



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:39 PM UTC

PDB ID : 5T8U / pdb_00005t8u
Title : Crystal structure of P. falciparum LipL1 in complex lipoate
Authors : Guerra, A.J.; Afanador, G.A.; Prigge, S.T.
Deposited on : 2016-09-08
Resolution : 2.32 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

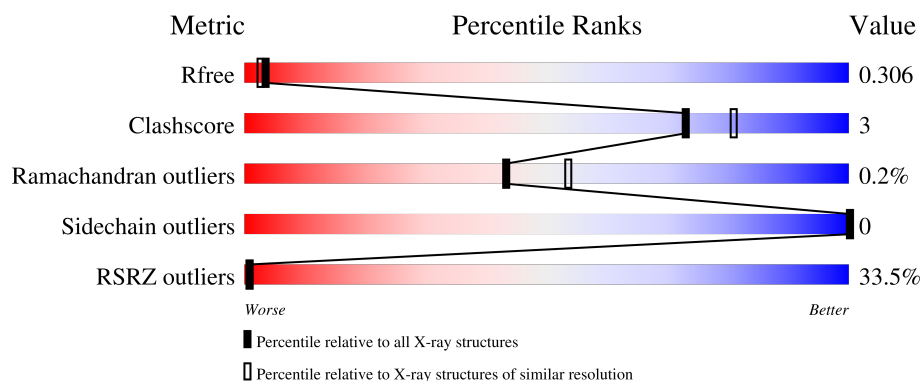
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	360	
1	B	360	

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 Lipoate-protein ligase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total 5293	C 1751	H 2569	N 457	O 509	S 7	0	0	0
1	B	336	Total 5308	C 1778	H 2546	N 466	O 511	S 7	0	0	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	-	expression tag	UNP Q8IEG9
A	12	HIS	-	expression tag	UNP Q8IEG9
A	13	HIS	-	expression tag	UNP Q8IEG9
A	14	HIS	-	expression tag	UNP Q8IEG9
A	15	HIS	-	expression tag	UNP Q8IEG9
A	16	HIS	-	expression tag	UNP Q8IEG9
A	17	HIS	-	expression tag	UNP Q8IEG9
A	18	GLU	-	expression tag	UNP Q8IEG9
A	19	LEU	-	expression tag	UNP Q8IEG9
A	?	-	LYS	deletion	UNP Q8IEG9
A	?	-	GLU	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ILE	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ILE	deletion	UNP Q8IEG9
A	?	-	LYS	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	LEU	deletion	UNP Q8IEG9
A	?	-	GLU	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ILE	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9

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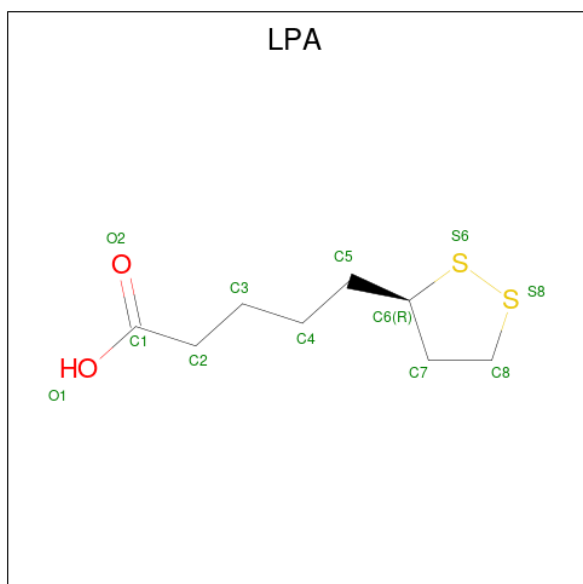
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	PHE	deletion	UNP Q8IEG9
A	?	-	GLN	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	LYS	deletion	UNP Q8IEG9
A	?	-	GLU	deletion	UNP Q8IEG9
A	?	-	GLN	deletion	UNP Q8IEG9
A	?	-	ILE	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ILE	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	THR	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	GLU	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
A	?	-	LEU	deletion	UNP Q8IEG9
A	?	-	ILE	deletion	UNP Q8IEG9
A	?	-	ASN	deletion	UNP Q8IEG9
B	11	GLY	-	expression tag	UNP Q8IEG9
B	12	HIS	-	expression tag	UNP Q8IEG9
B	13	HIS	-	expression tag	UNP Q8IEG9
B	14	HIS	-	expression tag	UNP Q8IEG9
B	15	HIS	-	expression tag	UNP Q8IEG9
B	16	HIS	-	expression tag	UNP Q8IEG9
B	17	HIS	-	expression tag	UNP Q8IEG9
B	18	GLU	-	expression tag	UNP Q8IEG9
B	19	LEU	-	expression tag	UNP Q8IEG9
B	?	-	LYS	deletion	UNP Q8IEG9
B	?	-	GLU	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	ILE	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	ILE	deletion	UNP Q8IEG9
B	?	-	LYS	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	LEU	deletion	UNP Q8IEG9
B	?	-	GLU	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	ILE	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	SER	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	PHE	deletion	UNP Q8IEG9
B	?	-	GLN	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	LYS	deletion	UNP Q8IEG9
B	?	-	GLU	deletion	UNP Q8IEG9
B	?	-	GLN	deletion	UNP Q8IEG9
B	?	-	ILE	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	ILE	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	THR	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	GLU	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9
B	?	-	LEU	deletion	UNP Q8IEG9
B	?	-	ILE	deletion	UNP Q8IEG9
B	?	-	ASN	deletion	UNP Q8IEG9

- Molecule 2 is LIPOIC ACID (CCD ID: LPA) (formula: $C_8H_{14}O_2S_2$).



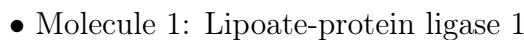
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			25	8	13	2	2		
2	B	1	Total	C	H	O	S	0	0
			25	8	13	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	44	Total	O	0	0
			44	44		

i

- Molecule 1: Lipoate-protein ligase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.24Å 120.24Å 134.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.57 – 2.32 48.57 – 2.32	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.57-2.32) 96.8 (48.57-2.32)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.11 _ 2558: ???)	Depositor
R, R_{free}	0.273 , 0.302 0.278 , 0.306	Depositor DCC
R_{free} test set	2317 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10735	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LPA

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	0.10	0/2783	0.29	0/3779
1	B	0.10	0/2821	0.27	0/3821
All	All	0.10	0/5604	0.28	0/7600

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	2724	2569	2630	16	0
1	B	2762	2546	2699	15	0
2	A	12	13	13	2	0
2	B	12	13	13	2	0
3	A	40	0	0	1	0
3	B	44	0	0	0	0
All	All	5594	5141	5355	35	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 3.

All (35) 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:A:401:LPA:C6	2:A:401:LPA:C7	1.98	1.41
2:B:401:LPA:C6	2:B:401:LPA:C7	1.98	1.41
1:B:29:ASN:N	1:B:257:ASP:OD2	2.22	0.73
1:A:56:ASN:OD1	1:A:57:THR:N	2.29	0.64
1:A:92:ILE:HG23	1:A:97:VAL:HB	1.84	0.59
1:A:285:THR:N	1:A:286:PRO:CD	2.67	0.58
1:A:233:GLU:OE2	3:A:501:HOH:O	2.18	0.56
1:B:156:VAL:HG11	1:B:212:ILE:HD13	1.87	0.56
1:B:40:ASN:O	1:B:44:ASN:ND2	2.36	0.53
1:B:236:LYS:HA	1:B:239:GLU:HG3	1.90	0.53
1:B:212:ILE:HD11	1:B:217:ILE:HD11	1.90	0.52
2:B:401:LPA:C7	2:B:401:LPA:C5	2.80	0.51
2:A:401:LPA:C7	2:A:401:LPA:C5	2.80	0.49
1:B:21:GLY:N	1:B:241:ASN:HD21	2.11	0.49
1:B:227:CYS:O	1:B:231:ILE:HG12	2.14	0.48
1:B:92:ILE:HG23	1:B:97:VAL:HB	1.96	0.47
1:A:267:GLU:OE2	1:A:271:TYR:OH	2.25	0.46
1:A:285:THR:O	1:A:286:PRO:C	2.58	0.46
1:A:316:ASN:OD1	1:A:331:LYS:NZ	2.32	0.45
1:A:277:ASP:OD1	1:A:278:TRP:N	2.50	0.44
1:B:35:ASN:ND2	1:B:70:ARG:O	2.50	0.44
1:B:212:ILE:CD1	1:B:217:ILE:HD11	2.47	0.44
1:B:239:GLU:O	1:B:241:ASN:N	2.49	0.44
1:B:102:ARG:NH2	1:B:105:GLY:O	2.50	0.44
1:A:77:ILE:HG22	1:A:81:GLN:HB2	2.00	0.43
1:A:169:ILE:O	1:A:170:LYS:C	2.61	0.43
1:A:162:SER:HA	1:A:178:THR:O	2.19	0.43
1:A:284:LYS:CB	1:A:286:PRO:HD2	2.48	0.43
1:A:29:ASN:OD1	1:A:30:GLN:N	2.52	0.43
1:B:156:VAL:HG12	1:B:212:ILE:HG21	2.01	0.42
1:A:114:GLY:O	1:A:182:ASN:N	2.42	0.41
1:B:181:ILE:HD11	1:B:226:LEU:HD22	2.02	0.41
1:B:175:HIS:CD2	1:B:175:HIS:C	2.98	0.41
1:A:185:LYS:HB2	1:A:214:LEU:HD21	2.03	0.40
1:A:73:ARG:HA	1:A:111:HIS:O	2.22	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	329/360 (91%)	312 (95%)	16 (5%)	1 (0%)	36	45
1	B	330/360 (92%)	312 (94%)	18 (6%)	0	100	100
All	All	659/720 (92%)	624 (95%)	34 (5%)	1 (0%)	43	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	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	305/338 (90%)	305 (100%)	0	100	100
1	B	310/338 (92%)	310 (100%)	0	100	100
All	All	615/676 (91%)	615 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	122	ASN
1	A	218	ASN

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Mol	Chain	Res	Type
1	A	219	ASN
1	A	241	ASN
1	A	245	ASN
1	A	325	ASN
1	A	335	ASN
1	B	290	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LPA	A	401	-	12,12,12	2.86	3 (25%)	14,14,14	1.59	3 (21%)
2	LPA	B	401	-	12,12,12	2.85	3 (25%)	14,14,14	1.66	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LPA	A	401	-	-	4/7/14/14	0/1/1/1
2	LPA	B	401	-	-	2/7/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	LPA	C7-C6	8.52	1.98	1.53
2	B	401	LPA	C7-C6	8.48	1.98	1.53
2	A	401	LPA	C6-S6	-3.26	1.54	1.80
2	B	401	LPA	C6-S6	-3.26	1.54	1.80
2	A	401	LPA	C7-C8	2.06	1.59	1.50
2	B	401	LPA	C7-C8	2.04	1.59	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	LPA	C8-S8-S6	3.08	105.39	94.48
2	A	401	LPA	C6-S6-S8	2.96	104.92	95.19
2	A	401	LPA	C8-S8-S6	2.92	104.83	94.48
2	B	401	LPA	C6-S6-S8	2.92	104.77	95.19
2	A	401	LPA	C3-C2-C1	-2.07	109.11	114.51
2	B	401	LPA	C3-C2-C1	-2.06	109.12	114.51

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	LPA	C4-C5-C6-S6
2	A	401	LPA	O2-C1-C2-C3
2	A	401	LPA	O1-C1-C2-C3
2	B	401	LPA	O2-C1-C2-C3
2	B	401	LPA	O1-C1-C2-C3
2	A	401	LPA	C4-C5-C6-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	LPA	2	0
2	B	401	LPA	2	0

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	A	333/360 (92%)	1.83	123 (36%)  	45, 83, 126, 164	33 (9%)
1	B	336/360 (93%)	1.61	101 (30%)  	52, 78, 122, 165	26 (7%)
All	All	669/720 (92%)	1.72	224 (33%)  	45, 81, 126, 165	59 (8%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	THR	6.6
1	B	209	ALA	6.1
1	A	242	TYR	6.0
1	A	320	ASP	6.0
1	B	248	PRO	5.5
1	A	77	ILE	5.5
1	A	21	GLY	5.3
1	B	194	PRO	5.3
1	A	286	PRO	5.2
1	A	283	GLY	5.1
1	B	283	GLY	5.1
1	A	55	ILE	5.0
1	B	278	TRP	4.9
1	B	200	ILE	4.8
1	B	21	GLY	4.8
1	A	156	VAL	4.8
1	B	320	ASP	4.7
1	A	321	CYS	4.6
1	A	278	TRP	4.6
1	A	221	ILE	4.6
1	A	218	ASN	4.5
1	B	286	PRO	4.5
1	A	212	ILE	4.4
1	B	311	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	58	ILE	4.3
1	A	185	LYS	4.2
1	A	78	GLY	4.2
1	B	151	ARG	4.1
1	A	284	LYS	4.1
1	B	282	TYR	4.0
1	B	241	ASN	4.0
1	A	186	ASN	4.0
1	A	150	GLY	4.0
1	A	282	TYR	4.0
1	B	340	TYR	3.9
1	B	84	TRP	3.9
1	B	57	THR	3.9
1	A	213	ASN	3.9
1	A	216	GLU	3.8
1	A	187	ILE	3.7
1	A	217	ILE	3.7
1	B	56	ASN	3.7
1	B	58	ILE	3.7
1	A	290	ASN	3.6
1	B	195	ASP	3.6
1	B	215	SER	3.5
1	B	223	CYS	3.5
1	A	188	LEU	3.5
1	B	156	VAL	3.5
1	A	183	LEU	3.5
1	A	338	ILE	3.4
1	B	284	LYS	3.4
1	B	221	ILE	3.4
1	A	339	LYS	3.3
1	A	289	GLN	3.3
1	B	337	ASP	3.3
1	A	23	LEU	3.3
1	B	172	VAL	3.3
1	A	264	LYS	3.3
1	A	57	THR	3.3
1	A	124	ASN	3.2
1	B	347	ILE	3.2
1	A	223	CYS	3.2
1	B	257	ASP	3.2
1	A	99	VAL	3.2
1	A	98	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	185	LYS	3.1
1	B	189	ASN	3.1
1	A	246	ILE	3.1
1	B	370	GLU	3.1
1	A	310	GLY	3.1
1	B	187	ILE	3.1
1	A	189	ASN	3.0
1	B	92	ILE	3.0
1	B	193	THR	3.0
1	A	169	ILE	3.0
1	B	196	LYS	3.0
1	A	318	PHE	2.9
1	A	353	ASN	2.9
1	B	91	ASN	2.9
1	A	178	THR	2.9
1	A	163	GLY	2.9
1	B	143	ASN	2.9
1	B	249	ASN	2.9
1	A	274	LEU	2.9
1	A	325	ASN	2.9
1	B	219	ASN	2.9
1	A	340	TYR	2.8
1	A	247	ILE	2.8
1	B	181	ILE	2.8
1	B	168	LYS	2.8
1	A	214	LEU	2.8
1	A	348	PHE	2.8
1	A	349	PHE	2.8
1	A	51	LYS	2.8
1	A	192	LEU	2.8
1	A	326	LEU	2.8
1	A	241	ASN	2.8
1	B	333	ILE	2.7
1	A	308	SER	2.7
1	B	220	ASN	2.7
1	A	84	TRP	2.7
1	A	219	ASN	2.7
1	A	181	ILE	2.7
1	A	315	GLY	2.7
1	B	75	ILE	2.7
1	B	303	LEU	2.7
1	A	54	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	124	ASN	2.6
1	A	244	THR	2.6
1	A	62	ASN	2.6
1	B	225	ASN	2.6
1	B	368	LEU	2.6
1	A	190	LYS	2.6
1	A	171	ASP	2.6
1	B	279	ASP	2.6
1	A	313	LYS	2.6
1	A	123	ASN	2.6
1	A	149	GLN	2.5
1	B	98	LEU	2.5
1	B	212	ILE	2.5
1	A	330	LEU	2.5
1	B	276	LYS	2.5
1	B	313	LYS	2.5
1	B	99	VAL	2.5
1	A	269	LEU	2.5
1	A	146	ALA	2.5
1	A	266	PRO	2.5
1	B	72	ASN	2.5
1	B	240	GLN	2.5
1	B	216	GLU	2.4
1	A	319	SER	2.4
1	B	54	ASN	2.4
1	B	236	LYS	2.4
1	A	301	LEU	2.4
1	A	72	ASN	2.4
1	A	220	ASN	2.4
1	B	258	GLN	2.4
1	B	343	GLU	2.4
1	A	148	THR	2.4
1	A	193	THR	2.4
1	B	304	PHE	2.4
1	B	312	ILE	2.4
1	A	275	LEU	2.4
1	A	90	LYS	2.4
1	A	75	ILE	2.4
1	A	303	LEU	2.4
1	B	269	LEU	2.4
1	A	293	TRP	2.4
1	B	280	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	335	ASN	2.3
1	B	171	ASP	2.3
1	A	262	ILE	2.3
1	A	347	ILE	2.3
1	B	53	LEU	2.3
1	B	113	LEU	2.3
1	B	184	GLU	2.3
1	A	182	ASN	2.3
1	A	225	ASN	2.3
1	A	92	ILE	2.3
1	B	59	GLU	2.3
1	A	322	LEU	2.3
1	B	321	CYS	2.3
1	A	257	ASP	2.3
1	B	182	ASN	2.3
1	A	96	GLY	2.3
1	A	238	TYR	2.3
1	A	211	THR	2.3
1	B	210	ARG	2.3
1	A	94	GLU	2.3
1	A	304	PHE	2.3
1	B	348	PHE	2.3
1	B	183	LEU	2.3
1	B	309	ASN	2.3
1	A	176	HIS	2.3
1	A	333	ILE	2.3
1	B	173	PHE	2.2
1	B	86	GLU	2.2
1	B	29	ASN	2.2
1	B	273	ASN	2.2
1	B	235	THR	2.2
1	B	272	TYR	2.2
1	B	307	VAL	2.2
1	A	314	ASP	2.2
1	A	281	CYS	2.2
1	B	149	GLN	2.2
1	B	217	ILE	2.2
1	A	158	ASP	2.2
1	A	249	ASN	2.2
1	A	86	GLU	2.2
1	B	264	LYS	2.2
1	B	297	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	188	LEU	2.1
1	A	288	PHE	2.1
1	A	263	THR	2.1
1	B	285	THR	2.1
1	A	60	LYS	2.1
1	A	312	ILE	2.1
1	A	317	ILE	2.1
1	A	305	PHE	2.1
1	A	369	GLN	2.1
1	B	365	SER	2.1
1	A	145	GLU	2.1
1	A	184	GLU	2.1
1	B	123	ASN	2.1
1	B	251	ILE	2.1
1	B	324	ILE	2.1
1	A	87	CYS	2.1
1	A	337	ASP	2.1
1	B	125	ILE	2.1
1	B	186	ASN	2.1
1	A	52	TYR	2.1
1	A	143	ASN	2.0
1	A	243	ASN	2.0
1	B	353	ASN	2.0
1	A	251	ILE	2.0
1	A	327	ILE	2.0
1	B	55	ILE	2.0
1	A	172	VAL	2.0
1	B	222	THR	2.0
1	B	369	GLN	2.0
1	B	88	ASN	2.0
1	B	192	LEU	2.0
1	A	125	ILE	2.0

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LPA	A	401	12/12	0.86	0.25	74,81,95,95	25
2	LPA	B	401	12/12	0.86	0.22	94,102,121,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.