

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 23, 2023 – 11:23 AM EDT

PDB ID : 3BUA

Title : Crystal Structure of TRF2 TRFH domain and APOLLO peptide complex Authors : Chen, Y.; Yang, Y.; van Overbeek, M.; Donigian, J.R.; Baciu, P.; de Lange,

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Deposited on : 2008-01-02

Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Xtriage (Phenix): 1.13

EDS: 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove) oteins) : Engh & Huber (2007)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

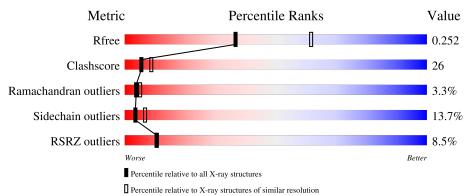
Validation Pipeline (wwPDB-VP) : 2.35

## 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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					
		20.4	8%					_
1	A	204		53%		38%	6%	••
			5%					
1	В	204		60%	o o	29%	8%	•••
			9%					
1	С	204		60%	ò	30%	8%	•••
			7%					
1	D	204		50%		39%	9%	
			11%					
2	E	36	14%	19%	6%	61%		

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Mol	Chain	Length	Quality of chain				
	Б	2.0	3%				
2	F'	36	17%	8% 8%		67%	
			19%				
2	G	36	17%	19%	8%	56%	
			6%				
2	Н	36	19%	11% •		67%	



# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7148 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 Telomeric repeat-binding factor 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	202	Total	С	N	О	S	0	0	0
1	A	202	1653	1050	291	302	10	0	U	
1	В	202	Total	С	N	О	S	0	0	0
1	Б	202	1653	1050	291	302	10	0	U	
1	С	202	Total	С	N	О	S	0	0	0
1		202	1653	1050	291	302	10	0	U	
1	D	202	Total	С	N	О	S	0	0	0
1	ע	202	1653	1050	291	302	10	U	U	U

• Molecule 2 is a protein called DNA cross-link repair 1B protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	14	Total C N O	0	0	0
2	ינו	14	113 77 19 17	0		0
2	F	12	Total C N O	0	0	0
2	I'	12	94 64 16 14	0		0
2	G	16	Total C N O	0	0	0
2	G	10	128 85 21 22	0		0
2	Н	12	Total C N O	0	0	0
	11	12	91 62 14 15	0	U	U

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	495	SER	THR	SEE REMARK 999	UNP Q9H816
F	495	SER	THR	SEE REMARK 999	UNP Q9H816
G	495	SER	THR	SEE REMARK 999	UNP Q9H816
Н	495	SER	THR	SEE REMARK 999	UNP Q9H816

• Molecule 3 is water.



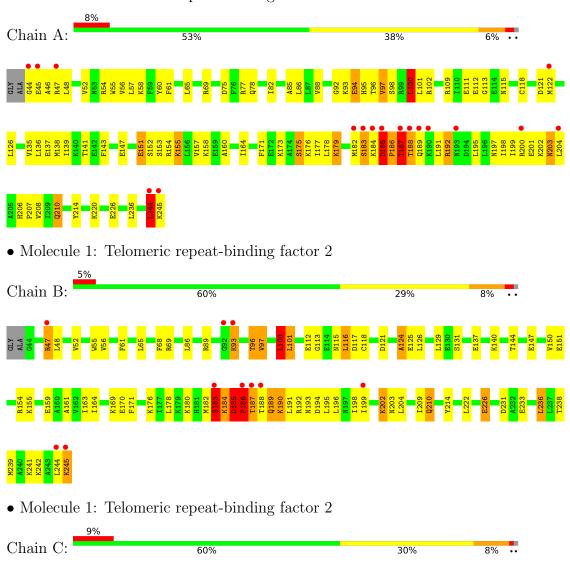
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	В	39	Total O 39 39	0	0
3	С	24	Total O 24 24	0	0
3	D	20	Total O 20 20	0	0
3	E	1	Total O 1 1	0	0
3	G	2	Total O 2 2	0	0



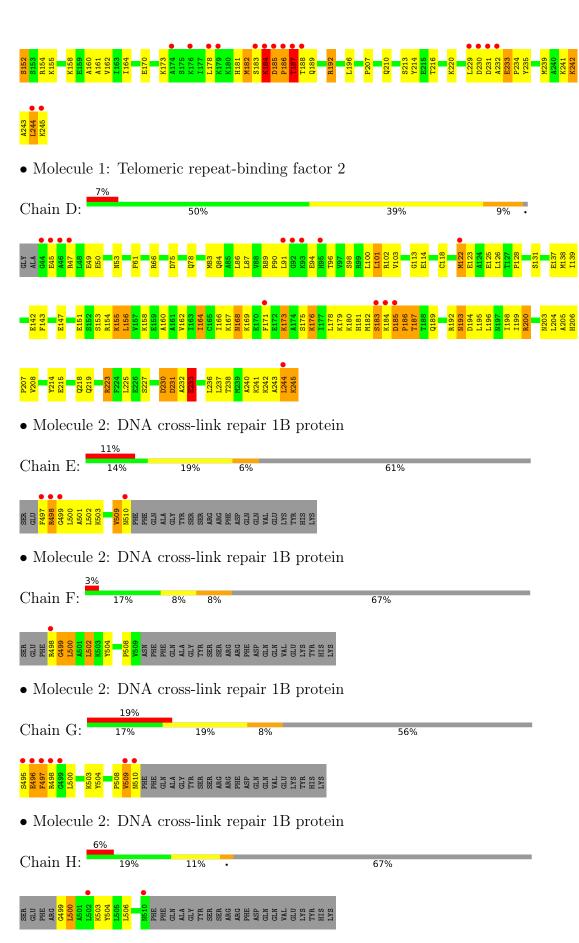
# 3 Residue-property plots (i)

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: Telomeric repeat-binding factor 2









# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 32 2 1	Depositor	
Cell constants	109.95Å 109.95Å 130.83Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor	
Resolution (Å)	50.00 - 2.50	Depositor	
resolution (A)	42.09 - 2.50	EDS	
% Data completeness	95.3 (50.00-2.50)	Depositor	
(in resolution range)	95.8 (42.09-2.50)	EDS	
$R_{merge}$	0.09	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.39  (at  2.51Å)	Xtriage	
Refinement program	CNS 1.1	Depositor	
$R, R_{free}$	0.229 , $0.254$	Depositor	
it, it <sub>free</sub>	0.228 , $0.252$	DCC	
$R_{free}$ test set	3201  reflections  (10.04%)	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage	
Anisotropy	0.059	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	$0.38 \; ,  46.6$	EDS	
L-test for twinning <sup>2</sup>	$< L > = 0.50, < L^2> = 0.33$	Xtriage	
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage	
$F_o, F_c$ correlation	0.94	EDS	
Total number of atoms	7148	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality (i)

### 5.1 Standard geometry (i)

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	Во	ond angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.37	0/1678	0.75	3/2249 (0.1%)
1	В	0.36	0/1678	0.73	$4/2249 \ (0.2\%)$
1	С	0.33	0/1678	0.70	2/2249 (0.1%)
1	D	0.37	0/1678	0.74	2/2249 (0.1%)
2	Е	0.51	0/115	0.87	0/155
2	F	0.36	0/95	0.79	1/128 (0.8%)
2	G	0.49	0/130	1.44	3/175 (1.7%)
2	Н	0.39	0/92	0.83	0/125
All	All	0.36	0/7144	0.75	$15/9579 \ (0.2\%)$

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
1	A	244	LEU	CA-CB-CG	13.30	145.90	115.30
2	G	509	VAL	CB-CA-C	8.99	128.48	111.40
1	A	185	ASP	N-CA-C	7.58	131.48	111.00
1	В	185	ASP	N-CA-C	7.11	130.20	111.00
1	A	100	LEU	CA-CB-CG	6.46	130.17	115.30

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	A	1653	0	1705	87	0
1	В	1653	0	1705	77	0
1	С	1653	0	1705	89	0
1	D	1653	0	1705	105	0
2	Е	113	0	124	8	0
2	F	94	0	109	6	0
2	G	128	0	135	14	0
2	Н	91	0	102	8	0
3	A	24	0	0	2	0
3	В	39	0	0	0	0
3	С	24	0	0	2	0
3	D	20	0	0	1	0
3	Е	1	0	0	0	0
3	G	2	0	0	0	0
All	All	7148	0	7290	373	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 26.

The worst 5 of 373 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:D:185:ASP:HB3	1:D:186:PRO:CD	1.74	1.17
2:G:508:PRO:HB2	2:G:510:ASN:ND2	1.64	1.11
1:D:185:ASP:HB3	1:D:186:PRO:HD3	1.17	1.10
1:A:185:ASP:O	1:A:189:GLN:HG3	1.52	1.10
1:C:93:LYS:HE3	1:C:95:HIS:ND1	1.69	1.05

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	ntiles
1	A	200/204~(98%)	187 (94%)	6 (3%)	7 (4%)	3	4
1	В	200/204 (98%)	183 (92%)	12 (6%)	5 (2%)	5	8
1	С	200/204~(98%)	178 (89%)	12 (6%)	10 (5%)	2	2
1	D	200/204 (98%)	185 (92%)	10 (5%)	5 (2%)	5	8
2	E	12/36 (33%)	11 (92%)	1 (8%)	0	100	100
2	F	10/36 (28%)	8 (80%)	2 (20%)	0	100	100
2	G	14/36 (39%)	11 (79%)	2 (14%)	1 (7%)	1	1
2	Н	10/36 (28%)	9 (90%)	1 (10%)	0	100	100
All	All	846/960 (88%)	772 (91%)	46 (5%)	28 (3%)	4	5

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ASP
1	A	186	PRO
1	В	183	SER
1	В	186	PRO
1	В	189	GLN

#### 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	182/182 (100%)	158 (87%)	24 (13%)	4 7
1	В	$182/182 \; (100\%)$	155 (85%)	27 (15%)	3 5
1	$\mathbf{C}$	$182/182\ (100\%)$	162 (89%)	20 (11%)	6 12
1	D	182/182 (100%)	154 (85%)	28 (15%)	2 5
2	E	12/32~(38%)	9 (75%)	3~(25%)	0 1
2	F	10/32~(31%)	8 (80%)	2 (20%)	1 2
2	G	14/32~(44%)	13 (93%)	1 (7%)	14 28
2	Н	10/32~(31%)	9 (90%)	1 (10%)	7 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	774/856 (90%)	668 (86%)	106 (14%)	3 7

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	125	GLU
1	D	45	GLU
2	Е	497	PHE
1	С	143	PHE
1	С	187	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	В	218	GLN
1	В	228	HIS
1	D	219	GLN
1	D	193	ASN
1	D	218	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 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>	$\# \mathrm{RSRZ} {>} 2$	$OWAB(A^2)$	Q < 0.9
1	A	202/204~(99%)	0.33	17 (8%) 11 11	29, 44, 72, 94	0
1	В	202/204~(99%)	0.26	10 (4%) 28 30	28, 43, 66, 86	0
1	С	202/204 (99%)	0.52	18 (8%) 9 9	29, 47, 78, 91	0
1	D	202/204 (99%)	0.39	14 (6%) 16 17	33, 56, 77, 88	0
2	E	14/36 (38%)	1.40	4 (28%) 0 0	35, 42, 78, 84	0
2	F	12/36 (33%)	0.64	1 (8%) 11 11	33, 42, 69, 83	0
2	G	16/36 (44%)	2.00	7 (43%) 0 0	33, 49, 82, 85	0
2	Н	12/36 (33%)	0.66	2 (16%) 1 1	38, 45, 59, 69	0
All	All	862/960 (89%)	0.43	73 (8%) 10 10	28, 48, 77, 94	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	510	ASN	8.0
2	Е	497	PHE	6.3
1	A	183	SER	6.3
2	G	495	SER	5.6
1	С	184	LYS	5.6

### 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 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.

