



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:58 PM GMT

PDB ID : 4QI2  
Title : X-ray structure of the ROQ domain from murine Roquin-1 in complex with a 23-mer Tnf-CDE RNA  
Authors : Janowski, R.; Schlundt, A.; Sattler, M.; Niessing, D.  
Deposited on : 2014-05-30  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
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

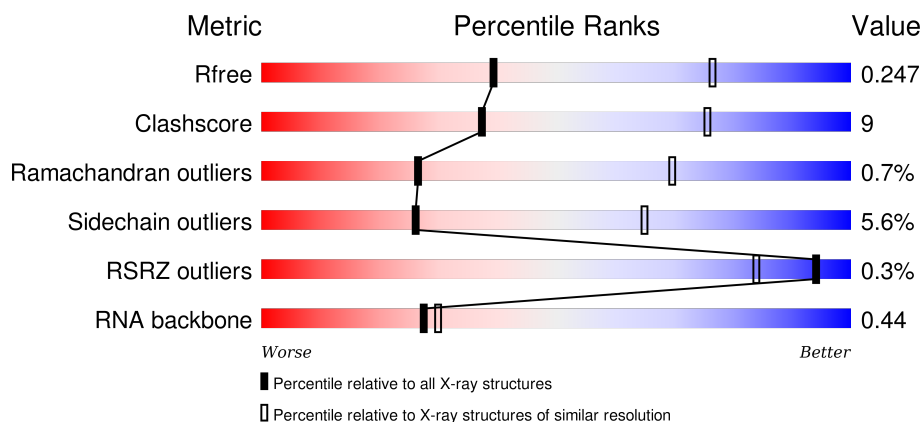
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	180	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 15%, orange 15%, yellow 12%, green 71%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>15%</span> <span>12%</span> <span>71%</span> </div> </div>
1	B	180	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 15%, orange 15%, yellow 17%, green 64%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>15%</span> <span>17%</span> <span>64%</span> </div> </div>
1	C	180	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 16%, orange 12%, yellow 12%, green 71%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>16%</span> <span>12%</span> <span>71%</span> </div> </div>
1	D	180	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 14%, orange 14%, yellow 14%, green 69%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>14%</span> <span>14%</span> <span>69%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
2	E	23	<div><div></div><div>30%30%17%•17%</div></div>
2	F	23	<div><div></div><div>30%26%17%•22%</div></div>
2	G	23	<div><div></div><div>35%35%9%•17%</div></div>
2	H	23	<div><div></div><div>35%30%•9%22%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6546 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 Roquin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1224	770	223	225	6			
1	B	153	Total	C	N	O	S	0	0	0
			1224	770	223	225	6			
1	C	152	Total	C	N	O	S	0	0	0
			1214	764	220	224	6			
1	D	154	Total	C	N	O	S	0	0	0
			1233	775	225	227	6			

- Molecule 2 is a RNA chain called RNA (5'-R(\*AP\*CP\*AP\*UP\*GP\*UP\*UP\*UP\*UP\*CP\*UP\*GP\*UP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	19	Total	C	N	O	P	0	0	0
			405	181	70	135	19			
2	F	18	Total	C	N	O	P	0	0	0
			383	171	65	129	18			
2	G	19	Total	C	N	O	P	0	0	0
			405	181	70	135	19			
2	H	18	Total	C	N	O	P	0	2	0
			426	190	72	144	20			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	7	Total	O	0	0
			7	7		
3	C	5	Total	O	0	0
			5	5		
3	D	5	Total	O	0	0
			5	5		

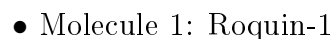
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	3	Total 3	O 3	0	0
3	F	3	Total 3	O 3	0	0
3	G	1	Total 1	O 1	0	0
3	H	1	Total 1	O 1	0	0

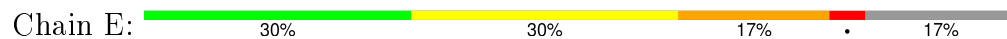


- Molecule 1: Roquin-1

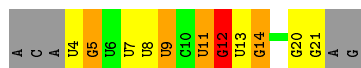
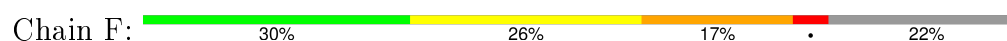




- Molecule 2: RNA (5'-R(\*AP\*CP\*AP\*UP\*GP\*UP\*UP\*UP\*UP\*CP\*UP\*GP\*UP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*AP\*G)-3')



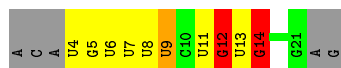
- Molecule 2: RNA (5'-R(\*AP\*CP\*AP\*UP\*GP\*UP\*UP\*UP\*UP\*CP\*UP\*GP\*UP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*AP\*G)-3')



- Molecule 2: RNA (5'-R(\*AP\*CP\*AP\*UP\*GP\*UP\*UP\*UP\*UP\*CP\*UP\*GP\*UP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*AP\*G)-3')



- Molecule 2: RNA (5'-R(\*AP\*CP\*AP\*UP\*GP\*UP\*UP\*UP\*UP\*CP\*UP\*GP\*UP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*AP\*G)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.56Å 60.41Å 84.37Å 105.68° 101.36° 95.72°	Depositor
Resolution (Å)	50.00 – 3.00 41.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-3.00) 86.6 (41.00-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.203 , 0.247 0.209 , 0.247	Depositor DCC
$R_{free}$ test set	1020 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.6	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19951 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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	0.65	0/1245	0.77	0/1677
1	B	0.61	0/1245	0.75	0/1677
1	C	0.58	0/1234	0.76	0/1662
1	D	0.58	0/1254	0.75	0/1689
2	E	0.58	0/452	0.92	1/702 (0.1%)
2	F	0.55	0/427	0.93	1/663 (0.2%)
2	G	0.57	0/452	0.90	2/702 (0.3%)
2	H	0.55	0/475	0.93	2/738 (0.3%)
All	All	0.60	0/6784	0.81	6/9510 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	12	G	C4'-C3'-O3'	5.98	124.95	113.00
2	H	14	G	O5'-P-OP2	-5.90	100.39	105.70
2	G	12	G	C4'-C3'-O3'	5.75	124.49	113.00
2	F	12	G	C4'-C3'-O3'	5.52	124.05	113.00
2	H	12	G	C4'-C3'-O3'	5.50	124.00	113.00

There are no chirality outliers.

There are no planarity outliers.

### 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	1224	0	1240	17	0
1	B	1224	0	1240	23	0
1	C	1214	0	1233	15	0
1	D	1233	0	1248	25	0
2	E	405	0	203	11	0
2	F	383	0	192	9	0
2	G	405	0	203	7	0
2	H	426	0	213	21	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	E	3	0	0	1	0
3	F	3	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	6546	0	5772	114	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 9.

The worst 5 of 114 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)
2:E:21:G:OP2	2:E:21:G:C8	1.66	1.46
2:E:21:G:OP2	2:E:21:G:H8	0.78	1.12
2:H:4[B]:U:O2	2:H:4[B]:U:H5'	1.63	0.98
2:H:4[B]:U:O2	2:H:4[B]:U:C5'	2.26	0.83
1:D:188:ARG:HH22	2:H:5[A]:G:H5'	1.52	0.74

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	151/180 (84%)	141 (93%)	9 (6%)	1 (1%)	26	70
1	B	151/180 (84%)	142 (94%)	8 (5%)	1 (1%)	26	70
1	C	150/180 (83%)	140 (93%)	9 (6%)	1 (1%)	26	70
1	D	152/180 (84%)	144 (95%)	7 (5%)	1 (1%)	26	70
All	All	604/720 (84%)	567 (94%)	33 (6%)	4 (1%)	26	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	PRO
1	B	176	PRO
1	C	176	PRO
1	D	176	PRO

### 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	134/156 (86%)	127 (95%)	7 (5%)	29	68
1	B	134/156 (86%)	125 (93%)	9 (7%)	20	57
1	C	133/156 (85%)	126 (95%)	7 (5%)	28	67
1	D	135/156 (86%)	128 (95%)	7 (5%)	29	68
All	All	536/624 (86%)	506 (94%)	30 (6%)	26	65

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

Mol	Chain	Res	Type
1	B	285	SER
1	C	188	ARG
1	D	275	THR
1	B	312	SER
1	C	208	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	318	GLN
1	C	193	GLN
1	D	236	GLN
1	B	289	GLN
1	D	289	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	18/23 (78%)	6 (33%)	1 (5%)
2	F	17/23 (73%)	6 (35%)	1 (5%)
2	G	18/23 (78%)	6 (33%)	1 (5%)
2	H	16/23 (69%)	4 (25%)	1 (6%)
All	All	69/92 (75%)	22 (31%)	4 (5%)

5 of 22 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	9	U
2	E	11	U
2	E	13	U
2	E	14	G
2	E	20	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	12	G
2	F	12	G
2	G	12	G
2	H	12	G

## 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 [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](#)

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	153/180 (85%)	-0.46	0 100 100	53, 69, 93, 144	13 (8%)
1	B	153/180 (85%)	-0.38	1 (0%) 89 70	50, 71, 95, 149	14 (9%)
1	C	152/180 (84%)	-0.32	0 100 100	59, 80, 106, 148	26 (17%)
1	D	154/180 (85%)	-0.37	1 (0%) 90 73	59, 82, 111, 166	36 (23%)
2	E	19/23 (82%)	-0.31	0 100 100	62, 72, 128, 137	1 (5%)
2	F	18/23 (78%)	-0.52	0 100 100	62, 71, 141, 146	0
2	G	19/23 (82%)	-0.52	0 100 100	71, 85, 157, 164	0
2	H	18/23 (78%)	-0.49	0 100 100	66, 75, 96, 151	0
All	All	686/812 (84%)	-0.39	2 (0%) 94 84	50, 75, 111, 166	90 (13%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	234	PHE	2.6
1	B	296	LEU	2.1

### 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.