



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 10:55 PM UTC

PDB ID : 5F5F / pdb_00005f5f
Title : X-ray structure of Roquin ROQ domain in complex with a Selex-derived hexa-loop RNA motif
Authors : Janowski, R.; Schlundt, A.; Sattler, M.; Niessing, D.
Deposited on : 2015-12-04
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

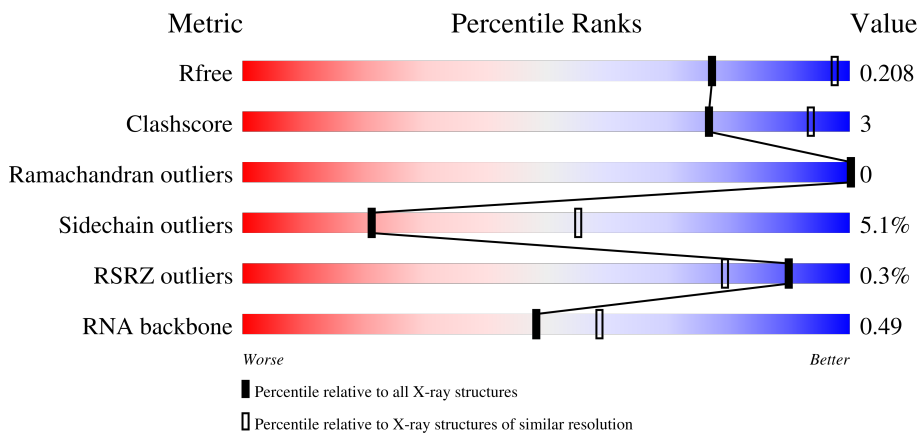
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 ≥ 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	190	 69% 9% • 20%
1	C	190	 69% 9% •• 20%
1	E	190	 72% 6% • 20%
1	G	190	 69% 7% • 22%

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Mol	Chain	Length	Quality of chain
2	B	20	 75% 15% 10%
2	D	20	 65% 30% 5%
2	F	20	 60% 35% 5%
2	H	20	 75% 25%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6577 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	152	Total 1212	C 763	N 219	O 224	S 6	0	0	0
1	C	152	Total 1215	C 765	N 219	O 225	S 6	0	1	0
1	E	152	Total 1212	C 763	N 219	O 224	S 6	0	0	0
1	G	148	Total 1181	C 745	N 213	O 217	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	20	Total 427	C 190	N 72	O 145	P 20	0	0	0
2	D	20	Total 427	C 190	N 72	O 145	P 20	0	0	0
2	F	20	Total 427	C 190	N 72	O 145	P 20	0	0	0
2	H	20	Total 427	C 190	N 72	O 145	P 20	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total 15	O 15	0	0
3	B	9	Total 9	O 9	0	0
3	C	11	Total 11	O 11	0	0
3	D	5	Total 5	O 5	0	0

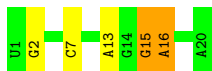
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	3	Total O 3 3	0	0
3	F	4	Total O 4 4	0	0
3	H	2	Total O 2 2	0	0

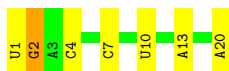
- Molecule 2: RNA (5'-R(P*UP*GP*AP*CP*UP*GP*CP*GP*UP*UP*UP*UP*AP*GP*GP*AP*GP*UP*UP*A)-3')

Chain B:  75% 15% 10%



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

Chain D:  65% 30% 5%



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

Chain F:  60% 35% 5%



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

Chain H:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.90Å 89.30Å 144.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.00) 99.9 (50.00-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.183 , 0.234 (Not available) , 0.208	Depositor DCC
R_{free} test set	952 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6577	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5026e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.11	1/1232 (0.1%)	1.11	4/1660 (0.2%)
1	C	1.14	2/1238 (0.2%)	1.18	7/1668 (0.4%)
1	E	1.02	2/1232 (0.2%)	1.17	5/1660 (0.3%)
1	G	0.91	1/1200 (0.1%)	1.09	3/1615 (0.2%)
2	B	0.70	1/476 (0.2%)	1.04	3/738 (0.4%)
2	D	0.58	0/476	0.96	1/738 (0.1%)
2	F	0.53	0/476	1.00	2/738 (0.3%)
2	H	0.48	0/476	0.96	2/738 (0.3%)
All	All	0.95	7/6806 (0.1%)	1.10	27/9555 (0.3%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	177	GLN	N-CA	5.68	1.53	1.46
1	G	236	GLN	CA-C	5.53	1.60	1.52
2	B	15	G	O3'-P	-5.30	1.53	1.61
1	C	199	MET	SD-CE	5.30	1.92	1.79
1	C	234	PHE	C-O	-5.26	1.18	1.24

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	GLN	N-CA-C	9.91	126.11	112.93
2	B	15	G	C2'-C3'-O3'	8.09	125.84	113.70
2	F	1	U	C2'-C3'-O3'	7.82	121.23	109.50
1	E	176	PRO	N-CA-C	7.51	124.22	113.47
1	E	178	GLN	CB-CA-C	6.58	120.13	109.07

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	1212	0	1232	8	1
1	C	1215	0	1237	5	1
1	E	1212	0	1232	3	0
1	G	1181	0	1204	14	0
2	B	427	0	213	0	0
2	D	427	0	212	13	0
2	F	427	0	211	9	0
2	H	427	0	213	0	0
3	A	15	0	0	1	0
3	B	9	0	0	0	0
3	C	11	0	0	0	0
3	D	5	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
3	H	2	0	0	0	0
All	All	6577	0	5754	36	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 3.

The worst 5 of 36 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:D:20:A:H2'	1:G:314:LYS:HD3	1.78	0.66
2:F:15:G:O2'	1:G:277:GLU:OE1	2.14	0.62
1:A:297:ARG:NH2	3:A:401:HOH:O	2.30	0.62
2:D:2:G:O2'	2:F:2:G:O2'	1.72	0.59
2:D:1:U:O4	1:G:314:LYS:NZ	2.32	0.58

All (1) 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:A:297:ARG:NH1	1:C:212:GLU:OE1[3_755]	2.19	0.01

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	150/190 (79%)	149 (99%)	1 (1%)	0	100	100
1	C	151/190 (80%)	151 (100%)	0	0	100	100
1	E	150/190 (79%)	149 (99%)	1 (1%)	0	100	100
1	G	146/190 (77%)	146 (100%)	0	0	100	100
All	All	597/760 (79%)	595 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	133/166 (80%)	126 (95%)	7 (5%)	20	54
1	C	134/166 (81%)	127 (95%)	7 (5%)	21	55
1	E	133/166 (80%)	125 (94%)	8 (6%)	17	50
1	G	129/166 (78%)	124 (96%)	5 (4%)	28	62
All	All	529/664 (80%)	502 (95%)	27 (5%)	21	55

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	175	ASN
1	E	233	ARG
1	G	208	LEU

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Mol	Chain	Res	Type
1	E	229	ARG
1	E	248	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	228	GLN
1	G	236	GLN
1	C	318	GLN
1	C	325	GLN
1	E	325	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	19/20 (95%)	4 (21%)	0
2	D	19/20 (95%)	3 (15%)	0
2	F	19/20 (95%)	2 (10%)	0
2	H	19/20 (95%)	3 (15%)	0
All	All	76/80 (95%)	12 (15%)	0

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	G
2	B	13	A
2	B	15	G
2	B	16	A
2	D	2	G

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](#)

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, 95th 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	152/190 (80%)	-0.47	0 100 100	34, 50, 84, 140	0
1	C	152/190 (80%)	-0.49	1 (0%) 84 66	35, 51, 91, 124	1 (0%)
1	E	152/190 (80%)	-0.43	1 (0%) 84 66	45, 66, 99, 119	0
1	G	148/190 (77%)	0.12	0 100 100	63, 90, 124, 142	0
2	B	20/20 (100%)	-1.16	0 100 100	39, 48, 83, 84	0
2	D	20/20 (100%)	-0.98	0 100 100	42, 51, 85, 128	1 (5%)
2	F	20/20 (100%)	-0.75	0 100 100	55, 67, 104, 119	1 (5%)
2	H	20/20 (100%)	-0.81	0 100 100	67, 79, 99, 120	0
All	All	684/840 (81%)	-0.39	2 (0%) 90 79	34, 63, 113, 142	3 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	326	THR	3.1
1	E	175	ASN	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 oligosaccharides 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.