



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:48 PM UTC

PDB ID : 8R5W / pdb_00008r5w
Title : Crystal structure of the three anaphylatoxin-like modules in fibulin-2
Authors : Sohail, A.A.; Koski, M.K.; Ruddock, L.W.
Deposited on : 2023-11-18
Resolution : 2.20 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

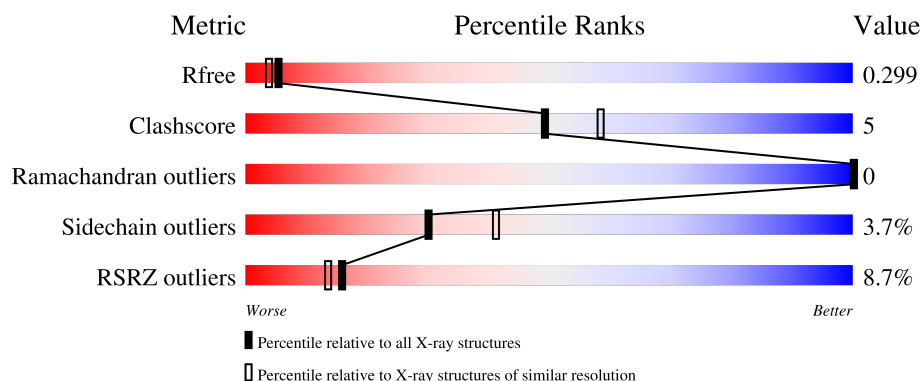
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	127	4% 79% 11% • 9%
1	B	127	9% 69% 16% • 14%
1	C	127	6% 76% 9% • 16%
1	D	127	9% 70% 13% • 17%
1	E	127	4% 77% 9% • 12%

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Mol	Chain	Length	Quality of chain
1	F	127	
1	G	127	
1	H	127	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6605 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 Fibulin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	2	0
			877	523	159	175	20			
1	B	109	Total	C	N	O	S	0	2	0
			814	486	144	165	19			
1	C	107	Total	C	N	O	S	0	0	0
			783	467	138	160	18			
1	D	106	Total	C	N	O	S	0	0	0
			789	470	143	157	19			
1	E	112	Total	C	N	O	S	0	0	0
			845	503	155	167	20			
1	F	110	Total	C	N	O	S	0	3	0
			827	494	149	165	19			
1	G	108	Total	C	N	O	S	0	0	0
			794	474	140	162	18			
1	H	104	Total	C	N	O	S	0	0	0
			768	457	135	157	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	initiating methionine	UNP P37889
A	420	HIS	-	expression tag	UNP P37889
A	421	HIS	-	expression tag	UNP P37889
A	422	HIS	-	expression tag	UNP P37889
A	423	HIS	-	expression tag	UNP P37889
A	424	HIS	-	expression tag	UNP P37889
A	425	HIS	-	expression tag	UNP P37889
A	426	MET	-	expression tag	UNP P37889
B	419	MET	-	initiating methionine	UNP P37889
B	420	HIS	-	expression tag	UNP P37889
B	421	HIS	-	expression tag	UNP P37889
B	422	HIS	-	expression tag	UNP P37889
B	423	HIS	-	expression tag	UNP P37889

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Chain	Residue	Modelled	Actual	Comment	Reference
B	424	HIS	-	expression tag	UNP P37889
B	425	HIS	-	expression tag	UNP P37889
B	426	MET	-	expression tag	UNP P37889
C	419	MET	-	initiating methionine	UNP P37889
C	420	HIS	-	expression tag	UNP P37889
C	421	HIS	-	expression tag	UNP P37889
C	422	HIS	-	expression tag	UNP P37889
C	423	HIS	-	expression tag	UNP P37889
C	424	HIS	-	expression tag	UNP P37889
C	425	HIS	-	expression tag	UNP P37889
C	426	MET	-	expression tag	UNP P37889
D	419	MET	-	initiating methionine	UNP P37889
D	420	HIS	-	expression tag	UNP P37889
D	421	HIS	-	expression tag	UNP P37889
D	422	HIS	-	expression tag	UNP P37889
D	423	HIS	-	expression tag	UNP P37889
D	424	HIS	-	expression tag	UNP P37889
D	425	HIS	-	expression tag	UNP P37889
D	426	MET	-	expression tag	UNP P37889
E	419	MET	-	initiating methionine	UNP P37889
E	420	HIS	-	expression tag	UNP P37889
E	421	HIS	-	expression tag	UNP P37889
E	422	HIS	-	expression tag	UNP P37889
E	423	HIS	-	expression tag	UNP P37889
E	424	HIS	-	expression tag	UNP P37889
E	425	HIS	-	expression tag	UNP P37889
E	426	MET	-	expression tag	UNP P37889
F	419	MET	-	initiating methionine	UNP P37889
F	420	HIS	-	expression tag	UNP P37889
F	421	HIS	-	expression tag	UNP P37889
F	422	HIS	-	expression tag	UNP P37889
F	423	HIS	-	expression tag	UNP P37889
F	424	HIS	-	expression tag	UNP P37889
F	425	HIS	-	expression tag	UNP P37889
F	426	MET	-	expression tag	UNP P37889
G	419	MET	-	initiating methionine	UNP P37889
G	420	HIS	-	expression tag	UNP P37889
G	421	HIS	-	expression tag	UNP P37889
G	422	HIS	-	expression tag	UNP P37889
G	423	HIS	-	expression tag	UNP P37889
G	424	HIS	-	expression tag	UNP P37889
G	425	HIS	-	expression tag	UNP P37889

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Chain	Residue	Modelled	Actual	Comment	Reference
G	426	MET	-	expression tag	UNP P37889
H	419	MET	-	initiating methionine	UNP P37889
H	420	HIS	-	expression tag	UNP P37889
H	421	HIS	-	expression tag	UNP P37889
H	422	HIS	-	expression tag	UNP P37889
H	423	HIS	-	expression tag	UNP P37889
H	424	HIS	-	expression tag	UNP P37889
H	425	HIS	-	expression tag	UNP P37889
H	426	MET	-	expression tag	UNP P37889

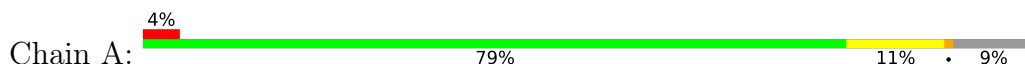
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	17	Total O 17 17	0	0
2	C	18	Total O 18 18	0	0
2	D	9	Total O 9 9	0	0
2	E	8	Total O 8 8	0	0
2	F	17	Total O 17 17	0	0
2	G	14	Total O 14 14	0	0
2	H	10	Total O 10 10	0	0

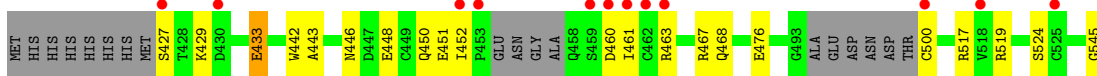
3 Residue-property plots [i](#)

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.

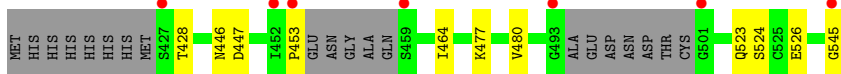
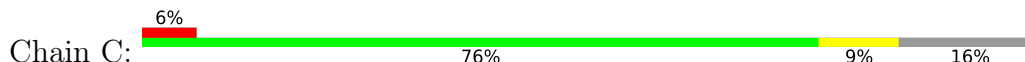
- Molecule 1: Fibulin-2



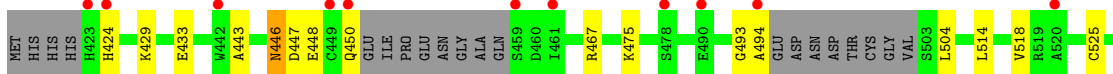
- Molecule 1: Fibulin-2



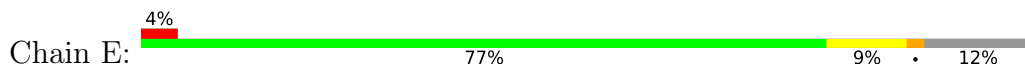
- Molecule 1: Fibulin-2



- Molecule 1: Fibulin-2



- Molecule 1: Fibulin-2



● Molecule 1: Fibulin-2

Chain F: 



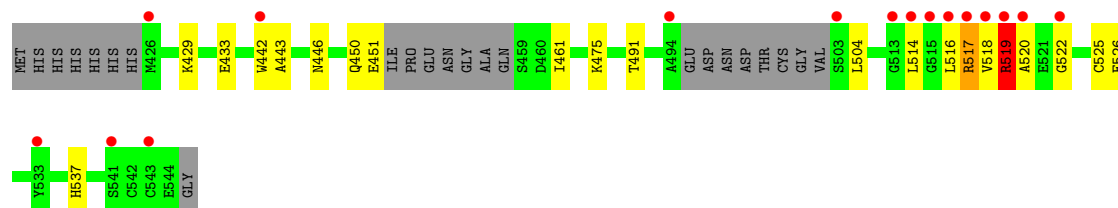
● Molecule 1: Fibulin-2

Chain G: 



● Molecule 1: Fibulin-2

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.68Å 34.51Å 106.89Å 90.00° 94.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.20 48.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.80-2.20) 99.8 (48.80-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.243 , 0.297 0.246 , 0.299	Depositor DCC
R_{free} test set	2716 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6605	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.83 % 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 6.6541e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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	0.65	0/894	1.11	0/1197
1	B	0.65	0/826	1.05	0/1106
1	C	0.64	0/788	1.12	2/1055 (0.2%)
1	D	0.60	0/797	1.12	2/1067 (0.2%)
1	E	0.61	0/856	1.09	0/1146
1	F	0.65	0/842	1.06	0/1127
1	G	0.67	0/800	1.09	0/1072
1	H	0.64	0/773	1.13	1/1034 (0.1%)
All	All	0.64	0/6576	1.10	5/8804 (0.1%)

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	H	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	537	HIS	CB-CG-CD2	-6.36	122.93	131.20
1	C	453	PRO	N-CA-CB	6.23	109.86	103.00
1	D	537	HIS	CB-CG-ND1	5.84	131.45	122.70
1	C	446	ASN	N-CA-C	5.31	120.62	113.72
1	H	537	HIS	CA-CB-CG	-5.29	108.52	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	519	ARG	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	877	0	802	9	0
1	B	814	0	764	14	1
1	C	783	0	726	7	0
1	D	789	0	728	7	0
1	E	845	0	770	11	0
1	F	827	0	784	11	0
1	G	794	0	740	12	0
1	H	768	0	713	17	1
2	A	15	0	0	1	0
2	B	17	0	0	2	0
2	C	18	0	0	1	0
2	D	9	0	0	0	0
2	E	8	0	0	0	0
2	F	17	0	0	1	0
2	G	14	0	0	1	0
2	H	10	0	0	0	0
All	All	6605	0	6027	67	1

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 5.

The worst 5 of 67 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:476:GLU:OE2	2:B:601:HOH:O	2.01	0.77
1:G:433:GLU:OE1	2:G:601:HOH:O	2.09	0.70
1:G:428:THR:HG21	1:H:518:VAL:HG22	1.76	0.67
1:A:523:GLN:HE22	1:B:427:SER:HB2	1.60	0.65
1:A:517:ARG:HG3	1:B:461:ILE:HD11	1.79	0.65

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ASP:OD2	1:H:522:GLY:O[1_454]	2.16	0.04

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	111/127 (87%)	109 (98%)	2 (2%)	0	100	100
1	B	105/127 (83%)	103 (98%)	2 (2%)	0	100	100
1	C	101/127 (80%)	99 (98%)	2 (2%)	0	100	100
1	D	100/127 (79%)	97 (97%)	3 (3%)	0	100	100
1	E	106/127 (84%)	105 (99%)	1 (1%)	0	100	100
1	F	107/127 (84%)	105 (98%)	2 (2%)	0	100	100
1	G	102/127 (80%)	102 (100%)	0	0	100	100
1	H	98/127 (77%)	96 (98%)	2 (2%)	0	100	100
All	All	830/1016 (82%)	816 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	99/106 (93%)	94 (95%)	5 (5%)	21	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	93/106 (88%)	89 (96%)	4 (4%)	26	35
1	C	88/106 (83%)	87 (99%)	1 (1%)	65	79
1	D	89/106 (84%)	82 (92%)	7 (8%)	11	13
1	E	95/106 (90%)	92 (97%)	3 (3%)	34	47
1	F	94/106 (89%)	94 (100%)	0	100	100
1	G	90/106 (85%)	87 (97%)	3 (3%)	33	45
1	H	87/106 (82%)	82 (94%)	5 (6%)	18	23
All	All	735/848 (87%)	707 (96%)	28 (4%)	30	40

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	450	GLN
1	H	526	GLU
1	E	451	GLU
1	H	517	ARG
1	D	525	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	440	GLN
1	F	507	GLN
1	F	468	GLN
1	G	440	GLN
1	B	530	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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	115/127 (90%)	0.75	5 (4%) 40 36	26, 52, 92, 112	2 (1%)
1	B	109/127 (85%)	0.71	12 (11%) 10 8	28, 48, 91, 123	2 (1%)
1	C	107/127 (84%)	0.63	7 (6%) 25 22	31, 49, 87, 102	0
1	D	106/127 (83%)	0.87	11 (10%) 11 9	38, 58, 95, 112	0
1	E	112/127 (88%)	0.85	5 (4%) 38 35	39, 56, 98, 119	0
1	F	110/127 (86%)	0.71	11 (10%) 12 10	26, 48, 86, 99	3 (2%)
1	G	108/127 (85%)	0.61	9 (8%) 17 15	33, 46, 83, 104	0
1	H	104/127 (81%)	1.02	16 (15%) 5 4	38, 57, 101, 118	0
All	All	871/1016 (85%)	0.77	76 (8%) 16 13	26, 52, 95, 123	7 (0%)

The worst 5 of 76 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	452	ILE	4.7
1	A	502	VAL	4.7
1	D	494	ALA	4.1
1	H	520	ALA	3.8
1	F	461	ILE	3.8

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.