

Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 10:03 AM EDT

:	8SH5
:	Crystal structure of 3'cap-independent translation enhancers (CITE) from Pea
	enation mosaic virus RNA 2 (PEMV2) with Fab BL3-6K170A
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	2023-04-13
:	2.75 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 (i) 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 (1)) were used in the production of this report:

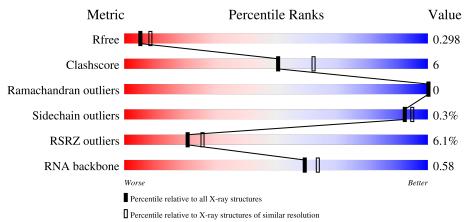
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.75 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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 <=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	Н	228	88%	11% •
2	L	215	3% 90%	10%
3	R	88	^{3%} 47% 49%	5%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5226 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 Fab BL3-6K170A heavy chain.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Н	225	Total 1678	$\begin{array}{c} \mathrm{C} \\ 1055 \end{array}$	N 287	O 330	S 6	0	0	0

• Molecule 2 is a protein called Fab BL3-6K170A light chain.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
2	L	215	Total 1639	C 1022	N 274	O 337	S 6	0	0	0

• Molecule 3 is a RNA chain called RNA (88-MER).

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
3	R	88	Total 1884	C 838	N 339	0 618	Р 89	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	39	А	G	conflict	GB 51979311
R	40	А	U	conflict	GB 51979311
R	41	А	U	conflict	GB 51979311
R	42	С	А	conflict	GB 51979311
R	43	А	U	conflict	GB 51979311
R	76	U	С	conflict	GB 51979311
R	79	С	А	conflict	GB 51979311

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	6	Total O 6 6	0	0



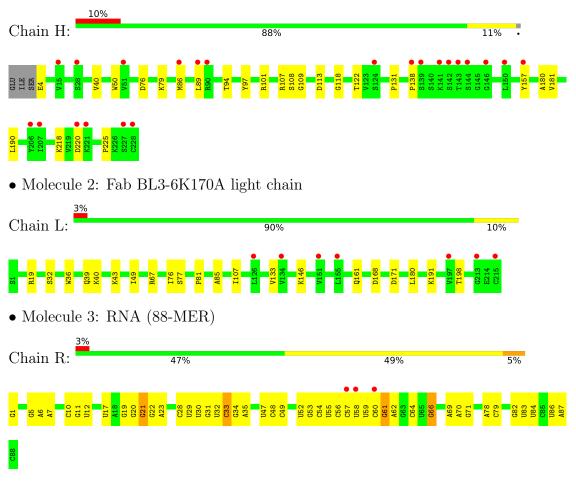
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	2	Total O 2 2	0	0
4	R	17	Total O 17 17	0	0



3 Residue-property plots (i)

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: Fab BL3-6K170A heavy chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	63.35Å 65.46 Å 89.82 Å	Depositor
a, b, c, α , β , γ	90.00° 110.29° 90.00°	Depositor
Resolution (Å)	59.42 - 2.75	Depositor
Resolution (A)	59.42 - 2.75	EDS
% Data completeness	97.3 (59.42-2.75)	Depositor
(in resolution range)	97.3(59.42-2.75)	EDS
R _{merge}	0.19	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.78 (at 2.77 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.251 , 0.297	Depositor
R, R_{free}	0.252 , 0.298	DCC
R_{free} test set	1600 reflections (9.07%)	wwPDB-VP
Wilson B-factor $(Å^2)$	61.7	Xtriage
Anisotropy	1.222	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.28 , 49.5	EDS
L-test for twinning ²	$< L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5226	wwPDB-VP
Average B, all atoms $(Å^2)$	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.31% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: GDP

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		
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Н	0.26	0/1719	0.50	0/2339	
2	L	0.26	0/1674	0.50	0/2273	
3	R	0.25	0/2074	0.86	3/3231~(0.1%)	
All	All	0.26	0/5467	0.67	3/7843~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	R	33	С	C2-N1-C1'	-6.81	111.31	118.80
3	R	33	С	C6-N1-C1'	5.81	127.77	120.80
3	R	66	G	N9-C4-C5	-5.24	103.30	105.40

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	Н	1678	0	1637	15	0
2	L	1639	0	1586	11	0
3	R	1884	0	952	28	0
4	Н	6	0	0	1	0
4	L	2	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	17	0	0	0	0
All	All	5226	0	4175	53	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 6.

All (53) 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:R:58:U:H2'	3:R:61:G:H21	1.57	0.70
1:H:40:VAL:HG12	1:H:50:TRP:HA	1.72	0.69
3:R:20:G:H4'	3:R:21:G:H5"	1.78	0.66
1:H:86:MET:HB2	1:H:89:LEU:HD21	1.82	0.60
1:H:94:THR:HG23	1:H:122:THR:HA	1.83	0.60
3:R:29:U:H2'	3:R:30:U:C6	2.37	0.59
2:L:81:PRO:HA	2:L:107:ILE:HD13	1.85	0.58
1:H:4:GLU:N	4:H:301:HOH:O	2.36	0.57
3:R:6:A:H2'	3:R:7:A:C8	2.40	0.56
1:H:108:SER:OG	1:H:109:GLY:N	2.39	0.56
1:H:131:PRO:HB3	1:H:157:TYR:HB3	1.87	0.56
2:L:36:TRP:HB2	2:L:49:ILE:HB	1.89	0.55
2:L:32:SER:OG	2:L:67:ARG:NH1	2.38	0.54
1:H:76:ASP:OD2	1:H:79:LYS:NZ	2.26	0.53
3:R:5:G:H2'	3:R:6:A:H8	1.72	0.53
1:H:180:ALA:HA	1:H:190:LEU:HB3	1.89	0.53
3:R:31:G:H2'	3:R:32:U:O4'	2.09	0.53
3:R:55:U:H2'	3:R:56:C:C6	2.44	0.52
3:R:70:A:H2'	3:R:71:G:C8	2.43	0.52
2:L:168:ASP:HB3	2:L:171:ASP:OD1	2.10	0.52
3:R:5:G:H2'	3:R:6:A:C8	2.45	0.51
2:L:19:ARG:HG3	2:L:77:SER:HA	1.91	0.51
2:L:133:VAL:HG13	2:L:180:LEU:HB3	1.93	0.51
3:R:29:U:H2'	3:R:30:U:H6	1.75	0.50
3:R:6:A:H2'	3:R:7:A:H8	1.76	0.50
3:R:30:U:H2'	3:R:31:G:C8	2.47	0.50
3:R:69:A:H2'	3:R:70:A:C8	2.48	0.49
3:R:30:U:H2'	3:R:31:G:H8	1.76	0.49
1:H:180:ALA:HB2	1:H:190:LEU:HD23	1.96	0.47
2:L:146:LYS:HB3	2:L:198:THR:OG1	2.14	0.47
3:R:83:U:H2'	3:R:84:U:C6	2.50	0.47
3:R:53:G:H2'	3:R:54:C:C6	2.49	0.47



Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:R:52:U:H2'	3:R:53:G:H8	1.81	0.46
2:L:40:LYS:HB2	2:L:43:LYS:HB2	1.97	0.46
3:R:11:G:H2'	3:R:12:U:C6	2.51	0.45
3:R:78:A:H2'	3:R:79:C:C6	2.51	0.45
3:R:82:G:H2'	3:R:83:U:C6	2.51	0.45
2:L:19:ARG:HA	2:L:76:ILE:O	2.16	0.44
2:L:39:GLN:O	2:L:85:ALA:HB1	2.17	0.44
1:H:181:VAL:HG11	2:L:161:GLN:HB3	1.99	0.44
1:H:218:LYS:NZ	1:H:220:ASP:OD2	2.51	0.44
3:R:28:C:H2'	3:R:29:U:C6	2.52	0.44
3:R:70:A:H2'	3:R:71:G:H8	1.80	0.44
3:R:32:U:H2'	3:R:33:C:C6	2.52	0.44
1:H:101:ARG:NH2	1:H:113:ASP:OD2	2.37	0.43
3:R:52:U:H2'	3:R:53:G:C8	2.55	0.42
3:R:53:G:H2'	3:R:54:C:H6	1.84	0.42
1:H:138:PRO:HG2	1:H:225:PRO:HB3	2.02	0.42
1:H:107:ARG:H	1:H:107:ARG:HG2	1.72	0.41
3:R:47:U:H2'	3:R:48:C:C6	2.55	0.41
3:R:86:U:H2'	3:R:87:A:C8	2.55	0.41
3:R:11:G:H2'	3:R:12:U:H6	1.86	0.41
1:H:97:TYR:O	1:H:118:GLY:HA2	2.20	0.40

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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	Perce	\mathbf{ntiles}
1	Н	223/228~(98%)	213~(96%)	10 (4%)	0	100	100
2	L	213/215~(99%)	207~(97%)	6 (3%)	0	100	100
All	All	436/443~(98%)	420 (96%)	16 (4%)	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 side chain 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	Н	186/189~(98%)	186 (100%)	0	100 100
2	L	189/189~(100%)	188 (100%)	1 (0%)	88 92
All	All	375/378~(99%)	374 (100%)	1 (0%)	92 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	191	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
2	L	139	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	86/88~(97%)	16 (18%)	0

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	10	С
3	R	17	U
3	R	19	G
3	R	21	G
3	R	22	G
3	R	23	А
3	R	34	G



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Mol	Chain	\mathbf{Res}	Type				
3	R	35	А				
3	R	49	С				
3	R	57	С				
3	R	59	U				
3	R	60	С				
3	R	61	G				
3	R	62	А				
3	R	64	С				
3	R	66	G				

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There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	Tuno	Chain	Chain	Chain	Chain	Res	Link	Bo	ond leng	ths	B	ond ang	les
	туре		nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2			
3	GDP	R	1	3	24,30,30	0.96	1 (4%)	30,47,47	1.22	4 (13%)			

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	GDP	R	1	3	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

\mathbf{N}	ſol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
	3	R	1	GDP	C6-N1	-2.40	1.34	1.37

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	R	1	GDP	PA-O3A-PB	-3.20	121.84	132.83
3	R	1	GDP	C3'-C2'-C1'	2.80	105.20	100.98
3	R	1	GDP	C5-C6-N1	2.31	118.03	113.95
3	R	1	GDP	C8-N7-C5	2.31	107.38	102.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	Н	225/228~(98%)	0.81	22 (9%) 7 8	68, 88, 117, 146	0
2	L	215/215~(100%)	0.56	7 (3%) 46 54	82, 95, 111, 125	0
3	R	87/88~(98%)	-0.20	3 (3%) 45 53	91, 103, 123, 152	0
All	All	527/531~(99%)	0.54	32 (6%) 21 26	68, 95, 116, 152	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	143	THR	12.1
1	Н	228	CYS	10.2
1	Н	227	SER	6.4
3	R	58	U	5.6
1	Н	144	SER	4.6
2	L	197	VAL	4.2
2	L	155	LEU	4.1
1	Н	142	SER	3.8
2	L	215	CYS	3.7
2	L	213	GLY	3.5
1	Н	138	PRO	3.3
1	Н	157	TYR	3.0
1	Н	141	LYS	2.9
1	Н	86	MET	2.8
1	Н	89	LEU	2.6
1	Н	150	LEU	2.4
1	Н	207	ILE	2.4
1	Н	221	LYS	2.3
1	Н	206	TYR	2.3
1	Н	146	GLY	2.3
1	Н	124	SER	2.3
1	Н	139	SER	2.2
2	L	151	VAL	2.2



Mol	Chain	Res	Type	RSRZ
3	R	60	C	2.2
1	Н	90	ARG	2.2
1	Н	28	SER	2.1
1	Н	220	ASP	2.1
2	L	134	VAL	2.1
1	Н	15	VAL	2.0
1	Н	51	VAL	2.0
3	R	57	С	2.0
2	L	126	LEU	2.0

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6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	$B-factors(Å^2)$	Q < 0.9
3	GDP	R	1	28/28	0.88	0.15	106,110,113,115	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.

