



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:27 AM GMT

PDB ID : 3UUX
Title : Crystal structure of yeast Fis1 in complex with Mdv1 fragment containing N-terminal extension and coiled coil domains
Authors : Zhang, Y.; Chan, N.C.; Gristick, H.; Chan, D.C.
Deposited on : 2011-11-28
Resolution : 3.90 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

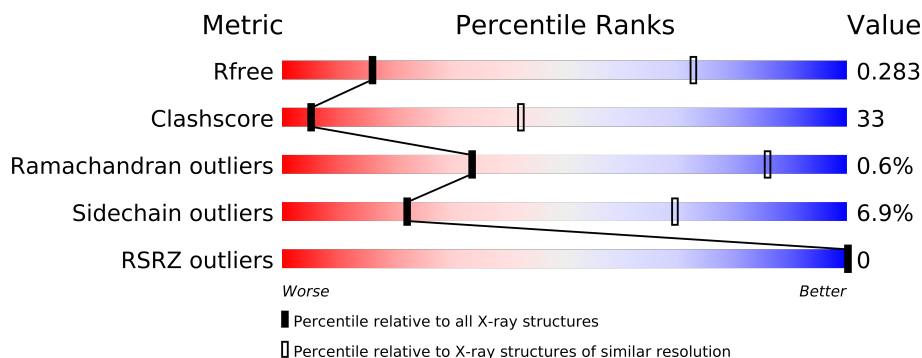
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.90 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))
R_{free}	66092	1022 (4.38-3.42)
Clashscore	79885	1173 (4.30-3.50)
Ramachandran outliers	78287	1118 (4.30-3.50)
Sidechain outliers	78261	1107 (4.30-3.50)
RSRZ outliers	66119	1000 (4.36-3.44)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	129	
1	C	129	
2	B	242	
2	D	242	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4076 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Mitochondria fission 1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1028	654	172	198	4			
1	C	125	Total	C	N	O	S	0	0	0
			1004	638	168	194	4			

- Molecule 2 is a protein called Mitochondrial division protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1013	641	164	206	2			
2	D	135	Total	C	N	O	S	0	0	0
			1031	651	169	209	2			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	MET	-	EXPRESSION TAG	UNP P47025
B	74	GLY	-	EXPRESSION TAG	UNP P47025
B	75	SER	-	EXPRESSION TAG	UNP P47025
B	76	SER	-	EXPRESSION TAG	UNP P47025
B	77	HIS	-	EXPRESSION TAG	UNP P47025
B	78	HIS	-	EXPRESSION TAG	UNP P47025
B	79	HIS	-	EXPRESSION TAG	UNP P47025
B	80	HIS	-	EXPRESSION TAG	UNP P47025
B	81	HIS	-	EXPRESSION TAG	UNP P47025
B	82	HIS	-	EXPRESSION TAG	UNP P47025
B	83	SER	-	EXPRESSION TAG	UNP P47025
B	84	SER	-	EXPRESSION TAG	UNP P47025
B	85	GLY	-	EXPRESSION TAG	UNP P47025
B	86	LEU	-	EXPRESSION TAG	UNP P47025
B	87	VAL	-	EXPRESSION TAG	UNP P47025
B	88	PRO	-	EXPRESSION TAG	UNP P47025

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Chain	Residue	Modelled	Actual	Comment	Reference
B	89	ARG	-	EXPRESSION TAG	UNP P47025
B	90	GLY	-	EXPRESSION TAG	UNP P47025
B	91	SER	-	EXPRESSION TAG	UNP P47025
B	92	HIS	-	EXPRESSION TAG	UNP P47025
B	93	MET	-	EXPRESSION TAG	UNP P47025
B	215	ALA	LYS	ENGINEERED MUTATION	UNP P47025
B	216	ALA	LYS	ENGINEERED MUTATION	UNP P47025
D	73	MET	-	EXPRESSION TAG	UNP P47025
D	74	GLY	-	EXPRESSION TAG	UNP P47025
D	75	SER	-	EXPRESSION TAG	UNP P47025
D	76	SER	-	EXPRESSION TAG	UNP P47025
D	77	HIS	-	EXPRESSION TAG	UNP P47025
D	78	HIS	-	EXPRESSION TAG	UNP P47025
D	79	HIS	-	EXPRESSION TAG	UNP P47025
D	80	HIS	-	EXPRESSION TAG	UNP P47025
D	81	HIS	-	EXPRESSION TAG	UNP P47025
D	82	HIS	-	EXPRESSION TAG	UNP P47025
D	83	SER	-	EXPRESSION TAG	UNP P47025
D	84	SER	-	EXPRESSION TAG	UNP P47025
D	85	GLY	-	EXPRESSION TAG	UNP P47025
D	86	LEU	-	EXPRESSION TAG	UNP P47025
D	87	VAL	-	EXPRESSION TAG	UNP P47025
D	88	PRO	-	EXPRESSION TAG	UNP P47025
D	89	ARG	-	EXPRESSION TAG	UNP P47025
D	90	GLY	-	EXPRESSION TAG	UNP P47025
D	91	SER	-	EXPRESSION TAG	UNP P47025
D	92	HIS	-	EXPRESSION TAG	UNP P47025
D	93	MET	-	EXPRESSION TAG	UNP P47025
D	215	ALA	LYS	ENGINEERED MUTATION	UNP P47025
D	216	ALA	LYS	ENGINEERED MUTATION	UNP P47025



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	174.68Å 174.68Å 167.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.51 – 3.90 19.81 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (123.51-3.90) 99.6 (19.81-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 3.94Å)	Xtriage
Refinement program	REFMAC 5.6.0111	Depositor
R, R_{free}	0.270 , 0.284 0.268 , 0.283	Depositor DCC
R_{free} test set	1178 reflections (10.89%)	DCC
Wilson B-factor (Å ²)	122.5	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 78.6	EDS
Estimated twinning fraction	0.000 for l,-k,h 0.028 for -h,-l,-k	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 11999 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4076	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.87	3/1048 (0.3%)	0.87	1/1417 (0.1%)
1	C	0.86	2/1024 (0.2%)	0.85	1/1388 (0.1%)
2	B	0.96	2/1023 (0.2%)	1.00	4/1382 (0.3%)
2	D	1.33	5/1042 (0.5%)	1.06	4/1407 (0.3%)
All	All	1.02	12/4137 (0.3%)	0.95	10/5594 (0.2%)

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
2	B	0	1
2	D	0	1
All	All	0	2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	218	SER	CB-OG	18.31	1.66	1.42
2	D	225	ALA	C-O	13.78	1.49	1.23
1	C	127	GLU	C-O	9.32	1.41	1.23
2	B	225	ALA	C-O	-9.14	1.05	1.23
1	C	44	ASN	CB-CG	-7.00	1.34	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	ASN	CB-CA-C	-7.88	94.63	110.40
2	B	161	LEU	CA-CB-CG	6.80	130.95	115.30
2	D	98	CYS	CA-CB-SG	-6.67	101.99	114.00
2	D	292	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	D	107	ASP	N-CA-C	-6.41	93.71	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	220	SER	Peptide
2	D	225	ALA	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1028	0	1001	70	0
1	C	1004	0	961	72	0
2	B	1013	0	975	70	0
2	D	1031	0	986	105	2
All	All	4076	0	3923	266	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

The worst 5 of 266 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:113:ILE:CG1	2:D:113:ILE:CD1	1.82	1.54
2:D:218:SER:OG	2:D:218:SER:CB	1.66	1.39
1:C:77:ARG:NH2	2:D:114:PRO:HD3	1.46	1.26
1:C:59:ARG:HD2	2:D:99:PHE:HD1	1.02	1.15
1:A:126:LYS:HB3	2:D:104:TYR:CE2	1.86	1.10

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:98:CYS:SG	2:D:98:CYS:SG[5_555]	1.04	1.16
2:D:218:SER:OG	2:D:292:ARG:NH2[5_555]	1.82	0.38

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	125/129 (97%)	118 (94%)	6 (5%)	1 (1%)	27	83
1	C	123/129 (95%)	115 (94%)	7 (6%)	1 (1%)	27	83
2	B	126/242 (52%)	118 (94%)	7 (6%)	1 (1%)	27	83
2	D	129/242 (53%)	119 (92%)	10 (8%)	0	100	100
All	All	503/742 (68%)	470 (93%)	30 (6%)	3 (1%)	33	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLY
1	C	34	GLY
2	B	217	ILE

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	109/116 (94%)	104 (95%)	5 (5%)	37	82
1	C	105/116 (90%)	100 (95%)	5 (5%)	35	81
2	B	110/217 (51%)	103 (94%)	7 (6%)	25	73
2	D	111/217 (51%)	98 (88%)	13 (12%)	8	43
All	All	435/666 (65%)	405 (93%)	30 (7%)	22	69

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	9	THR

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Mol	Chain	Res	Type
1	C	112	GLN
2	D	266	GLU
1	C	95	MET
2	D	95	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	285	ASN
1	C	28	GLN
2	D	231	GLN
2	B	243	GLN
1	C	112	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	127/129 (98%)	-0.08	0 100 100	101, 123, 134, 138	0
1	C	125/129 (96%)	0.01	0 100 100	108, 124, 135, 145	0
2	B	132/242 (54%)	-0.21	0 100 100	104, 128, 138, 145	0
2	D	135/242 (55%)	-0.09	0 100 100	108, 133, 146, 152	0
All	All	519/742 (69%)	-0.09	0 100 100	101, 127, 142, 152	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.