	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 oligosaccharides 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.