



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:12 pm BST

PDB ID : 2QY2
Title : Characterization of a trifunctional mimivirus mRNA capping enzyme and crystal structure of the RNA triphosphatase domain.
Authors : Shuman, S.; Benarroch, D.; Smith, P.
Deposited on : 2007-08-13
Resolution : 2.00 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

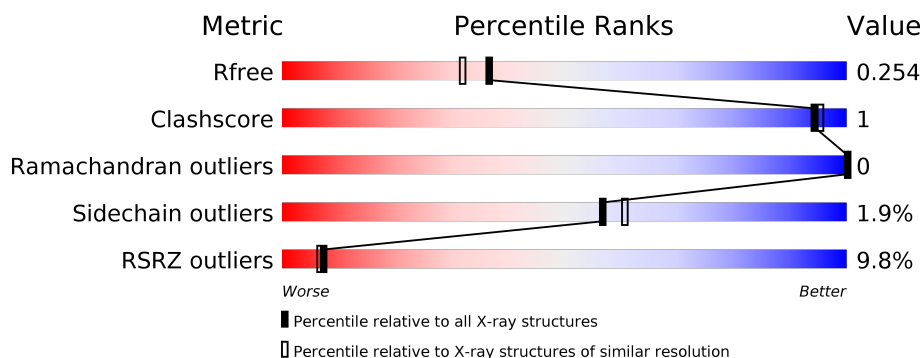
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	238	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>
1	B	238	<div> <div>16%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4228 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 Probable mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	17	0
			1980	1257	322	396	5			
1	B	217	Total	C	N	O	S	0	13	0
			1882	1199	303	374	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q5UQX1
B	1000	SER	-	EXPRESSION TAG	UNP Q5UQX1

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



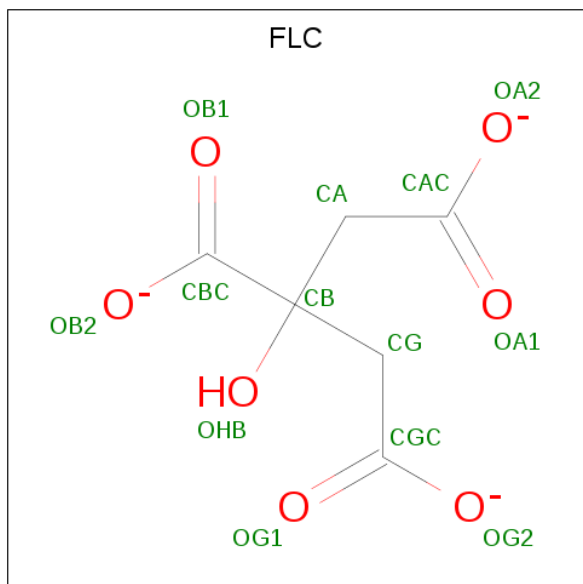
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7^-$).

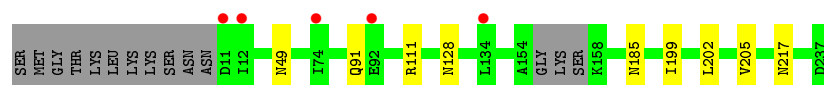



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		

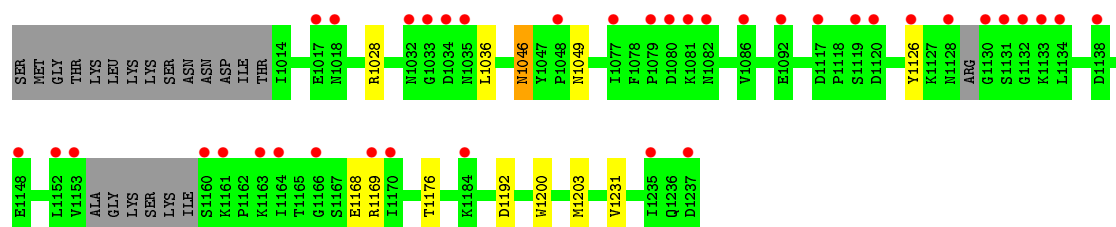
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total	O	0	0
			235	235		
4	B	110	Total	O	0	0
			110	110		

- Molecule 1: Probable mRNA-capping enzyme



- Chain B:  16% 86% 5% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	154.46 Å 154.46 Å 39.62 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.09 – 2.00 19.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (34.09-2.00) 93.6 (19.60-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.01 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.252 0.212 , 0.254	Depositor DCC
R_{free} test set	3631 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4228	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, ACT

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	0.67	0/2013	0.75	0/2722
1	B	0.69	0/1914	0.70	0/2585
All	All	0.68	0/3927	0.72	0/5307

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91[B]	GLN	Mainchain

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	1980	0	1953	5	0
1	B	1882	0	1857	5	0
2	A	8	0	6	0	0
3	B	13	0	5	0	0
4	A	235	0	0	3	0
4	B	110	0	0	1	0
All	All	4228	0	3821	10	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 1.

All (10) 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:1046:ASN:H	1:B:1046:ASN:HD22	1.22	0.82
1:B:1176[B]:THR:HG23	1:B:1192:ASP:HB3	1.74	0.69
1:A:185:ASN:HD22	1:A:217:ASN:HD22	1.42	0.68
1:A:111[B]:ARG:NH1	4:A:1020:HOH:O	2.33	0.61
1:B:1046:ASN:N	1:B:1046:ASN:HD22	1.97	0.55
1:A:199:ILE:HG23	4:A:1225:HOH:O	2.14	0.47
1:A:49:ASN:ND2	4:A:1151:HOH:O	2.44	0.46
1:B:1200:TRP:O	1:B:1203:MET:HG2	2.17	0.45
1:B:1028:ARG:HD3	4:B:1341:HOH:O	2.17	0.43
1:A:202:LEU:O	1:A:205[B]:VAL:HG22	2.17	0.43

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	237/238 (100%)	234 (99%)	3 (1%)	0	100	100
1	B	224/238 (94%)	214 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	461/476 (97%)	448 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	232/227 (102%)	231 (100%)	1 (0%)	91	93
1	B	221/227 (97%)	213 (96%)	8 (4%)	35	34
All	All	453/454 (100%)	444 (98%)	9 (2%)	57	58

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

Mol	Chain	Res	Type
1	A	128	ASN
1	B	1036	LEU
1	B	1046	ASN
1	B	1049	ASN
1	B	1126	TYR
1	B	1168	GLU
1	B	1169	ARG
1	B	1231[A]	VAL
1	B	1231[B]	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	185	ASN
1	A	236	GLN
1	B	1046	ASN
1	B	1128	ASN

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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	A	1003	-	1,3,3	2.09	1 (100%)	0,3,3	0.00	-
2	ACT	A	1002	-	1,3,3	1.71	0	0,3,3	0.00	-
3	FLC	B	1238	-	3,12,12	0.96	0	3,17,17	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	B	1238	-	-	0/6/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	ACT	CH3-C	2.09	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	91[B]:GLN	C	92:GLU	N	0.93

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	224/238 (94%)	0.02	5 (2%) 62 60	19, 31, 52, 98	0
1	B	217/238 (91%)	0.99	38 (17%) 1 1	28, 53, 94, 109	0
All	All	441/476 (92%)	0.50	43 (9%) 7 7	19, 42, 89, 109	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1034	ASP	5.7
1	B	1033	GLY	5.2
1	B	1080	ASP	4.9
1	B	1048	PRO	4.7
1	B	1237	ASP	4.5
1	B	1079	PRO	4.3
1	B	1128	ASN	4.3
1	B	1153	VAL	4.1
1	B	1130	GLY	4.0
1	B	1134	LEU	4.0
1	A	11	ASP	3.9
1	B	1169	ARG	3.9
1	B	1117	ASP	3.6
1	B	1035	ASN	3.5
1	B	1092	GLU	3.2
1	B	1132	GLY	3.1
1	B	1018	ASN	3.1
1	B	1160	SER	3.1
1	B	1161	LYS	3.1
1	B	1166	GLY	3.0
1	B	1170	ILE	3.0
1	B	1163	LYS	2.9
1	A	92	GLU	2.9
1	B	1082	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1152	LEU	2.8
1	B	1131	SER	2.8
1	B	1138	ASP	2.7
1	B	1032	ASN	2.6
1	A	12	ILE	2.5
1	A	74	ILE	2.4
1	B	1081[A]	LYS	2.4
1	B	1133	LYS	2.4
1	B	1184	LYS	2.4
1	B	1148	GLU	2.3
1	A	134	LEU	2.3
1	B	1120	ASP	2.3
1	B	1077	ILE	2.3
1	B	1086	VAL	2.2
1	B	1164	ILE	2.1
1	B	1017	GLU	2.1
1	B	1119	SER	2.1
1	B	1235	ILE	2.1
1	B	1126	TYR	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FLC	B	1238	13/13	0.57	0.34	93,95,96,98	0
2	ACT	A	1003	4/4	0.76	0.16	71,72,73,73	0
2	ACT	A	1002	4/4	0.93	0.19	47,54,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.