



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:11 pm BST

PDB ID : 5WWF
Title : Crystal structure of hnRNPA2B1 in complex with RNA
Authors : Wu, B.X.; Su, S.C.; Ma, J.B.
Deposited on : 2017-01-01
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 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 : 2.11
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) : 2.11

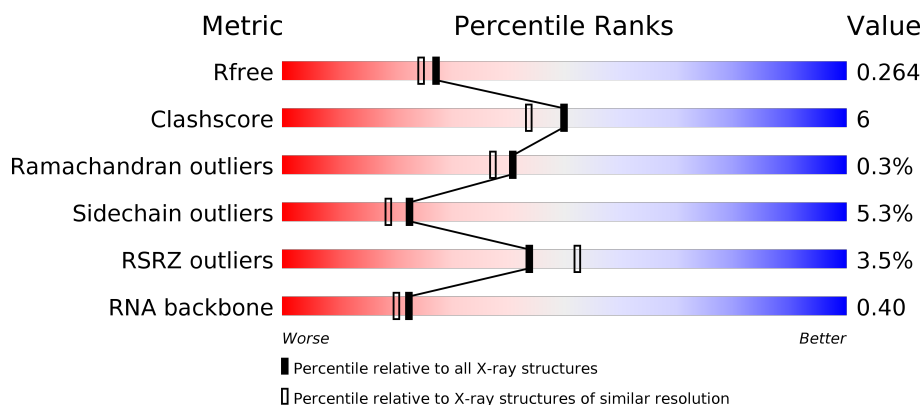
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)
RNA backbone	3102	1060 (2.60-1.72)

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 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	184	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>...</div> </div> </div>
1	C	184	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>...</div> </div> </div>
2	B	10	<div> <div>50%</div> <div>20%</div> <div>30%</div> </div>
2	D	10	<div> <div>40%</div> <div>30%</div> <div>30%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3393 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 Heterogeneous nuclear ribonucleoproteins A2/B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	4	0
			1466	919	266	275	6			
1	C	176	Total	C	N	O	S	0	3	0
			1441	905	262	269	5			

- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	0	0
			209	94	43	63	9			
2	D	10	Total	C	N	O	P	0	0	0
			217	98	46	64	9			

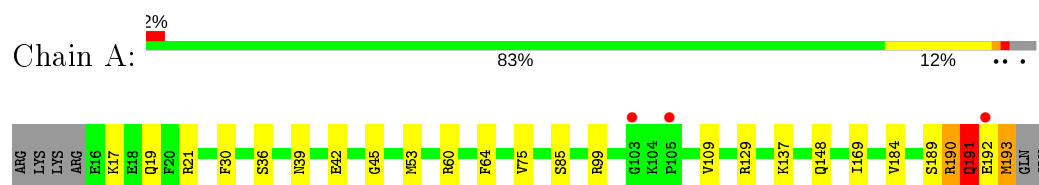
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	3	Total	O	0	0
			3	3		
3	C	20	Total	O	0	0
			20	20		
3	D	2	Total	O	0	0
			2	2		

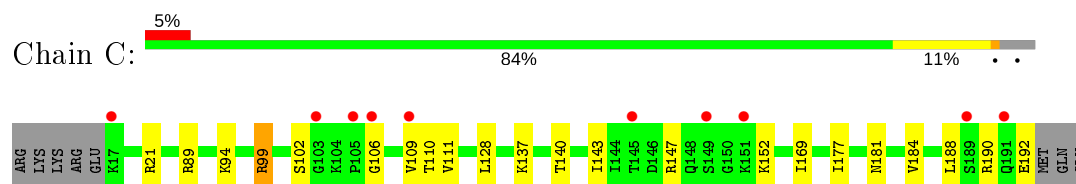
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Heterogeneous nuclear ribonucleoproteins A2/B1



- Molecule 1: Heterogeneous nuclear ribonucleoproteins A2/B1



- Molecule 2: RNA



- Molecule 2: RNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.35Å 38.30Å 107.93Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	30.00 – 2.15 29.65 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.15) 92.9 (29.65-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.203 , 0.258 0.211 , 0.264	Depositor DCC
R_{free} test set	1081 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3393	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% 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, 0.333 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	0.79	0/1498	0.95	3/2006 (0.1%)
1	C	0.65	0/1473	0.84	3/1973 (0.2%)
2	B	0.91	1/235 (0.4%)	1.03	3/366 (0.8%)
2	D	0.56	0/244	1.04	2/380 (0.5%)
All	All	0.73	1/3450 (0.0%)	0.92	11/4725 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	G	O3'-P	-7.27	1.52	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	C	O5'-P-OP1	-10.72	96.05	105.70
2	D	9	G	O5'-P-OP2	-6.45	99.90	105.70
2	B	3	G	O5'-P-OP1	-6.41	99.93	105.70
2	D	9	G	O5'-P-OP1	6.33	118.29	110.70
2	B	10	C	O5'-P-OP2	5.52	117.33	110.70
1	A	60	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	21	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	A	129	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	147	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	C	147	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	190	ARG	C-N-CA	5.09	134.42	121.70

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	1466	0	1441	23	0
1	C	1441	0	1421	11	0
2	B	209	0	107	6	0
2	D	217	0	112	2	0
3	A	35	0	0	1	0
3	B	3	0	0	0	0
3	C	20	0	0	1	0
3	D	2	0	0	0	0
All	All	3393	0	3081	37	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 6.

All (37) 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:A:191:GLN:H	1:A:192:GLU:CG	1.88	0.86
1:A:192:GLU:HB3	1:A:193:MET:C	1.96	0.85
1:A:190:ARG:N	1:A:191:GLN:HB2	1.92	0.84
1:A:190:ARG:CA	1:A:191:GLN:HB2	2.10	0.82
1:C:109:VAL:HG12	1:C:111:VAL:HG13	1.67	0.75
1:A:190:ARG:HB2	1:A:191:GLN:HB2	1.69	0.74
1:A:191:GLN:N	1:A:192:GLU:HA	2.03	0.73
1:A:190:ARG:CB	1:A:191:GLN:HB2	2.21	0.69
1:A:191:GLN:H	1:A:192:GLU:HG2	1.57	0.69
1:A:191:GLN:H	1:A:192:GLU:HG3	1.59	0.67
1:A:189:SER:O	1:A:193:MET:HB2	1.95	0.66
1:C:109:VAL:CG1	1:C:111:VAL:HG13	2.29	0.61
2:B:3:G:H5"	2:B:3:G:H8	1.67	0.60
1:A:190:ARG:N	1:A:191:GLN:CB	2.66	0.57
1:C:188:LEU:HB3	1:C:192:GLU:HA	1.90	0.54
1:A:191:GLN:N	1:A:192:GLU:CA	2.71	0.53
1:A:53[B]:MET:CE	2:B:3:G:C8	2.95	0.49
2:B:3:G:H5"	2:B:3:G:C8	2.47	0.48
1:A:21:ARG:HA	1:A:75:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:LEU:HD13	1:C:192:GLU:HG3	1.94	0.47
1:C:128:LEU:HD23	1:C:177:ILE:HG21	1.97	0.46
1:C:94:LYS:HE3	3:C:213:HOH:O	2.15	0.46
1:C:99:ARG:NH2	2:D:2:A:O2'	2.49	0.45
1:C:143:ILE:HG21	1:C:152:LYS:HD3	1.98	0.45
1:A:190:ARG:O	1:A:193:MET:HB3	2.17	0.45
1:C:106:GLY:HA2	1:C:109:VAL:HG23	1.98	0.45
1:A:53[B]:MET:HE3	2:B:3:G:C8	2.52	0.44
1:A:53[B]:MET:HE1	2:B:3:G:C8	2.51	0.44
1:A:36:SER:HA	1:A:39[B]:ASN:OD1	2.18	0.43
1:A:169:ILE:HG22	1:A:184:VAL:HG21	2.00	0.42
1:A:99:ARG:NH1	2:B:2:A:C8	2.88	0.42
2:D:2:A:H1'	2:D:3:G:N7	2.36	0.41
1:A:42:GLU:HA	1:A:45:GLY:O	2.21	0.41
1:A:53[B]:MET:HG2	1:A:64:PHE:CE2	2.55	0.41
1:A:39[B]:ASN:HB3	3:A:213:HOH:O	2.21	0.41
1:C:109:VAL:HG12	1:C:110:THR:N	2.35	0.41
1:C:169:ILE:HG22	1:C:184:VAL:HG21	2.03	0.40

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	180/184 (98%)	175 (97%)	4 (2%)	1 (1%)	25	18
1	C	177/184 (96%)	170 (96%)	7 (4%)	0	100	100
All	All	357/368 (97%)	345 (97%)	11 (3%)	1 (0%)	41	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	GLN

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	156/158 (99%)	147 (94%)	9 (6%)	20	15
1	C	153/158 (97%)	146 (95%)	7 (5%)	27	23
All	All	309/316 (98%)	293 (95%)	16 (5%)	22	19

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	19	GLN
1	A	30	PHE
1	A	85	SER
1	A	109	VAL
1	A	137	LYS
1	A	148	GLN
1	A	191	GLN
1	A	193	MET
1	C	89	ARG
1	C	99	ARG
1	C	102	SER
1	C	137	LYS
1	C	140	THR
1	C	181	ASN
1	C	190	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	43	GLN

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Mol	Chain	Res	Type
1	A	172	GLN
1	A	191	GLN
1	C	108	HIS
1	C	181	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	9/10 (90%)	4 (44%)	0
2	D	9/10 (90%)	6 (66%)	0
All	All	18/20 (90%)	10 (55%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	A
2	B	8	A
2	B	9	G
2	B	10	C
2	D	2	A
2	D	3	G
2	D	4	G
2	D	8	A
2	D	9	G
2	D	10	C

There are no RNA pucker outliers to report.

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers

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	178/184 (96%)	0.08	3 (1%) 70 76	8, 22, 44, 64	0
1	C	176/184 (95%)	0.43	10 (5%) 23 32	18, 33, 62, 84	0
2	B	10/10 (100%)	-0.77	0 100 100	19, 21, 50, 55	0
2	D	10/10 (100%)	-0.58	0 100 100	30, 36, 38, 38	0
All	All	374/388 (96%)	0.20	13 (3%) 44 52	8, 28, 55, 84	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	189	SER	6.3
1	C	151	LYS	5.9
1	A	105	PRO	4.2
1	A	192	GLU	3.9
1	C	105	PRO	3.7
1	C	17	LYS	3.4
1	C	191	GLN	3.0
1	C	103	GLY	2.8
1	C	106	GLY	2.4
1	A	103	GLY	2.2
1	C	149	SER	2.2
1	C	109	VAL	2.1
1	C	145	THR	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.