



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 09:27 AM GMT

PDB ID : 1FT8
Title : CRYSTAL STRUCTURE OF THE RNA-BINDING DOMAIN OF THE
MRNA EXPORT FACTOR TAP
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Deposited on : 2000-09-12
Resolution : 3.15 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

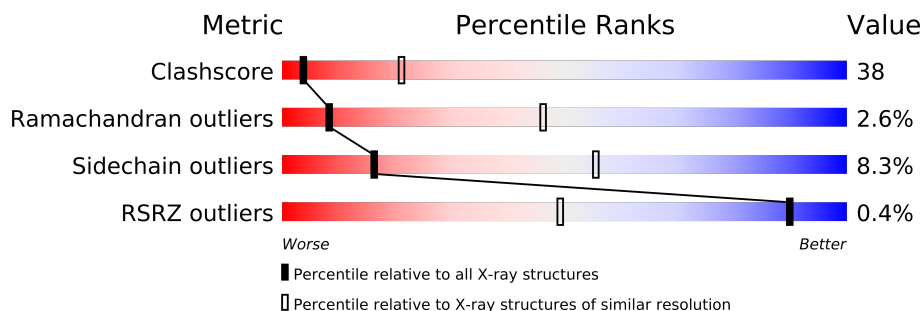
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.15 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))
Clashscore	79885	1681 (3.22-3.10)
Ramachandran outliers	78287	1639 (3.22-3.10)
Sidechain outliers	78261	1638 (3.22-3.10)
RSRZ outliers	66119	1361 (3.22-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	271	
1	B	271	
1	C	271	
1	D	271	
1	E	271	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6913 atoms, of which 0 are hydrogen and 0 are deuterium.

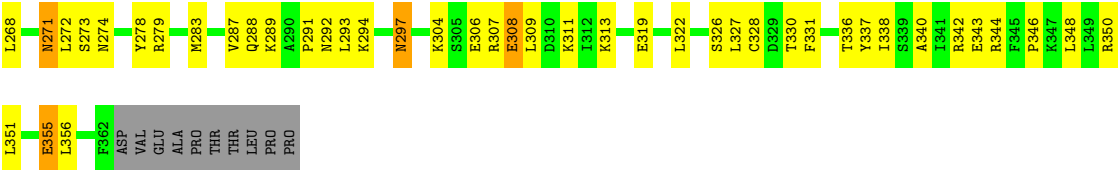
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TIP ASSOCIATING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1961	1245	343	366	7			
1	B	165	Total	C	N	O	S	0	0	0
			1323	831	232	255	5			
1	C	244	Total	C	N	O	S	0	0	0
			1973	1253	346	367	7			
1	D	162	Total	C	N	O	S	0	0	0
			1302	818	229	250	5			
1	E	44	Total	C	N	O	S	0	0	0
			354	236	54	62	2			

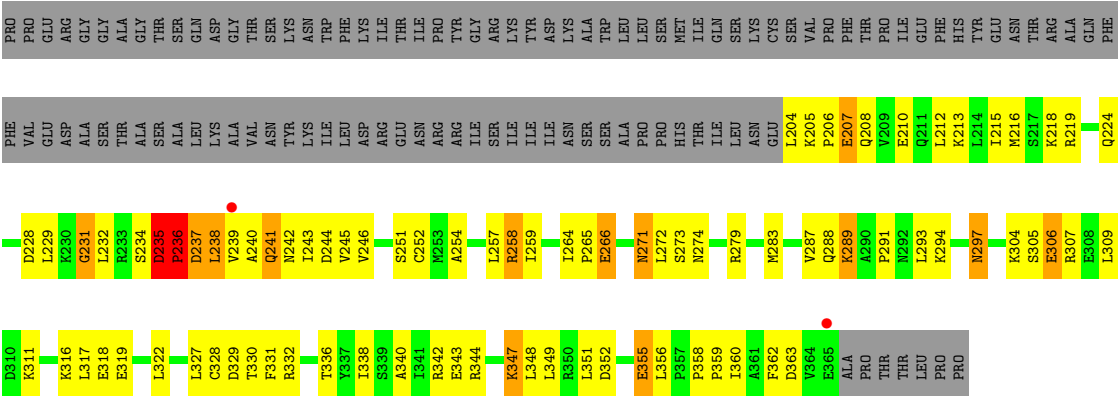
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
A	226	VAL	ALA	ENGINEERED	UNP Q9UBU9
B	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
B	226	VAL	ALA	ENGINEERED	UNP Q9UBU9
C	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
C	226	VAL	ALA	ENGINEERED	UNP Q9UBU9
D	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
D	226	VAL	ALA	ENGINEERED	UNP Q9UBU9
E	119	TRP	CYS	ENGINEERED	UNP Q9UBU9
E	226	VAL	ALA	ENGINEERED	UNP Q9UBU9



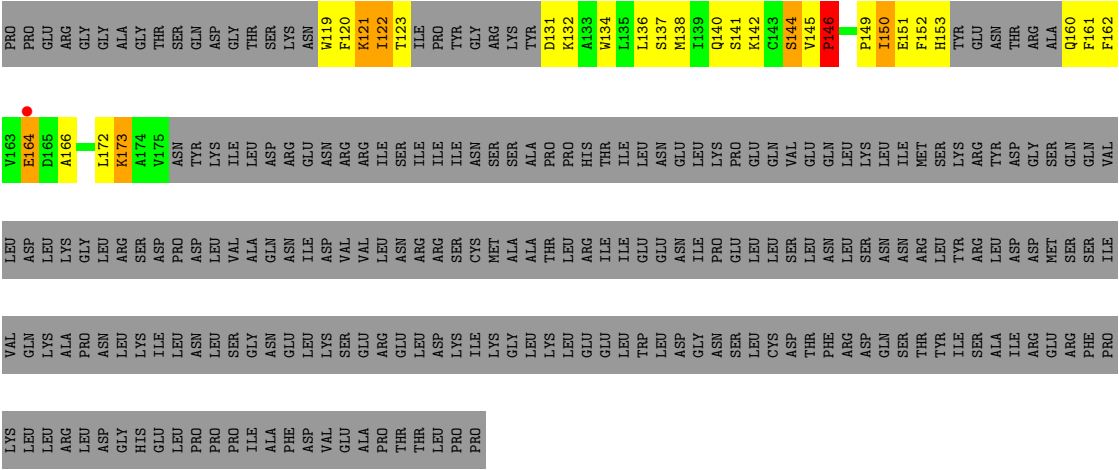
• Molecule 1: TIP ASSOCIATING PROTEIN

Chain D:



• Molecule 1: TIP ASSOCIATING PROTEIN

Chain E:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.92Å 139.92Å 206.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15 29.94 – 3.16	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.15) 99.6 (29.94-3.16)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.10 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.303 , 0.303 0.302 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 35832 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6913	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.73	4/1996 (0.2%)	0.91	10/2696 (0.4%)
1	B	0.60	1/1340 (0.1%)	0.79	2/1808 (0.1%)
1	C	0.75	7/2008 (0.3%)	0.98	8/2711 (0.3%)
1	D	0.61	1/1318 (0.1%)	0.92	8/1777 (0.5%)
1	E	0.72	0/363	0.95	2/489 (0.4%)
All	All	0.69	13/7025 (0.2%)	0.92	30/9481 (0.3%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	ASP	CB-CG	-11.57	1.27	1.51
1	C	228	ASP	CB-CG	-10.18	1.30	1.51
1	A	164	GLU	CB-CG	-10.11	1.32	1.52
1	C	165	ASP	CB-CG	-9.04	1.32	1.51
1	C	164	GLU	CB-CG	-7.82	1.37	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	ASP	CB-CG-OD1	-19.55	100.71	118.30
1	A	165	ASP	CB-CG-OD2	-18.87	101.32	118.30
1	C	165	ASP	CB-CG-OD2	-18.30	101.83	118.30
1	C	155	GLU	OE1-CD-OE2	-8.83	112.70	123.30
1	C	165	ASP	CB-CG-OD1	8.22	125.70	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1961	0	2003	171	0
1	B	1323	0	1363	107	0
1	C	1973	0	2013	135	0
1	D	1302	0	1345	113	0
1	E	354	0	349	50	1
All	All	6913	0	7073	536	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 536 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:LYS:HD2	1:A:273:SER:OG	1.29	1.32
1:B:323:ASP:HB2	1:C:177:TYR:CE2	1.78	1.19
1:C:119:TRP:HZ3	1:C:150:ILE:CD1	1.56	1.19
1:E:144:SER:O	1:E:145:VAL:HG23	1.39	1.19
1:E:145:VAL:HG22	1:E:146:PRO:CD	1.73	1.17

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:142:LYS:NZ	1:E:142:LYS:NZ[8_665]	1.44	0.76

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	238/271 (88%)	213 (90%)	20 (8%)	5 (2%)	11 53
1	B	163/271 (60%)	149 (91%)	10 (6%)	4 (2%)	9 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	240/271 (89%)	216 (90%)	17 (7%)	7 (3%)	7	42
1	D	160/271 (59%)	139 (87%)	16 (10%)	5 (3%)	7	40
1	E	38/271 (14%)	35 (92%)	2 (5%)	1 (3%)	8	46
All	All	839/1355 (62%)	752 (90%)	65 (8%)	22 (3%)	8	46

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	PRO
1	C	157	THR
1	C	236	PRO
1	C	238	LEU
1	C	308	GLU

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	222/245 (91%)	201 (90%)	21 (10%)	12	45
1	B	152/245 (62%)	143 (94%)	9 (6%)	28	72
1	C	222/245 (91%)	205 (92%)	17 (8%)	18	60
1	D	150/245 (61%)	137 (91%)	13 (9%)	15	52
1	E	39/245 (16%)	34 (87%)	5 (13%)	6	27
All	All	785/1225 (64%)	720 (92%)	65 (8%)	16	55

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	367	PRO
1	C	172	LEU
1	E	121	LYS
1	C	122	ILE
1	C	156	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	263	ASN
1	B	297	ASN
1	D	297	ASN
1	B	271	ASN
1	C	156	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	242/271 (89%)	-0.05	0	100 100	55, 66, 89, 109	0
1	B	165/271 (60%)	-0.04	0	100 100	49, 63, 82, 97	0
1	C	244/271 (90%)	0.05	0	100 100	55, 74, 106, 106	0
1	D	162/271 (59%)	0.01	2 (1%)	75 23	52, 65, 85, 100	0
1	E	44/271 (16%)	0.52	1 (2%)	57 11	89, 94, 94, 94	0
All	All	857/1355 (63%)	0.02	3 (0%)	90 49	49, 68, 106, 109	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	164	GLU	2.9
1	D	239	VAL	2.3
1	D	365	GLU	2.1

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 carbohydrates 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.