



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:32 AM UTC

PDB ID : 6DED / pdb_00006ded
Title : Crystal structure of the C-terminal ARM domain of Homo sapiens SPIN90 (SH3-protein interacting with Nck), residues 351-722
Authors : Nolen, B.J.; Luan, Q.
Deposited on : 2018-05-11
Resolution : 2.20 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 ⓘ 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

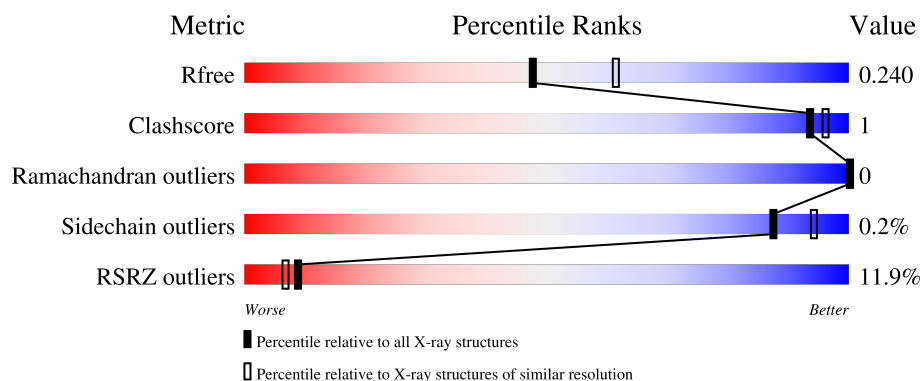
1 Overall quality at a glance

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	373	13% 86% 10%
1	B	373	9% 89% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5686 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 NCK-interacting protein with SH3 domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2655	1699	457	475	24			
1	B	344	Total	C	N	O	S	0	0	0
			2708	1729	467	488	24			

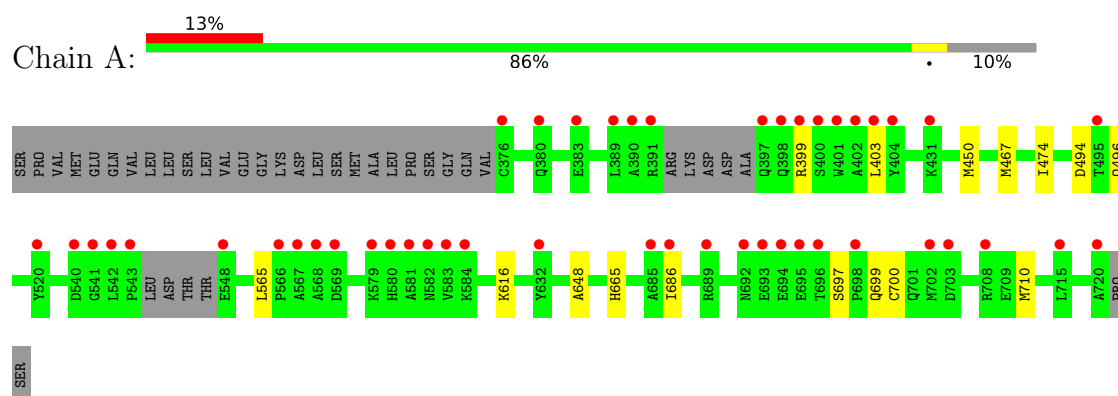
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		
2	B	173	Total	O	0	0
			173	173		

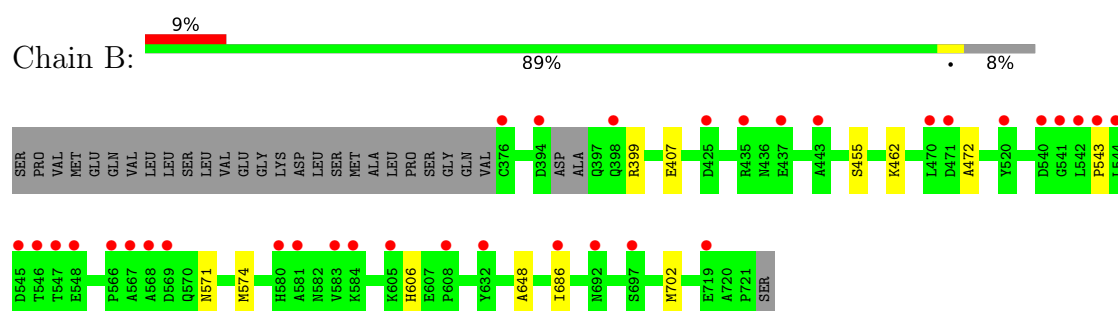
3 Residue-property plots

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: NCK-interacting protein with SH3 domain



- Molecule 1: NCK-interacting protein with SH3 domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.36Å 76.17Å 92.26Å 90.00° 93.12° 90.00°	Depositor
Resolution (Å)	35.70 – 2.20 35.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (35.70-2.20) 98.9 (35.70-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.239 0.218 , 0.240	Depositor DCC
R_{free} test set	2559 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5686	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% 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 [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	0.29	0/2707	0.67	0/3669
1	B	0.29	0/2761	0.68	1/3744 (0.0%)
All	All	0.29	0/5468	0.68	1/7413 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	543	PRO	N-CA-CB	6.48	110.39	103.52

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	2655	0	2678	9	0
1	B	2708	0	2709	7	0
2	A	150	0	0	0	0
2	B	173	0	0	1	0
All	All	5686	0	5387	15	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 1.

All (15) 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:A:648:ALA:HB2	1:A:686:ILE:HD13	1.71	0.72
1:B:648:ALA:HB2	1:B:686:ILE:HD13	1.71	0.70
1:A:699:GLN:HG3	1:B:702:MET:HE1	1.80	0.63
1:A:494:ASP:OD1	1:A:496:GLN:NE2	2.35	0.59
1:B:462:LYS:NZ	2:B:804:HOH:O	2.36	0.58
1:A:403:LEU:HD11	1:A:450:MET:HB3	1.91	0.53
1:A:565:LEU:O	1:A:616:LYS:NZ	2.41	0.51
1:B:407:GLU:OE2	1:B:455:SER:OG	2.26	0.49
1:A:665:HIS:CG	1:A:710:MET:HG2	2.48	0.47
1:A:697:SER:OG	1:A:700:CYS:SG	2.73	0.46
1:A:467:MET:HB3	1:A:474:ILE:HG21	1.99	0.45
1:B:571:ASN:HB3	1:B:574:MET:HB2	1.99	0.45
1:B:648:ALA:HB2	1:B:686:ILE:CD1	2.43	0.44
1:A:399:ARG:HD2	1:A:399:ARG:HA	1.88	0.42
1:B:472:ALA:HB2	1:B:606:HIS:HB3	2.03	0.40

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	330/373 (88%)	327 (99%)	3 (1%)	0	100	100
1	B	340/373 (91%)	337 (99%)	3 (1%)	0	100	100
All	All	670/746 (90%)	664 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	290/330 (88%)	290 (100%)	0	100	100
1	B	293/330 (89%)	292 (100%)	1 (0%)	86	93
All	All	583/660 (88%)	582 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	399	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	GLN
1	A	492	GLN
1	A	525	HIS
1	B	419	HIS
1	B	449	GLN
1	B	492	GLN
1	B	525	HIS
1	B	549	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	336/373 (90%)	0.73	47 (13%) 6 4	27, 42, 83, 121	0
1	B	344/373 (92%)	0.61	34 (9%) 13 10	26, 41, 78, 123	0
All	All	680/746 (91%)	0.67	81 (11%) 9 7	26, 41, 80, 123	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	ASP	7.3
1	B	545	ASP	7.1
1	B	567	ALA	7.1
1	B	394	ASP	6.2
1	A	567	ALA	5.3
1	B	569	ASP	5.1
1	A	541	GLY	5.0
1	B	547	THR	5.0
1	B	544	LEU	4.8
1	A	720	ALA	4.7
1	B	608	PRO	4.4
1	B	546	THR	4.3
1	A	376	CYS	4.2
1	B	568	ALA	4.2
1	B	541	GLY	4.1
1	A	397	GLN	4.0
1	B	566	PRO	4.0
1	B	580	HIS	4.0
1	A	398	GLN	4.0
1	A	548	GLU	4.0
1	A	401	TRP	3.8
1	A	580	HIS	3.7
1	A	686	ILE	3.6
1	A	520	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	425	ASP	3.5
1	B	583	VAL	3.4
1	A	400	SER	3.4
1	A	404	TYR	3.4
1	B	543	PRO	3.4
1	B	632	TYR	3.3
1	A	568	ALA	3.3
1	A	403	LEU	3.3
1	B	376	CYS	3.2
1	A	399	ARG	3.0
1	B	435	ARG	3.0
1	A	689	ARG	2.9
1	A	566	PRO	2.9
1	A	582	ASN	2.9
1	A	380	GLN	2.9
1	A	632	TYR	2.9
1	A	389	LEU	2.9
1	A	543	PRO	2.8
1	A	391	ARG	2.8
1	B	548	GLU	2.7
1	A	579	LYS	2.7
1	B	398	GLN	2.7
1	B	605	LYS	2.7
1	A	402	ALA	2.7
1	A	540	ASP	2.6
1	B	542	LEU	2.6
1	B	692	ASN	2.6
1	A	692	ASN	2.5
1	B	540	ASP	2.5
1	A	581	ALA	2.5
1	A	698	PRO	2.5
1	A	583	VAL	2.5
1	A	685	ALA	2.5
1	B	686	ILE	2.4
1	A	584	LYS	2.4
1	B	437	GLU	2.4
1	B	719	GLU	2.4
1	A	693	GLU	2.4
1	B	520	TYR	2.3
1	A	708	ARG	2.3
1	A	390	ALA	2.3
1	B	470	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	703	ASP	2.2
1	A	431	LYS	2.2
1	A	696	THR	2.2
1	A	702	MET	2.2
1	A	695	GLU	2.2
1	A	542	LEU	2.2
1	A	383	GLU	2.2
1	B	471	ASP	2.1
1	B	443	ALA	2.1
1	A	715	LEU	2.1
1	A	495	THR	2.1
1	B	697	SER	2.1
1	B	581	ALA	2.1
1	B	584	LYS	2.1
1	A	694	GLU	2.1

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.