

Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 02:22 PM EST

PDB ID : 2NQC

Title : Crystal structure of ig-like domain 23 from human filamin C

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Deposited on : 2006-10-31

Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

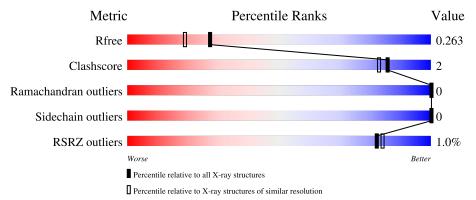
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	
1	Δ	138	67%	30%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 768 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 Filamin-C.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	97	Total 689	C 434	N 116	O 136	S 3	13	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2441	GLY	-	expression tag	UNP Q14315
A	2442	SER	-	expression tag	UNP Q14315
A	2443	HIS	-	expression tag	UNP Q14315
A	2444	MET	-	expression tag	UNP Q14315
A	2445	ALA	-	expression tag	UNP Q14315
A	2446	SER	-	expression tag	UNP Q14315
A	2447	MET	-	expression tag	UNP Q14315
A	2448	THR	-	expression tag	UNP Q14315
A	2449	GLY	-	expression tag	UNP Q14315
A	2450	GLY	-	expression tag	UNP Q14315
A	2451	GLN	-	expression tag	UNP Q14315
A	2452	GLN	-	expression tag	UNP Q14315
A	2453	MET	-	expression tag	UNP Q14315
A	2454	GLY	-	expression tag	UNP Q14315
A	2455	ARG	-	expression tag	UNP Q14315
A	2456	GLY	-	expression tag	UNP Q14315
A	2457	SER	-	expression tag	UNP Q14315
A	2458	GLY	_	expression tag	UNP Q14315
A	2459	SER	-	expression tag	UNP Q14315
A	2460	HIS	-	expression tag	UNP Q14315
A	2461	MET	_	expression tag	UNP Q14315
A	2462	ALA	-	expression tag	UNP Q14315
A	2463	SER	-	expression tag	UNP Q14315
A	2464	MET	-	expression tag	UNP Q14315
A	2465	THR	-	expression tag	UNP Q14315
A	2466	GLY	-	expression tag	UNP Q14315
A	2467	GLY	-	expression tag	UNP Q14315

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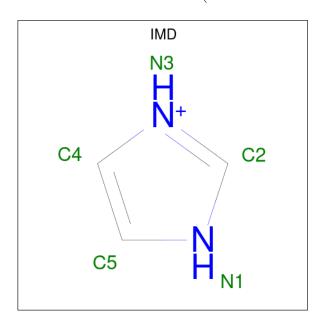
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Chain	Residue	Modelled	Actual	Comment	Reference
A	2468	GLN	-	expression tag	UNP Q14315
A	2469	GLN	-	expression tag	UNP Q14315
A	2470	MET	-	expression tag	UNP Q14315
A	2471	GLY	-	expression tag	UNP Q14315
A	2472	ARG	-	expression tag	UNP Q14315
A	2473	GLY	-	expression tag	UNP Q14315
A	2474	SER	-	expression tag	UNP Q14315

• Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ni 1 1	0	0

 \bullet Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $\mathrm{C_3H_5N_2}).$



\mathbf{M}	ol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	}	A	1	Total C N 5 3 2	0	0
3	}	A	1	Total C N 5 3 2	0	0

 \bullet Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$





Mo	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

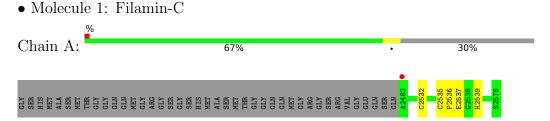
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	52.14Å 52.14Å 69.22Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.17 - 2.05	Depositor
resolution (A)	27.47 - 2.05	EDS
% Data completeness	97.5 (45.17 - 2.05)	Depositor
(in resolution range)	97.5 (27.47-2.05)	EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	2.81 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.237	Depositor
it, it _{free}	0.195 , 0.263	DCC
R_{free} test set	329 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 54.0	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	768	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.55% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, GOL, IMD

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).

Mal	Chain	Bon	d lengths	Bond	angles
Mol Chain		RMSZ	# Z > 5	RMSZ	$\mid \# Z > 5 \mid$
1	A	0.65	1/705~(0.1%)	0.65	0/960

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	A	2537	GLU	CB-CG	8.52	1.68	1.52

There are no bond angle outliers.

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	689	0	681	2	0
2	A	1	0	0	0	0
3	A	10	0	8	1	0
4	A	12	0	16	0	0
5	A	56	0	0	0	0
All	All	768	0	705	3	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 2.



All (3) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:2535:CYS:HB3	1:A:2536:PRO:HD2	1.90	0.53
1:A:2532:CYS:SG	1:A:2539:HIS:HB3	2.52	0.50
3:A:201:IMD:H2	3:A:301:IMD:H4	2.02	0.42

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	95/138 (69%)	93 (98%)	2 (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	ysed Rotameric		Percentiles	
1	A	74/102 (72%)	74 (100%)	0	100 100	

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



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)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Iol Type Chain Res	Chain	Dec	Link	Tiple Bo		ond lengths		Bond angles		
MIOI		nes	Les Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
3	IMD	A	201	2	3,5,5	0.52	0	4,5,5	0.80	0	
4	GOL	A	401	-	5,5,5	0.30	0	5,5,5	0.31	0	
3	IMD	A	301	2	3,5,5	0.34	0	4,5,5	0.94	0	
4	GOL	A	501	-	5,5,5	0.45	0	5,5,5	0.19	0	

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	A	201	2	-	_	0/1/1/1
4	GOL	A	501	-	-	4/4/4/4	-
4	GOL	A	401	-	-	4/4/4/4	-
3	IMD	A	301	2	-	-	0/1/1/1

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	401	GOL	C1-C2-C3-O3
4	A	501	GOL	O1-C1-C2-C3
4	A	501	GOL	C1-C2-C3-O3
4	A	501	GOL	O2-C2-C3-O3
4	A	401	GOL	O1-C1-C2-O2
4	A	401	GOL	O1-C1-C2-C3
4	A	401	GOL	O2-C2-C3-O3
4	A	501	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	IMD	1	0
3	A	301	IMD	1	0

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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q<0.9
1	A	97/138 (70%)	-0.02	1 (1%) 82 84	32, 40, 50, 59	3 (3%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	A	2482	ALA	6.9	

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	GOL	A	401	6/6	0.75	0.20	67,69,69,70	0
4	GOL	A	501	6/6	0.93	0.29	67,69,70,71	0
3	IMD	A	301	5/5	0.99	0.11	39,39,40,40	0
2	NI	A	101	1/1	0.99	0.09	36,36,36,36	0
3	IMD	A	201	5/5	0.99	0.10	34,37,38,40	0



6.5 Other polymers (i)

There are no such residues in this entry.

