



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 9IJX / pdb_00009ijx
Title : Crystal structure of the mouse Spef1 coiled-coil domain
Authors : Ren, J.; Li, D.; Feng, W.
Deposited on : 2024-06-25
Resolution : 2.45 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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

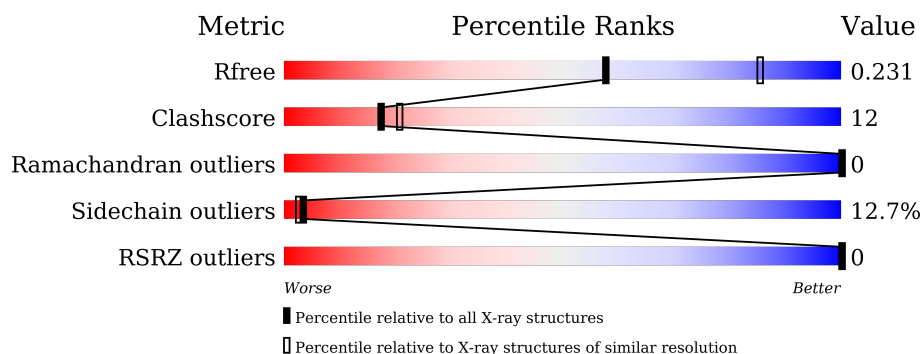
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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	69	<div> <div>54%</div> <div>17%</div> <div>•</div> <div>25%</div> </div>
1	B	69	<div> <div>49%</div> <div>16%</div> <div>•</div> <div>30%</div> </div>
1	C	69	<div> <div>52%</div> <div>23%</div> <div>•</div> <div>22%</div> </div>
1	D	69	<div> <div>45%</div> <div>22%</div> <div>•</div> <div>32%</div> </div>
1	E	69	<div> <div>45%</div> <div>28%</div> <div>6%</div> <div>22%</div> </div>
1	F	69	<div> <div>41%</div> <div>19%</div> <div>•</div> <div>38%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2445 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 Sperm flagellar protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	52	Total	C	N	O	S	0	0	0
			422	264	77	80	1			
1	B	48	Total	C	N	O	S	0	0	0
			395	246	74	74	1			
1	C	54	Total	C	N	O	S	0	0	0
			445	278	81	85	1			
1	D	47	Total	C	N	O	S	0	0	0
			389	241	74	73	1			
1	E	54	Total	C	N	O	S	0	0	0
			436	273	81	81	1			
1	F	43	Total	C	N	O	S	0	0	0
			358	222	68	67	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	GLY	-	expression tag	UNP Q99JL1
A	167	PRO	-	expression tag	UNP Q99JL1
A	168	GLY	-	expression tag	UNP Q99JL1
A	169	SER	-	expression tag	UNP Q99JL1
B	166	GLY	-	expression tag	UNP Q99JL1
B	167	PRO	-	expression tag	UNP Q99JL1
B	168	GLY	-	expression tag	UNP Q99JL1
B	169	SER	-	expression tag	UNP Q99JL1
C	166	GLY	-	expression tag	UNP Q99JL1
C	167	PRO	-	expression tag	UNP Q99JL1
C	168	GLY	-	expression tag	UNP Q99JL1
C	169	SER	-	expression tag	UNP Q99JL1
D	166	GLY	-	expression tag	UNP Q99JL1
D	167	PRO	-	expression tag	UNP Q99JL1
D	168	GLY	-	expression tag	UNP Q99JL1
D	169	SER	-	expression tag	UNP Q99JL1
E	166	GLY	-	expression tag	UNP Q99JL1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	167	PRO	-	expression tag	UNP Q99JL1
E	168	GLY	-	expression tag	UNP Q99JL1
E	169	SER	-	expression tag	UNP Q99JL1
F	166	GLY	-	expression tag	UNP Q99JL1
F	167	PRO	-	expression tag	UNP Q99JL1
F	168	GLY	-	expression tag	UNP Q99JL1
F	169	SER	-	expression tag	UNP Q99JL1

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: Sperm flagellar protein 1

Chain A: 



- Molecule 1: Sperm flagellar protein 1

Chain B: 



- Molecule 1: Sperm flagellar protein 1

Chain C: 



- Molecule 1: Sperm flagellar protein 1

Chain D: 



- Molecule 1: Sperm flagellar protein 1

Chain E: 



- Molecule 1: Sperm flagellar protein 1

Chain F: 

GLY	PRO	GLY	SER	TYR	ASN	GLN	ALA	LEU	GLN	GLY	ASP	PRO	SER	PHE	VAL	LEU	Q183	I184	A185	E186	L191	L192	E196	T197	V200	L201	Q202	M203	K204	L208	R218	D221	R225	LEU	GLN	GLN	ALA	GLU	ARG	LYS	GLN	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	60.15Å 104.36Å 72.27Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	26.09 – 2.45 26.09 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.9 (26.09-2.45) 95.9 (26.09-2.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.44Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.195 , 0.234 0.191 , 0.231	Depositor DCC
R_{free} test set	15063 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.379 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.369 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.459 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.459 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.378 for h,-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2445	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.81% 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	1.07	0/424	1.68	0/568
1	B	1.05	0/395	1.65	0/528
1	C	1.05	0/447	1.66	0/599
1	D	1.02	0/389	1.65	0/519
1	E	1.06	0/438	1.65	0/587
1	F	1.07	0/358	1.66	0/477
All	All	1.05	0/2451	1.66	0/3278

There are no bond length outliers.

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	422	0	437	8	0
1	B	395	0	420	9	0
1	C	445	0	467	10	0
1	D	389	0	416	12	0
1	E	436	0	460	18	0
1	F	358	0	384	10	0
All	All	2445	0	2584	62	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 12.

All (62) 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:213:GLN:HA	1:A:213:GLN:OE1	1.77	0.85
1:E:200:VAL:O	1:E:203:MET:HG2	1.81	0.81
1:B:186:GLU:O	1:B:189:GLN:HG2	1.86	0.76
1:D:225:ARG:O	1:D:228:GLN:CG	2.43	0.66
1:D:183:GLN:O	1:D:187:LYS:HD3	1.98	0.62
1:D:225:ARG:O	1:D:228:GLN:HG3	1.99	0.62
1:C:197:THR:O	1:C:201:LEU:HD23	1.99	0.62
1:A:197:THR:O	1:A:201:LEU:HD23	2.00	0.61
1:E:197:THR:O	1:E:201:LEU:HD23	2.00	0.61
1:E:214:LEU:O	1:E:217:VAL:HG22	2.01	0.60
1:A:214:LEU:O	1:A:217:VAL:HG22	2.03	0.58
1:B:186:GLU:HA	1:B:189:GLN:NE2	2.19	0.58
1:B:186:GLU:HG2	1:B:187:LYS:N	2.19	0.58
1:E:200:VAL:HA	1:E:203:MET:SD	2.45	0.57
1:B:188:GLU:O	1:B:192:LEU:HG	2.05	0.56
1:A:196:GLU:O	1:A:200:VAL:HG13	2.06	0.55
1:C:202:GLN:O	1:C:205:VAL:HG22	2.06	0.54
1:E:183:GLN:O	1:E:187:LYS:HD3	2.08	0.54
1:F:221:ASP:O	1:F:225:ARG:HG3	2.07	0.54
1:F:204:LYS:O	1:F:208:LEU:HD23	2.08	0.54
1:D:188:GLU:O	1:D:192:LEU:HD23	2.08	0.53
1:C:178:PRO:O	1:C:181:VAL:HG12	2.07	0.53
1:E:178:PRO:O	1:E:181:VAL:HG12	2.09	0.53
1:D:225:ARG:O	1:D:228:GLN:HG2	2.09	0.52
1:E:204:LYS:O	1:E:208:LEU:HD23	2.10	0.52
1:A:204:LYS:O	1:A:208:LEU:HD23	2.10	0.52
1:B:196:GLU:O	1:B:200:VAL:HG13	2.10	0.51
1:D:225:ARG:C	1:D:228:GLN:HG2	2.36	0.51
1:A:218:ARG:O	1:A:222:LEU:HD23	2.11	0.50
1:E:218:ARG:O	1:E:222:LEU:HD23	2.12	0.50
1:D:218:ARG:O	1:D:222:LEU:HD23	2.11	0.49
1:B:218:ARG:O	1:B:222:LEU:HD23	2.12	0.49
1:C:215:LYS:NZ	1:D:216:ASN:OD1	2.25	0.48
1:E:196:GLU:O	1:E:200:VAL:HG12	2.14	0.48
1:C:196:GLU:O	1:C:200:VAL:HG12	2.14	0.47
1:F:196:GLU:OE2	1:F:196:GLU:HA	2.14	0.47
1:B:188:GLU:OE2	1:B:191:LEU:HD22	2.16	0.46
1:E:177:ASP:OD1	1:E:178:PRO:HD2	2.15	0.46
1:E:183:GLN:O	1:E:187:LYS:CD	2.65	0.45
1:B:186:GLU:HA	1:B:189:GLN:HE21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:THR:O	1:F:200:VAL:HG12	2.17	0.45
1:D:197:THR:O	1:D:200:VAL:HG12	2.17	0.44
1:E:180:PHE:CD1	1:E:180:PHE:N	2.84	0.44
1:F:183:GLN:HG2	1:F:184:ILE:N	2.33	0.43
1:C:204:LYS:HE2	1:D:205:VAL:HG11	2.00	0.43
1:E:226:LEU:CD1	1:F:225:ARG:O	2.66	0.43
1:B:191:LEU:C	1:B:191:LEU:HD23	2.44	0.43
1:E:219:ILE:HD13	1:F:218:ARG:HD3	1.99	0.43
1:D:225:ARG:HA	1:D:228:GLN:HG2	2.01	0.43
1:E:187:LYS:HD2	1:E:187:LYS:N	2.34	0.43
1:C:178:PRO:HA	1:C:181:VAL:HG12	2.01	0.43
1:E:201:LEU:HB3	1:F:201:LEU:HB3	2.01	0.43
1:F:191:LEU:C	1:F:191:LEU:HD23	2.44	0.42
1:C:214:LEU:HD23	1:C:214:LEU:HA	1.89	0.42
1:D:183:GLN:HG2	1:D:184:ILE:N	2.34	0.42
1:C:219:ILE:O	1:C:223:SER:HB2	2.20	0.42
1:A:211:LEU:HD13	1:A:211:LEU:HA	1.91	0.42
1:C:202:GLN:O	1:C:205:VAL:CG2	2.67	0.42
1:E:211:LEU:HD13	1:E:211:LEU:HA	1.90	0.41
1:E:214:LEU:O	1:E:217:VAL:CG2	2.66	0.41
1:F:191:LEU:HD23	1:F:192:LEU:N	2.36	0.41
1:A:214:LEU:O	1:A:217:VAL:CG2	2.68	0.40

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	50/69 (72%)	49 (98%)	1 (2%)	0	100	100
1	B	46/69 (67%)	44 (96%)	2 (4%)	0	100	100
1	C	52/69 (75%)	51 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	45/69 (65%)	44 (98%)	1 (2%)	0	100	100
1	E	52/69 (75%)	50 (96%)	2 (4%)	0	100	100
1	F	41/69 (59%)	40 (98%)	1 (2%)	0	100	100
All	All	286/414 (69%)	278 (97%)	8 (3%)	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	47/62 (76%)	41 (87%)	6 (13%)	3	2
1	B	44/62 (71%)	37 (84%)	7 (16%)	2	1
1	C	51/62 (82%)	44 (86%)	7 (14%)	3	2
1	D	44/62 (71%)	40 (91%)	4 (9%)	7	7
1	E	49/62 (79%)	42 (86%)	7 (14%)	2	2
1	F	41/62 (66%)	37 (90%)	4 (10%)	6	6
All	All	276/372 (74%)	241 (87%)	35 (13%)	3	2

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	GLU
1	A	200	VAL
1	A	206	LYS
1	A	207	ARG
1	A	211	LEU
1	A	213	GLN
1	B	186	GLU
1	B	191	LEU
1	B	199	GLN
1	B	200	VAL

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Mol	Chain	Res	Type
1	B	203	MET
1	B	206	LYS
1	B	211	LEU
1	C	186	GLU
1	C	200	VAL
1	C	207	ARG
1	C	211	LEU
1	C	213	GLN
1	C	223	SER
1	C	227	GLN
1	D	188	GLU
1	D	196	GLU
1	D	207	ARG
1	D	227	GLN
1	E	179	SER
1	E	180	PHE
1	E	187	LYS
1	E	191	LEU
1	E	200	VAL
1	E	207	ARG
1	E	211	LEU
1	F	186	GLU
1	F	191	LEU
1	F	196	GLU
1	F	203	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	189	GLN
1	C	228	GLN
1	D	213	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 [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	52/69 (75%)	-1.41	0 100 100	77, 97, 117, 123	0
1	B	48/69 (69%)	-1.56	0 100 100	76, 108, 120, 125	0
1	C	54/69 (78%)	-1.57	0 100 100	67, 93, 114, 120	0
1	D	47/69 (68%)	-1.31	0 100 100	66, 104, 159, 169	0
1	E	54/69 (78%)	-1.57	0 100 100	65, 88, 109, 121	0
1	F	43/69 (62%)	-1.51	0 100 100	61, 87, 120, 128	0
All	All	298/414 (71%)	-1.49	0 100 100	61, 94, 128, 169	0

There are no RSRZ outliers to report.

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.