wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:04 PM GMT

PDB ID	:	1N9S
Title	:	Crystal structure of yeast SmF in spacegroup P43212
Authors	:	Collins, B.M.; Cubeddu, L.; Naidoo, N.; Harrop, S.J.; Kornfeld, G.D.; Dawes, I.W.; Curmi, P.M.G.; Mabbutt, B.C.
Deposited on	:	2002-11-26
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

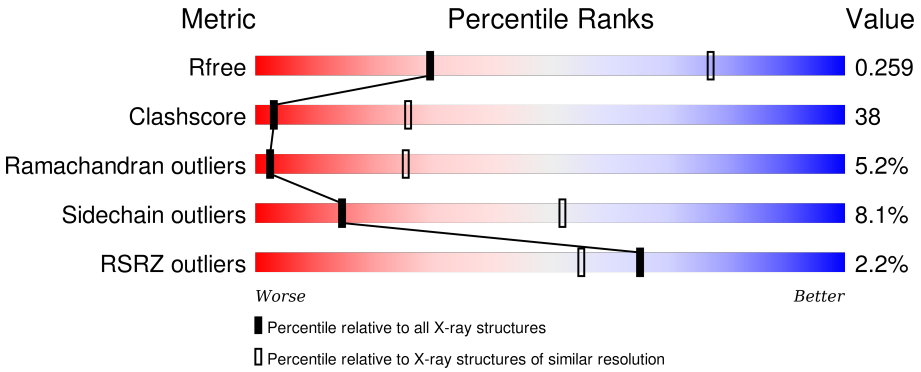
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 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 <=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	93	3% 28% 38% 8% 27%
1	B	93	% 27% 41% 5% 27%
1	C	93	3% 39% 31% 6% • 20%
1	D	93	% 27% 42% 8% 24%
1	E	93	2% 29% 34% 9% • 27%

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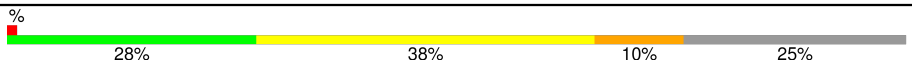
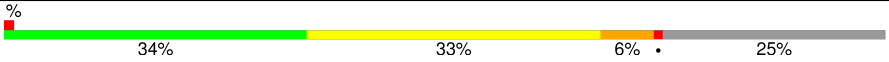
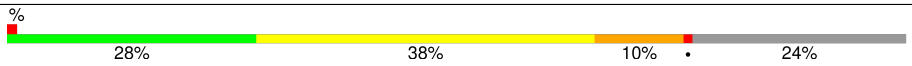
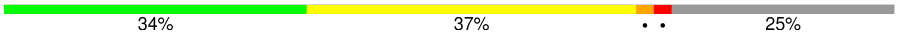
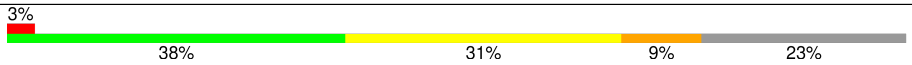
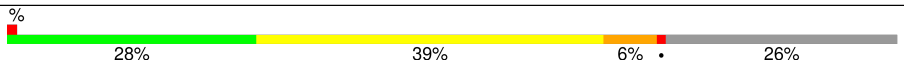
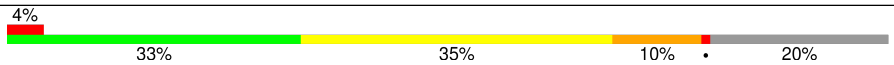
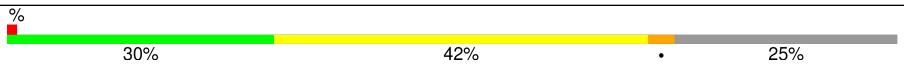
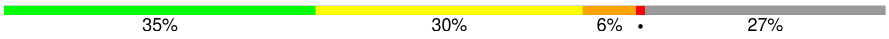
Mol	Chain	Length	Quality of chain
1	F	93	
1	G	93	
1	H	93	
1	I	93	
1	J	93	
1	K	93	
1	L	93	
1	M	93	
1	N	93	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7887 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 Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	68	Total 544	C 346	N 96	O 102	0	0	0
1	B	68	Total 544	C 346	N 96	O 102	0	0	0
1	C	74	Total 593	C 380	N 104	O 109	0	0	0
1	D	71	Total 571	C 366	N 100	O 105	0	0	0
1	E	68	Total 544	C 346	N 96	O 102	0	0	0
1	F	70	Total 562	C 360	N 98	O 104	0	0	0
1	G	70	Total 562	C 360	N 98	O 104	0	0	0
1	H	71	Total 571	C 366	N 100	O 105	0	0	0
1	I	70	Total 562	C 360	N 98	O 104	0	0	0
1	J	72	Total 578	C 371	N 101	O 106	0	0	0
1	K	69	Total 555	C 355	N 97	O 103	0	0	0
1	L	74	Total 593	C 380	N 104	O 109	0	0	0
1	M	70	Total 562	C 360	N 98	O 104	0	0	0
1	N	68	Total 546	C 351	N 95	O 100	0	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP P54999

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP P54999
A	-4	HIS	-	EXPRESSION TAG	UNP P54999
A	-3	HIS	-	EXPRESSION TAG	UNP P54999
A	-2	HIS	-	EXPRESSION TAG	UNP P54999
A	-1	HIS	-	EXPRESSION TAG	UNP P54999
A	0	HIS	-	EXPRESSION TAG	UNP P54999
A	75	SER	CYS	ENGINEERED	UNP P54999
B	-6	MET	-	EXPRESSION TAG	UNP P54999
B	-5	HIS	-	EXPRESSION TAG	UNP P54999
B	-4	HIS	-	EXPRESSION TAG	UNP P54999
B	-3	HIS	-	EXPRESSION TAG	UNP P54999
B	-2	HIS	-	EXPRESSION TAG	UNP P54999
B	-1	HIS	-	EXPRESSION TAG	UNP P54999
B	0	HIS	-	EXPRESSION TAG	UNP P54999
B	75	SER	CYS	ENGINEERED	UNP P54999
C	-6	MET	-	EXPRESSION TAG	UNP P54999
C	-5	HIS	-	EXPRESSION TAG	UNP P54999
C	-4	HIS	-	EXPRESSION TAG	UNP P54999
C	-3	HIS	-	EXPRESSION TAG	UNP P54999
C	-2	HIS	-	EXPRESSION TAG	UNP P54999
C	-1	HIS	-	EXPRESSION TAG	UNP P54999
C	0	HIS	-	EXPRESSION TAG	UNP P54999
C	75	SER	CYS	ENGINEERED	UNP P54999
D	-6	MET	-	EXPRESSION TAG	UNP P54999
D	-5	HIS	-	EXPRESSION TAG	UNP P54999
D	-4	HIS	-	EXPRESSION TAG	UNP P54999
D	-3	HIS	-	EXPRESSION TAG	UNP P54999
D	-2	HIS	-	EXPRESSION TAG	UNP P54999
D	-1	HIS	-	EXPRESSION TAG	UNP P54999
D	0	HIS	-	EXPRESSION TAG	UNP P54999
D	75	SER	CYS	ENGINEERED	UNP P54999
E	-6	MET	-	EXPRESSION TAG	UNP P54999
E	-5	HIS	-	EXPRESSION TAG	UNP P54999
E	-4	HIS	-	EXPRESSION TAG	UNP P54999
E	-3	HIS	-	EXPRESSION TAG	UNP P54999
E	-2	HIS	-	EXPRESSION TAG	UNP P54999
E	-1	HIS	-	EXPRESSION TAG	UNP P54999
E	0	HIS	-	EXPRESSION TAG	UNP P54999
E	75	SER	CYS	ENGINEERED	UNP P54999
F	-6	MET	-	EXPRESSION TAG	UNP P54999
F	-5	HIS	-	EXPRESSION TAG	UNP P54999
F	-4	HIS	-	EXPRESSION TAG	UNP P54999

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	HIS	-	EXPRESSION TAG	UNP P54999
F	-2	HIS	-	EXPRESSION TAG	UNP P54999
F	-1	HIS	-	EXPRESSION TAG	UNP P54999
F	0	HIS	-	EXPRESSION TAG	UNP P54999
F	75	SER	CYS	ENGINEERED	UNP P54999
G	-6	MET	-	EXPRESSION TAG	UNP P54999
G	-5	HIS	-	EXPRESSION TAG	UNP P54999
G	-4	HIS	-	EXPRESSION TAG	UNP P54999
G	-3	HIS	-	EXPRESSION TAG	UNP P54999
G	-2	HIS	-	EXPRESSION TAG	UNP P54999
G	-1	HIS	-	EXPRESSION TAG	UNP P54999
G	0	HIS	-	EXPRESSION TAG	UNP P54999
G	75	SER	CYS	ENGINEERED	UNP P54999
H	-6	MET	-	EXPRESSION TAG	UNP P54999
H	-5	HIS	-	EXPRESSION TAG	UNP P54999
H	-4	HIS	-	EXPRESSION TAG	UNP P54999
H	-3	HIS	-	EXPRESSION TAG	UNP P54999
H	-2	HIS	-	EXPRESSION TAG	UNP P54999
H	-1	HIS	-	EXPRESSION TAG	UNP P54999
H	0	HIS	-	EXPRESSION TAG	UNP P54999
H	75	SER	CYS	ENGINEERED	UNP P54999
I	-6	MET	-	EXPRESSION TAG	UNP P54999
I	-5	HIS	-	EXPRESSION TAG	UNP P54999
I	-4	HIS	-	EXPRESSION TAG	UNP P54999
I	-3	HIS	-	EXPRESSION TAG	UNP P54999
I	-2	HIS	-	EXPRESSION TAG	UNP P54999
I	-1	HIS	-	EXPRESSION TAG	UNP P54999
I	0	HIS	-	EXPRESSION TAG	UNP P54999
I	75	SER	CYS	ENGINEERED	UNP P54999
J	-6	MET	-	EXPRESSION TAG	UNP P54999
J	-5	HIS	-	EXPRESSION TAG	UNP P54999
J	-4	HIS	-	EXPRESSION TAG	UNP P54999
J	-3	HIS	-	EXPRESSION TAG	UNP P54999
J	-2	HIS	-	EXPRESSION TAG	UNP P54999
J	-1	HIS	-	EXPRESSION TAG	UNP P54999
J	0	HIS	-	EXPRESSION TAG	UNP P54999
J	75	SER	CYS	ENGINEERED	UNP P54999
K	-6	MET	-	EXPRESSION TAG	UNP P54999
K	-5	HIS	-	EXPRESSION TAG	UNP P54999
K	-4	HIS	-	EXPRESSION TAG	UNP P54999
K	-3	HIS	-	EXPRESSION TAG	UNP P54999
K	-2	HIS	-	EXPRESSION TAG	UNP P54999

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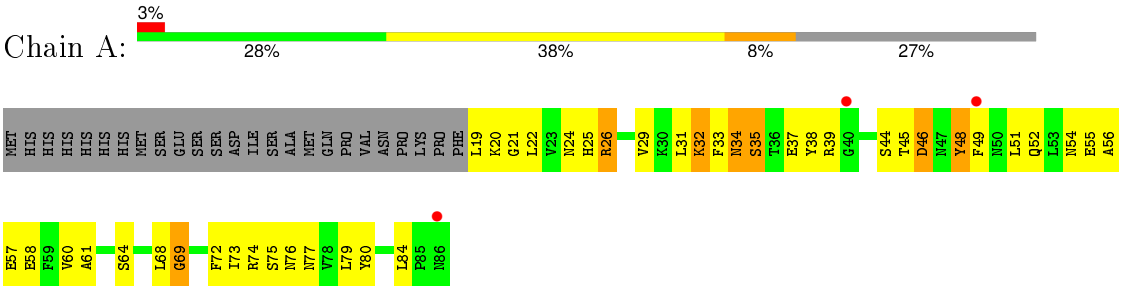
Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	EXPRESSION TAG	UNP P54999
K	0	HIS	-	EXPRESSION TAG	UNP P54999
K	75	SER	CYS	ENGINEERED	UNP P54999
L	-6	MET	-	EXPRESSION TAG	UNP P54999
L	-5	HIS	-	EXPRESSION TAG	UNP P54999
L	-4	HIS	-	EXPRESSION TAG	UNP P54999
L	-3	HIS	-	EXPRESSION TAG	UNP P54999
L	-2	HIS	-	EXPRESSION TAG	UNP P54999
L	-1	HIS	-	EXPRESSION TAG	UNP P54999
L	0	HIS	-	EXPRESSION TAG	UNP P54999
L	75	SER	CYS	ENGINEERED	UNP P54999
M	-6	MET	-	EXPRESSION TAG	UNP P54999
M	-5	HIS	-	EXPRESSION TAG	UNP P54999
M	-4	HIS	-	EXPRESSION TAG	UNP P54999
M	-3	HIS	-	EXPRESSION TAG	UNP P54999
M	-2	HIS	-	EXPRESSION TAG	UNP P54999
M	-1	HIS	-	EXPRESSION TAG	UNP P54999
M	0	HIS	-	EXPRESSION TAG	UNP P54999
M	75	SER	CYS	ENGINEERED	UNP P54999
N	-6	MET	-	EXPRESSION TAG	UNP P54999
N	-5	HIS	-	EXPRESSION TAG	UNP P54999
N	-4	HIS	-	EXPRESSION TAG	UNP P54999
N	-3	HIS	-	EXPRESSION TAG	UNP P54999
N	-2	HIS	-	EXPRESSION TAG	UNP P54999
N	-1	HIS	-	EXPRESSION TAG	UNP P54999
N	0	HIS	-	EXPRESSION TAG	UNP P54999
N	75	SER	CYS	ENGINEERED	UNP P54999

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

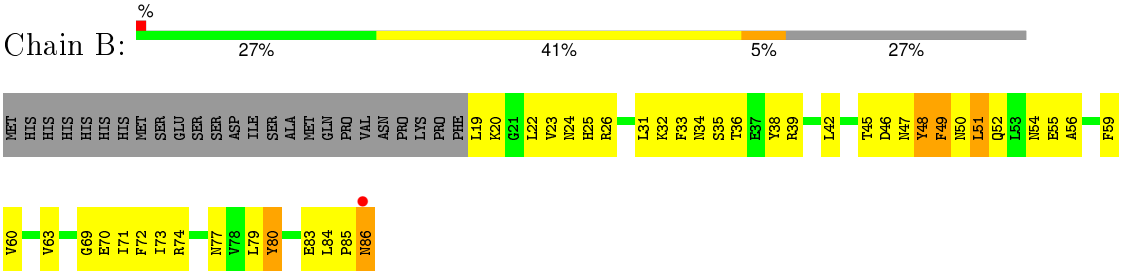
- Molecule 1: Small nuclear ribonucleoprotein F

Chain A:



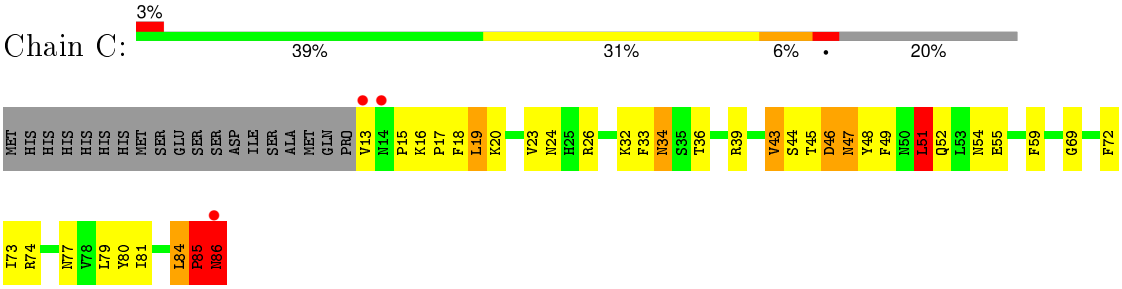
- Molecule 1: Small nuclear ribonucleoprotein F

Chain B:



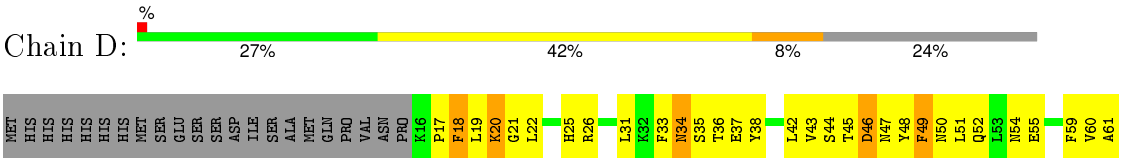
- Molecule 1: Small nuclear ribonucleoprotein F

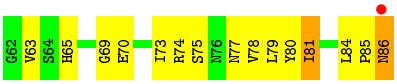
Chain C:



- Molecule 1: Small nuclear ribonucleoprotein F

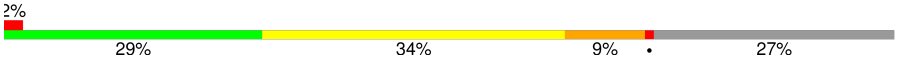
Chain D:

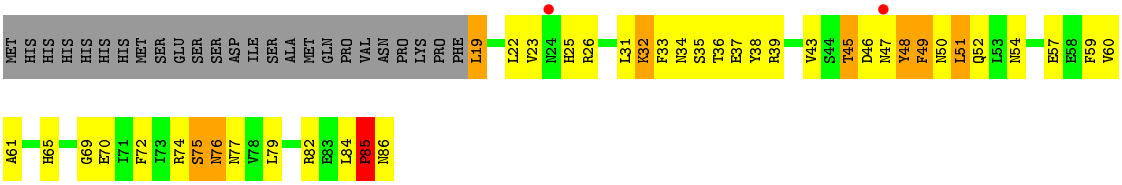




• Molecule 1: Small nuclear ribonucleoprotein F

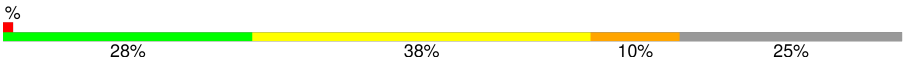
Chain E:

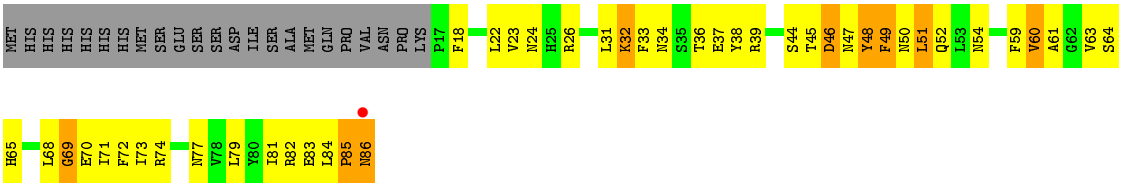




• Molecule 1: Small nuclear ribonucleoprotein F

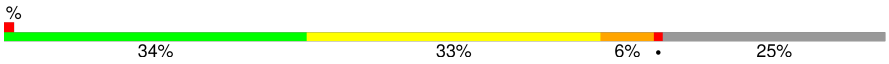
Chain F:

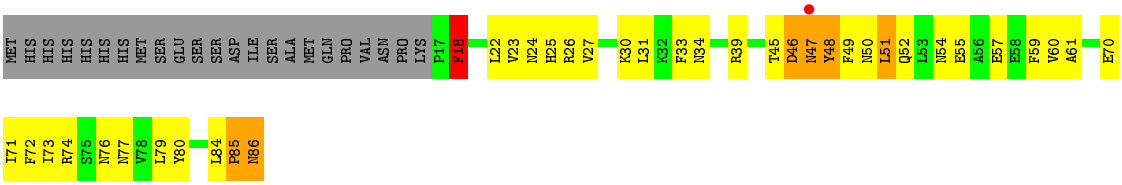




• Molecule 1: Small nuclear ribonucleoprotein F

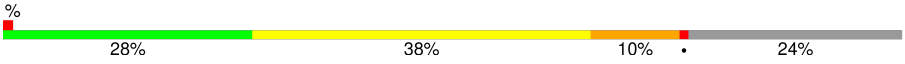
Chain G:





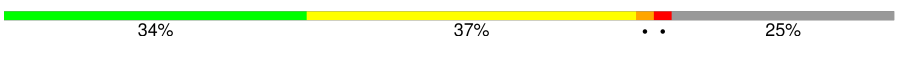
• Molecule 1: Small nuclear ribonucleoprotein F

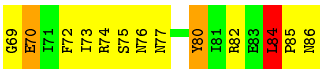
Chain H:



• Molecule 1: Small nuclear ribonucleoprotein F

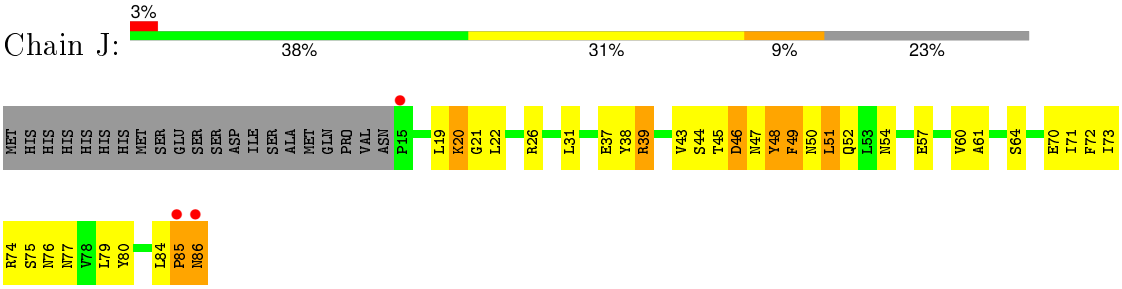
Chain I:





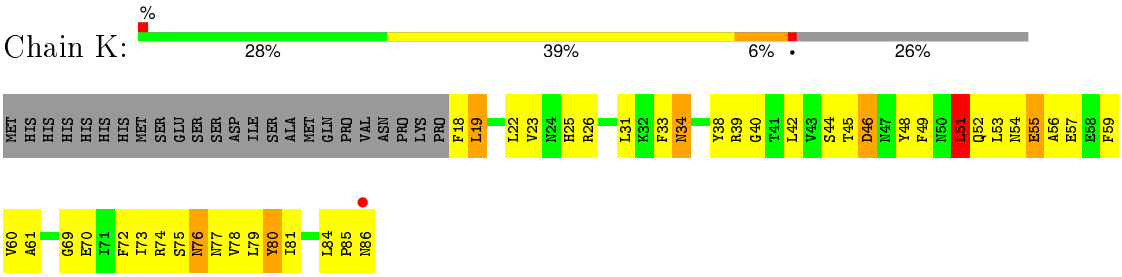
• Molecule 1: Small nuclear ribonucleoprotein F

Chain J:



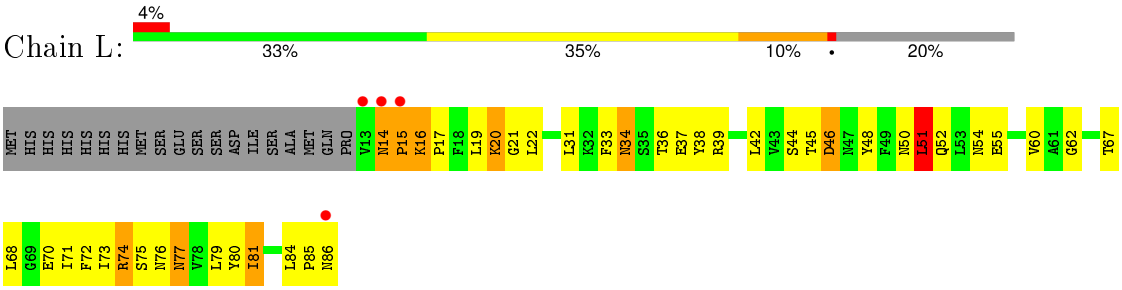
• Molecule 1: Small nuclear ribonucleoprotein F

Chain K:



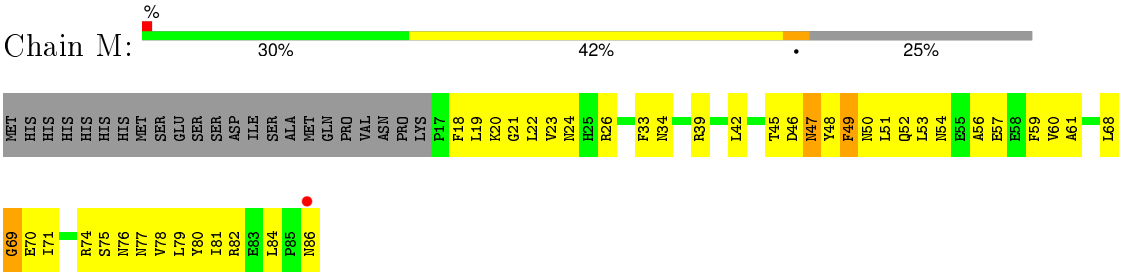
• Molecule 1: Small nuclear ribonucleoprotein F

Chain L:



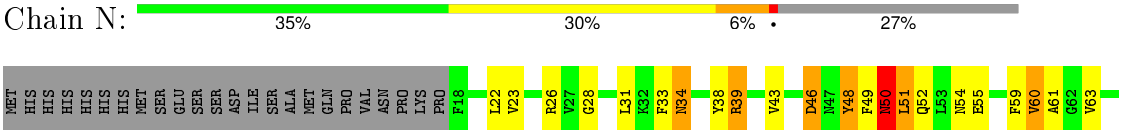
• Molecule 1: Small nuclear ribonucleoprotein F

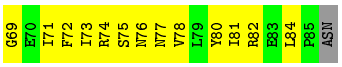
Chain M:



• Molecule 1: Small nuclear ribonucleoprotein F

Chain N:




G69
E70
I71
F72
I73
R74
S75
N76
N77
V78
L79
Y80
I81
R82
E83
L84
P85
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.64Å 105.64Å 235.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 46.32 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-3.50) 98.3 (46.32-3.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.51 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.292 , 0.297 0.255 , 0.259	Depositor DCC
R_{free} test set	876 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	108.6	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 86.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 17266 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7887	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.94	0/553	1.01	1/746 (0.1%)
1	B	0.91	0/553	1.06	0/746
1	C	1.02	2/605 (0.3%)	1.09	4/818 (0.5%)
1	D	1.12	1/582 (0.2%)	1.13	4/785 (0.5%)
1	E	1.05	0/553	1.19	2/746 (0.3%)
1	F	1.11	0/573	1.23	4/773 (0.5%)
1	G	1.15	1/573 (0.2%)	1.11	1/773 (0.1%)
1	H	1.26	2/582 (0.3%)	1.20	1/785 (0.1%)
1	I	1.11	0/573	1.17	3/773 (0.4%)
1	J	1.18	0/590	1.15	1/796 (0.1%)
1	K	1.10	0/565	1.21	3/762 (0.4%)
1	L	1.23	1/605 (0.2%)	1.22	3/818 (0.4%)
1	M	1.18	1/573 (0.2%)	1.16	0/773
1	N	1.20	1/556 (0.2%)	1.22	4/751 (0.5%)
All	All	1.12	9/8036 (0.1%)	1.16	31/10845 (0.3%)

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	I	0	1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	13	VAL	CB-CG2	7.20	1.68	1.52
1	C	13	VAL	N-CA	6.45	1.59	1.46
1	H	34	ASN	CB-CG	6.27	1.65	1.51
1	H	60	VAL	CB-CG2	-6.01	1.40	1.52
1	N	60	VAL	CB-CG2	-5.71	1.40	1.52

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	46	ASP	CB-CG-OD2	9.21	126.59	118.30
1	N	39	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	C	86	ASN	N-CA-C	-7.55	90.62	111.00
1	G	46	ASP	CB-CG-OD2	7.16	124.74	118.30
1	E	85	PRO	CA-C-N	-7.15	101.48	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	84	LEU	Peptide

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	544	0	538	51	0
1	B	544	0	538	43	0
1	C	593	0	589	46	0
1	D	571	0	567	61	0
1	E	544	0	538	46	0
1	F	562	0	555	51	2
1	G	562	0	555	60	0
1	H	571	0	567	50	2
1	I	562	0	555	49	0
1	J	578	0	575	62	2
1	K	555	0	547	56	0
1	L	593	0	589	49	2
1	M	562	0	555	47	0
1	N	546	0	541	42	0
All	All	7887	0	7809	599	4

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 38.

The worst 5 of 599 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:J:49:PHE:CZ	1:K:74:ARG:HG2	1.58	1.37
1:J:19:LEU:O	1:J:21:GLY:N	1.64	1.29
1:H:85:PRO:O	1:H:86:ASN:ND2	1.65	1.28
1:J:49:PHE:CD1	1:K:74:ARG:HD3	1.73	1.23
1:D:42:LEU:HD21	1:D:45:THR:OG1	1.41	1.19

All (4) 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	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:LYS:NZ	1:L:86:ASN:ND2[6_455]	1.83	0.37
1:F:83:GLU:OE1	1:J:20:LYS:NZ[4_555]	1.90	0.30
1:H:83:GLU:OE1	1:L:20:LYS:NZ[6_455]	2.01	0.19
1:F:83:GLU:OE2	1:J:20:LYS:NZ[4_555]	2.13	0.07

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	66/93 (71%)	57 (86%)	6 (9%)	3 (4%)	3 30
1	B	66/93 (71%)	57 (86%)	5 (8%)	4 (6%)	2 21
1	C	72/93 (77%)	60 (83%)	6 (8%)	6 (8%)	1 13
1	D	69/93 (74%)	56 (81%)	8 (12%)	5 (7%)	1 17
1	E	66/93 (71%)	53 (80%)	7 (11%)	6 (9%)	1 11
1	F	68/93 (73%)	58 (85%)	7 (10%)	3 (4%)	3 30
1	G	68/93 (73%)	59 (87%)	6 (9%)	3 (4%)	3 30
1	H	69/93 (74%)	61 (88%)	4 (6%)	4 (6%)	2 23
1	I	68/93 (73%)	57 (84%)	9 (13%)	2 (3%)	6 42
1	J	70/93 (75%)	62 (89%)	6 (9%)	2 (3%)	6 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	K	67/93 (72%)	54 (81%)	9 (13%)	4 (6%)	2 21
1	L	72/93 (77%)	59 (82%)	10 (14%)	3 (4%)	3 32
1	M	68/93 (73%)	58 (85%)	8 (12%)	2 (3%)	6 42
1	N	66/93 (71%)	58 (88%)	5 (8%)	3 (4%)	3 30
All	All	955/1302 (73%)	809 (85%)	96 (10%)	50 (5%)	2 25

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	LYS
1	B	85	PRO
1	C	47	ASN
1	C	84	LEU
1	D	20	LYS

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	59/84 (70%)	52 (88%)	7 (12%)	6 31
1	B	59/84 (70%)	50 (85%)	9 (15%)	3 21
1	C	65/84 (77%)	61 (94%)	4 (6%)	23 63
1	D	62/84 (74%)	60 (97%)	2 (3%)	46 80
1	E	59/84 (70%)	53 (90%)	6 (10%)	9 40
1	F	61/84 (73%)	56 (92%)	5 (8%)	14 51
1	G	61/84 (73%)	58 (95%)	3 (5%)	31 70
1	H	62/84 (74%)	54 (87%)	8 (13%)	5 27
1	I	61/84 (73%)	57 (93%)	4 (7%)	21 61
1	J	63/84 (75%)	58 (92%)	5 (8%)	15 53
1	K	60/84 (71%)	55 (92%)	5 (8%)	14 50
1	L	65/84 (77%)	60 (92%)	5 (8%)	16 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	61/84 (73%)	58 (95%)	3 (5%)	31 70
1	N	59/84 (70%)	56 (95%)	3 (5%)	29 69
All	All	857/1176 (73%)	788 (92%)	69 (8%)	15 52

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	74	ARG
1	H	26	ARG
1	M	49	PHE
1	F	86	ASN
1	G	86	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	76	ASN
1	J	76	ASN
1	M	34	ASN
1	F	77	ASN
1	H	34	ASN

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

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, 95^{th} 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	68/93 (73%)	0.11	3 (4%) 38 29	36, 48, 62, 68	0
1	B	68/93 (73%)	-0.11	1 (1%) 76 67	32, 48, 65, 70	0
1	C	74/93 (79%)	0.13	3 (4%) 41 32	34, 47, 64, 72	0
1	D	71/93 (76%)	-0.29	1 (1%) 78 68	30, 48, 60, 65	0
1	E	68/93 (73%)	-0.08	2 (2%) 55 45	32, 47, 62, 65	0
1	F	70/93 (75%)	-0.23	1 (1%) 78 68	26, 47, 61, 70	0
1	G	70/93 (75%)	-0.09	1 (1%) 78 68	35, 48, 63, 66	0
1	H	71/93 (76%)	-0.08	1 (1%) 78 68	31, 43, 59, 64	0
1	I	70/93 (75%)	-0.28	0 100 100	30, 43, 58, 66	0
1	J	72/93 (77%)	-0.18	3 (4%) 40 31	30, 45, 59, 61	0
1	K	69/93 (74%)	-0.23	1 (1%) 78 68	33, 47, 59, 62	0
1	L	74/93 (79%)	-0.14	4 (5%) 29 23	31, 43, 56, 63	0
1	M	70/93 (75%)	-0.30	1 (1%) 78 68	29, 42, 59, 65	0
1	N	68/93 (73%)	-0.33	0 100 100	28, 43, 62, 68	0
All	All	983/1302 (75%)	-0.15	22 (2%) 65 55	26, 46, 62, 72	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	13	VAL	8.4
1	C	86	ASN	6.0
1	L	86	ASN	5.7
1	J	86	ASN	5.6
1	K	86	ASN	3.8

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 carbohydrates 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.