



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:24 AM UTC

PDB ID : 1X2H / pdb_00001x2h
Title : Crystal Structure of Lipate-Protein Ligase A from Escherichia coli complexed with lipoic acid
Authors : Fujiwara, K.; Toma, S.; Okamura-Ikeda, K.; Motokawa, Y.; Nakagawa, A.; Taniguchi, H.
Deposited on : 2005-04-23
Resolution : 2.91 Å(reported)

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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

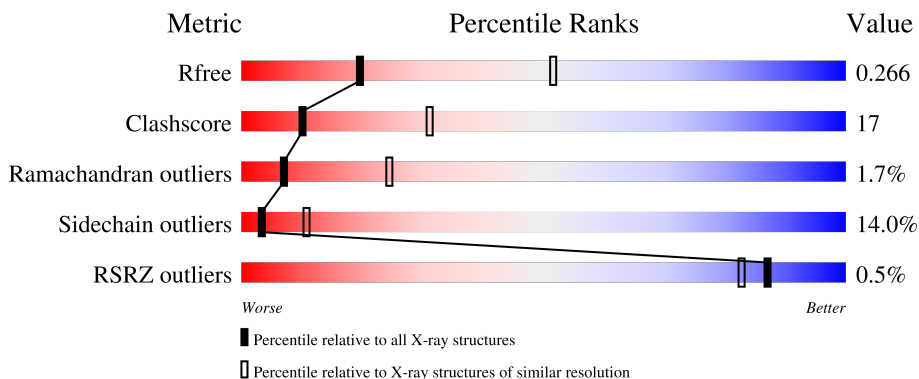
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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 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	337	% 57% 31% 9% ..
1	B	337	64% 28% 6% .
1	C	337	% 56% 36% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7937 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.

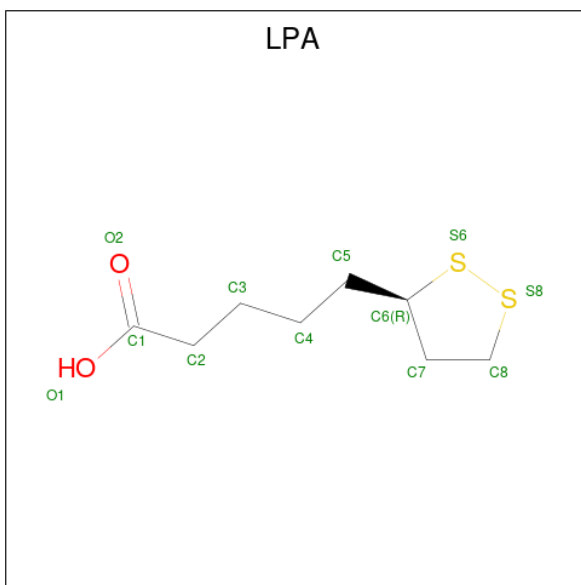
- Molecule 1 is a protein called Lipoate-protein ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	Se	0	0	0
			2614	1644	466	493	6	5			
1	B	330	Total	C	N	O	S	Se	0	0	0
			2614	1644	466	493	6	5			
1	C	337	Total	C	N	O	S	Se	0	0	0
			2663	1673	476	503	6	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MSE	MET	modified residue	UNP P32099
A	60	MSE	MET	modified residue	UNP P32099
A	89	MSE	MET	modified residue	UNP P32099
A	306	MSE	MET	modified residue	UNP P32099
A	332	MSE	MET	modified residue	UNP P32099
B	27	MSE	MET	modified residue	UNP P32099
B	60	MSE	MET	modified residue	UNP P32099
B	89	MSE	MET	modified residue	UNP P32099
B	306	MSE	MET	modified residue	UNP P32099
B	332	MSE	MET	modified residue	UNP P32099
C	27	MSE	MET	modified residue	UNP P32099
C	60	MSE	MET	modified residue	UNP P32099
C	89	MSE	MET	modified residue	UNP P32099
C	306	MSE	MET	modified residue	UNP P32099
C	332	MSE	MET	modified residue	UNP P32099

- Molecule 2 is LIPOIC ACID (CCD ID: LPA) (formula: C₈H₁₄O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			12	8	2	2		
2	B	1	Total	C	O	S	0	0
			12	8	2	2		

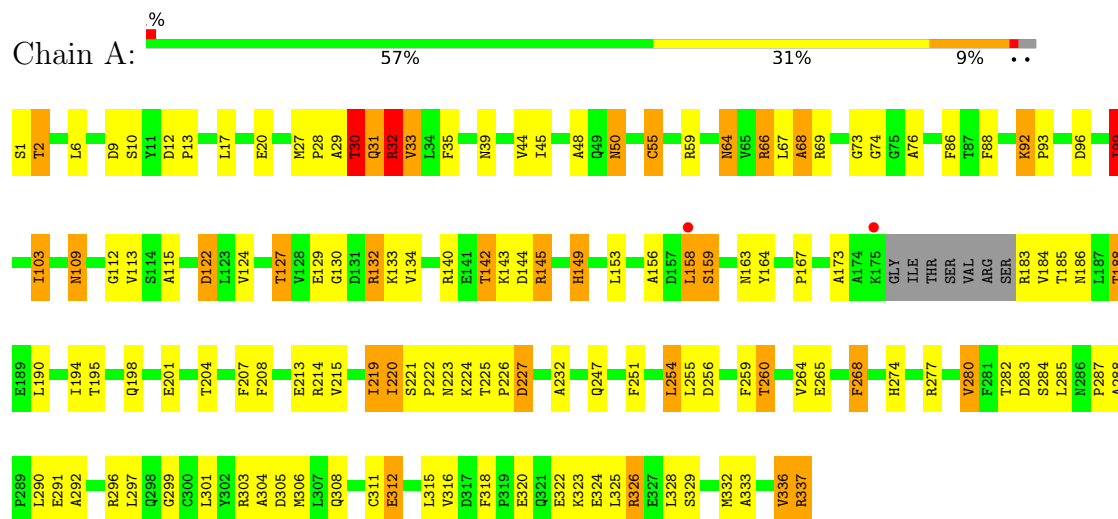
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	8	Total	O	0	0
			8	8		
3	C	3	Total	O	0	0
			3	3		

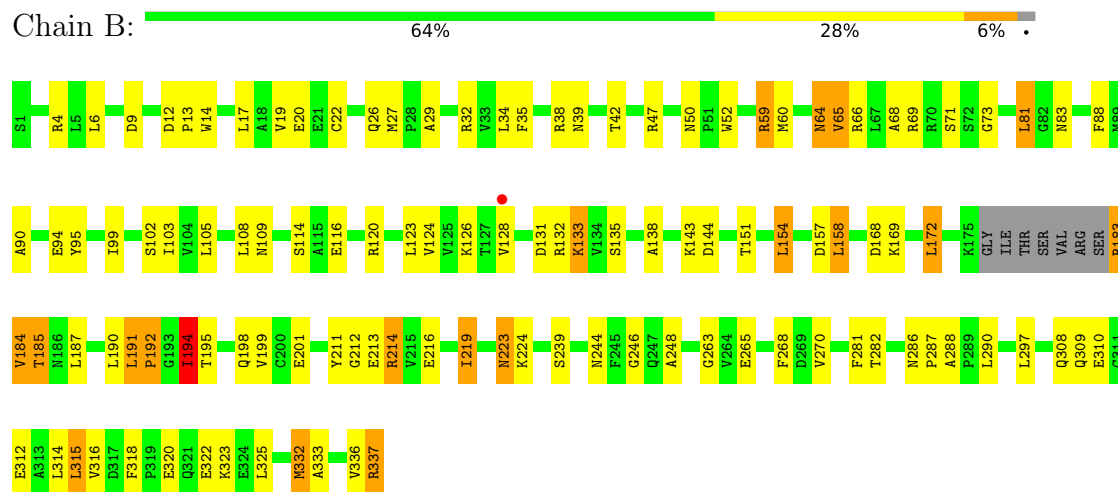
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Lipoate-protein ligase A



• Molecule 1: Lipoate-protein ligase A



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P287	S182	L108	S1
P288	R183	N109	T2
P289	V184	A110	L3
E290	T185	R111	R4
E291	N186	G112	L5
A292	L187	V113	
L293	T188	S114	W14
A294	E189	A117	L17
G295	L190	S118	A18
L296	L191	G119	V19
L297	G192	R120	
Q298	N194	N121	F24
R303	T195	V124	R25
L307	H196	V125	Q26
	E197	K126	M27
	Q198	T127	R32
E310	T204	V128	
C311	E205	E129	F35
V316	A206	G130	
	F207	D131	T42
E320	E213	R132	
G321	E216	K133	T45
E322	A217	V134	G46
R326		S135	R47
E327	L220	E141	E54
A330	T225	T142	C55
M331	E233	K143	R66
A333	T234	R145	L67
	F235	G146	A68
V336	A236	F147	R69
R337	R237	H148	
		H149	G73
	E242	G150	
	H253	T151	L81
	D256	L152	G82
	E257	L153	N83
	T260	L154	T84
	V264	N155	C85
	L266	A156	F86
	H267	D157	T87
	F268	R160	F88
	K272	L161	M89
	A277	A162	A90
	R278	N163	G91
	E279		R92
			P93
			E94
			Y95
			T99
			I103
			V104
			L105
			N106
			A107

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.20Å 111.60Å 289.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.67 – 2.91 66.67 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.1 (66.67-2.91) 97.1 (66.67-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.271 0.184 , 0.266	Depositor DCC
R_{free} test set	1572 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7937	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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	1.22	5/2665 (0.2%)	1.29	24/3601 (0.7%)
1	B	1.14	3/2665 (0.1%)	1.29	18/3601 (0.5%)
1	C	1.11	6/2715 (0.2%)	1.24	15/3670 (0.4%)
All	All	1.16	14/8045 (0.2%)	1.27	57/10872 (0.5%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	MSE	SE-CE	6.75	2.15	1.95
1	C	89	MSE	SE-CE	-6.70	1.75	1.95
1	C	2	THR	CA-CB	6.30	1.64	1.53
1	C	332	MSE	SE-CE	6.16	2.13	1.95
1	A	48	ALA	CA-CB	-5.85	1.45	1.53

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	LYS	N-CA-C	-7.24	99.57	110.28
1	B	318	PHE	CA-C-N	-7.07	111.21	119.05
1	B	318	PHE	C-N-CA	-7.07	111.21	119.05
1	A	30	THR	N-CA-C	-6.95	104.61	113.23
1	A	312	GLU	N-CA-C	6.52	120.49	112.54

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	2614	0	2551	101	0
1	B	2614	0	2551	77	0
1	C	2663	0	2605	104	0
2	A	12	0	13	0	0
2	B	12	0	13	1	0
3	A	11	0	0	2	0
3	B	8	0	0	2	0
3	C	3	0	0	1	0
All	All	7937	0	7733	270	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 17.

The worst 5 of 270 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:B:332:MSE:SE	1:B:332:MSE:CE	2.15	1.42
1:B:158:LEU:HD12	1:B:158:LEU:H	1.17	1.04
1:A:282:THR:HG21	1:A:290:LEU:HD12	1.39	1.03
1:C:286:ASN:HB3	3:C:338:HOH:O	1.59	0.99
1:C:89:MSE:HE3	1:C:145:ARG:HB2	1.40	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	326/337 (97%)	301 (92%)	20 (6%)	5 (2%)	8	27
1	B	326/337 (97%)	305 (94%)	16 (5%)	5 (2%)	8	27
1	C	335/337 (99%)	297 (89%)	31 (9%)	7 (2%)	5	20
All	All	987/1011 (98%)	903 (92%)	67 (7%)	17 (2%)	7	24

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	THR
1	B	81	LEU
1	B	212	GLY
1	B	246	GLY
1	C	94	GLU

5.3.2 Protein sidechains ⓘ

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	276/277 (100%)	235 (85%)	41 (15%)	3	9
1	B	276/277 (100%)	239 (87%)	37 (13%)	4	12
1	C	282/277 (102%)	243 (86%)	39 (14%)	3	11
All	All	834/831 (100%)	717 (86%)	117 (14%)	3	11

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	172	LEU
1	C	307	LEU
1	B	315	LEU
1	C	290	LEU
1	C	180	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	50	ASN
1	C	198	GLN
1	C	253	HIS
1	C	247	GLN
1	A	267	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](#)

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	B	338	-	12,12,12	0.93	0	14,14,14	1.78	4 (28%)
2	LPA	A	338	-	12,12,12	0.76	0	14,14,14	1.44	1 (7%)

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	B	338	-	-	5/7/14/14	0/1/1/1
2	LPA	A	338	-	-	1/7/14/14	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	LPA	C3-C2-C1	-4.38	103.07	114.51
2	A	338	LPA	C6-S6-S8	3.38	106.28	95.19
2	B	338	LPA	O2-C1-C2	-2.31	115.77	123.09
2	B	338	LPA	C4-C3-C2	-2.24	104.90	113.13
2	B	338	LPA	O1-C1-C2	2.21	120.98	114.00

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	338	LPA	C3-C4-C5-C6
2	B	338	LPA	C1-C2-C3-C4
2	B	338	LPA	C3-C4-C5-C6
2	B	338	LPA	C2-C3-C4-C5
2	B	338	LPA	O2-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	338	LPA	1	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 [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	325/337 (96%)	-0.42	2 (0%) 85 81	16, 34, 53, 80	0
1	B	325/337 (96%)	-0.39	1 (0%) 90 87	19, 33, 63, 83	0
1	C	332/337 (98%)	-0.20	2 (0%) 85 81	23, 41, 73, 79	0
All	All	982/1011 (97%)	-0.34	5 (0%) 87 83	16, 35, 67, 83	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	VAL	2.5
1	A	175	LYS	2.2
1	C	194	ILE	2.1
1	A	158	LEU	2.0
1	C	193	GLY	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](#)

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($\text{\AA}^2$)	Q<0.9
2	LPA	A	338	12/12	0.88	0.22	74,78,82,84	0
2	LPA	B	338	12/12	0.93	0.15	74,76,79,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.