wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2HGN
Title	:	NMR structure of the third qRRM domain of human hnRNP F
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This is a wwPDB NMR 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

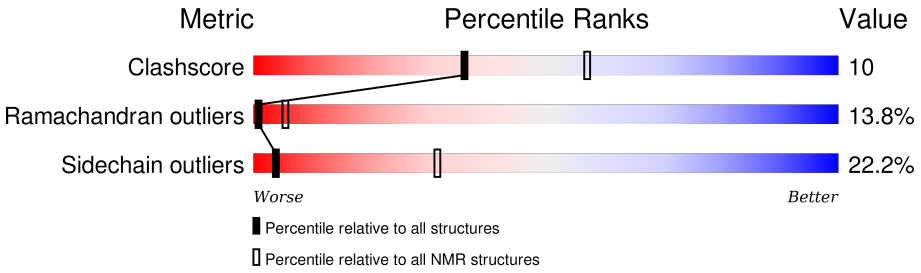
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	139	28% 22% 5% • • 42%

2 Ensemble composition and analysis

This entry contains 15 models. Model 4 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:289-A:365 (77)	0.32	4

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12
2	13, 14, 15
Single-model clusters	1

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1237 atoms, of which 602 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Heterogeneous nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	81	1237	396	602	114	121	4	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	CLONING ARTIFACT	UNP P52597
A	244	GLY	-	CLONING ARTIFACT	UNP P52597
A	245	SER	-	CLONING ARTIFACT	UNP P52597
A	246	SER	-	CLONING ARTIFACT	UNP P52597
A	247	HIS	-	EXPRESSION TAG	UNP P52597
A	248	HIS	-	EXPRESSION TAG	UNP P52597
A	249	HIS	-	EXPRESSION TAG	UNP P52597
A	250	HIS	-	EXPRESSION TAG	UNP P52597
A	251	HIS	-	EXPRESSION TAG	UNP P52597
A	252	HIS	-	EXPRESSION TAG	UNP P52597
A	253	SER	-	CLONING ARTIFACT	UNP P52597
A	254	SER	-	CLONING ARTIFACT	UNP P52597
A	255	GLY	-	CLONING ARTIFACT	UNP P52597
A	256	LEU	-	CLONING ARTIFACT	UNP P52597
A	257	VAL	-	CLONING ARTIFACT	UNP P52597
A	258	PRO	-	CLONING ARTIFACT	UNP P52597
A	259	ARG	-	CLONING ARTIFACT	UNP P52597
A	260	GLY	-	CLONING ARTIFACT	UNP P52597
A	261	SER	-	CLONING ARTIFACT	UNP P52597
A	262	HIS	-	CLONING ARTIFACT	UNP P52597
A	263	MET	-	CLONING ARTIFACT	UNP P52597
A	264	ALA	-	CLONING ARTIFACT	UNP P52597
A	265	SER	-	CLONING ARTIFACT	UNP P52597
A	266	MET	-	CLONING ARTIFACT	UNP P52597
A	267	THR	-	CLONING ARTIFACT	UNP P52597
A	268	GLY	-	CLONING ARTIFACT	UNP P52597
A	269	GLY	-	CLONING ARTIFACT	UNP P52597
A	270	GLN	-	CLONING ARTIFACT	UNP P52597
A	271	GLN	-	CLONING ARTIFACT	UNP P52597
A	272	MET	-	CLONING ARTIFACT	UNP P52597
A	273	GLY	-	CLONING ARTIFACT	UNP P52597

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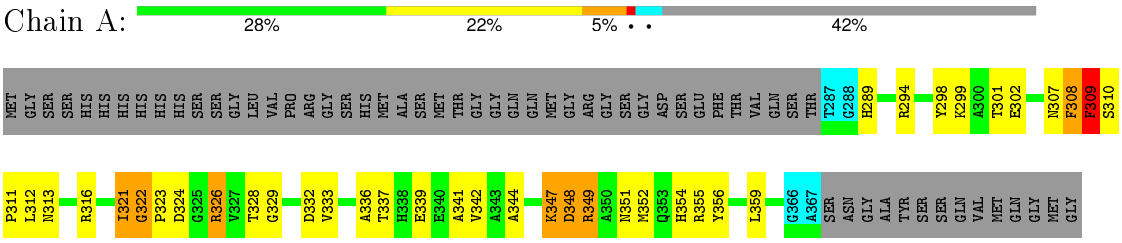
Chain	Residue	Modelled	Actual	Comment	Reference
A	274	ARG	-	CLONING ARTIFACT	UNP P52597
A	275	GLY	-	CLONING ARTIFACT	UNP P52597
A	276	SER	-	CLONING ARTIFACT	UNP P52597

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

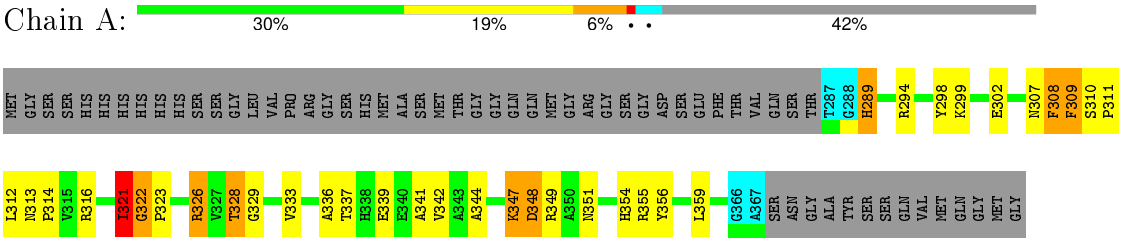
- Molecule 1: Heterogeneous nuclear ribonucleoprotein F



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: Heterogeneous nuclear ribonucleoprotein F



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
Cyana	structure solution	2.1
AMBER	refinement	7.0

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 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 (average) 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	0.75±0.01	0±0/631 (0.0±0.0%)	1.41±0.03	6±2/857 (0.7±0.2%)
All	All	0.75	0/9465 (0.0%)	1.41	84/12855 (0.7%)

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	Planarity
1	A	0.0±0.0	6.0±1.3
All	All	0	90

There are no bond-length outliers.

5 of 21 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	326	ARG	NE-CZ-NH1	9.66	125.13	120.30	13	11
1	A	294	ARG	NE-CZ-NH1	7.95	124.27	120.30	4	11
1	A	349	ARG	NE-CZ-NH1	7.66	124.13	120.30	5	6
1	A	308	PHE	CB-CG-CD1	-6.65	116.14	120.80	8	1
1	A	361	LEU	CB-CG-CD1	6.55	122.14	111.00	15	1

There are no chirality outliers.

5 of 24 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	349	ARG	Peptide,Sidechain	15
1	A	336	ALA	Peptide	15
1	A	309	PHE	Sidechain,Peptide	10

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	351	ASN	Peptide	5
1	A	362	ASN	Peptide	4

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	615	584	584	12±2
All	All	9225	8760	8760	184

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 10.

5 of 36 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:309:PHE:CD1	1:A:344:ALA:HB1	0.75	2.16	10	15
1:A:309:PHE:CE1	1:A:359:LEU:HD22	0.69	2.22	13	8
1:A:312:LEU:HD11	1:A:344:ALA:HB2	0.64	1.69	10	15
1:A:312:LEU:CD1	1:A:344:ALA:HB2	0.62	2.25	13	14
1:A:308:PHE:CZ	1:A:359:LEU:HD11	0.59	2.33	11	13

6.3 Torsion angles

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	77/139 (55%)	54±2 (70±3%)	13±2 (17±3%)	11±2 (14±2%)	1 5
All	All	1155/2085 (55%)	804 (70%)	192 (17%)	159 (14%)	1 5

5 of 22 unique Ramachandran outliers are listed below. They are sorted by the frequency of

occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	337	THR	15
1	A	348	ASP	15
1	A	322	GLY	15
1	A	311	PRO	13
1	A	354	HIS	13

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	66/112 (59%)	51±2 (78±3%)	15±2 (22±3%)	4	31
All	All	990/1680 (59%)	770 (78%)	220 (22%)	4	31

5 of 31 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	302	GLU	15
1	A	347	LYS	15
1	A	307	ASN	15
1	A	308	PHE	15
1	A	309	PHE	15

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided