



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:17 AM UTC

PDB ID : 3BUA / pdb_00003bua
Title : Crystal Structure of TRF2 TRFH domain and APOLLO peptide complex
Authors : Chen, Y.; Yang, Y.; van Overbeek, M.; Donigian, J.R.; Baciou, P.; de Lange, T.; Lei, M.
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

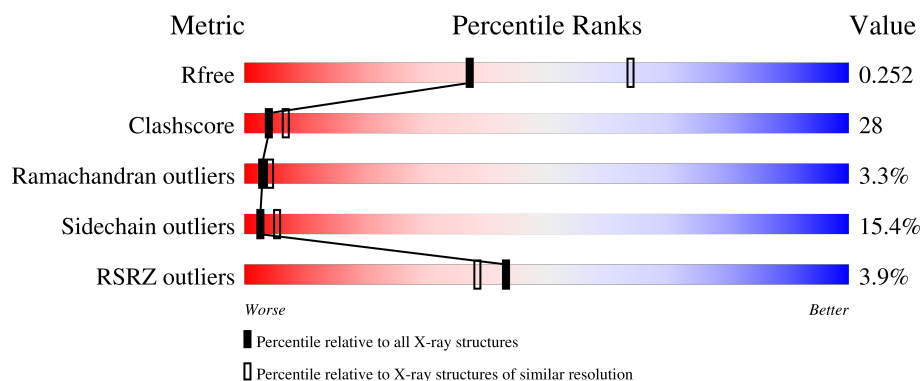
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	204	3% 49% 39% 9% ..
1	B	204	3% 55% 29% 12% ..
1	C	204	4% 58% 26% 12% ..
1	D	204	2% 45% 42% 10% ..
2	E	36	6% 14% 17% 6% 61%

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Mol	Chain	Length	Quality of chain
2	F	36	3%11%14%8%67%
2	G	36	11%17%14%11%•56%
2	H	36	3%14%14%••67%

2 Entry composition

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	A	202	Total	C	N	O	S	0	0	0
			1653	1050	291	302	10			
1	B	202	Total	C	N	O	S	0	0	0
			1653	1050	291	302	10			
1	C	202	Total	C	N	O	S	0	0	0
			1653	1050	291	302	10			
1	D	202	Total	C	N	O	S	0	0	0
			1653	1050	291	302	10			

- 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
			113	77	19	17			
2	F	12	Total	C	N	O	0	0	0
			94	64	16	14			
2	G	16	Total	C	N	O	0	0	0
			128	85	21	22			
2	H	12	Total	C	N	O	0	0	0
			91	62	14	15			

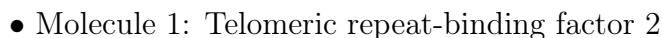
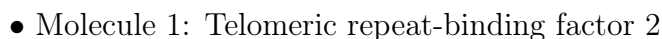
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	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
H	495	SER	THR	SEE REMARK 999	UNP Q9H816

- Molecule 3 is water.

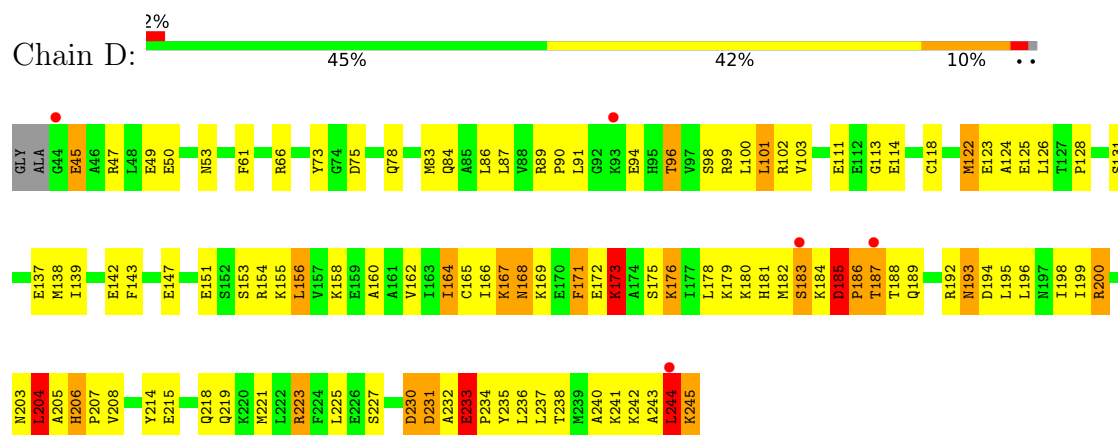
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	0	0
3	B	39	Total 39	O 39	0	0
3	C	24	Total 24	O 24	0	0
3	D	20	Total 20	O 20	0	0
3	E	1	Total 1	O 1	0	0
3	G	2	Total 2	O 2	0	0

- Molecule 1: Telomeric repeat-binding factor 2

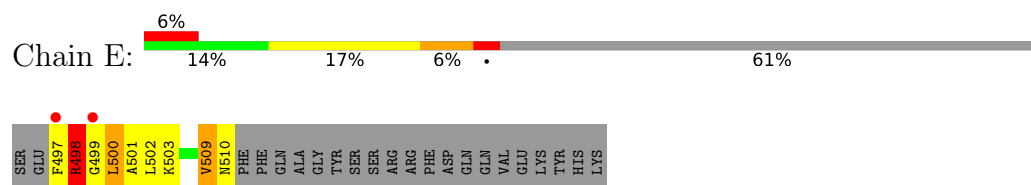




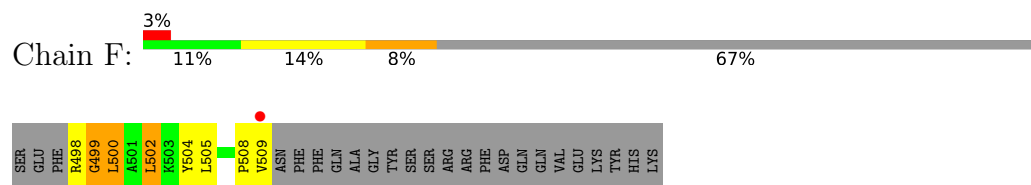
- Molecule 1: Telomeric repeat-binding factor 2



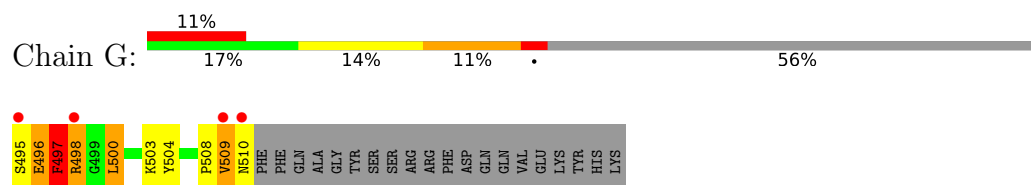
- Molecule 2: DNA cross-link repair 1B protein



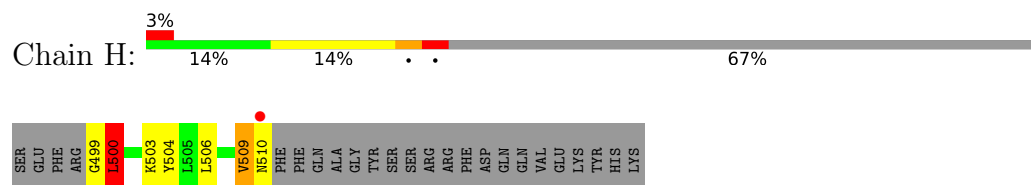
- Molecule 2: DNA cross-link repair 1B protein



- Molecule 2: DNA cross-link repair 1B protein



- Molecule 2: DNA cross-link repair 1B protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.95Å 109.95Å 130.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.50) 95.8 (50.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.254 0.228 , 0.252	Depositor DCC
R_{free} test set	3201 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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.

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	0.44	1/1678 (0.1%)	1.14	19/2249 (0.8%)
1	B	0.43	0/1678	1.16	18/2249 (0.8%)
1	C	0.39	0/1678	1.14	14/2249 (0.6%)
1	D	0.45	0/1678	1.18	19/2249 (0.8%)
2	E	0.64	0/115	1.43	2/155 (1.3%)
2	F	0.38	0/95	0.96	1/128 (0.8%)
2	G	0.59	0/130	2.13	8/175 (4.6%)
2	H	0.56	0/92	1.28	3/125 (2.4%)
All	All	0.44	1/7144 (0.0%)	1.19	84/9579 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ASP	C-O	-5.62	1.17	1.24

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	THR	N-CA-C	-12.75	98.65	112.93
1	B	188	THR	N-CA-C	-11.78	98.16	111.82
2	G	496	GLU	N-CA-C	11.67	127.02	109.63
2	G	509	VAL	CB-CA-C	10.48	128.48	111.29
1	B	185	ASP	CA-C-N	-10.13	107.17	119.84

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	1653	0	1705	92	0
1	B	1653	0	1705	85	0
1	C	1653	0	1705	92	0
1	D	1653	0	1705	115	0
2	E	113	0	124	8	0
2	F	94	0	109	8	0
2	G	128	0	135	14	0
2	H	91	0	102	9	0
3	A	24	0	0	2	0
3	B	39	0	0	0	0
3	C	24	0	0	2	0
3	D	20	0	0	1	0
3	E	1	0	0	0	0
3	G	2	0	0	0	0
All	All	7148	0	7290	399	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 28.

The worst 5 of 399 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: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	Percentiles	
1	A	200/204 (98%)	187 (94%)	6 (3%)	7 (4%)	3	4
1	B	200/204 (98%)	183 (92%)	12 (6%)	5 (2%)	4	7
1	C	200/204 (98%)	178 (89%)	12 (6%)	10 (5%)	1	2
1	D	200/204 (98%)	185 (92%)	10 (5%)	5 (2%)	4	7
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	H	10/36 (28%)	9 (90%)	1 (10%)	0	100	100
All	All	846/960 (88%)	772 (91%)	46 (5%)	28 (3%)	3	4

5 of 28 Ramachandran outliers are listed below:

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

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	182/182 (100%)	154 (85%)	28 (15%)	2	5
1	B	182/182 (100%)	153 (84%)	29 (16%)	2	5
1	C	182/182 (100%)	157 (86%)	25 (14%)	3	7
1	D	182/182 (100%)	153 (84%)	29 (16%)	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%)	13	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	10/32 (31%)	8 (80%)	2 (20%)	1	2
All	All	774/856 (90%)	655 (85%)	119 (15%)	2	5

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	45	GLU
1	D	245	LYS
1	C	152	SER
1	D	244	LEU
2	H	510	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	84	GLN
1	D	218	GLN
1	D	219	GLN
1	D	193	ASN
1	B	181	HIS

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 oligosaccharides 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, 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	202/204 (99%)	0.13	6 (2%) 52 48	29, 44, 72, 94	0
1	B	202/204 (99%)	0.07	6 (2%) 52 48	28, 43, 66, 86	0
1	C	202/204 (99%)	0.21	9 (4%) 38 33	29, 47, 78, 91	0
1	D	202/204 (99%)	0.33	5 (2%) 58 54	33, 56, 77, 88	0
2	E	14/36 (38%)	0.89	2 (14%) 6 5	35, 42, 78, 84	0
2	F	12/36 (33%)	0.60	1 (8%) 17 15	33, 42, 69, 83	0
2	G	16/36 (44%)	1.10	4 (25%) 2 1	33, 49, 82, 85	0
2	H	12/36 (33%)	0.38	1 (8%) 17 15	38, 45, 59, 69	0
All	All	862/960 (89%)	0.22	34 (3%) 43 38	28, 48, 77, 94	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	510	ASN	6.0
1	C	232	ALA	4.4
2	G	509	VAL	4.0
1	A	182	MET	4.0
2	E	497	PHE	3.9

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 oligosaccharides 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.