



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 16, 2024 – 12:07 AM JST

PDB ID : 8JJ9  
Title : Human FAM91A1 N terminal domain in complex with TBC1D23  
Authors : Deng, H.Q.; Zhang, S.T.; Jia, D.  
Deposited on : 2023-05-29  
Resolution : 2.51 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

<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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

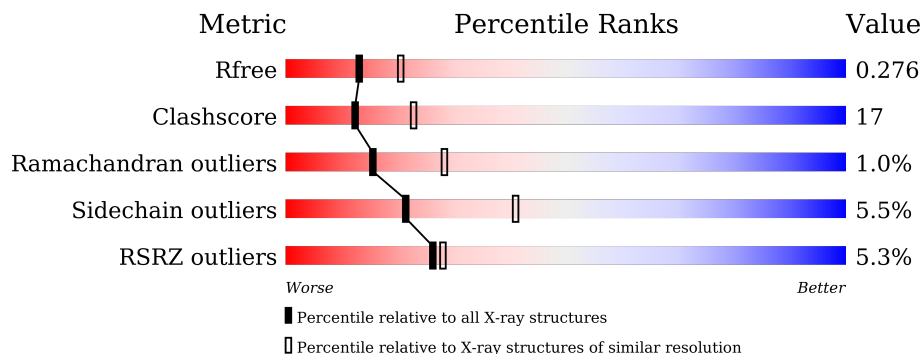
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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))
$R_{free}$	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  $\geq 3$ , 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	312	 5% (poor fit), 63% (0 outliers), 31% (1 outlier), 5% (2 outliers), 5% (3+ outliers)
1	B	312	 3% (poor fit), 58% (0 outliers), 32% (1 outlier), 5% (2 outliers), 5% (3+ outliers)
2	C	21	 29% (poor fit), 57% (0 outliers), 38% (1 outlier), 5% (2 outliers), 5% (3+ outliers)
2	D	21	 14% (poor fit), 52% (0 outliers), 43% (1 outlier), 5% (2 outliers), 5% (3+ outliers)

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5398 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 Protein FAM91A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	298	2443	1564	419	447	13	0	0	0
1	B	299	2460	1577	421	449	13	0	0	0

- Molecule 2 is a protein called TBC1 domain family member 23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	21	166	104	34	28	0	0	0
2	D	20	160	101	33	26	0	0	0

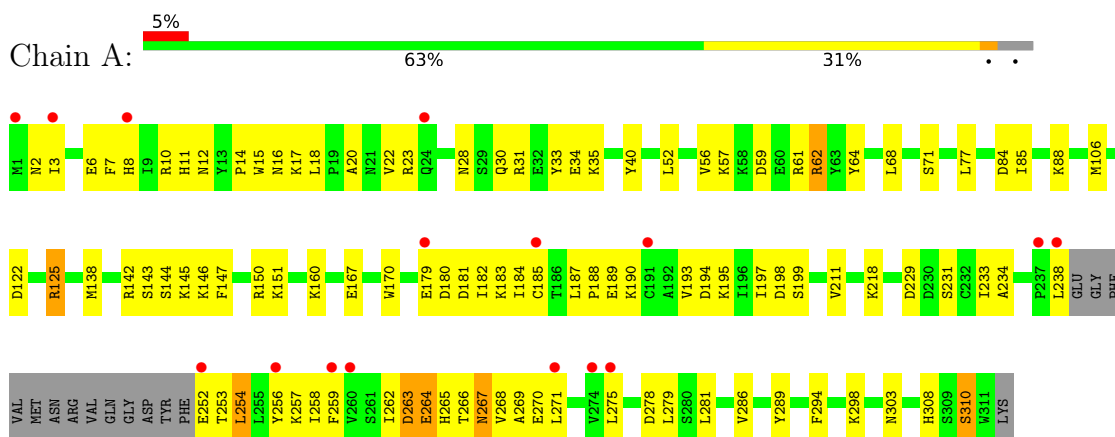
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total 81	O 81	0	0
3	B	84	Total 84	O 84	0	0
3	C	1	Total 1	O 1	0	0
3	D	3	Total 3	O 3	0	0

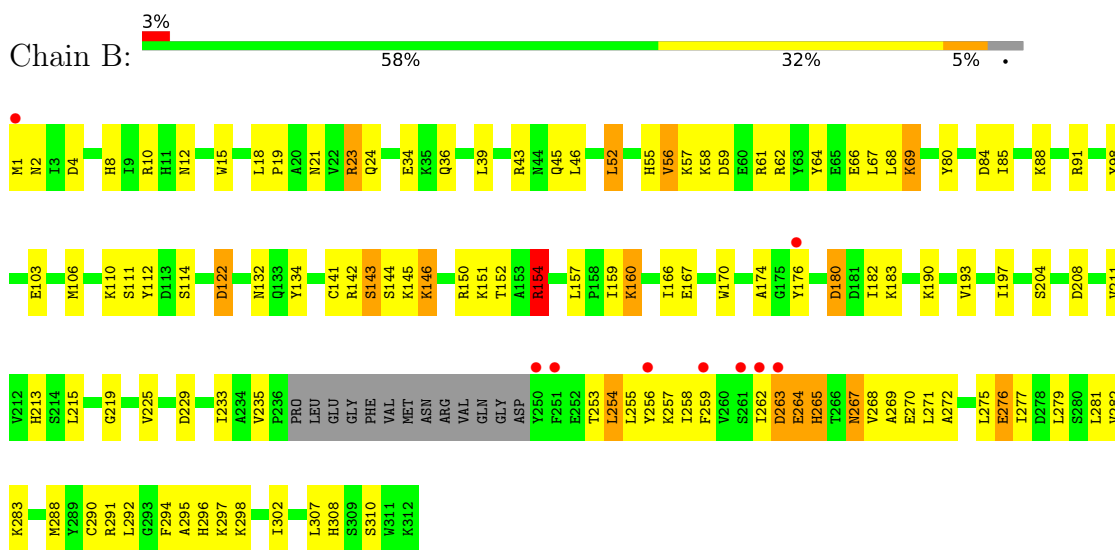
### 3 Residue-property plots [i](#)

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: Protein FAM91A1



- Molecule 1: Protein FAM91A1

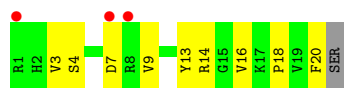


- Molecule 2: TBC1 domain family member 23



- Molecule 2: TBC1 domain family member 23

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.21Å 93.56Å 111.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.01 – 2.51 69.18 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.01-2.51) 99.9 (69.18-2.51)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.225 , 0.277 0.224 , 0.276	Depositor DCC
$R_{free}$ test set	1598 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5398	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9866e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	0/2497	0.68	1/3380 (0.0%)
1	B	0.56	0/2515	0.69	2/3402 (0.1%)
2	C	0.55	0/170	0.70	0/227
2	D	0.45	0/164	0.74	0/219
All	All	0.55	0/5346	0.69	3/7228 (0.0%)

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	2
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	154	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	B	52	LEU	CB-CG-CD2	-5.25	102.08	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	B	264	GLU	Peptide
1	B	276	GLU	Peptide

## 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	2443	0	2449	83	0
1	B	2460	0	2462	80	0
2	C	166	0	172	11	0
2	D	160	0	167	12	0
3	A	81	0	0	6	0
3	B	84	0	0	4	0
3	C	1	0	0	0	0
3	D	3	0	0	4	0
All	All	5398	0	5250	177	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 17.

The worst 5 of 177 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:B:69:LYS:NZ	3:B:401:HOH:O	1.92	1.03
1:A:190:LYS:NZ	2:C:13:TYR:OH	1.94	1.00
1:A:198:ASP:OD2	2:C:14:ARG:NH2	1.95	0.99
2:D:20:PHE:HB2	3:D:101:HOH:O	1.74	0.87
1:A:15:TRP:CG	1:A:30:GLN:HG3	2.16	0.80

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	294/312 (94%)	279 (95%)	11 (4%)	4 (1%)	11	20
1	B	295/312 (95%)	284 (96%)	9 (3%)	2 (1%)	22	39
2	C	19/21 (90%)	19 (100%)	0	0	100	100
2	D	18/21 (86%)	15 (83%)	3 (17%)	0	100	100
All	All	626/666 (94%)	597 (95%)	23 (4%)	6 (1%)	15	28

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	A	267	ASN
1	B	263	ASP
1	A	264	GLU
1	B	265	HIS

### 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	274/286 (96%)	264 (96%)	10 (4%)	35	61
1	B	275/286 (96%)	256 (93%)	19 (7%)	15	30
2	C	19/19 (100%)	16 (84%)	3 (16%)	2	4
2	D	18/19 (95%)	18 (100%)	0	100	100
All	All	586/610 (96%)	554 (94%)	32 (6%)	21	41

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	292	LEU
2	C	9	VAL
1	B	23	ARG
1	B	10	ARG
2	C	11	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	45	GLN
1	B	132	ASN

### 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<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	298/312 (95%)	0.41	16 (5%) 25 27	11, 34, 66, 84	0
1	B	299/312 (95%)	0.33	9 (3%) 50 53	9, 29, 58, 75	0
2	C	21/21 (100%)	1.52	6 (28%) 0 0	34, 57, 71, 77	0
2	D	20/21 (95%)	1.12	3 (15%) 2 2	33, 48, 68, 88	0
All	All	638/666 (95%)	0.43	34 (5%) 26 28	9, 32, 65, 88	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	PHE	6.5
1	B	250	TYR	5.7
2	C	9	VAL	5.6
1	A	238	LEU	5.4
2	D	8	ARG	4.7

### 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.