



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9H45  
Title : Crystal Structure of Hfq V22A  
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Deposited on : 2024-10-17  
Resolution : 2.08 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](mailto: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>.

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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	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40



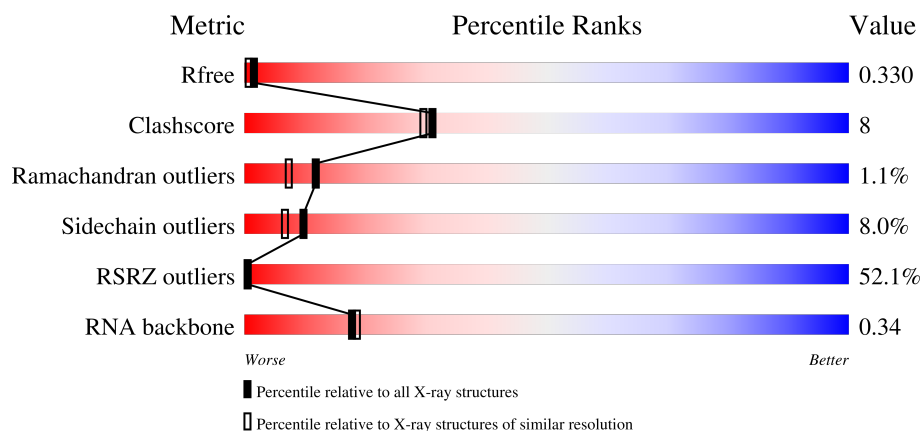
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	7574 (2.10-2.06)
Clashscore	180529	8325 (2.10-2.06)
Ramachandran outliers	177936	8271 (2.10-2.06)
Sidechain outliers	177891	8272 (2.10-2.06)
RSRZ outliers	164620	7574 (2.10-2.06)
RNA backbone	3690	1067 (2.46-1.70)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	102	<div> <div>37%</div> <div>49%</div> <div>14%</div> <div>•</div> <div>36%</div> </div>
1	B	102	<div> <div>25%</div> <div>46%</div> <div>15%</div> <div>•</div> <div>38%</div> </div>
1	C	102	<div> <div>37%</div> <div>48%</div> <div>13%</div> <div>•</div> <div>38%</div> </div>
1	D	102	<div> <div>39%</div> <div>42%</div> <div>17%</div> <div>•</div> <div>40%</div> </div>

*Continued on next page...*



Mol	Chain	Length	Quality of chain
1	E	102	<p>35% 43% 15% 38%</p>
1	F	102	<p>28% 47% 15% 37%</p>
2	Q	18	<p>28% 61% 11%</p>





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 RNA-binding protein Hfq.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total 517	C 332	N 91	O 93	S 1	0	0	0
1	B	63	Total 502	C 324	N 88	O 89	S 1	0	0	0
1	C	63	Total 502	C 324	N 88	O 89	S 1	0	0	0
1	D	61	Total 491	C 318	N 86	O 86	S 1	0	0	0
1	E	63	Total 502	C 324	N 88	O 89	S 1	0	0	0
1	F	64	Total 525	C 339	N 94	O 91	S 1	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	VAL	engineered mutation	UNP P0A6X3
B	22	ALA	VAL	engineered mutation	UNP P0A6X3
C	22	ALA	VAL	engineered mutation	UNP P0A6X3
D	22	ALA	VAL	engineered mutation	UNP P0A6X3
E	22	ALA	VAL	engineered mutation	UNP P0A6X3
F	22	ALA	VAL	engineered mutation	UNP P0A6X3

- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP\*AP)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	18	Total 396	C 180	N 90	O 108	P 18	0	0	0

- Molecule 3 is water.



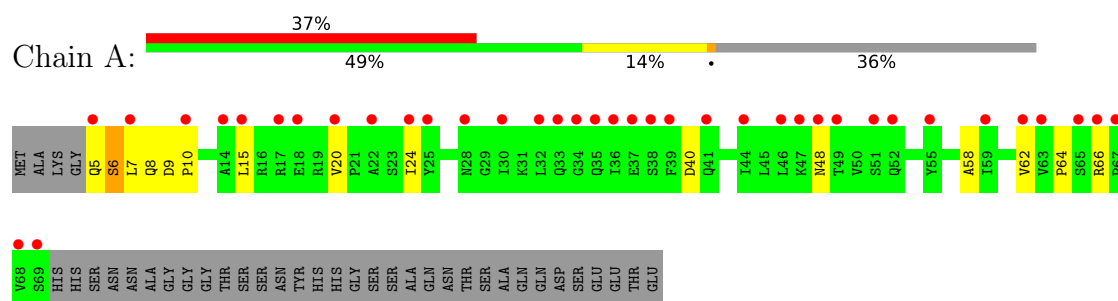
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total 36	O 36	0	0
3	B	39	Total 39	O 39	0	0
3	C	31	Total 31	O 31	0	0
3	D	38	Total 38	O 38	0	0
3	E	41	Total 41	O 41	0	0
3	F	43	Total 43	O 43	0	0
3	Q	54	Total 54	O 54	0	0



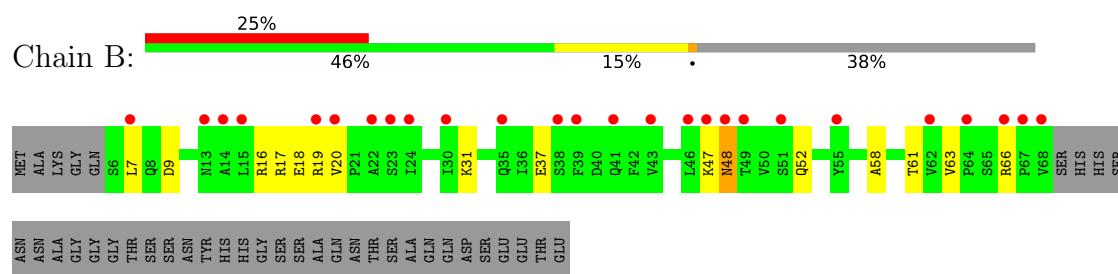
### 3 Residue-property plots

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. 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. 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.

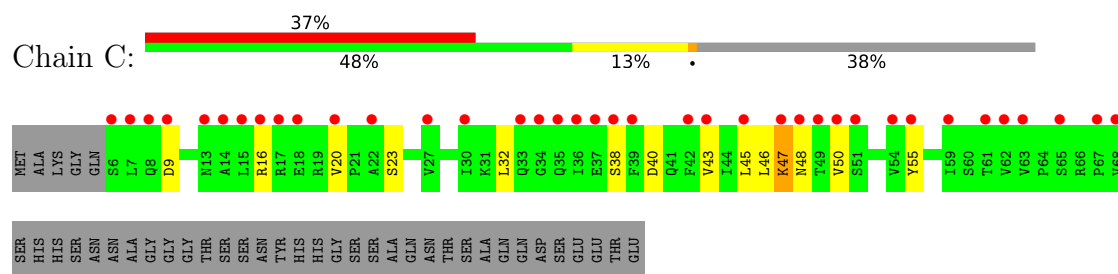
#### • Molecule 1: RNA-binding protein Hfq



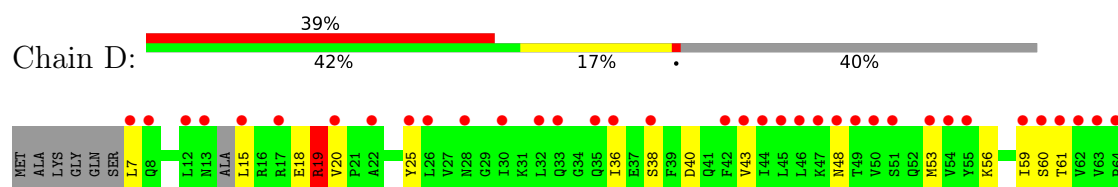
#### • Molecule 1: RNA-binding protein Hfq



#### • Molecule 1: RNA-binding protein Hfq



#### • Molecule 1: RNA-binding protein Hfq









## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.25Å 67.15Å 84.58Å 90.00° 104.64° 90.00°	Depositor
Resolution (Å)	56.24 – 2.08 56.24 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.0 (56.24-2.08) 99.1 (56.24-2.08)	Depositor EDS
$R_{merge}$	0.51	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.08Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.274 , 0.323 0.290 , 0.330	Depositor DCC
$R_{free}$ test set	1879 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	3717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.29	0/526	0.54	0/713
1	B	0.33	0/511	0.57	0/693
1	C	0.47	0/511	0.73	0/693
1	D	0.55	0/499	0.70	0/675
1	E	0.44	0/511	0.65	0/693
1	F	0.47	0/540	0.71	0/730
2	Q	0.40	0/449	1.10	5/698 (0.7%)
All	All	0.43	0/3547	0.74	5/4895 (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	D	0	1
1	E	0	2
All	All	0	3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	4	A	P-O3'-C3'	-7.62	110.55	119.70
2	Q	18	A	OP1-P-OP2	-7.25	108.72	119.60
2	Q	17	A	OP1-P-O3'	6.47	119.43	105.20
2	Q	13	A	P-O3'-C3'	-6.43	111.98	119.70
2	Q	10	A	P-O3'-C3'	-6.04	112.45	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	D	19	ARG	Sidechain
1	E	16	ARG	Sidechain
1	E	66	ARG	Sidechain

## 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	517	0	539	14	0
1	B	502	0	526	7	0
1	C	502	0	526	10	0
1	D	491	0	515	13	0
1	E	502	0	526	9	0
1	F	525	0	560	13	0
2	Q	396	0	199	2	0
3	A	36	0	0	3	0
3	B	39	0	0	1	1
3	C	31	0	0	1	0
3	D	38	0	0	4	0
3	E	41	0	0	1	1
3	F	43	0	0	0	0
3	Q	54	0	0	1	0
All	All	3717	0	3391	55	1

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 8.

The worst 5 of 55 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:F:15:LEU:HD13	1:F:20:VAL:HG13	1.47	0.94
1:F:68:VAL:HG23	1:F:68:VAL:O	1.93	0.69
1:A:7:LEU:HD13	1:C:45:LEU:HD21	1.77	0.67
1:F:15:LEU:HD13	1:F:20:VAL:CG1	2.25	0.64
1:A:7:LEU:HD23	1:C:40:ASP:HB3	1.85	0.59

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-



metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:211:HOH:O	3:E:229:HOH:O[1_545]	1.96	0.24

## 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	63/102 (62%)	60 (95%)	2 (3%)	1 (2%)	8	4
1	B	61/102 (60%)	58 (95%)	2 (3%)	1 (2%)	8	4
1	C	61/102 (60%)	59 (97%)	1 (2%)	1 (2%)	8	4
1	D	57/102 (56%)	54 (95%)	3 (5%)	0	100	100
1	E	61/102 (60%)	58 (95%)	2 (3%)	1 (2%)	8	4
1	F	64/102 (63%)	61 (95%)	3 (5%)	0	100	100
All	All	367/612 (60%)	350 (95%)	13 (4%)	4 (1%)	12	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	ASN
1	A	48	ASN
1	B	48	ASN
1	E	48	ASN

### 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	60/88 (68%)	58 (97%)	2 (3%)	33	34
1	B	58/88 (66%)	52 (90%)	6 (10%)	6	3
1	C	58/88 (66%)	53 (91%)	5 (9%)	8	5
1	D	57/88 (65%)	52 (91%)	5 (9%)	8	5
1	E	58/88 (66%)	52 (90%)	6 (10%)	6	3
1	F	61/88 (69%)	56 (92%)	5 (8%)	9	6
All	All	352/528 (67%)	323 (92%)	29 (8%)	10	6

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	18	GLU
1	F	37	GLU
1	D	60	SER
1	F	17[A]	ARG
1	D	40	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Q	17/18 (94%)	7 (41%)	0

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Q	2	A
2	Q	5	A
2	Q	8	A
2	Q	9	A
2	Q	11	A

There are no RNA pucker outliers to report.



## 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 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](#)

**Warning:** The R factor obtained from EDS is 0.3321, which does not match the depositor's R factor of 0.274. Please interpret the results in this section carefully.

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	65/102 (63%)	2.25	38 (58%) 0 0	10, 26, 47, 79	0
1	B	63/102 (61%)	2.11	26 (41%) 1 1	8, 21, 43, 64	0
1	C	63/102 (61%)	2.45	38 (60%) 0 0	6, 24, 41, 54	0
1	D	61/102 (59%)	2.43	40 (65%) 0 0	4, 25, 41, 55	0
1	E	63/102 (61%)	2.27	36 (57%) 0 0	10, 23, 44, 65	0
1	F	64/102 (62%)	2.12	29 (45%) 1 1	9, 24, 44, 71	2 (3%)
2	Q	18/18 (100%)	1.09	0 100 100	15, 24, 29, 30	0
All	All	397/630 (63%)	2.22	207 (52%) 0 0	4, 24, 47, 79	2 (0%)

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	VAL	6.7
1	C	68	VAL	6.7
1	A	68	VAL	6.0
1	D	49	THR	5.9
1	E	6	SER	5.9

### 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.