



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2016 – 08:27 AM EDT

PDB ID : 5DV7
Title : Crystal Structure of NF90 tandem dsRBDs with dsRNA
Authors : Jayachandran, U.; Grey, H.; Cook, A.G.
Deposited on : 2015-09-21
Resolution : 3.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

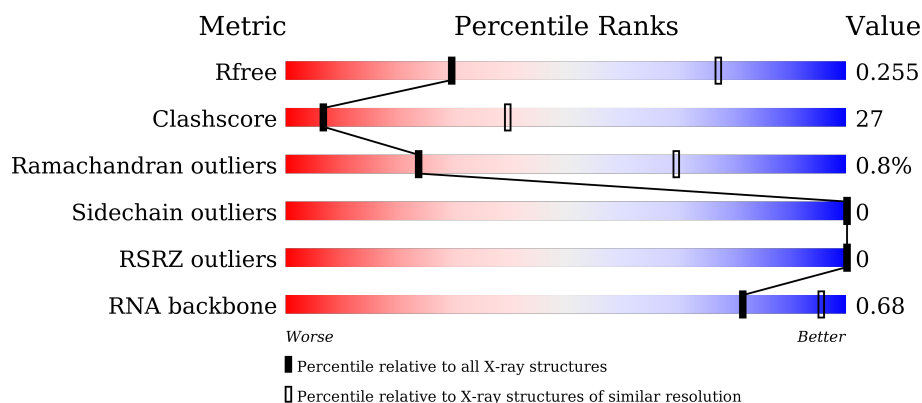
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	18	<div> <div>11%</div> <div>83%</div> <div>6%</div> </div>
2	B	18	<div> <div>28%</div> <div>72%</div> </div>
3	C	700	<div> <div>13%</div> <div>7%</div> <div>80%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1637 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 RNA chain called RNA (5'-R(*CP*CP*AP*GP*CP*AP*UP*UP*AP*UP*GP*AP*AP*AP*GP*UP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	18	Total	C	N	O	P	0	0	0
			383	173	72	121	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	P	0	0	0
			374	169	61	127	17			

- Molecule 3 is a protein called Interleukin enhancer-binding factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			879	548	156	171	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		

THR	GLY	THR	GLN	P443
PRO	GLY	PRO	GLY	P444
VAL	P519	VAL	P520	A445
VAL	ASN	VAL	ASN	T452
ARG	ALA	ARG	ALA	A453
GLY	GLY	GLY	GLY	V457
GLY	PRO	GLY	PRO	A458
LYS	TYR	LYS	LYS	L467
PHE	GLY	PHE	GLY	PRO
ALA	SER	ALA	ALA	THR
ALA	TYR	ALA	ALA	GLY
LYS	GLY	LYS	LYS	ALA
PRO	TYR	PRO	TYR	GLU
SER	SER	SER	SER	GLY
ASN	ASN	ASN	ASN	ARG
SER	SER	SER	GLY	ASP
ALA	ALA	PHE	K583	SER
THR	THR	GLY	R594	SER
ALA	ALA	MET	F555	LYS
GLY	GLY	GLY	V556	GLY
TYR	TYR	GLY	K557	GLU
SER	SER	PRO	E558	ASP
ASP	ASP	MET	V559	SER
PHE	PHE	HIS	E560	ALA
PHE	PHE	ASN	V561	GLU
THR	THR	GLU	D562	GLU
ASP	ASP	VAL	G563	SER
CYS	CYS	PRO	Q564	ASP
TYR	TYR	PRO	K565	GLY
GLY	GLY	PRO	F566	LYS
THR	THR	PRO	ASN	ALA
HIS	HIS	ASN	A569	ALA
ASP	ASP	ILE	G570	ILE
PHE	PHE	ARG	S571	VAL
GLY	GLY	GLY	D572	ALA
ALA	ALA	ARG	V575	PRO
SER	SER	GLY	Y579	PRO
		GLY	Y579	VAL
		GLY	Y579	VAL
		ASN	A584	GLU
		ILE	F589	ALA
		ARG	P590	VAL
		GLY	ASP	SER
		ARG	THR	ASN
		GLY	PRO	PRO
		ARG	PRO	SER
		GLY	LEU	SER
		ARG	ALA	VAL
		ARG	LEU	VAL
		GLY	PHE	PHE
		PHE	GLY	PRO
		GLY	ALA	PRO
		GLY	ASN	SER
		ALA	LYS	ASP
		ASN	LYS	ALA
		HIS	LYS	ALA
		GLY	THR	THR
		GLY	ARG	GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	100.10Å 100.10Å 108.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.41 – 3.50 45.41 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.41-3.50) 100.0 (45.41-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.239 , 0.273 0.226 , 0.255	Depositor DCC
R_{free} test set	704 reflections (4.61%)	DCC
Wilson B-factor (Å ²)	127.0	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.0	EDS
Estimated twinning fraction	0.057 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 7977 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1637	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.77	1/429 (0.2%)	1.02	1/667 (0.1%)
2	B	0.76	0/416	1.01	0/645
3	C	0.52	0/893	0.68	1/1222 (0.1%)
All	All	0.65	1/1738 (0.1%)	0.87	2/2534 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	A	N9-C4	-5.09	1.34	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	519	PRO	N-CA-CB	5.80	110.26	103.30
1	A	3	A	C8-N9-C4	5.51	108.00	105.80

There are no chirality outliers.

There are no planarity outliers.

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	383	0	196	22	0
2	B	374	0	193	16	0
3	C	879	0	715	38	0
4	C	1	0	0	0	0
All	All	1637	0	1104	74	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 27.

The worst 5 of 74 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)
3:C:544:ILE:HD11	3:C:558:GLU:CB	1.92	1.00
2:B:18:G:O2'	3:C:549:GLY:O	1.89	0.90
3:C:561:VAL:N	3:C:564:GLN:O	2.06	0.87
3:C:561:VAL:O	3:C:563:GLY:N	2.09	0.85
3:C:560:GLU:HA	3:C:565:LYS:HA	1.60	0.82

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
3	C	133/700 (19%)	120 (90%)	12 (9%)	1 (1%)	24 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	562	ASP

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	
3	C	65/575 (11%)	65 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
3	C	527	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	17/18 (94%)	1 (5%)	0
2	B	17/18 (94%)	0	0
All	All	34/36 (94%)	1 (2%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	C

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 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 ⓘ

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	18/18 (100%)	-0.58	0 100 100	98, 123, 215, 218	0
2	B	18/18 (100%)	-0.53	0 100 100	84, 123, 212, 228	0
3	C	137/700 (19%)	-0.34	0 100 100	75, 126, 183, 200	0
All	All	173/736 (23%)	-0.39	0 100 100	75, 125, 193, 228	0

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 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.