



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 02:07 PM JST

PDB ID : 6LPH
Title : the Sufu-Fu complex crystal structure
Authors : Hua, L.; Geng, W.
Deposited on : 2020-01-10
Resolution : 1.91 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	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)	:	2.16

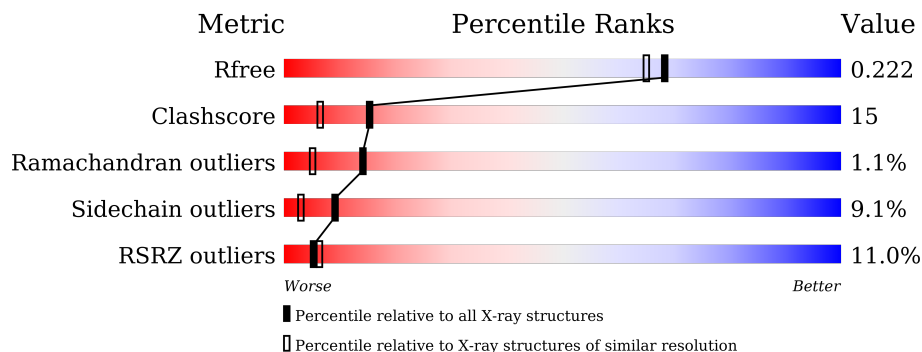
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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}	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 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	258	
2	B	28	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2278 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 Suppressor of fused homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			1930	1224	333	364	9			

- Molecule 2 is a protein called Serine/threonine-protein kinase fused.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	28	Total	C	N	O	S	0	0	0
			203	123	38	39	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	361	ALA	-	expression tag	UNP P23647
B	362	ALA	-	expression tag	UNP P23647
B	388	ALA	-	expression tag	UNP P23647

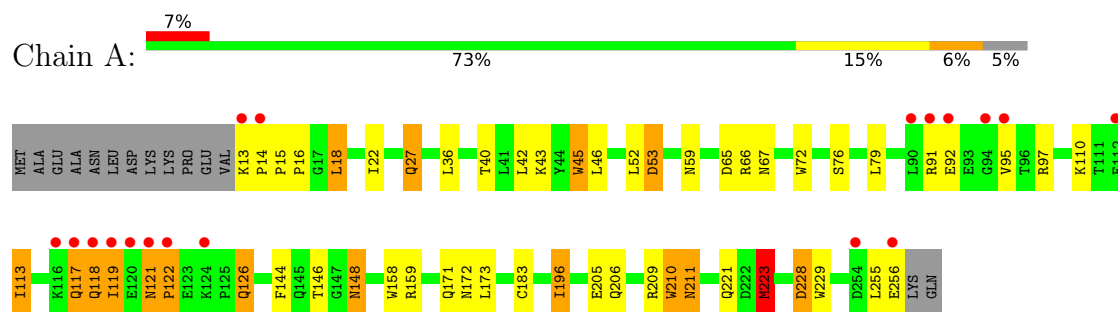
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		
3	B	9	Total	O	0	0
			9	9		

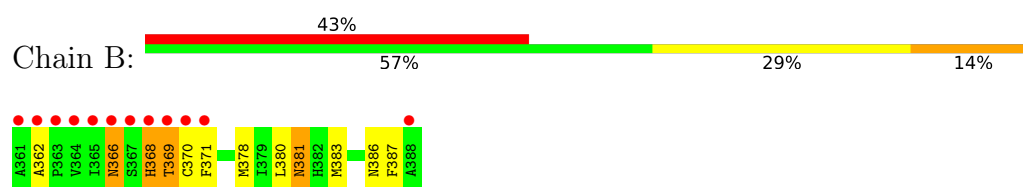
3 Residue-property plots

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: Suppressor of fused homolog



- Molecule 2: Serine/threonine-protein kinase fused



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.15Å 68.42Å 56.14Å 90.00° 97.49° 90.00°	Depositor
Resolution (Å)	55.67 – 1.91 32.10 – 1.92	Depositor EDS
% Data completeness (in resolution range)	97.5 (55.67-1.91) 98.0 (32.10-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.148 , 0.220 0.146 , 0.222	Depositor DCC
R_{free} test set	1056 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2278	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.68% 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

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	0.74	5/1981 (0.3%)	0.79	3/2702 (0.1%)
2	B	0.73	0/207	0.80	0/281
All	All	0.74	5/2188 (0.2%)	0.79	3/2983 (0.1%)

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	2
2	B	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	TRP	CD2-CE2	6.79	1.49	1.41
1	A	72	TRP	CD2-CE2	6.13	1.48	1.41
1	A	158	TRP	CD2-CE2	5.56	1.48	1.41
1	A	210	TRP	CD2-CE2	5.45	1.47	1.41
1	A	229	TRP	CD2-CE2	5.07	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	171	GLN	CB-CA-C	-5.60	99.20	110.40
1	A	223	MET	CG-SD-CE	-5.42	91.52	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ASN	Peptide
1	A	122	PRO	Peptide
2	B	370	CYS	Peptide

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	1930	0	1844	49	0
2	B	203	0	173	17	0
3	A	136	0	0	13	0
3	B	9	0	0	0	0
All	All	2278	0	2017	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 15.

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:118:GLN:CB	1:A:126:GLN:HE22	1.57	1.17
1:A:146:THR:OG1	3:A:301:HOH:O	1.63	1.13
1:A:183:CYS:HB3	3:A:342:HOH:O	1.44	1.12
1:A:118:GLN:HB2	1:A:126:GLN:HE22	1.19	1.06
1:A:18:LEU:HD11	2:B:387:PHE:CZ	2.02	0.94
1:A:118:GLN:HB3	1:A:126:GLN:HE22	1.35	0.89
1:A:206:GLN:HE22	1:A:209:ARG:HH21	1.17	0.88
1:A:255:LEU:HA	1:A:256:GLU:CB	2.04	0.88
1:A:118:GLN:CB	1:A:126:GLN:NE2	2.39	0.86
2:B:368:HIS:HD2	2:B:369:THR:N	1.74	0.85
2:B:368:HIS:HA	2:B:369:THR:CB	2.05	0.85
2:B:368:HIS:HA	2:B:369:THR:CG2	2.07	0.84
2:B:368:HIS:HA	2:B:369:THR:HG22	1.60	0.83
2:B:368:HIS:HA	2:B:369:THR:HB	1.61	0.82
2:B:368:HIS:CD2	2:B:368:HIS:C	2.52	0.82
2:B:371:PHE:HB2	2:B:378:MET:O	1.81	0.79
1:A:118:GLN:HB2	1:A:126:GLN:NE2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLN:HB3	1:A:126:GLN:NE2	1.97	0.76
1:A:173:LEU:HD22	1:A:196:ILE:HG23	1.68	0.76
1:A:117:GLN:HB3	3:A:391:HOH:O	1.86	0.75
1:A:91:ARG:CZ	3:A:304:HOH:O	2.32	0.75
2:B:368:HIS:CA	2:B:369:THR:HG22	2.16	0.75
1:A:18:LEU:HD11	2:B:387:PHE:CE1	2.22	0.74
2:B:368:HIS:CD2	2:B:369:THR:N	2.56	0.73
1:A:66:ARG:O	1:A:228:ASP:HB2	1.89	0.72
2:B:366:ASN:OD1	2:B:366:ASN:N	2.18	0.67
2:B:368:HIS:CB	2:B:369:THR:HG22	2.29	0.63
1:A:173:LEU:HD22	1:A:196:ILE:CG2	2.29	0.62
1:A:45:TRP:HZ3	1:A:53:ASP:OD2	1.84	0.60
1:A:22:ILE:HD12	2:B:383:MET:SD	2.42	0.60
1:A:18:LEU:CD1	2:B:387:PHE:CE1	2.85	0.60
1:A:92:GLU:O	1:A:95:VAL:HG12	2.01	0.60
1:A:228:ASP:OD2	3:A:302:HOH:O	2.17	0.59
1:A:79:LEU:HD23	1:A:144:PHE:HE1	1.68	0.58
1:A:255:LEU:CA	1:A:256:GLU:CB	2.82	0.57
1:A:79:LEU:HD23	1:A:144:PHE:CE1	2.40	0.56
1:A:43:LYS:HG2	1:A:45:TRP:CH2	2.41	0.56
1:A:118:GLN:HG2	1:A:119:ILE:HD13	1.88	0.55
1:A:210:TRP:O	1:A:211:ASN:HB3	2.06	0.54
1:A:228:ASP:CG	3:A:302:HOH:O	2.45	0.54
1:A:91:ARG:NH2	3:A:304:HOH:O	2.41	0.53
1:A:14:PRO:HB3	3:A:435:HOH:O	2.08	0.53
1:A:206:GLN:NE2	1:A:209:ARG:HH21	1.97	0.52
2:B:381:ASN:HD21	2:B:386:ASN:HD21	1.57	0.51
1:A:14:PRO:HA	3:A:416:HOH:O	2.10	0.51
1:A:159:ARG:H	1:A:172:ASN:ND2	2.10	0.50
1:A:67:ASN:HB3	1:A:223:MET:HG2	1.94	0.50
1:A:97:ARG:HD2	3:A:425:HOH:O	2.11	0.50
1:A:148:ASN:N	3:A:301:HOH:O	2.41	0.49
1:A:15:PRO:HD3	3:A:416:HOH:O	2.12	0.49
1:A:27:GLN:HE21	1:A:27:GLN:HA	1.78	0.49
1:A:52:LEU:HD13	1:A:76:SER:HB2	1.95	0.48
1:A:15:PRO:HA	1:A:16:PRO:HD3	1.80	0.46
1:A:65:ASP:HB2	3:A:303:HOH:O	2.16	0.45
1:A:13:LYS:HA	1:A:14:PRO:HD3	1.88	0.44
1:A:59:ASN:OD1	1:A:110:LYS:NZ	2.42	0.44
1:A:40:THR:HG21	1:A:52:LEU:O	2.17	0.44
1:A:113:ILE:HD12	1:A:113:ILE:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TRP:CD1	1:A:46:LEU:HG	2.53	0.43
2:B:371:PHE:CB	2:B:378:MET:O	2.60	0.42
1:A:40:THR:CG2	1:A:52:LEU:O	2.68	0.41
1:A:45:TRP:CD1	1:A:45:TRP:C	2.94	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	242/258 (94%)	237 (98%)	4 (2%)	1 (0%)	34	24
2	B	26/28 (93%)	22 (85%)	2 (8%)	2 (8%)	1	0
All	All	268/286 (94%)	259 (97%)	6 (2%)	3 (1%)	14	5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	PRO
2	B	369	THR
2	B	362	ALA

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	210/228 (92%)	193 (92%)	17 (8%)	11	4
2	B	21/24 (88%)	17 (81%)	4 (19%)	1	0
All	All	231/252 (92%)	210 (91%)	21 (9%)	9	3

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	27	GLN
1	A	36	LEU
1	A	42	LEU
1	A	113	ILE
1	A	117	GLN
1	A	118	GLN
1	A	119	ILE
1	A	121	ASN
1	A	126	GLN
1	A	148	ASN
1	A	196	ILE
1	A	205	GLU
1	A	211	ASN
1	A	221	GLN
1	A	223	MET
1	A	228	ASP
2	B	366	ASN
2	B	368	HIS
2	B	380	LEU
2	B	381	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	83	HIS
1	A	118	GLN
1	A	126	GLN
1	A	134	ASN
1	A	172	ASN
1	A	177	GLN
1	A	206	GLN
2	B	368	HIS

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Mol	Chain	Res	Type
2	B	381	ASN
2	B	382	HIS

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](#)

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	244/258 (94%)	0.11	18 (7%) 14 16	10, 19, 49, 81	2 (0%)
2	B	28/28 (100%)	3.82	12 (42%) 0 0	20, 32, 55, 58	9 (32%)
All	All	272/286 (95%)	0.50	30 (11%) 5 6	10, 20, 55, 81	11 (4%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	365	ILE	20.0
2	B	361	ALA	18.7
1	A	119	ILE	14.0
2	B	369	THR	13.3
1	A	120	GLU	10.8
2	B	368	HIS	10.5
2	B	362	ALA	8.9
2	B	364	VAL	7.8
2	B	363	PRO	7.5
2	B	366	ASN	6.8
2	B	371	PHE	5.5
2	B	367	SER	5.3
1	A	121	ASN	5.1
2	B	370	CYS	5.0
1	A	13	LYS	4.4
1	A	122	PRO	4.4
1	A	254	ASP	4.0
1	A	90	LEU	4.0
1	A	118	GLN	3.9
2	B	388	ALA	3.5
1	A	14	PRO	3.5
1	A	256	GLU	3.3
1	A	94	GLY	3.2
1	A	112	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	116	LYS	2.5
1	A	117	GLN	2.4
1	A	92	GLU	2.2
1	A	91	ARG	2.1
1	A	95	VAL	2.0
1	A	124	LYS	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.