



Full wwPDB EM Validation Report ⓘ

Jun 2, 2026 – 04:14 PM JST

PDB ID : 9VFS / pdb_00009vfs
EMDB ID : EMD-65034
Title : Structure of Coxsackievirus A6 Altered-particles
Authors : Ke, X.; Li, X.; Liu, Z.; Liu, K.; Yan, X.; Shu, B.; Zhang, C.
Deposited on : 2025-06-11
Resolution : 2.49 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

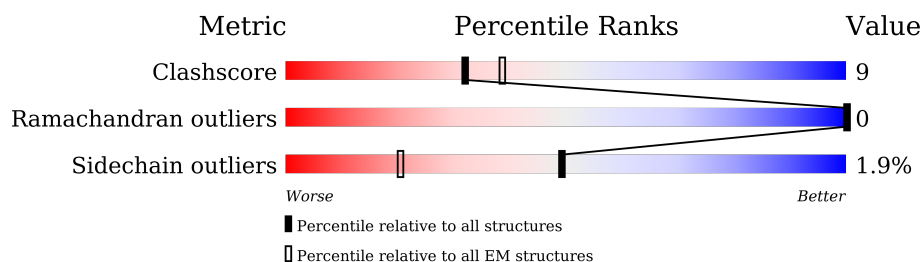
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.49 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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	305	
2	B	256	
3	C	240	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5379 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	229	Total	C	N	O	S	0	0
			1792	1137	313	330	12		

- Molecule 2 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	241	Total	C	N	O	S	0	0
			1864	1197	310	350	7		

- Molecule 3 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	225	Total	C	N	O	S	0	0
			1723	1101	281	332	9		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	51465	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

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	0.30	0/1844	0.34	0/2518
2	B	0.28	0/1921	0.33	0/2636
3	C	0.28	0/1767	0.31	0/2422
All	All	0.29	0/5532	0.33	0/7576

There are no bond length outliers.

There are no bond angle outliers.

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	1792	0	1718	29	0
2	B	1864	0	1793	38	0
3	C	1723	0	1699	39	0
All	All	5379	0	5210	91	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 9.

All (91) 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)
3:C:91:ASN:OD1	3:C:104:ARG:NH2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:VAL:HG11	1:A:104:TRP:HB2	1.72	0.71
2:B:83:PRO:HG2	2:B:213:ASN:H	1.54	0.70
2:B:13:VAL:HA	2:B:26:GLN:HA	1.74	0.69
1:A:86:VAL:HG11	1:A:248:MET:HE2	1.76	0.68
1:A:215:LEU:HD12	1:A:216:GLN:HG2	1.81	0.63
2:B:113:ASN:HB2	2:B:235:PRO:HG2	1.80	0.63
1:A:83:ALA:HB2	1:A:249:ARG:HB2	1.83	0.61
2:B:188:ARG:HE	3:C:161:SER:HB3	1.67	0.60
1:A:260:PRO:HB3	2:B:176:GLN:HB2	1.84	0.59
1:A:263:SER:HB3	2:B:173:PRO:HD3	1.84	0.58
1:A:119:GLU:OE2	1:A:266:TYR:OH	2.21	0.58
3:C:173:THR:HG22	3:C:174:HIS:H	1.67	0.58
3:C:107:THR:HG22	3:C:174:HIS:HB3	1.87	0.56
3:C:50:GLU:HA	3:C:217:ALA:HB2	1.88	0.56
1:A:200:TYR:O	1:A:218:GLY:HA2	2.05	0.56
2:B:83:PRO:O	2:B:87:ASN:ND2	2.40	0.55
2:B:68:THR:HG22	2:B:237:THR:HG23	1.89	0.55
3:C:170:ILE:HD11	3:C:222:PHE:HE1	1.72	0.55
2:B:155:PRO:HB3	2:B:160:GLN:HB2	1.89	0.55
3:C:170:ILE:HG13	3:C:171:SER:H	1.71	0.55
2:B:188:ARG:NH1	3:C:122:SER:O	2.41	0.54
3:C:88:PRO:HA	3:C:94:TRP:HB3	1.90	0.54
2:B:101:LEU:HB2	2:B:248:SER:HB2	1.90	0.53
2:B:149:ASP:OD1	2:B:152:HIS:ND1	2.42	0.53
3:C:202:VAL:HB	3:C:206:THR:HG23	1.91	0.53
2:B:186:ASN:HB3	2:B:189:THR:HG22	1.92	0.52
1:A:108:VAL:HG23	1:A:109:MET:HG3	1.92	0.51
1:A:194:THR:HG22	2:B:202:ALA:O	2.10	0.51
2:B:99:HIS:CG	2:B:247:PHE:HB3	2.46	0.51
2:B:101:LEU:HB3	2:B:205:PHE:HB3	1.92	0.51
2:B:188:ARG:NH2	3:C:157:PHE:O	2.44	0.51
3:C:126:THR:HG23	3:C:201:VAL:HB	1.93	0.51
2:B:144:GLN:H	2:B:144:GLN:CD	2.19	0.50
3:C:202:VAL:HG21	3:C:208:THR:HG22	1.94	0.50
1:A:91:VAL:HG22	1:A:102:THR:HG22	1.93	0.49
2:B:176:GLN:HE22	3:C:101:GLN:HG3	1.77	0.49
3:C:50:GLU:OE2	3:C:116:THR:OG1	2.29	0.49
1:A:108:VAL:HG12	1:A:248:MET:HE1	1.95	0.49
2:B:37:GLU:HB3	2:B:198:PRO:HG3	1.95	0.48
2:B:119:GLN:HG2	2:B:225:LYS:HB2	1.95	0.48
3:C:128:LYS:HB2	3:C:198:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLN:O	1:A:223:ASN:ND2	2.35	0.48
1:A:135:ASN:ND2	1:A:136:LEU:O	2.46	0.48
2:B:122:LEU:HB2	2:B:185:ILE:HB	1.96	0.47
2:B:82:PHE:CE2	2:B:108:MET:HG2	2.50	0.47
1:A:142:PRO:O	1:A:178:LEU:HB2	2.15	0.47
2:B:104:SER:HB2	2:B:245:SER:HA	1.97	0.47
2:B:168:LEU:HD12	2:B:172:ILE:HG13	1.97	0.46
1:A:249:ARG:NH1	3:C:18:ASP:OD1	2.49	0.46
2:B:102:TYR:CE1	2:B:104:SER:HB3	2.50	0.46
3:C:109:TRP:HB3	3:C:224:LEU:HD23	1.97	0.45
1:A:187:VAL:HA	3:C:24:ILE:HD11	1.98	0.45
2:B:37:GLU:OE2	3:C:35:HIS:NE2	2.50	0.45
3:C:94:TRP:O	3:C:97:THR:OG1	2.35	0.45
3:C:7:LYS:O	3:C:10:THR:HG23	2.17	0.45
3:C:89:GLY:HA3	3:C:109:TRP:CZ2	2.51	0.45
2:B:52:LYS:HA	2:B:52:LYS:HD2	1.71	0.45
1:A:185:VAL:HB	3:C:24:ILE:HG23	1.99	0.44
3:C:53:LEU:HD21	3:C:94:TRP:CD2	2.52	0.44
3:C:77:VAL:HG22	3:C:78:ASP:H	1.82	0.44
1:A:159:ASP:OD1	1:A:159:ASP:N	2.49	0.44
3:C:69:ILE:HB	3:C:212:ILE:HB	2.00	0.44
3:C:24:ILE:HD12	3:C:25:LEU:N	2.33	0.44
1:A:267:MET:HE2	1:A:267:MET:HB3	1.77	0.44
2:B:72:LYS:H	2:B:75:SER:HG	1.62	0.43
3:C:133:TYR:HB2	3:C:165:LEU:HD21	2.00	0.43
3:C:231:ASP:OD1	3:C:231:ASP:N	2.48	0.43
3:C:89:GLY:O	3:C:104:ARG:NE	2.50	0.43
2:B:82:PHE:O	2:B:85:VAL:HG12	2.19	0.43
1:A:250:ILE:HG22	1:A:253:VAL:HB	1.99	0.42
1:A:256:TRP:CD1	3:C:39:GLU:HB2	2.53	0.42
2:B:48:THR:HA	2:B:51:ASP:OD2	2.20	0.42
1:A:248:MET:HE3	1:A:250:ILE:HD11	2.01	0.42
1:A:109:MET:HE1	1:A:198:TRP:HB3	2.00	0.42
1:A:125:ARG:NH2	3:C:31:THR:O	2.39	0.41
1:A:260:PRO:HB2	2:B:172:ILE:HB	2.01	0.41
1:A:189:PHE:CZ	1:A:191:SER:HB3	2.54	0.41
1:A:285:ARG:NH2	3:C:55:VAL:O	2.49	0.41
2:B:63:PHE:CD1	2:B:241:ALA:HB2	2.56	0.41
3:C:88:PRO:HA	3:C:94:TRP:CB	2.50	0.41
3:C:13:PHE:CE2	3:C:15:THR:HG22	2.56	0.41
2:B:61:ASN:OD1	2:B:245:SER:OG	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:HD11	2:B:177:ALA:HB2	2.03	0.41
3:C:113:LEU:HD11	3:C:170:ILE:HD13	2.02	0.41
1:A:182:PRO:HA	1:A:183:PRO:HD2	1.99	0.40
2:B:142:ASN:OD1	2:B:142:ASN:N	2.54	0.40
2:B:53:PRO:HB3	2:B:248:SER:OG	2.21	0.40
3:C:87:ASP:OD2	3:C:87:ASP:N	2.55	0.40
2:B:127:ILE:HG12	2:B:180:PHE:CD2	2.57	0.40
3:C:104:ARG:HD3	3:C:104:ARG:HA	1.94	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 PDB entries followed by that with respect to all EM entries.

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	227/305 (74%)	211 (93%)	16 (7%)	0	100	100
2	B	239/256 (93%)	229 (96%)	10 (4%)	0	100	100
3	C	221/240 (92%)	211 (96%)	10 (4%)	0	100	100
All	All	687/801 (86%)	651 (95%)	36 (5%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	194/260 (75%)	191 (98%)	3 (2%)	57	80
2	B	203/218 (93%)	198 (98%)	5 (2%)	42	69
3	C	194/206 (94%)	191 (98%)	3 (2%)	57	80
All	All	591/684 (86%)	580 (98%)	11 (2%)	49	76

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

Mol	Chain	Res	Type
1	A	134	SER
1	A	237	THR
1	A	253	VAL
2	B	37	GLU
2	B	44	SER
2	B	52	LYS
2	B	84	ASP
2	B	139	THR
3	C	24	ILE
3	C	42	SER
3	C	65	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	A	135	ASN
1	A	184	GLN
2	B	15	GLN
2	B	30	ASN
2	B	87	ASN
2	B	109	HIS
2	B	160	GLN
2	B	176	GLN
2	B	244	ASN
3	C	48	GLN
3	C	140	GLN
3	C	172	ASN

5.3.3 RNA ⓘ

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.