



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID : 2RBL  
Title : High resolution design of a protein loop  
Authors : Hu, X.; Wang, H.; Ke, H.; Kuhlman, B.  
Deposited on : 2007-09-19  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

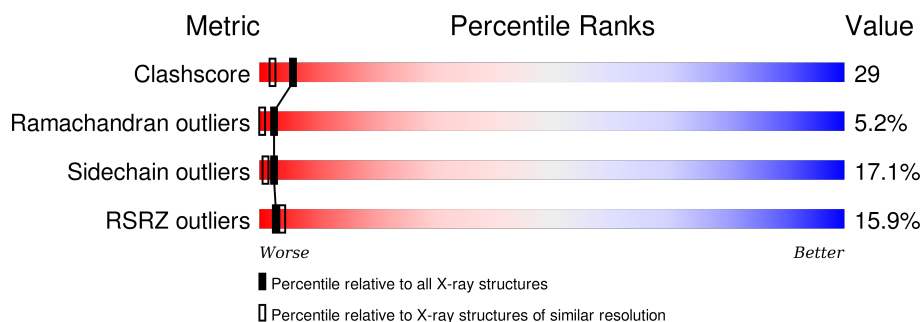
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	104	
1	B	104	
1	M	104	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2009 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 Tenascin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	0	0
			693	428	110	153	2			
1	B	89	Total	C	N	O	S	0	0	0
			693	428	110	153	2			
1	M	80	Total	C	N	O	S	0	0	0
			623	386	99	137	1			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	801	MET	-	INITIATING METHIONINE	UNP P24821
A	824	SER	PHE	ENGINEERED	UNP P24821
A	825	MET	LYS	ENGINEERED	UNP P24821
A	826	GLN	PRO	ENGINEERED	UNP P24821
A	828	SER	ALA	ENGINEERED	UNP P24821
A	829	GLN	GLU	ENGINEERED	UNP P24821
A	830	LEU	ILE	ENGINEERED	UNP P24821
A	831	GLU	ASP	ENGINEERED	UNP P24821
A	894	ALA	-	EXPRESSION TAG	UNP P24821
A	895	ALA	-	EXPRESSION TAG	UNP P24821
A	896	ALA	-	EXPRESSION TAG	UNP P24821
A	897	LEU	-	EXPRESSION TAG	UNP P24821
A	898	GLU	-	EXPRESSION TAG	UNP P24821
A	899	HIS	-	EXPRESSION TAG	UNP P24821
A	900	HIS	-	EXPRESSION TAG	UNP P24821
A	901	HIS	-	EXPRESSION TAG	UNP P24821
A	902	HIS	-	EXPRESSION TAG	UNP P24821
A	903	HIS	-	EXPRESSION TAG	UNP P24821
A	904	HIS	-	EXPRESSION TAG	UNP P24821
B	801	MET	-	INITIATING METHIONINE	UNP P24821
B	824	SER	PHE	ENGINEERED	UNP P24821
B	825	MET	LYS	ENGINEERED	UNP P24821
B	826	GLN	PRO	ENGINEERED	UNP P24821

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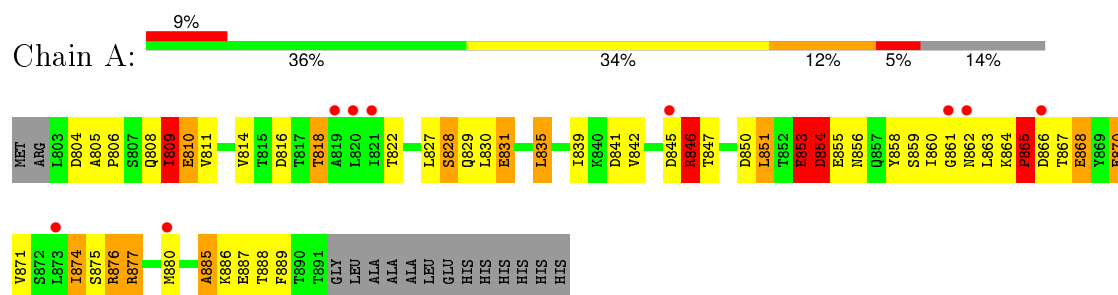
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Chain	Residue	Modelled	Actual	Comment	Reference
B	828	SER	ALA	ENGINEERED	UNP P24821
B	829	GLN	GLU	ENGINEERED	UNP P24821
B	830	LEU	ILE	ENGINEERED	UNP P24821
B	831	GLU	ASP	ENGINEERED	UNP P24821
B	894	ALA	-	EXPRESSION TAG	UNP P24821
B	895	ALA	-	EXPRESSION TAG	UNP P24821
B	896	ALA	-	EXPRESSION TAG	UNP P24821
B	897	LEU	-	EXPRESSION TAG	UNP P24821
B	898	GLU	-	EXPRESSION TAG	UNP P24821
B	899	HIS	-	EXPRESSION TAG	UNP P24821
B	900	HIS	-	EXPRESSION TAG	UNP P24821
B	901	HIS	-	EXPRESSION TAG	UNP P24821
B	902	HIS	-	EXPRESSION TAG	UNP P24821
B	903	HIS	-	EXPRESSION TAG	UNP P24821
B	904	HIS	-	EXPRESSION TAG	UNP P24821
M	801	MET	-	INITIATING METHIONINE	UNP P24821
M	824	SER	PHE	ENGINEERED	UNP P24821
M	825	MET	LYS	ENGINEERED	UNP P24821
M	826	GLN	PRO	ENGINEERED	UNP P24821
M	828	SER	ALA	ENGINEERED	UNP P24821
M	829	GLN	GLU	ENGINEERED	UNP P24821
M	830	LEU	ILE	ENGINEERED	UNP P24821
M	831	GLU	ASP	ENGINEERED	UNP P24821
M	894	ALA	-	EXPRESSION TAG	UNP P24821
M	895	ALA	-	EXPRESSION TAG	UNP P24821
M	896	ALA	-	EXPRESSION TAG	UNP P24821
M	897	LEU	-	EXPRESSION TAG	UNP P24821
M	898	GLU	-	EXPRESSION TAG	UNP P24821
M	899	HIS	-	EXPRESSION TAG	UNP P24821
M	900	HIS	-	EXPRESSION TAG	UNP P24821
M	901	HIS	-	EXPRESSION TAG	UNP P24821
M	902	HIS	-	EXPRESSION TAG	UNP P24821
M	903	HIS	-	EXPRESSION TAG	UNP P24821
M	904	HIS	-	EXPRESSION TAG	UNP P24821

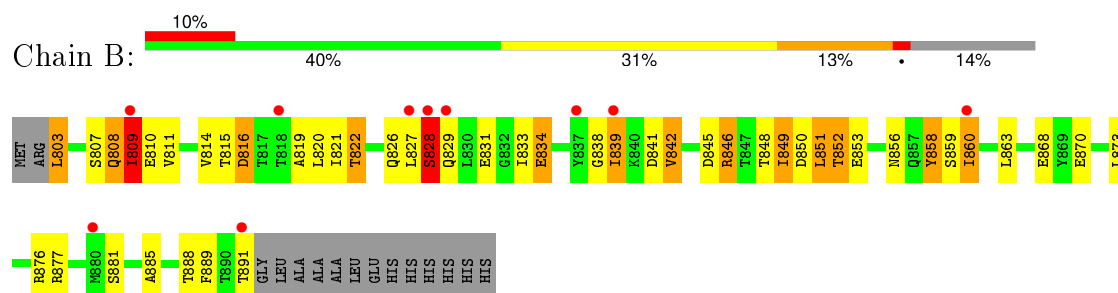
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

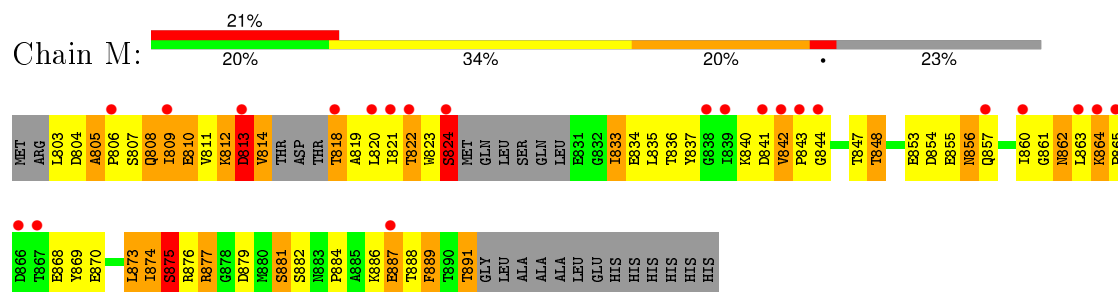
#### • Molecule 1: Tenascin



#### • Molecule 1: Tenascin



#### • Molecule 1: Tenascin



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.20 Å 137.20 Å 86.68 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 49.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 85.7 (49.00-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.250 , 0.300 0.287 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.2	EDS
Estimated twinning fraction	0.005 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.024 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.017 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 15756 reflections (0.013%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.93	18/702 (2.6%)	1.78	19/955 (2.0%)
1	B	1.88	12/702 (1.7%)	1.78	18/955 (1.9%)
1	M	2.15	12/630 (1.9%)	1.51	13/854 (1.5%)
All	All	1.99	42/2034 (2.1%)	1.70	50/2764 (1.8%)

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
1	B	0	1
1	M	0	1
All	All	0	3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	813	ASP	CG-OD2	18.24	1.67	1.25
1	M	810	GLU	CD-OE1	14.98	1.42	1.25
1	M	810	GLU	CD-OE2	14.96	1.42	1.25
1	M	813	ASP	CG-OD1	13.50	1.56	1.25
1	M	856	ASN	CG-OD1	10.46	1.47	1.24

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	877	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	B	876	ARG	NE-CZ-NH1	-9.80	115.40	120.30
1	A	854	ASP	CB-CG-OD1	9.09	126.48	118.30
1	M	876	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	B	816	ASP	CB-CG-OD1	-8.32	110.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	885	ALA	Peptide
1	B	858	TYR	Mainchain
1	M	856	ASN	Sidechain

## 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	693	0	671	43	0
1	B	693	0	671	39	0
1	M	623	0	599	53	0
All	All	2009	0	1941	115	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 29.

The worst 5 of 115 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:M:813:ASP:CG	1:M:813:ASP:OD2	1.67	1.33
1:B:829:GLN:HG3	1:B:877:ARG:NH2	1.55	1.22
1:A:831:GLU:HB3	1:B:829:GLN:NE2	1.56	1.20
1:B:829:GLN:CG	1:B:877:ARG:HH21	1.58	1.15
1:A:831:GLU:HB3	1:B:829:GLN:HE21	0.93	1.07

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	87/104 (84%)	77 (88%)	6 (7%)	4 (5%)	3	1
1	B	87/104 (84%)	77 (88%)	6 (7%)	4 (5%)	3	1
1	M	74/104 (71%)	59 (80%)	10 (14%)	5 (7%)	1	0
All	All	248/312 (80%)	213 (86%)	22 (9%)	13 (5%)	2	0

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	809	ILE
1	A	828	SER
1	A	846	ARG
1	M	808	GLN
1	M	809	ILE

### 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	81/92 (88%)	70 (86%)	11 (14%)	5	2
1	B	81/92 (88%)	72 (89%)	9 (11%)	8	4
1	M	72/92 (78%)	52 (72%)	20 (28%)	0	0
All	All	234/276 (85%)	194 (83%)	40 (17%)	2	1

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	881	SER
1	M	813	ASP
1	M	877	ARG
1	M	803	LEU
1	M	814	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	856	ASN
1	B	826	GLN
1	B	829	GLN
1	M	857	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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	89/104 (85%)	0.80	9 (10%) 9 12	40, 54, 70, 74	0
1	B	89/104 (85%)	0.96	10 (11%) 7 9	45, 55, 69, 77	0
1	M	80/104 (76%)	1.51	22 (27%) 1 1	42, 53, 62, 69	0
All	All	258/312 (82%)	1.08	41 (15%) 3 4	40, 54, 69, 77	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	863	LEU	6.4
1	M	844	GLY	6.1
1	M	820	LEU	4.3
1	M	821	ILE	4.3
1	M	842	VAL	4.2

### 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 carbohydrates 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.