



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1M1C
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 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

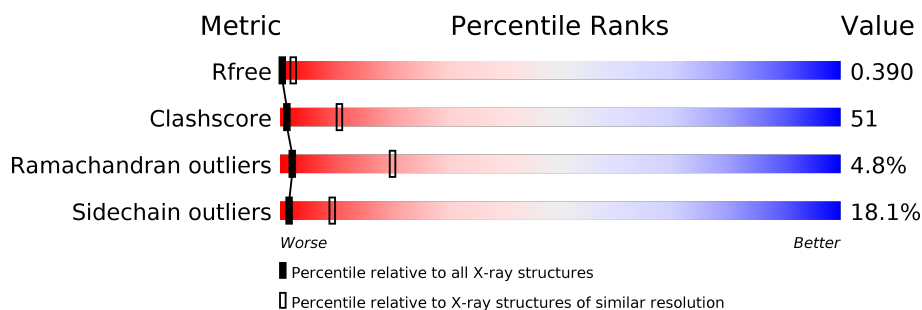
1 Overall quality at a glance

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 $\leq 5\%$.

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.

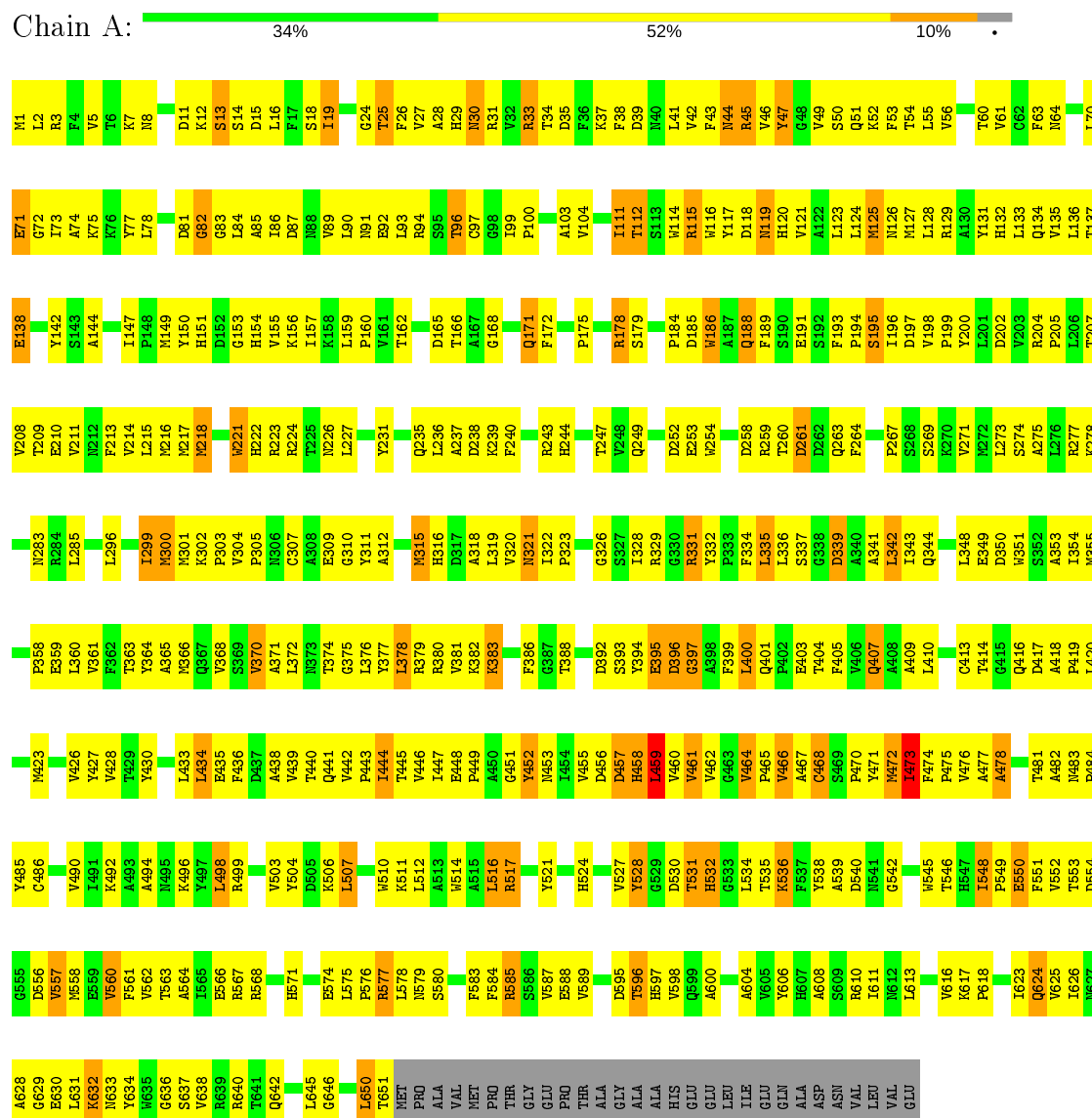
- Molecule 1 is a protein called Major coat protein.

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 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. 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. 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



GLU	Y594	H524	G463	Y394	S327	P284	L201	L133	E65	M1
PRO	D595	F525	G464	E395	R329	R265	D202	Q134	G66	L2
THR	Y596	R526	V464	D396	G330	P286	R203	V135	S67	R3
ALA	H597	V527	P465	G397	R331	K270	R204	L136	S68	F4
GLY	V598	V466	V466	G397	R332	K271	P205	T137	V6	T5
ALA	Q599	D530	A467	L400	R333	Y332	L206	E138	T6	T6
ALA	A600	T531	C468	Q461	F334	M272	T207	Q139	E71	K7
HIS	G601	H532	S469	P402	F334	L273	V208	G140	G72	M8
GLU	A602	G533	P470	E403	L335	S274	T209	Q141	I73	S9
GLU	H603	L534	Y471	E403	L336	A275	E210	Q142	Q10	Q10
LEU	A604	T535	Y472	V406	S337	L276	V211	S143	K75	D11
ILE	V605	K536	I473	Q407	G338	R277	N212	A144	K12	K12
GLU	Y606	F537	F474	A408	D339	K278	F213	G145	S13	S13
GLN	H607	Y538	P475	A409	A340	Y279	V214	D146	Y77	Y77
ALA	A608	A539	V476	L410	A341	V280	L215	I147	S14	S14
ASP	S609	A477	A477	L410	L342	N281	M216	P148	D15	D15
ASN	R610	T544	F478	C413	I343	H282	M217	M149	F17	F17
VAL	I611	W545	F479	T414	T414	N283	M218	Y150	S18	S18
LEU	W612	T546	D480	G415	G415	R284	S219	H151	I88	I88
VAL	L613	H547	T481	Q416	L348	L285	K220	D152	I89	I89
GLU	W615	I548	A482	D417	W351	Y286	K221	G153	V89	V89
	V616	P549	M483	A418	S352	N287	H222	H154	N91	N91
	W617	E550	P484	P419	A353	Q288	R223	V155	E92	E92
	P618	F551	Y485	L420	I354	R224	R224	K156	L93	L93
		V552	C486		T291	T225	T225	I157	R94	R94
		T553	G487	M423	A292	N226	N226	K158	S95	S95
			M488	S424	A293	L227	L227	L159	T96	T96
			F489	D425	Q294	A228	A228	P160	C97	C97
			V490	V426	E359	L229	L229	V161	G98	G98
			V500	Y427	L360	L296	D230	T162	I99	I99
			K492	V428	A297	A297	Y231	I163	V32	V32
			A493	T429	F362	Q298		D164	R33	R33
			A494	Y430	T363	L299	P234	D165		
			M495	P431	Y364	M300	Q235		K37	K37
			K496		A365	N301	L236		F38	F38
			Y497	L434	M366	K302	A237	Q171	D39	D39
			L498	E435	Q367	P303	D238	F172		
			R499	P436	V368	V304	K239	A173	V42	V42
			K500	D437	S369	P305	F240	W174	F43	F43
			A501	A438	V370	N306	A241	P175	N44	N44
			A502		A371	C307	Y242		S113	S113
			V503	V442	L372	A308	R243	R178	W114	W114
			Y504	P443	G375	E309	T247	S179	R115	R115
			D505	I444	L376	G310	V248	T180	W116	W116
			K506	T445	Y377	Y311	V249	D181	Y117	Y117
			L507	T446	Y377	A312	Q249		D118	D118
			E508	I447	L378	W313	D250	P184	Q51	Q51
			A509	E448	R379	L314	A251	D185	H120	H120
			W510	P449	R380	M315	D252	W186	V121	V121
				A450	V381	H316	E253	A187	A122	A122
			A513	G451	K382	D317	W254	Q188	L123	L123
			W514	Y452	K383	A318	I255	F189	L124	L124
			R517	N453	T384	V320	E256	S190	G57	G57
			V518	I454	G385	N321	G257		N126	N126
			A519	V455	F386	I322	D258	S195	P59	P59
			W520	D456		P323	R259	I196	L128	L128
			Y521	D457	I390	F324	T260	D197	R129	R129
			T523	H488	D391	F325	D261	V198	A130	A130
				L459	D392	D262	D262	P199	F63	F63
				V460	S393	G326	Q263	Y200	H132	H132

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 47.85 – 3.28	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.50) 22.6 (47.85-3.28)	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 0.390 , 0.390	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 , -17.0	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	0.59	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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.29	0/5289	0.57	4/7212 (0.1%)
1	B	0.29	0/5289	0.60	4/7212 (0.1%)
All	All	0.29	0/10578	0.59	8/14424 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	HIS	N-CA-C	-8.36	88.42	111.00
1	A	452	TYR	N-CA-C	-7.01	92.06	111.00
1	B	492	LYS	N-CA-C	-5.83	95.27	111.00
1	B	474	PHE	N-CA-C	5.65	126.25	111.00
1	B	613	LEU	N-CA-C	5.56	126.02	111.00

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	470	0
1	B	5151	0	5012	579	0
All	All	10302	0	10024	1036	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 51.

The worst 5 of 1036 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%)	5	34
1	B	649/680 (95%)	540 (83%)	63 (10%)	46 (7%)	1	12
All	All	1298/1360 (95%)	1137 (88%)	99 (8%)	62 (5%)	2	20

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%)	462 (84%)	88 (16%)	2	14
1	B	550/573 (96%)	439 (80%)	111 (20%)	1	6
All	All	1100/1146 (96%)	901 (82%)	199 (18%)	1	9

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	ASP
1	B	156	LYS
1	B	586	SER
1	B	15	ASP
1	B	78	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	HIS
1	B	10	GLN
1	B	599	GLN
1	A	597	HIS
1	A	624	GLN

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 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](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.