Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2022 – 12:39 pm GMT

PDB ID	:	6HAU
Title	:	KSHV PAN RNA Mta-response element fragment complexed with the globular domain of herpesvirus saimiri ORF57
Authors	:	Tunnicliffe, R.B.; Levy, C.; Ruiz Nivia, H.D.; Sandri-Goldin, R.M.; Golovanov, A.P.
Deposited on	:	2018-08-08
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

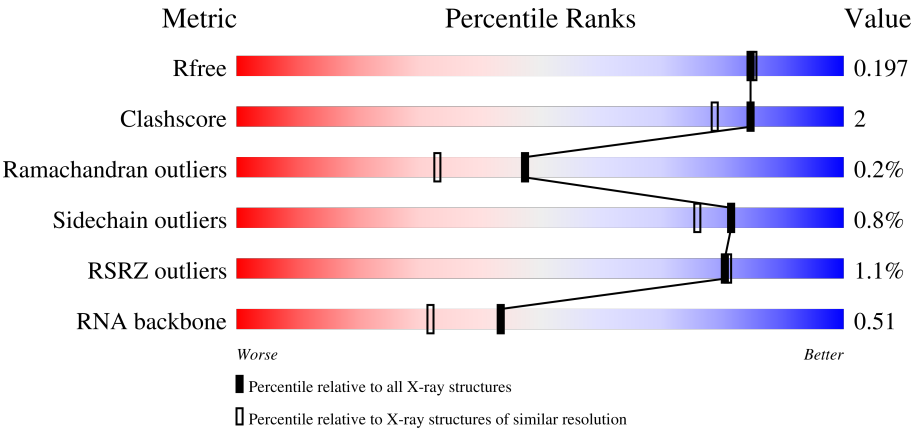
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

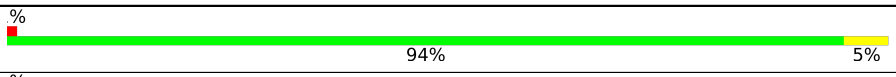
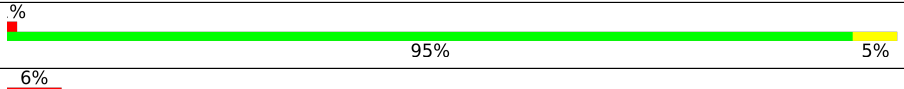
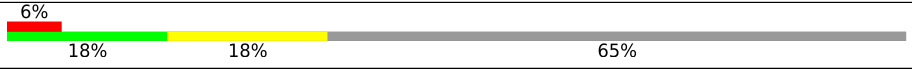
The reported resolution of this entry is 1.86 Å.

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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)
RNA backbone	3102	1026 (2.40-1.32)

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	A	273	
1	B	273	
2	D	17	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9666 atoms, of which 4664 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 mRNA export factor ICP27 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	273	Total	C	H	N	O	S	0	16	0
			4508	1426	2286	372	406	18			
1	B	273	Total	C	H	N	O	S	0	20	0
			4536	1436	2312	368	402	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	GLY	-	expression tag	UNP P13199
B	145	GLY	-	expression tag	UNP P13199

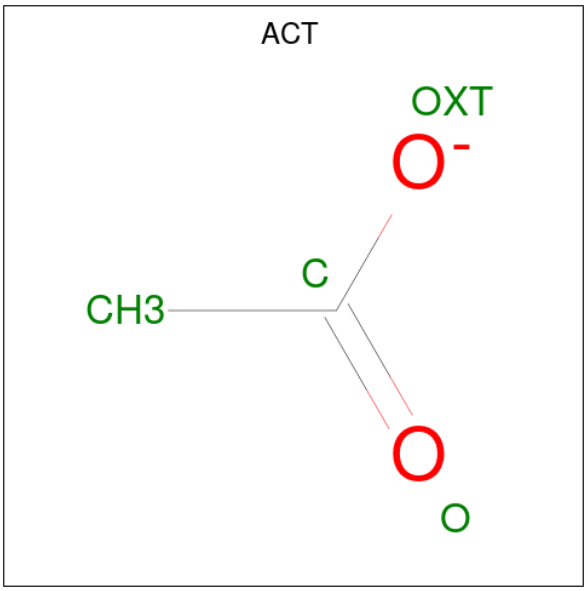
- Molecule 2 is a RNA chain called MRE fragment of PAN RNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	6	Total	C	H	N	O	P	0	0	0
			182	55	63	16	43	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H O 7 2 3 2	0	0

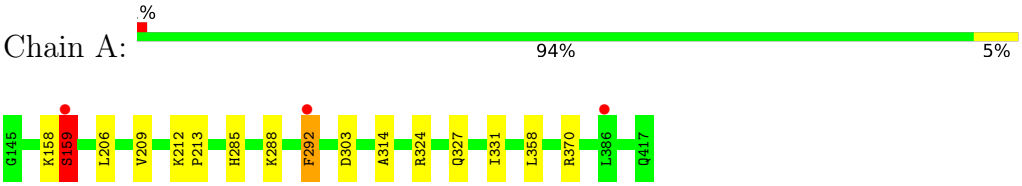
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	181	Total O 181 181	0	0
5	B	241	Total O 241 241	0	0
5	D	9	Total O 9 9	0	0

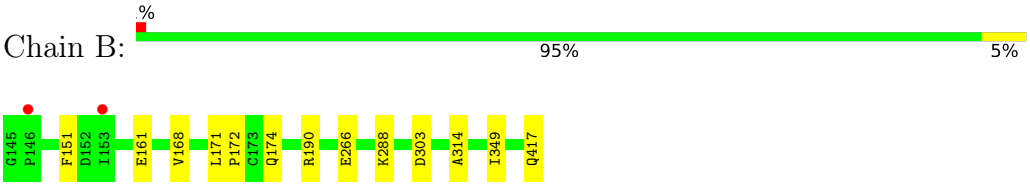
3 Residue-property plots (i)

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.

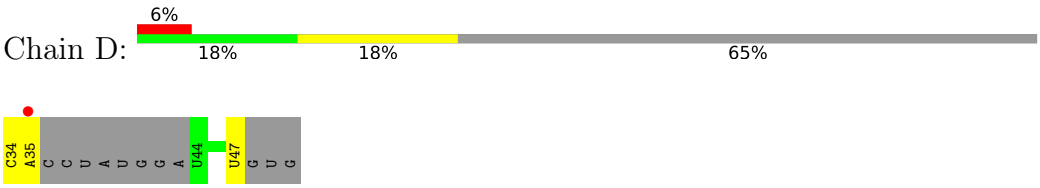
• Molecule 1: mRNA export factor ICP27 homolog



• Molecule 1: mRNA export factor ICP27 homolog



• Molecule 2: MRE fragment of PAN RNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.66Å 105.26Å 118.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.71 – 1.86 78.71 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (78.71-1.86) 94.8 (78.71-1.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.158 , 0.197 0.158 , 0.197	Depositor DCC
R_{free} test set	3123 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9666	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.37	0/2326	0.57	0/3159
1	B	0.41	0/2368	0.58	1/3221 (0.0%)
2	D	0.31	0/130	0.86	0/197
All	All	0.39	0/4824	0.59	1/6577 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	190	ARG	NE-CZ-NH1	5.52	123.06	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2222	2286	2221	12	0
1	B	2224	2312	2212	10	0
2	D	119	63	65	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	4	3	3	0	0
5	A	181	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	241	0	0	3	0
5	D	9	0	0	1	0
All	All	5002	4664	4501	21	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 2.

All (21) 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:159[B]:SER:O	5:A:601:HOH:O	1.68	1.11
1:B:303[A]:ASP:OD1	5:B:601:HOH:O	1.94	0.86
1:B:417:GLN:O	5:B:602:HOH:O	1.98	0.81
1:A:285:HIS:ND1	5:A:602:HOH:O	2.26	0.68
1:A:314:ALA:O	1:B:288:LYS:NZ	2.28	0.67
1:B:168:VAL:O	1:B:168:VAL:HG23	2.02	0.59
1:B:171:LEU:HB3	1:B:172:PRO:HD2	1.88	0.56
1:A:288:LYS:NZ	1:B:314:ALA:O	2.39	0.55
1:A:324:ARG:HG2	1:A:358:LEU:HD21	1.90	0.52
2:D:47:U:O3'	5:D:102:HOH:O	2.09	0.49
1:B:174:GLN:OE1	5:B:603:HOH:O	2.20	0.48
1:A:292:PHE:CZ	1:A:303[B]:ASP:OD1	2.68	0.46
1:A:285:HIS:CD2	5:A:741:HOH:O	2.69	0.45
1:B:266:GLU:HB3	1:B:349[B]:ILE:HG22	1.99	0.45
1:A:212:LYS:HB2	1:A:213:PRO:HD3	1.99	0.44
1:A:331:ILE:HB	1:B:151:PHE:HB3	2.01	0.42
1:A:158:LYS:O	1:A:159[B]:SER:O	2.36	0.41
1:A:324:ARG:O	1:A:327[B]:GLN:HG2	2.20	0.41
1:B:168:VAL:O	1:B:168:VAL:CG2	2.67	0.41
1:A:206:LEU:O	1:A:209:VAL:HG12	2.21	0.41
2:D:34:C:H2'	2:D:35:A:H5'	2.03	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	287/273 (105%)	282 (98%)	3 (1%)	2 (1%)	22 9
1	B	291/273 (107%)	285 (98%)	6 (2%)	0	100 100
All	All	578/546 (106%)	567 (98%)	9 (2%)	2 (0%)	47 26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159[A]	SER
1	A	159[B]	SER

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	261/247 (106%)	257 (98%)	4 (2%)	65 53
1	B	267/247 (108%)	266 (100%)	1 (0%)	91 89
All	All	528/494 (107%)	523 (99%)	5 (1%)	81 72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159[A]	SER
1	A	159[B]	SER
1	A	292	PHE
1	A	370	ARG
1	B	161	GLU

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

Mol	Chain	Res	Type
1	A	285	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	4/17 (23%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
4	ACT	B	502	-	1,3,3	4.82	1 (100%)	0,3,3	-	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	502	ACT	CH3-C	4.82	1.54	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)

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, 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	OWAB(Å^2)	Q<0.9
1	A	273/273 (100%)	0.05	3 (1%) 80 81	21, 35, 61, 90	0
1	B	273/273 (100%)	0.04	2 (0%) 87 88	17, 27, 65, 101	0
2	D	6/17 (35%)	0.71	1 (16%) 1 1	57, 81, 119, 134	0
All	All	552/563 (98%)	0.05	6 (1%) 80 81	17, 32, 65, 134	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	LEU	4.5
1	A	159[A]	SER	3.4
1	A	292	PHE	3.1
1	B	146	PRO	3.0
2	D	35	A	2.6
1	B	153	ILE	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
4	ACT	B	502	4/4	0.57	0.23	51,61,73,73	0
3	ZN	A	501	1/1	0.94	0.07	37,37,37,37	0
3	ZN	B	501	1/1	0.98	0.11	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.