



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 07:40 pm GMT

PDB ID : 1SHF
Title : CRYSTAL STRUCTURE OF THE SH3 DOMAIN IN HUMAN FYN; COMPARISON OF THE THREE-DIMENSIONAL STRUCTURES OF SH3 DOMAINS IN TYROSINE KINASES AND SPECTRIN
Authors : Noble, M.; Musacchio, A.; Saraste, M.; Wierenga, R.
Deposited on : 1993-05-19
Resolution : 1.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

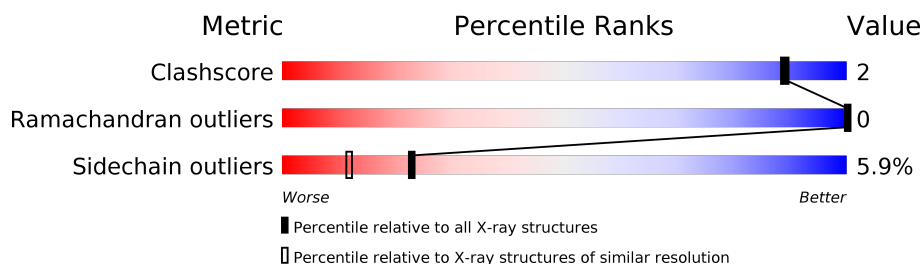
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	59	 69% 22% 7% •
1	B	59	 75% 19% 5% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 956 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 FYN TYROSINE KINASE SH3 DOMAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	59	Total	C	N	O	0	0	0
			478	305	74	99			
1	B	59	Total	C	N	O	0	0	0
			478	305	74	99			

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 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.

Note EDS was not executed.

• Molecule 1: FYN TYROSINE KINASE SH3 DOMAIN

Chain A: 



• Molecule 1: FYN TYROSINE KINASE SH3 DOMAIN

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.70Å 48.60Å 43.00Å 90.00° 98.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	956	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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	1.36	8/491 (1.6%)	1.90	15/668 (2.2%)
1	B	1.28	5/491 (1.0%)	1.92	13/668 (1.9%)
All	All	1.32	13/982 (1.3%)	1.91	28/1336 (2.1%)

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	A	0	1
1	B	0	2
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLU	CD-OE1	9.29	1.35	1.25
1	B	116	GLU	CD-OE2	7.89	1.34	1.25
1	B	94	GLU	CD-OE2	7.58	1.33	1.25
1	B	107	GLU	CD-OE1	6.76	1.33	1.25
1	A	116	GLU	CD-OE2	6.60	1.32	1.25
1	A	129	GLU	CD-OE2	6.45	1.32	1.25
1	B	98	GLU	CD-OE2	6.39	1.32	1.25
1	A	94	GLU	CD-OE1	5.99	1.32	1.25
1	A	123	ARG	CD-NE	-5.98	1.36	1.46
1	A	98	GLU	CD-OE1	5.93	1.32	1.25
1	A	134	PRO	N-CD	5.61	1.55	1.47
1	A	121	GLU	CD-OE2	5.59	1.31	1.25
1	B	129	GLU	CD-OE2	5.42	1.31	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ARG	NE-CZ-NH2	-19.73	110.43	120.30
1	B	123	ARG	NE-CZ-NH1	15.79	128.19	120.30
1	A	123	ARG	NE-CZ-NH1	-15.04	112.78	120.30
1	A	96	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	B	132	TYR	CB-CG-CD1	-12.56	113.46	121.00
1	A	123	ARG	CD-NE-CZ	10.81	138.74	123.60
1	B	132	TYR	CB-CG-CD2	9.10	126.46	121.00
1	A	118	ASP	CB-CG-OD2	-8.95	110.25	118.30
1	B	118	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	96	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	142	ASP	CB-CG-OD1	-7.27	111.76	118.30
1	A	127	THR	C-N-CA	-6.41	108.85	122.30
1	A	92	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	A	100	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	100	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	142	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	92	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	A	99	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	123	ARG	CD-NE-CZ	5.60	131.44	123.60
1	B	92	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	132	TYR	CB-CG-CD1	-5.38	117.78	121.00
1	B	99	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	A	99	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	91	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	96	ARG	CD-NE-CZ	5.12	130.77	123.60
1	B	118	ASP	N-CA-CB	-5.11	101.39	110.60
1	B	91	TYR	CB-CG-CD1	5.11	124.07	121.00
1	A	118	ASP	CB-CG-OD1	5.11	122.90	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain
1	B	118	ASP	Mainchain
1	B	123	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	478	0	436	3	0
1	B	478	0	436	1	0
All	All	956	0	872	4	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 (4) 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:95:ALA:HB1	1:B:100:ASP:HB2	1.96	0.47
1:A:120:TRP:O	1:A:132:TYR:HA	2.20	0.42
1:A:141:VAL:O	1:A:142:ASP:HB2	2.19	0.42
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.86	0.41

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	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
1	B	57/59 (97%)	57 (100%)	0	0	100	100
All	All	114/118 (97%)	113 (99%)	1 (1%)	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	51/51 (100%)	49 (96%)	2 (4%)	37	26
1	B	51/51 (100%)	47 (92%)	4 (8%)	15	6
All	All	102/102 (100%)	96 (94%)	6 (6%)	23	12

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	121	GLU
1	B	86	LEU
1	B	96	ARG
1	B	123	ARG
1	B	129	GLU

Some 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 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.