



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:22 PM UTC

PDB ID : 7UZT / pdb_00007uzt
Title : Crystal structure of the human astrovirus MLB1 capsid protein spike domain at 1.86-Å resolution
Authors : Delgado-Cunningham, K.; DuBois, R.
Deposited on : 2022-05-09
Resolution : 1.86 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
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

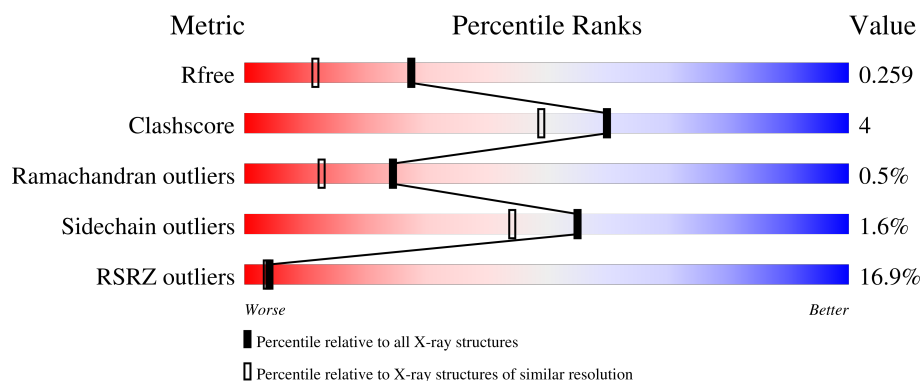
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	266	
1	B	266	
1	C	266	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5271 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 Capsid polypeptide VP90.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	1	0
			1667	1089	264	303	11			
1	B	214	Total	C	N	O	S	0	1	0
			1684	1097	267	309	11			
1	C	214	Total	C	N	O	S	0	2	0
			1689	1100	267	311	11			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	MET	-	initiating methionine	UNP B6UYJ1
A	389	HIS	-	expression tag	UNP B6UYJ1
A	390	HIS	-	expression tag	UNP B6UYJ1
A	391	HIS	-	expression tag	UNP B6UYJ1
A	392	HIS	-	expression tag	UNP B6UYJ1
A	393	HIS	-	expression tag	UNP B6UYJ1
A	394	HIS	-	expression tag	UNP B6UYJ1
A	395	HIS	-	expression tag	UNP B6UYJ1
A	396	HIS	-	expression tag	UNP B6UYJ1
A	397	HIS	-	expression tag	UNP B6UYJ1
A	398	HIS	-	expression tag	UNP B6UYJ1
B	388	MET	-	initiating methionine	UNP B6UYJ1
B	389	HIS	-	expression tag	UNP B6UYJ1
B	390	HIS	-	expression tag	UNP B6UYJ1
B	391	HIS	-	expression tag	UNP B6UYJ1
B	392	HIS	-	expression tag	UNP B6UYJ1
B	393	HIS	-	expression tag	UNP B6UYJ1
B	394	HIS	-	expression tag	UNP B6UYJ1
B	395	HIS	-	expression tag	UNP B6UYJ1
B	396	HIS	-	expression tag	UNP B6UYJ1
B	397	HIS	-	expression tag	UNP B6UYJ1
B	398	HIS	-	expression tag	UNP B6UYJ1
C	388	MET	-	initiating methionine	UNP B6UYJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	389	HIS	-	expression tag	UNP B6UYJ1
C	390	HIS	-	expression tag	UNP B6UYJ1
C	391	HIS	-	expression tag	UNP B6UYJ1
C	392	HIS	-	expression tag	UNP B6UYJ1
C	393	HIS	-	expression tag	UNP B6UYJ1
C	394	HIS	-	expression tag	UNP B6UYJ1
C	395	HIS	-	expression tag	UNP B6UYJ1
C	396	HIS	-	expression tag	UNP B6UYJ1
C	397	HIS	-	expression tag	UNP B6UYJ1
C	398	HIS	-	expression tag	UNP B6UYJ1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	64	Total O 64 64	0	0
2	B	94	Total O 94 94	0	0
2	C	73	Total O 73 73	0	0



HIS
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.10Å 77.11Å 75.44Å 90.00° 110.71° 90.00°	Depositor
Resolution (Å)	47.66 – 1.86 47.66 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.66-1.86) 98.0 (47.66-1.86)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.242 , 0.260 0.241 , 0.259	Depositor DCC
R_{free} test set	2015 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5271	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.67% 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	0.65	1/1716 (0.1%)	0.95	1/2337 (0.0%)
1	B	0.63	0/1734	0.93	2/2362 (0.1%)
1	C	0.56	0/1742	0.88	2/2373 (0.1%)
All	All	0.61	1/5192 (0.0%)	0.92	5/7072 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	563	VAL	C-N	-6.28	1.25	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	499	ASP	CB-CA-C	5.79	119.78	110.16
1	C	618	PHE	CA-CB-CG	5.31	119.11	113.80
1	B	499	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	492	GLU	CB-CA-C	-5.17	100.48	109.32
1	A	452	PHE	CA-CB-CG	5.11	118.91	113.80

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	1667	0	1641	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1684	0	1652	8	0
1	C	1689	0	1656	16	0
2	A	64	0	0	0	0
2	B	94	0	0	0	0
2	C	73	0	0	1	0
All	All	5271	0	4949	43	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 4.

All (43) 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:435:PHE:HD2	1:A:474:VAL:CG1	1.98	0.77
1:C:480:MET:HE2	1:C:482:LEU:HD21	1.69	0.75
1:A:435:PHE:HD2	1:A:474:VAL:HG11	1.54	0.72
1:C:606:ASN:O	1:C:607:GLU:HB2	1.90	0.70
1:C:431:MET:HE2	1:C:476:VAL:HG21	1.75	0.69
1:A:529[A]:LEU:HD21	1:A:623:LEU:HD13	1.75	0.68
1:B:529:LEU:HD21	1:B:623:LEU:HD23	1.80	0.61
1:A:480:MET:HE2	1:A:482:LEU:HD21	1.87	0.57
1:C:457:SER:HA	1:C:469:LYS:HD3	1.85	0.57
1:A:435:PHE:CD2	1:A:474:VAL:HG11	2.39	0.56
1:C:473:MET:HE2	1:C:587:PHE:CE2	2.41	0.55
1:A:542:ASN:HA	1:A:576:LEU:O	2.07	0.55
1:C:431:MET:HE2	1:C:476:VAL:CG2	2.37	0.54
1:A:435:PHE:HD2	1:A:474:VAL:HG12	1.74	0.53
1:C:450:LEU:HD13	1:C:547:VAL:HG11	1.91	0.52
1:C:451:LEU:HD23	1:C:472:SER:HB2	1.97	0.46
1:A:458:LYS:CE	1:A:541:PHE:HB2	2.46	0.46
1:C:548:TYR:CD2	1:C:569:GLN:HA	2.51	0.45
1:A:473:MET:HB3	1:A:578:TYR:CZ	2.51	0.45
1:C:450:LEU:HD13	1:C:547:VAL:CG1	2.45	0.45
1:B:420:SER:HA	1:B:490:THR:HG21	1.99	0.45
1:B:641:TRP:O	1:B:642:GLU:C	2.60	0.45
1:B:431:MET:SD	1:B:588:MET:HG3	2.57	0.45
1:B:544:ALA:HA	1:B:574:LYS:O	2.17	0.44
1:A:480:MET:CE	1:A:482:LEU:HD21	2.47	0.44
1:A:503:VAL:HB	1:A:511:ALA:HB3	2.00	0.44
1:A:626:LEU:HD12	1:A:631:TRP:HE1	1.83	0.43
1:C:448:MET:O	1:C:450:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:MET:HE3	1:A:481:TRP:CH2	2.54	0.43
1:A:588:MET:HE3	1:A:588:MET:HB3	1.79	0.43
1:A:458:LYS:HE2	1:A:541:PHE:HB2	2.00	0.43
1:A:440:ILE:HD11	1:A:450:LEU:HD21	2.02	0.42
1:A:642:GLU:HB3	1:B:521:ALA:HA	2.01	0.42
1:A:597:PHE:HE1	1:A:599:ILE:HD11	1.85	0.41
1:C:455:ASN:OD1	2:C:701:HOH:O	2.21	0.41
1:B:529:LEU:HD22	1:B:590:VAL:HG22	2.02	0.41
1:A:505:VAL:HG23	1:A:510:VAL:HG21	2.01	0.41
1:C:598:THR:HA	1:C:602:TYR:O	2.21	0.41
1:B:612:GLY:O	1:C:607:GLU:HG2	2.21	0.41
1:C:473:MET:HB3	1:C:578:TYR:CZ	2.56	0.41
1:A:596:SER:HA	1:A:604:VAL:O	2.21	0.40
1:A:425:PRO:HA	1:A:497:PHE:CE1	2.56	0.40
1:C:525:ARG:HB3	1:C:615:LEU:HD23	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	204/266 (77%)	198 (97%)	5 (2%)	1 (0%)	24	13
1	B	209/266 (79%)	199 (95%)	9 (4%)	1 (0%)	24	13
1	C	210/266 (79%)	203 (97%)	6 (3%)	1 (0%)	24	13
All	All	623/798 (78%)	600 (96%)	20 (3%)	3 (0%)	24	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	GLU
1	B	607	GLU

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Mol	Chain	Res	Type
1	C	607	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	182/227 (80%)	178 (98%)	4 (2%)	45	32
1	B	184/227 (81%)	181 (98%)	3 (2%)	55	44
1	C	185/227 (82%)	183 (99%)	2 (1%)	65	57
All	All	551/681 (81%)	542 (98%)	9 (2%)	55	44

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	453	GLN
1	A	484	LYS
1	A	499	ASP
1	A	614	GLU
1	B	450	LEU
1	B	475	LEU
1	B	536	LYS
1	C	565	LEU
1	C	600	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	466	HIS
1	B	507	ASN
1	B	524	ASN
1	B	542	ASN
1	C	487	ASN
1	C	606	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](#)

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

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	211/266 (79%)	1.65	77 (36%) 1 0	10, 25, 40, 52	1 (0%)
1	B	214/266 (80%)	0.70	17 (7%) 18 19	8, 17, 27, 34	1 (0%)
1	C	214/266 (80%)	0.74	14 (6%) 25 27	13, 21, 34, 39	2 (0%)
All	All	639/798 (80%)	1.03	108 (16%) 4 4	8, 21, 35, 52	4 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	GLY	4.6
1	A	541	PHE	4.5
1	A	447	TYR	4.5
1	A	578	TYR	4.3
1	A	575	THR	4.2
1	C	445	GLY	4.0
1	A	543	PHE	3.9
1	A	499	ASP	3.9
1	A	573	ASN	3.9
1	B	445	GLY	3.8
1	A	495	GLY	3.8
1	A	581	ILE	3.8
1	A	563	VAL	3.7
1	A	646	ALA	3.6
1	A	571	GLU	3.5
1	A	498	GLY	3.5
1	A	574	LYS	3.4
1	A	580	ALA	3.4
1	B	570	TRP	3.4
1	B	439	GLU	3.3
1	A	542	ASN	3.3
1	A	505	VAL	3.3
1	A	579	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	440	ILE	3.2
1	A	570	TRP	3.1
1	B	447	TYR	3.1
1	A	457	SER	3.1
1	A	576	LEU	3.0
1	C	498	GLY	3.0
1	A	507	ASN	2.9
1	A	607	GLU	2.9
1	A	440	ILE	2.9
1	A	613	LEU	2.9
1	A	477	ASP	2.9
1	A	494	ASP	2.9
1	A	538	ILE	2.9
1	A	537	ASN	2.8
1	A	459	VAL	2.8
1	A	496	VAL	2.8
1	A	564	VAL	2.8
1	A	608	GLY	2.8
1	A	448	MET	2.8
1	B	477	ASP	2.7
1	C	450	LEU	2.7
1	A	547	VAL	2.7
1	A	554	VAL	2.7
1	A	572	ALA	2.6
1	A	540	THR	2.6
1	A	475	LEU	2.6
1	A	506	ASP	2.6
1	A	544	ALA	2.6
1	A	446	LYS	2.6
1	B	571	GLU	2.6
1	A	600	GLN	2.5
1	A	439	GLU	2.5
1	A	536	LYS	2.5
1	A	497	PHE	2.5
1	B	450	LEU	2.5
1	B	464	GLY	2.5
1	A	568	ALA	2.5
1	A	567	VAL	2.5
1	A	582	PRO	2.5
1	A	500	VAL	2.4
1	A	503	VAL	2.4
1	A	424	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	627	TYR	2.4
1	A	545	ALA	2.4
1	C	446	LYS	2.4
1	A	629	PHE	2.3
1	A	644	ILE	2.3
1	B	610	GLY	2.3
1	A	458	LYS	2.3
1	A	546	THR	2.3
1	A	577	THR	2.3
1	A	514	ILE	2.3
1	B	500	VAL	2.3
1	A	588	MET	2.3
1	A	614	GLU	2.3
1	C	505	VAL	2.3
1	A	422	PRO	2.2
1	C	420	SER	2.2
1	B	644	ILE	2.2
1	B	448	MET	2.2
1	C	573	ASN	2.2
1	A	533	ARG	2.2
1	C	563	VAL	2.2
1	C	577	THR	2.2
1	B	627	TYR	2.1
1	A	539	GLN	2.1
1	C	499	ASP	2.1
1	C	522	PRO	2.1
1	C	580	ALA	2.1
1	A	468	ILE	2.1
1	A	486	PHE	2.1
1	A	597	PHE	2.1
1	A	618	PHE	2.1
1	A	510	VAL	2.1
1	A	604	VAL	2.1
1	A	450	LEU	2.1
1	A	595	ALA	2.1
1	B	478	ARG	2.1
1	C	618	PHE	2.0
1	A	431	MET	2.0
1	B	588	MET	2.0
1	A	584	ASP	2.0
1	C	440	ILE	2.0
1	A	476	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	554	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.