Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:21 pm BST

PDB ID	:	5AMQ
Title	:	Structure of the La Crosse Bunyavirus polymerase in complex with the 3' and 5' viral RNA
Authors	:	Reguera, J.; Gerlach, P.; Cusack, S.
Deposited on	:	2015-03-12
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

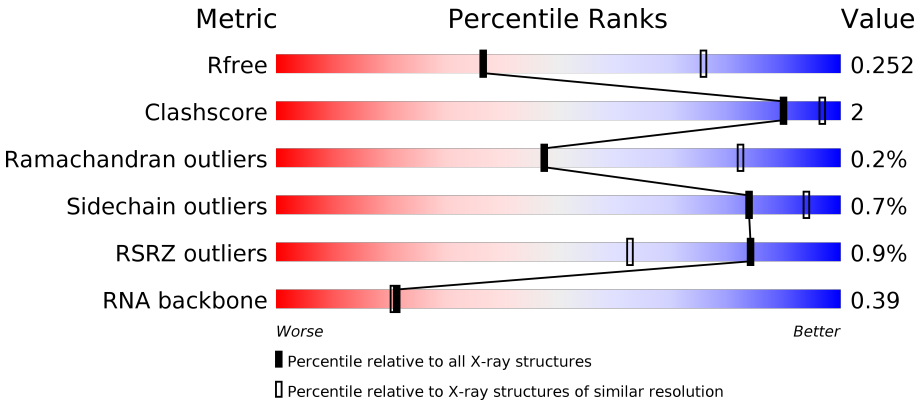
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 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 <=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	2263	% 70% . 26%
2	B	16	75% 25%
3	C	10	60% 40%
4	c	8	63% 38%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14334 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 RNA POLYMERASE L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1666	13618	8719	2269	2542	88	0	0	0

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	16	334	151	56	112	15	0	0	0

- Molecule 3 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	10	216	96	39	71	10	0	0	0

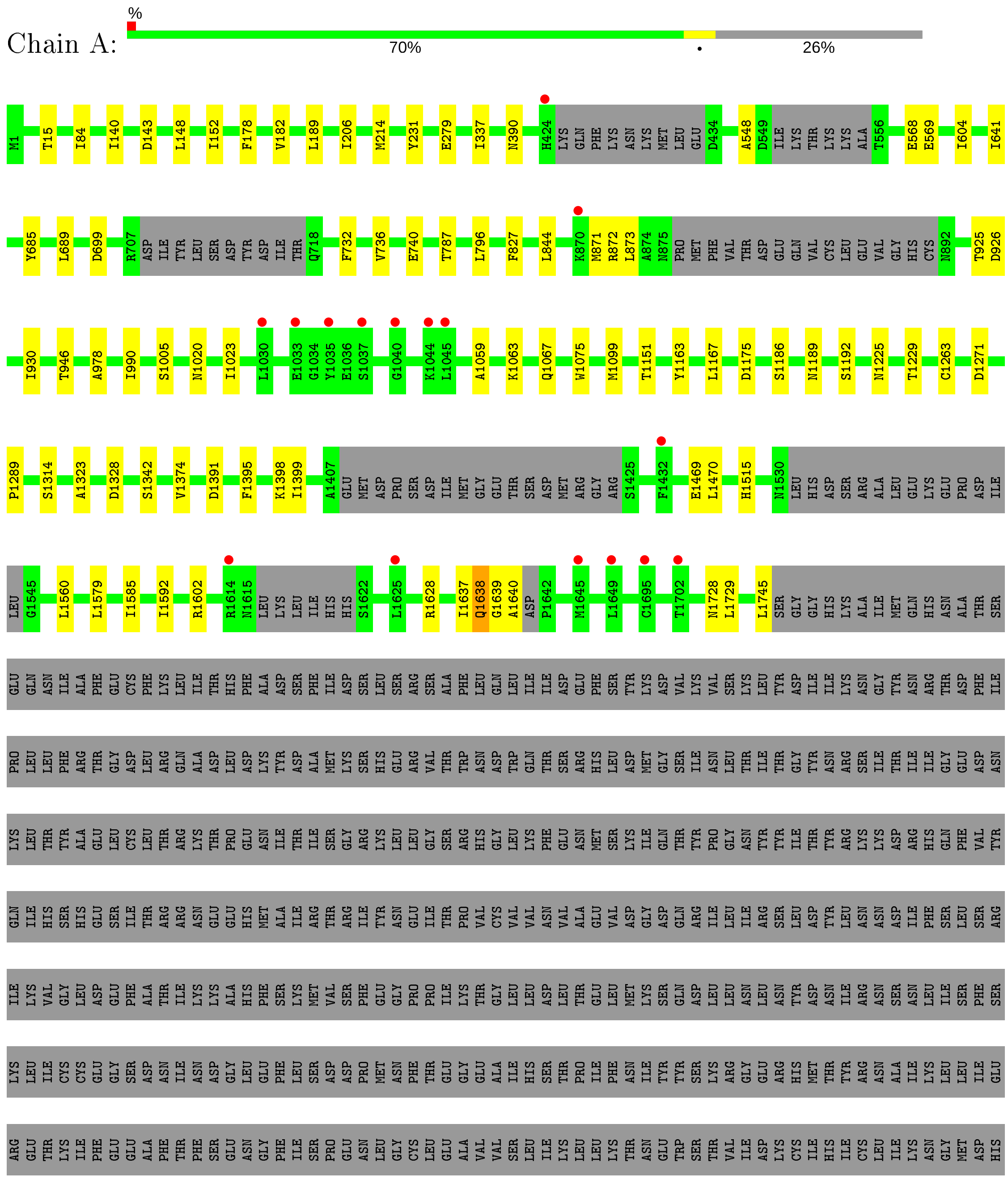
- Molecule 4 is a RNA chain called RNA.

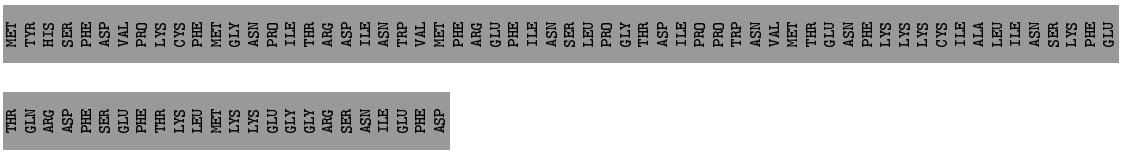
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	c	8	166	76	31	52	7	0	0	0

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 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.

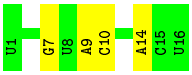
- Molecule 1: RNA POLYMERASE L





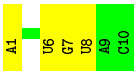
- Molecule 2: RNA

Chain B:



- Molecule 3: RNA

Chain C:



- Molecule 4: RNA

Chain c:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.00Å 141.10Å 165.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.17 – 3.00 49.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.17-3.00) 99.1 (49.17-3.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.192 , 0.252 0.194 , 0.252	Depositor DCC
R_{free} test set	2407 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	80.9	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14334	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.39	0/13890	0.61	3/18721 (0.0%)
2	B	0.33	0/372	0.69	0/577
3	C	0.70	1/241 (0.4%)	0.64	0/372
4	c	0.25	0/185	0.85	2/286 (0.7%)
All	All	0.40	1/14688 (0.0%)	0.61	5/19956 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	A	OP3-P	-9.73	1.49	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	568	GLU	N-CA-C	13.17	146.55	111.00
1	A	569	GLU	N-CA-CB	-7.70	96.74	110.60
4	c	9	G	C5'-C4'-O4'	6.69	117.12	109.10
1	A	568	GLU	CB-CA-C	-5.68	99.04	110.40
4	c	9	G	C5'-C4'-C3'	5.60	124.96	116.00

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	13618	0	13692	52	0
2	B	334	0	172	0	0
3	C	216	0	108	0	0
4	c	166	0	89	0	0
All	All	14334	0	14061	52	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 2.

All (52) 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:1639:GLY:O	1:A:1640:ALA:O	1.78	1.00
1:A:1063:LYS:HD3	1:A:1067:GLN:OE1	1.76	0.86
1:A:84:ILE:HD11	1:A:148:LEU:HD21	1.60	0.83
1:A:1063:LYS:HD3	1:A:1067:GLN:CD	1.99	0.83
1:A:1063:LYS:CD	1:A:1067:GLN:OE1	2.33	0.75
1:A:1063:LYS:CD	1:A:1067:GLN:CD	2.57	0.73
1:A:1628:ARG:HG2	1:A:1637:ILE:HD11	1.73	0.69
1:A:1225:ASN:O	1:A:1229:THR:HG23	1.92	0.69
1:A:1628:ARG:HG2	1:A:1637:ILE:CD1	2.24	0.68
1:A:1063:LYS:HD2	1:A:1067:GLN:NE2	2.11	0.66
1:A:1398:LYS:HB3	1:A:1560:LEU:HD22	1.77	0.66
1:A:685:TYR:CE2	1:A:689:LEU:HD11	2.33	0.62
1:A:1059:ALA:HB3	1:A:1189:ASN:HB3	1.82	0.62
1:A:1398:LYS:CB	1:A:1560:LEU:HD22	2.31	0.61
1:A:1063:LYS:NZ	1:A:1067:GLN:OE1	2.36	0.54
1:A:1063:LYS:HD2	1:A:1067:GLN:CD	2.30	0.51
1:A:189:LEU:HD12	1:A:231:TYR:HB2	1.93	0.50
1:A:214:MET:HE3	1:A:796:LEU:HD11	1.94	0.50
1:A:140:ILE:HD11	1:A:152:ILE:HD12	1.94	0.49
1:A:990:ILE:HD12	1:A:1186:SER:HB2	1.93	0.49
1:A:978:ALA:HB2	1:A:1151:THR:HG22	1.94	0.49
1:A:1314:SER:HG	1:A:1515:HIS:CE1	2.31	0.49
1:A:1637:ILE:O	1:A:1639:GLY:N	2.46	0.49
1:A:1323:ALA:HB1	1:A:1328:ASP:HB2	1.96	0.48
1:A:871:MET:O	1:A:873:LEU:N	2.48	0.47
1:A:1395:PHE:CE1	1:A:1399:ILE:HD11	2.50	0.46
1:A:214:MET:CE	1:A:796:LEU:HD11	2.46	0.46
1:A:1637:ILE:HG22	1:A:1638:GLN:N	2.31	0.45
1:A:1163:TYR:CE2	1:A:1167:LEU:HD11	2.52	0.45
1:A:1163:TYR:CZ	1:A:1167:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ILE:HG23	1:A:337:ILE:O	2.17	0.44
1:A:844:LEU:HD13	1:A:946:THR:HG22	1.99	0.44
1:A:787:THR:HG22	1:A:787:THR:O	2.17	0.43
1:A:1637:ILE:CG2	1:A:1638:GLN:N	2.80	0.43
1:A:925:THR:HG22	1:A:926:ASP:H	1.83	0.43
1:A:827:PHE:CE2	1:A:930:ILE:HD13	2.54	0.43
1:A:178:PHE:CZ	1:A:182:VAL:HG21	2.54	0.42
1:A:206:ILE:HD13	1:A:1099:MET:HB2	2.01	0.41
1:A:1469:GLU:HG2	1:A:1470:LEU:HD13	2.02	0.41
1:A:1020:ASN:O	1:A:1023:ILE:N	2.52	0.41
1:A:214:MET:HE3	1:A:1075:TRP:HE1	1.86	0.41
1:A:1602:ARG:NH2	1:A:1728:ASN:O	2.53	0.41
1:A:1637:ILE:HG22	1:A:1639:GLY:H	1.86	0.41
1:A:1637:ILE:C	1:A:1639:GLY:N	2.73	0.41
1:A:1289:PRO:HG3	1:A:1729:LEU:HA	2.03	0.41
1:A:1263:CYS:SG	1:A:1271:ASP:CG	2.99	0.41
1:A:1374:VAL:HG22	1:A:1592:ILE:HD12	2.03	0.41
1:A:604:ILE:HD11	1:A:641:ILE:HD13	2.02	0.41
1:A:1398:LYS:HB3	1:A:1560:LEU:CD2	2.50	0.40
1:A:1579:LEU:HA	1:A:1585:ILE:HD11	2.04	0.40
1:A:925:THR:HG22	1:A:926:ASP:N	2.36	0.40
1:A:736:VAL:HG22	1:A:740:GLU:HB2	2.04	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	1646/2263 (73%)	1568 (95%)	74 (4%)	4 (0%)	47 82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1638	GLN
1	A	548	ALA
1	A	872	ARG
1	A	1175	ASP

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	1538/2087 (74%)	1527 (99%)	11 (1%)	84 94

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	143	ASP
1	A	279	GLU
1	A	390	ASN
1	A	699	ASP
1	A	732	PHE
1	A	1005	SER
1	A	1192	SER
1	A	1342	SER
1	A	1391	ASP
1	A	1745	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	15/16 (93%)	4 (26%)	1 (6%)
3	C	9/10 (90%)	3 (33%)	0
4	c	7/8 (87%)	2 (28%)	0
All	All	31/34 (91%)	9 (29%)	1 (3%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	7	G
2	B	9	A
2	B	10	C
2	B	14	A
3	C	6	U
3	C	7	G
3	C	8	U
4	c	10	C
4	c	16	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	10	C

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	143:ASP	C	144:ARG	N	2.76

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, 95^{th} 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	1666/2263 (73%)	-0.13	16 (0%) 82 59	53, 84, 143, 189	0
2	B	16/16 (100%)	-0.40	0 100 100	76, 83, 93, 95	0
3	C	10/10 (100%)	-0.32	0 100 100	67, 76, 81, 84	0
4	c	8/8 (100%)	-0.69	0 100 100	85, 89, 97, 100	0
All	All	1700/2297 (74%)	-0.14	16 (0%) 84 63	53, 84, 143, 189	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1045	LEU	3.3
1	A	1035	TYR	3.2
1	A	1625	LEU	2.6
1	A	1645	MET	2.6
1	A	1040	GLY	2.5
1	A	1695	CYS	2.4
1	A	1037	SER	2.3
1	A	870	LYS	2.3
1	A	1702	THR	2.2
1	A	1614	ARG	2.2
1	A	1044	LYS	2.1
1	A	1033	GLU	2.1
1	A	1649	LEU	2.1
1	A	424	HIS	2.1
1	A	1432	PHE	2.0
1	A	1030	LEU	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 (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.