



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1M1C / pdb_00001m1c
Title : Structure of the L-A virus
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Deposited on : 2002-06-18
Resolution : 3.50 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

<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

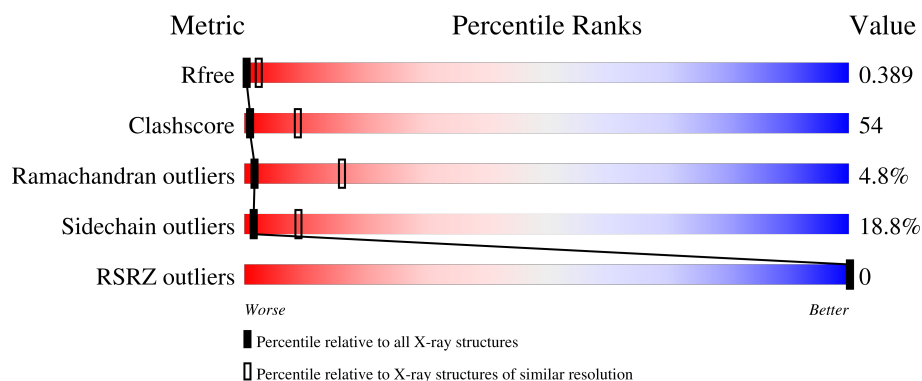
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

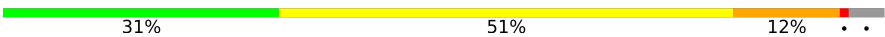
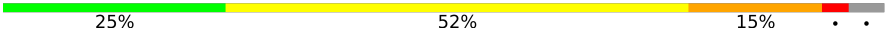
The reported resolution of this entry is 3.50 Å.

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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	680	
1	B	680	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10302 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.

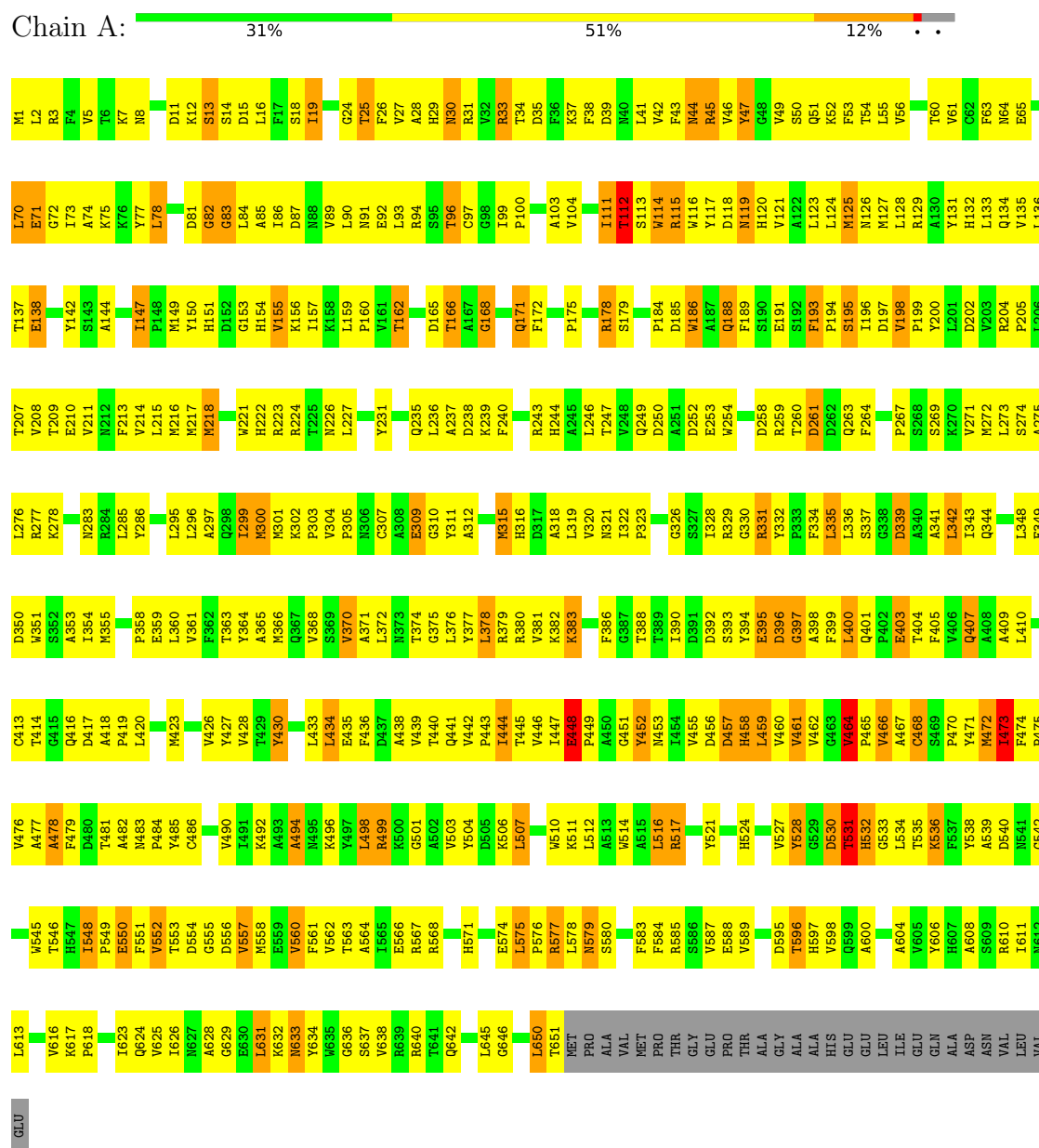
- Molecule 1 is a protein called Major coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5151	3302	871	955	23			
1	B	651	Total	C	N	O	S	0	0	0
			5151	3302	871	955	23			

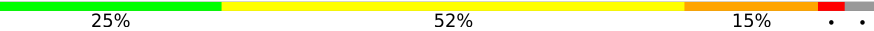
3 Residue-property plots

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: Major coat protein



- Molecule 1: Major coat protein

Chain B:  25% 52% 15% . .

PRO	V589	D522	H458	D391	L328	D263	P199	L133	E65	M1
THR		T523	L459	D392	R329	F264	T200	Q134	G66	L2
GLY	T593	H524	Y460	S393	G330	R265	L201	V135	S67	R3
GLU	Y594	F525		R331	G331	P266	D202	L136	S68	F4
PRO	D595	K526	Y463	E395	Y332		V203	L137	V69	Y5
THR	T596	V527	Y464	D396	P333	W272	R204	E138	L70	T6
ALA	H597		P465	G397	F334	L273	P205	Q139	K7	K7
GLY	V598	D530	Y466		L335	S274	L206	G140	E71	M8
ALA	Q599	T531	A467	L400	L336	A275	T207	Q141	G72	S9
ALA	A600	H532	C468	Q401	S337	L276	V208	Y142	I73	
HIS	G601	G533	S469	P402	G338	R277	T209	S143	A74	Q10
GLU	A602	L534	P470	E403	D339	K278	E210	K75	K12	D11
GLU	H603	T535	Y471		A340	V279	V211	G145	S13	K12
LEU	A604	K536	M472	V405	A341	V280	W212	D146	S14	S14
ILE	F537	L473	I473	Q407	L342	N281	F213	I147	D15	D15
GLU	Y606	F538	F474	A408	L343	H282	V214	P148	L16	L16
GLN	A539	A539	P475	A409	Q344	K283	L215	M149	F17	F17
ALA	A608		Y476	L410	A345	R284	M216	Y150	S18	S18
ASP	S609	D543	A477		T346	L285	M217	H151	D87	D87
ASN	R610	T544	A478	Q413	A347	Y286	W218	D152	N88	N88
VAL	I611	W545	F479	T414	L348	Q288	S219	G153	H89	H89
LEU	N612	T546	D480	Q415	L349		K220	H154	L90	L90
VAL	L613	H547	T481	Q416			W221	V155	E92	E92
GLU	D614	P549	A482	D417	S352	T291	H222	K156	L93	L93
	Y615	E549	N483	A418	A353	A292	R223	L157	R94	F26
	V616	E550	P484	P419	T354	K293	R224	K158	S95	V27
	K617	F551	Y485	L420	K355	Q294	T225	L159	T96	A28
	P618	V552				L295	K226	P160	C97	H29
		T553	N488	N423	P358	N296	L227	V161	G98	N30
	G622	W558	F489	S424	F359	A297	A228	T162	I99	R31
	I623	E559	V490	D425	L360	Q298	L229	I163	P100	Y32
	Q624	V560	I491	V426	V361	T299	D230	D184	R33	
	V625	K492	K492	Y427	F362	K300	Y231	D165		
	I626	F561	A493	V428	T363	K301	P234	T170	K37	K37
	N627	V562	N494	T429	Y364	K302	Q235	Q171	F38	F38
	A628	T563	N495	V430	A365	L236	F172	S106	D39	
	G629	A564	K496	P431	K366	V304	A173	Y109		
	E630	T565	Y497	L434	Q367	P305	K237	H110	V42	V42
	L631		L498	E435	V368	K306	D238	I111	F43	F43
	K632	R568	R499	E436	S369	C307	K239	T112	M44	M44
	N633	A569	K500	F436	V370	A308	F240	S113	R45	R45
	Y634	R570	G501	D437	A371	E309	A241	W114	V46	V46
	N635	H571	A502	A438	L372	G310	Y242	S115	Y47	Y47
	G636	F572	V503			Y311	R243	W116	G48	G48
	S637	V573	Y504	V442	G375	A312		T117	V49	V49
	V638	E574	D505	P443	L376	K313	T247	D118	S50	S50
	R639	L575	K506	L444	Y377	L314	V248	N119	Q51	Q51
	R640	P576	L507	T445	L378	K315	Q249	H120	K52	K52
	T641	R577	E508	V446	R379	H316	D250	Y121	F53	F53
	Q642	L578	A509	L447	R380	D317	A251	A122	T54	T54
	Q643	N579	V510	E448	V381	A318	D252	L123	L55	L55
	G644	S580		P449	K382	L319	E253	Q188	V56	V56
	L650	P581	A450	A450	K383	V320	W254	F189	G57	G57
	T651	A582	G451	G451	T384	N321	T255	S190	N58	N58
		F583	Y452	Y452	G385	T322	E256	E191	P59	P59
		R584	R517	V453	F386	P323			T60	T60
	PRO	R585	V518	T454	G387	K324	R259	S195	V61	V61
	ALA	S586	A519	V455	T388	F325	T260	I196	G62	G62
	VAL	V587	G520	D456	T389	G326	D261	D197	F63	F63
	MET	E588	Y521	D457	L390	S327	D262	V198	N64	N64

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	407.00Å 403.20Å 572.00Å 90.00° 90.46° 90.00°	Depositor
Resolution (Å)	30.00 – 3.50 30.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.50) 26.4 (30.00-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.31 (at 3.25Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.266 , 0.268 0.389 , 0.389	Depositor DCC
R_{free} test set	96853 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.064 for k,h,-l 0.065 for -k,-h,-l 0.067 for h,-k,-l	Xtriage
F_o, F_c correlation	0.30	EDS
Total number of atoms	10302	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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	0.35	0/5289	0.96	29/7212 (0.4%)
1	B	0.34	0/5289	0.96	27/7212 (0.4%)
All	All	0.35	0/10578	0.96	56/14424 (0.4%)

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	613	LEU	N-CA-C	13.81	126.02	110.97
1	A	532	HIS	N-CA-C	-12.56	88.42	108.90
1	A	452	TYR	N-CA-C	-12.26	92.06	108.24
1	B	493	ALA	N-CA-C	9.23	123.72	109.60
1	B	615	TYR	N-CA-C	-9.20	101.82	113.23

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	5151	0	5012	503	0
1	B	5151	0	5012	603	0
All	All	10302	0	10024	1092	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 54.

The worst 5 of 1092 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:16:LEU:HB2	1:B:363:THR:HG21	1.23	1.14
1:B:445:THR:HG23	1:B:446:VAL:H	1.05	1.14
1:A:15:ASP:HB2	1:A:608:ALA:HB1	1.25	1.13
1:A:144:ALA:HB3	1:A:165:ASP:HA	1.26	1.10
1:B:376:LEU:HB3	1:B:464:VAL:HG21	1.31	1.10

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	649/680 (95%)	597 (92%)	36 (6%)	16 (2%)	4	28
1	B	649/680 (95%)	540 (83%)	63 (10%)	46 (7%)	1	10
All	All	1298/1360 (95%)	1137 (88%)	99 (8%)	62 (5%)	2	16

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	397	GLY
1	A	473	ILE
1	A	531	THR
1	A	536	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	550/573 (96%)	457 (83%)	93 (17%)	2	13
1	B	550/573 (96%)	436 (79%)	114 (21%)	1	6
All	All	1100/1146 (96%)	893 (81%)	207 (19%)	1	9

5 of 207 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	121	VAL
1	B	320	VAL
1	B	616	VAL
1	B	164	ASP
1	B	249	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	GLN
1	B	401	GLN
1	B	154	HIS
1	B	283	ASN
1	B	547	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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	651/680 (95%)	-1.18	0 100 100	16, 54, 114, 169	0
1	B	651/680 (95%)	-1.20	0 100 100	14, 60, 127, 167	0
All	All	1302/1360 (95%)	-1.19	0 100 100	14, 57, 125, 169	0

There are no RSRZ outliers to report.

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.