wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2023 – 02:33 PM EDT

PDB ID	:	3RW6
Title	:	Structure of nuclear RNA export factor TAP bound to CTE RNA
Authors	:	Teplova, M.; Khin, N.W.; Patel, D.J.; Izaurralde, E.
Deposited on	:	2011-05-07
Resolution	:	2.30 Å(reported)

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

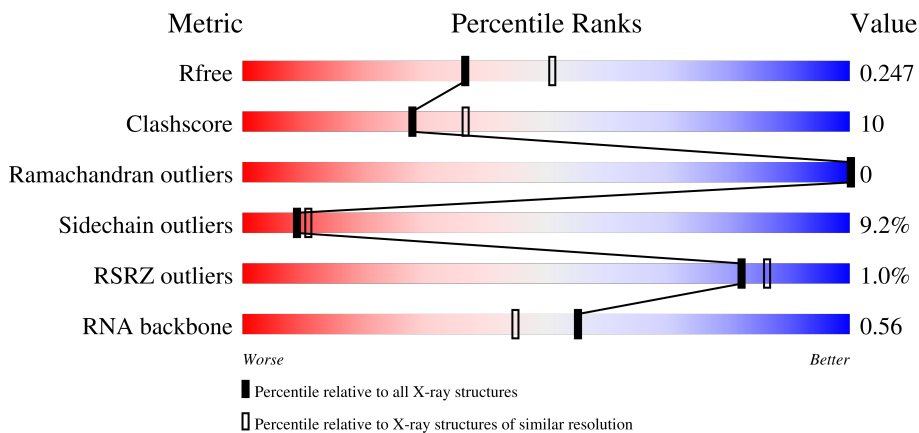|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.247
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		9.2%
RSRZ outliers		1.0%
RNA backbone		0.56

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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	267	64% / 25% · 8%
1	B	267	60% / 28% · 9%
2	F	62	68% / 26% / 6%
2	H	62	65% / 29% / 5% ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6786 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 Nuclear RNA export factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	1	0
			1989	1263	347	372	7			
1	B	244	Total	C	N	O	S	0	1	0
			1982	1257	347	371	7			

- Molecule 2 is a RNA chain called constitutive transport element(CTE)of Mason-Pfizer monkey virus RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	62	Total	C	N	O	P	0	0	0
			1340	595	250	431	64			
2	F	62	Total	C	N	O	P	0	0	0
			1340	595	250	431	64			

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	H	39	Total	O	0	0
			39	39		
3	F	30	Total	O	0	0
			30	30		
3	B	41	Total	O	0	0
			41	41		

3 Residue-property plots ⓘ

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.
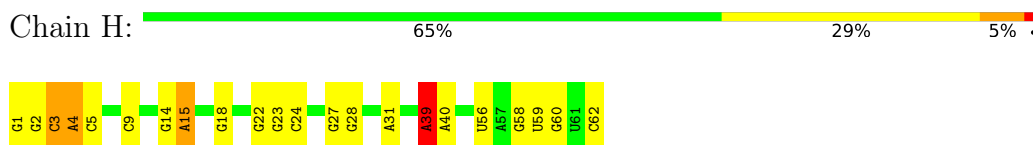
- Molecule 1: Nuclear RNA export factor 1
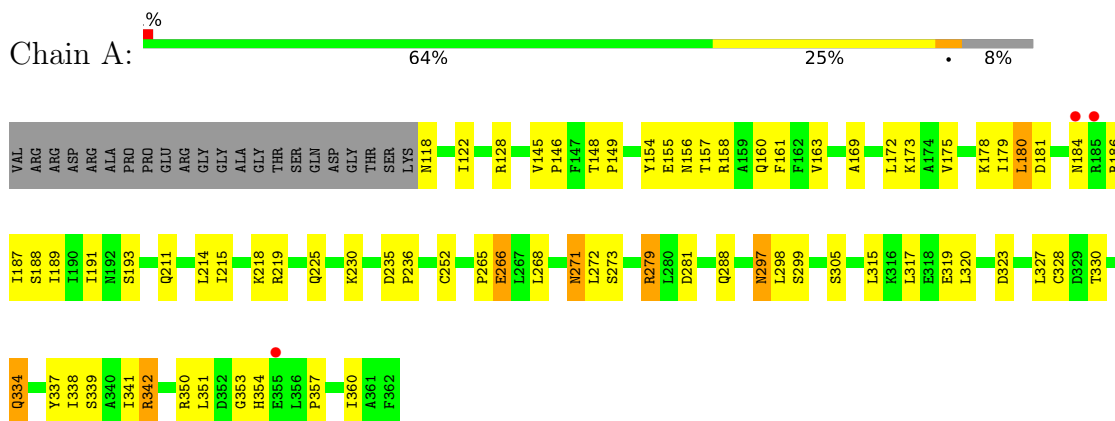
- Molecule 1: Nuclear RNA export factor 1
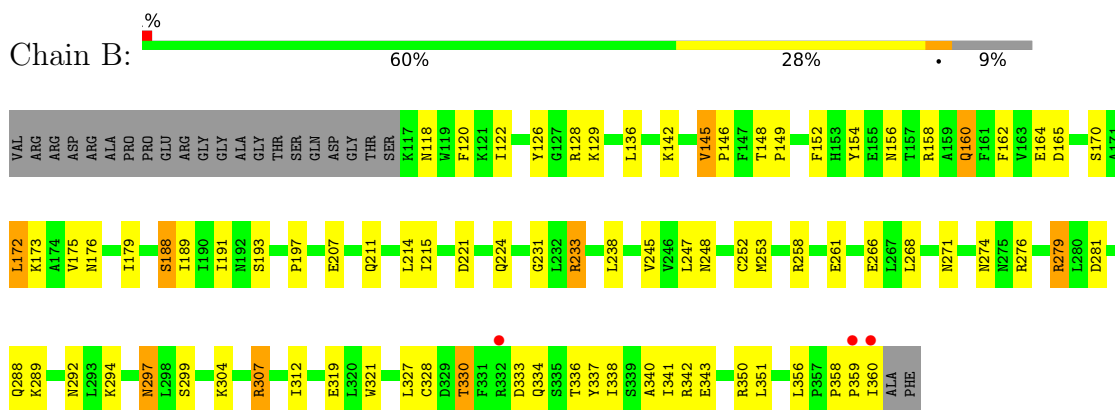
- Molecule 2: constitutive transport element(CTE)of Mason-Pfizer monkey virus RNA

- Molecule 2: constitutive transport element(CTE)of Mason-Pfizer monkey virus RNA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.41Å 117.05Å 84.77Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	37.87 – 2.30 37.87 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (37.87-2.30) 96.5 (37.87-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.5_2	Depositor
R, R_{free}	0.203 , 0.256 0.198 , 0.247	Depositor DCC
R_{free} test set	2257 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 28.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6786	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CCC, GTP

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	0.42	0/2028	0.58	0/2741
1	B	0.42	1/2020 (0.0%)	0.56	0/2729
2	F	0.71	0/1444	1.25	5/2250 (0.2%)
2	H	0.73	1/1444 (0.1%)	1.28	9/2250 (0.4%)
All	All	0.56	2/6936 (0.0%)	0.95	14/9970 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	56	U	O3'-P	-7.17	1.52	1.61
1	B	238	LEU	C-N	-5.12	1.22	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	28	G	N9-C1'-C2'	-9.21	101.86	112.00
2	H	39	A	P-O5'-C5'	-8.20	107.79	120.90
2	H	31	A	O4'-C1'-N9	-6.30	103.16	108.20
2	F	24	C	O5'-P-OP2	6.18	118.12	110.70
2	H	39	A	C5'-C4'-C3'	-6.15	106.15	116.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASN	Peptide

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	1989	0	2034	48	0
1	B	1982	0	2033	56	0
2	F	1340	0	671	10	0
2	H	1340	0	671	9	0
3	A	25	0	0	1	0
3	B	41	0	0	3	0
3	F	30	0	0	0	0
3	H	39	0	0	1	0
All	All	6786	0	5409	119	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 10.

The worst 5 of 119 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:327:LEU:O	1:A:330:THR:HG22	1.56	1.05
1:A:180:LEU:HD21	1:A:184:ASN:HA	1.36	1.03
1:B:327:LEU:O	1:B:330:THR:HG22	1.76	0.86
2:H:39:A:H8	2:H:39:A:H5"	1.42	0.85
2:H:39:A:H5"	2:H:39:A:C8	2.19	0.77

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	244/267 (91%)	231 (95%)	13 (5%)	0	100	100
1	B	243/267 (91%)	237 (98%)	6 (2%)	0	100	100
All	All	487/534 (91%)	468 (96%)	19 (4%)	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	225/240 (94%)	205 (91%)	20 (9%)	9	11
1	B	225/240 (94%)	204 (91%)	21 (9%)	9	10
All	All	450/480 (94%)	409 (91%)	41 (9%)	9	11

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	258	ARG
1	B	307	ARG
1	B	268	LEU
1	B	279	ARG
1	B	330	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	140	GLN
1	B	160	GLN
1	B	297	ASN
1	B	198	HIS
1	B	271	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	60/62 (96%)	8 (13%)	1 (1%)
2	H	60/62 (96%)	7 (11%)	1 (1%)
All	All	120/124 (96%)	15 (12%)	2 (1%)

5 of 15 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	H	3	C
2	H	4	A
2	H	14	G
2	H	15	A
2	H	18	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	39	A
2	F	15	A

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

4 non-standard protein/DNA/RNA residues 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	CCC	H	62	2	20,25,26	2.69	4 (20%)	28,38,41	1.53	6 (21%)
2	GTP	F	1	2	24,30,34	1.16	2 (8%)	30,47,54	1.31	4 (13%)
2	CCC	F	62	2	20,25,26	2.64	4 (20%)	28,38,41	1.53	6 (21%)
2	GTP	H	1	2	24,30,34	1.15	2 (8%)	30,47,54	1.35	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
2	CCC	H	62	2	-	0/7/35/36	0/3/3/3
2	GTP	F	1	2	-	3/12/32/38	0/3/3/3
2	CCC	F	62	2	-	1/7/35/36	0/3/3/3
2	GTP	H	1	2	-	6/12/32/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	62	CCC	C5-C4	-7.11	1.26	1.42
2	F	62	CCC	C5-C4	-7.05	1.26	1.42
2	H	62	CCC	C6-C5	-6.43	1.20	1.35
2	F	62	CCC	C6-C5	-6.38	1.20	1.35
2	H	62	CCC	C6-N1	-6.23	1.22	1.38

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	62	CCC	O3'-C3'-C2'	3.84	112.12	105.08
2	F	62	CCC	O2'-C2'-C3'	3.59	111.65	105.08
2	H	1	GTP	PA-O3A-PB	-3.54	120.68	132.83
2	F	62	CCC	O3'-C3'-C2'	3.42	111.35	105.08
2	H	62	CCC	C6-C5-C4	3.12	122.54	117.50

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	GTP	C5'-O5'-PA-O2A
2	F	1	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	F	1	GTP	C3'-C4'-C5'-O5'
2	H	1	GTP	PA-O3A-PB-O1B
2	H	1	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	245/267 (91%)	-0.13	3 (1%)	79	83	32, 49, 66, 78	0
1	B	244/267 (91%)	-0.22	3 (1%)	79	83	30, 43, 70, 107	0
2	F	60/62 (96%)	-0.30	0	100	100	29, 42, 85, 90	0
2	H	60/62 (96%)	-0.43	0	100	100	27, 38, 91, 100	0
All	All	609/658 (92%)	-0.21	6 (0%)	82	86	27, 45, 75, 107	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	ILE	7.7
1	A	355	GLU	3.5
1	B	359	PRO	3.3
1	B	332	ARG	2.5
1	A	185	ARG	2.2

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

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(Å^2)	Q<0.9
2	GTP	H	1	28/32	0.81	0.17	69,84,110,113	0
2	CCC	H	62	23/24	0.81	0.23	93,98,100,100	0
2	CCC	F	62	23/24	0.82	0.15	92,96,96,97	0
2	GTP	F	1	28/32	0.86	0.17	72,86,115,125	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.