



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 07:48 PM EDT

PDB ID : 2F44
Title : Crystal Structure of the Zinc-bound Shank SAM domain
Authors : Baron, M.K.; Bowie, J.U.; Faham, S.
Deposited on : 2005-11-22
Resolution : 2.40 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 : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

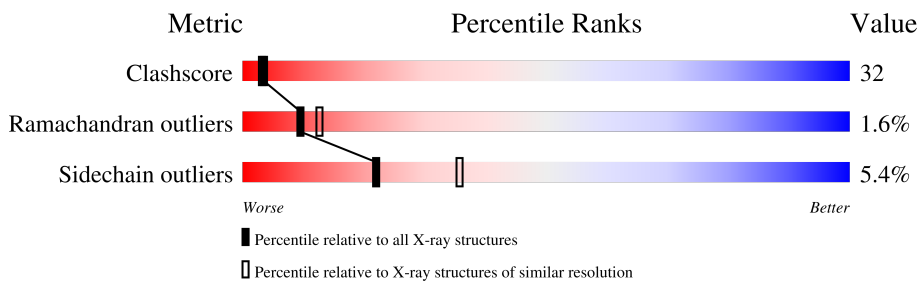
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	76	 53% 30% 14%
1	B	76	 43% 34% 7% 16%
1	C	76	 50% 30% 18%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 1658 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 SH3 and multiple ankyrin repeat domains 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	65	542	341	100	100	1	0	0	0
1	B	64	534	336	99	99		0	0	0
1	C	62	517	325	96	96		0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9JLU4
A	56	GLU	MET	engineered mutation	UNP Q9JLU4
A	69	ARG	-	cloning artifact	UNP Q9JLU4
A	70	ARG	-	cloning artifact	UNP Q9JLU4
A	71	HIS	-	expression tag	UNP Q9JLU4
A	72	HIS	-	expression tag	UNP Q9JLU4
A	73	HIS	-	expression tag	UNP Q9JLU4
A	74	HIS	-	expression tag	UNP Q9JLU4
A	75	HIS	-	expression tag	UNP Q9JLU4
A	76	HIS	-	expression tag	UNP Q9JLU4
B	1	MET	-	initiating methionine	UNP Q9JLU4
B	56	GLU	MET	engineered mutation	UNP Q9JLU4
B	69	ARG	-	cloning artifact	UNP Q9JLU4
B	70	ARG	-	cloning artifact	UNP Q9JLU4
B	71	HIS	-	expression tag	UNP Q9JLU4
B	72	HIS	-	expression tag	UNP Q9JLU4
B	73	HIS	-	expression tag	UNP Q9JLU4
B	74	HIS	-	expression tag	UNP Q9JLU4
B	75	HIS	-	expression tag	UNP Q9JLU4
B	76	HIS	-	expression tag	UNP Q9JLU4
C	1	MET	-	initiating methionine	UNP Q9JLU4
C	56	GLU	MET	engineered mutation	UNP Q9JLU4
C	69	ARG	-	cloning artifact	UNP Q9JLU4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	70	ARG	-	cloning artifact	UNP Q9JLU4
C	71	HIS	-	expression tag	UNP Q9JLU4
C	72	HIS	-	expression tag	UNP Q9JLU4
C	73	HIS	-	expression tag	UNP Q9JLU4
C	74	HIS	-	expression tag	UNP Q9JLU4
C	75	HIS	-	expression tag	UNP Q9JLU4
C	76	HIS	-	expression tag	UNP Q9JLU4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	28	Total O 28 28	0	0
4	B	15	Total O 15 15	0	0
4	C	16	Total O 16 16	0	0

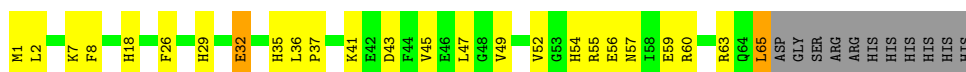
3 Residue-property plots [i](#)

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. 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. 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: SH3 and multiple ankyrin repeat domains 3

Chain A: 



- Molecule 1: SH3 and multiple ankyrin repeat domains 3

Chain B: 



- Molecule 1: SH3 and multiple ankyrin repeat domains 3

Chain C: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	104.82Å 104.82Å 40.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1658	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

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: ZN, CL

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	0.38	0/554	0.66	1/746 (0.1%)
1	B	0.41	0/546	0.63	0/736
1	C	0.34	0/529	0.54	0/713
All	All	0.38	0/1629	0.61	1/2195 (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	A	65	LEU	CA-CB-CG	5.57	128.10	115.30

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	542	0	522	27	0
1	B	534	0	510	46	0
1	C	517	0	491	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	1	0
4	A	28	0	0	14	0
4	B	15	0	0	16	0
4	C	16	0	0	14	0
All	All	1658	0	1523	100	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 32.

All (100) 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:2:LEU:HD21	1:B:4:LEU:HB2	1.38	1.02
1:B:2:LEU:HD22	1:B:5:TRP:CD1	1.95	1.01
1:A:59:GLU:HG3	1:A:63:ARG:HH22	1.22	0.98
1:B:12:ASP:HA	4:B:269:HOH:O	1.62	0.97
1:C:54:HIS:HA	4:C:262:HOH:O	1.65	0.97
1:C:12:ASP:HA	4:C:260:HOH:O	1.64	0.96
1:A:47:LEU:HD22	4:A:271:HOH:O	1.70	0.91
1:A:26:PHE:HA	4:A:271:HOH:O	1.69	0.90
1:A:59:GLU:HG3	1:A:63:ARG:NH2	1.90	0.87
1:B:15:GLU:HB2	4:B:269:HOH:O	1.73	0.85
1:A:54:HIS:HD2	4:A:277:HOH:O	1.62	0.83
1:A:57:ASN:ND2	4:A:277:HOH:O	2.16	0.78
1:B:2:LEU:HD23	1:B:4:LEU:H	1.48	0.78
1:C:25:ARG:HB2	4:C:273:HOH:O	1.85	0.77
1:B:2:LEU:CD2	1:B:4:LEU:H	2.00	0.74
1:C:57:ASN:ND2	4:C:262:HOH:O	2.22	0.72
1:A:29:HIS:HB2	4:A:271:HOH:O	1.89	0.72
1:A:59:GLU:HB2	4:A:261:HOH:O	1.88	0.71
1:B:2:LEU:HD23	1:B:4:LEU:N	2.04	0.71
1:B:2:LEU:HD23	1:B:2:LEU:C	2.11	0.70
1:B:36:LEU:HB3	1:B:62:LEU:HD21	1.74	0.69
1:B:2:LEU:HD21	1:B:4:LEU:CB	2.19	0.67
1:C:15:GLU:HB2	4:C:260:HOH:O	1.95	0.67
1:C:63:ARG:NH1	4:C:265:HOH:O	2.27	0.67
1:B:2:LEU:CD2	1:B:4:LEU:HB2	2.22	0.67
1:B:13:TRP:O	1:B:16:SER:HB3	1.96	0.65
1:A:52:VAL:O	1:A:56:GLU:HG2	1.97	0.65
1:B:2:LEU:CD2	1:B:5:TRP:CD1	2.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LEU:HB2	1:A:37:PRO:HD3	1.80	0.64
1:C:51:ARG:HG3	3:C:258:CL:CL	2.34	0.64
1:A:55:ARG:NH1	4:A:272:HOH:O	2.32	0.63
1:B:7:LYS:NZ	4:B:266:HOH:O	2.31	0.62
1:A:59:GLU:CG	1:A:63:ARG:HH22	2.06	0.62
1:B:23:ARG:HB3	4:B:270:HOH:O	2.01	0.60
1:A:54:HIS:HA	4:A:277:HOH:O	2.01	0.60
1:A:32:GLU:HG2	1:A:35:HIS:CE1	2.39	0.58
1:A:2:LEU:HD11	1:A:36:LEU:HD12	1.86	0.58
1:B:51:ARG:HH21	1:B:51:ARG:HG3	1.68	0.58
1:B:40:THR:OG1	1:B:42:GLU:HG2	2.04	0.57
1:A:45:VAL:CG2	4:A:272:HOH:O	2.53	0.57
1:A:45:VAL:HG22	4:A:272:HOH:O	2.04	0.57
1:B:11:GLY:O	4:B:270:HOH:O	2.18	0.56
1:B:23:ARG:HD2	4:B:270:HOH:O	2.05	0.56
1:B:36:LEU:HB2	1:B:37:PRO:HD3	1.86	0.56
1:C:54:HIS:CD2	4:C:262:HOH:O	2.58	0.56
1:B:23:ARG:CD	4:B:270:HOH:O	2.53	0.56
1:C:36:LEU:HB2	1:C:37:PRO:HD3	1.88	0.56
1:B:25:ARG:HB3	4:B:271:HOH:O	2.05	0.55
1:C:61:ALA:C	1:C:63:ARG:H	2.09	0.55
1:C:51:ARG:HH21	1:C:51:ARG:HG2	1.73	0.54
1:B:2:LEU:CD2	1:B:4:LEU:N	2.68	0.54
1:B:11:GLY:C	4:B:270:HOH:O	2.45	0.53
1:B:17:ILE:CD1	1:B:19:LEU:HD12	2.38	0.53
1:C:24:ASP:OD2	1:C:24:ASP:C	2.47	0.52
1:B:30:GLU:HG2	4:B:266:HOH:O	2.09	0.51
1:B:2:LEU:HD22	1:B:5:TRP:HD1	1.69	0.51
1:B:23:ARG:NH2	4:B:269:HOH:O	2.44	0.51
1:A:41:LYS:O	1:A:45:VAL:HG23	2.11	0.51
1:B:23:ARG:CB	4:B:270:HOH:O	2.59	0.50
1:B:2:LEU:HD23	1:B:5:TRP:H	1.75	0.50
1:A:18:HIS:HA	4:A:263:HOH:O	2.12	0.50
1:A:54:HIS:CD2	4:A:277:HOH:O	2.49	0.50
1:C:5:TRP:CH2	1:C:13:TRP:HB2	2.46	0.49
1:B:41:LYS:O	1:B:45:VAL:HG23	2.12	0.49
1:C:15:GLU:CG	4:C:260:HOH:O	2.60	0.49
1:C:5:TRP:HB2	1:C:33:GLY:HA3	1.93	0.49
1:C:52:VAL:O	1:C:56:GLU:HG2	2.13	0.49
1:C:61:ALA:C	1:C:63:ARG:N	2.64	0.49
1:B:21:GLU:HG2	4:B:268:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LEU:CD2	1:B:2:LEU:C	2.83	0.47
1:B:42:GLU:H	1:B:42:GLU:CD	2.17	0.46
1:C:24:ASP:HB3	4:C:266:HOH:O	2.15	0.46
1:C:5:TRP:HH2	1:C:13:TRP:CD1	2.32	0.46
1:C:12:ASP:CA	4:C:260:HOH:O	2.41	0.46
1:C:15:GLU:CB	4:C:260:HOH:O	2.60	0.46
1:A:49:VAL:CG1	1:A:55:ARG:HG2	2.46	0.45
1:B:62:LEU:O	1:B:63:ARG:C	2.53	0.45
1:B:64:GLN:O	1:B:65:LEU:HD23	2.15	0.45
1:B:25:ARG:NH1	1:B:47:LEU:C	2.69	0.45
1:B:43:ASP:O	1:B:47:LEU:HG	2.17	0.45
1:B:51:ARG:HG3	1:B:51:ARG:NH2	2.30	0.45
1:B:5:TRP:HB2	1:B:33:GLY:HA3	1.98	0.44
1:B:17:ILE:HD11	1:B:19:LEU:HD12	1.98	0.44
1:C:25:ARG:NE	4:C:273:HOH:O	2.50	0.44
1:A:43:ASP:O	1:A:47:LEU:HG	2.18	0.44
1:B:13:TRP:HA	1:B:16:SER:HB3	2.00	0.44
1:A:1:MET:HB2	4:A:283:HOH:O	2.17	0.44
1:C:60:ARG:CG	4:C:265:HOH:O	2.65	0.43
1:A:55:ARG:NH2	4:A:258:HOH:O	2.50	0.43
1:A:57:ASN:OD1	1:A:60:ARG:NH2	2.51	0.42
1:B:38:ALA:C	4:B:265:HOH:O	2.57	0.42
1:A:7:LYS:HE3	1:A:8:PHE:CZ	2.54	0.42
1:C:2:LEU:N	4:C:268:HOH:O	2.52	0.42
1:A:32:GLU:HG2	1:A:35:HIS:ND1	2.34	0.42
1:C:62:LEU:O	1:C:63:ARG:HB2	2.21	0.41
1:B:19:LEU:HA	4:B:268:HOH:O	2.19	0.41
1:C:51:ARG:HG2	1:C:51:ARG:NH2	2.35	0.41
1:B:2:LEU:CD2	1:B:5:TRP:HD1	2.30	0.41
1:C:49:VAL:O	1:C:55:ARG:NH1	2.53	0.41
1:B:11:GLY:CA	4:B:270:HOH:O	2.69	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	63/76 (83%)	61 (97%)	2 (3%)	0	100	100
1	B	62/76 (82%)	56 (90%)	4 (6%)	2 (3%)	4	3
1	C	60/76 (79%)	57 (95%)	2 (3%)	1 (2%)	9	11
All	All	185/228 (81%)	174 (94%)	8 (4%)	3 (2%)	9	13

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	B	62	LEU
1	B	63	ARG

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	57/67 (85%)	55 (96%)	2 (4%)	36	55
1	B	56/67 (84%)	52 (93%)	4 (7%)	14	23
1	C	54/67 (81%)	51 (94%)	3 (6%)	21	34
All	All	167/201 (83%)	158 (95%)	9 (5%)	22	36

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	65	LEU
1	B	2	LEU
1	B	25	ARG
1	B	42	GLU
1	B	59	GLU
1	C	2	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	21	GLU
1	C	59	GLU

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.