



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2023 – 05:52 AM EDT

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

<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 : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

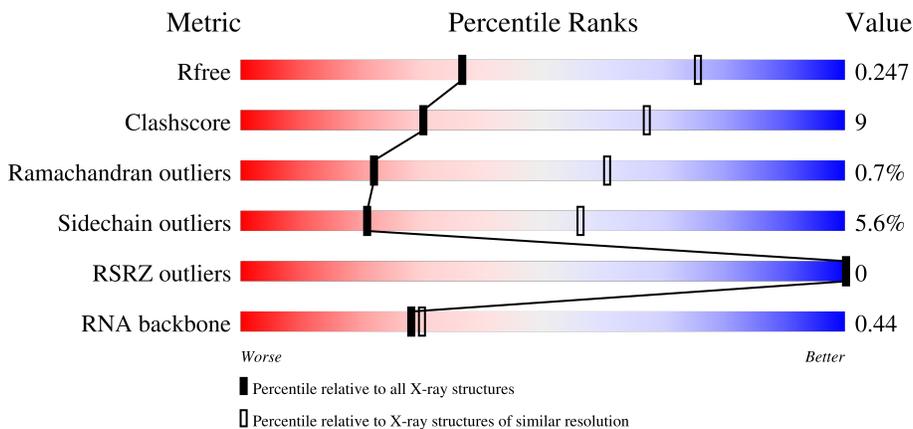
# 1 Overall quality at a glance

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.



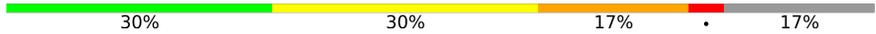
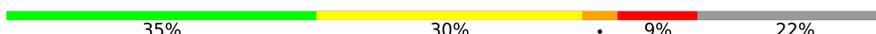
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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  $\leq 5\%$ . 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	 71% 12% • 15%
1	B	180	 64% 17% • 15%
1	C	180	 71% 12% • 16%
1	D	180	 69% 14% • 14%

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Mol	Chain	Length	Quality of chain
2	E	23	 30% 30% 17% . 17%
2	F	23	 30% 26% 17% . 22%
2	G	23	 35% 35% 9% . 17%
2	H	23	 35% 30% . 9% 22%

## 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
			Total	C	N	O	S			
1	A	153	Total 1224	C 770	N 223	O 225	S 6	0	0	0
1	B	153	Total 1224	C 770	N 223	O 225	S 6	0	0	0
1	C	152	Total 1214	C 764	N 220	O 224	S 6	0	0	0
1	D	154	Total 1233	C 775	N 225	O 227	S 6	0	0	0

- 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
			Total	C	N	O	P			
2	E	19	Total 405	C 181	N 70	O 135	P 19	0	0	0
2	F	18	Total 383	C 171	N 65	O 129	P 18	0	0	0
2	G	19	Total 405	C 181	N 70	O 135	P 19	0	0	0
2	H	18	Total 426	C 190	N 72	O 144	P 20	0	2	0

- Molecule 3 is water.

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

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

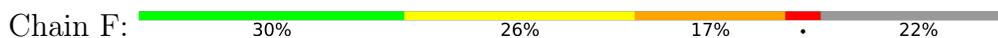




- Molecule 2: RNA (5'-R(\*AP\*CP\*AP\*UP\*GP\*UP\*UP\*UP\*UP\*CP\*UP\*GP\*UP\*GP\*AP\*AP\*AP\*AP\*CP\*GP\*GP\*AP\*G)-3')



- 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) 95.8 (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)	Xtrriage
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 (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.6	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage'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, 0.333 respectively for untwinned datasets, and 0.375, 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:C8	2:E:21:G:OP2	1.66	1.46
2:E:21:G:OP2	2:E:21:G:H8	0.78	1.12
2:H:4[B]:U:H5'	2:H:4[B]:U:O2	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%)	22	60
1	B	151/180 (84%)	142 (94%)	8 (5%)	1 (1%)	22	60
1	C	150/180 (83%)	140 (93%)	9 (6%)	1 (1%)	22	60
1	D	152/180 (84%)	144 (95%)	7 (5%)	1 (1%)	22	60
All	All	604/720 (84%)	567 (94%)	33 (6%)	4 (1%)	22	60

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 [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	134/156 (86%)	127 (95%)	7 (5%)	23	59
1	B	134/156 (86%)	125 (93%)	9 (7%)	16	49
1	C	133/156 (85%)	126 (95%)	7 (5%)	22	58
1	D	135/156 (86%)	128 (95%)	7 (5%)	23	59
All	All	536/624 (86%)	506 (94%)	30 (6%)	21	56

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

Mol	Chain	Res	Type
1	B	301	ASP
1	D	275	THR
1	C	208	LEU
1	D	301	ASP
1	D	229	ARG

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

such sidechains are listed below:

Mol	Chain	Res	Type
1	D	193	GLN
1	D	302	GLN
1	D	318	GLN
1	D	289	GLN
1	B	318	GLN

### 5.3.3 RNA [i](#)

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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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%)	-0.52	0 100 100	53, 69, 93, 144	13 (8%)
1	B	153/180 (85%)	-0.48	0 100 100	50, 71, 95, 149	14 (9%)
1	C	152/180 (84%)	-0.42	0 100 100	59, 80, 106, 148	26 (17%)
1	D	154/180 (85%)	-0.40	0 100 100	59, 82, 111, 166	36 (23%)
2	E	19/23 (82%)	-0.70	0 100 100	62, 72, 128, 137	1 (5%)
2	F	18/23 (78%)	-0.71	0 100 100	62, 71, 141, 146	0
2	G	19/23 (82%)	-0.83	0 100 100	71, 85, 157, 164	0
2	H	18/23 (78%)	-0.75	0 100 100	66, 75, 96, 151	0
All	All	686/812 (84%)	-0.49	0 100 100	50, 75, 111, 166	90 (13%)

There are no RSRZ outliers to report.

### 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.