



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5QZW / pdb_00005qzw
Title : PanDDA analysis group deposition – Auto-refined data of Aar2/RNaseH for ground state model 47
Authors : Weiss, M.S.; Wollenhaupt, J.; Metz, A.; Barthel, T.; Lima, G.M.A.; Heine, A.; Mueller, U.; Klebe, G.
Deposited on : 2020-02-12
Resolution : 1.36 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 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
Xtriage (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

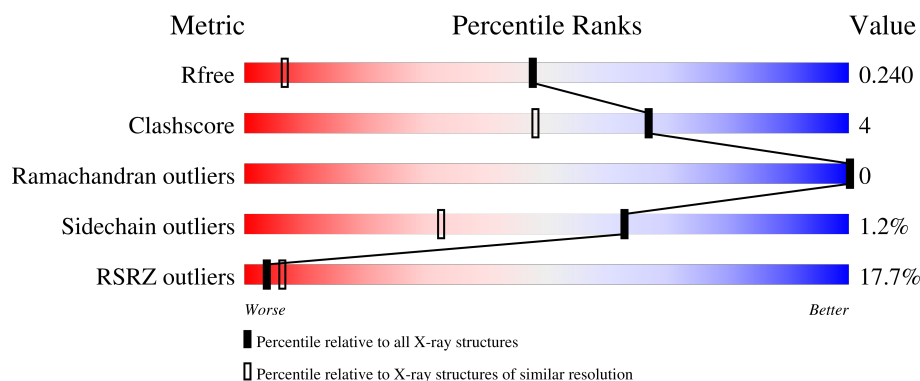
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.36 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	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	258	
2	B	308	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4768 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	2002	1283	335	372	12	0	12	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	GLY	-	expression tag	UNP P33334
A	1834	ALA	-	expression tag	UNP P33334
A	1835	MET	-	expression tag	UNP P33334

- Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	300	2580	1654	421	485	20	17	9	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	-	linker	UNP P32357
B	167	SER	-	linker	UNP P32357
B	168	SER	-	linker	UNP P32357
B	169	SER	-	linker	UNP P32357
B	170	SER	-	linker	UNP P32357

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	94	Total 94	O 94	0	0
3	B	92	Total 92	O 92	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.52Å 82.03Å 93.96Å 90.00° 108.83° 90.00°	Depositor
Resolution (Å)	43.77 – 1.36 43.77 – 1.36	Depositor EDS
% Data completeness (in resolution range)	97.9 (43.77-1.36) 98.1 (43.77-1.36)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.8.0238, PHENIX 1.16.3549	Depositor
R, R_{free}	0.226 , 0.227 0.235 , 0.240	Depositor DCC
R_{free} test set	6575 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4768	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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	1.01	1/2049 (0.0%)	1.16	1/2775 (0.0%)
2	B	1.07	1/2651 (0.0%)	1.19	1/3581 (0.0%)
All	All	1.05	2/4700 (0.0%)	1.18	2/6356 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	ILE	C-O	9.00	1.35	1.24
1	A	2059	ILE	C-O	-5.02	1.18	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2066	LYS	CB-CA-C	-5.79	101.79	110.88
2	B	317	LEU	CA-C-O	-5.11	112.12	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	54[A]	MET	Peptide

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	2002	0	2029	11	0
2	B	2580	0	2450	24	0
3	A	94	0	0	3	0
3	B	92	0	0	4	0
All	All	4768	0	4479	33	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 4.

All (33) 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:2062:GLU:O	1:A:2066:LYS:HG2	1.77	0.84
1:A:2069:VAL:O	3:A:2101:HOH:O	1.94	0.84
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.42	0.68
2:B:50:ASP:HB3	3:B:483:HOH:O	1.96	0.66
2:B:277:GLU:CD	2:B:277:GLU:H	2.09	0.61
1:A:1907:GLN:HG2	2:B:195:MET:HE3	1.83	0.60
1:A:1938:LYS:NZ	3:A:2102:HOH:O	2.26	0.59
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.85	0.58
2:B:275:LEU:CD2	2:B:283:LEU:HD13	2.34	0.57
2:B:51:ASN:OD1	2:B:53:SER:HB2	2.03	0.57
2:B:70:GLN:HB3	2:B:81:MET:CE	2.35	0.57
1:A:1835:MET:HE1	1:A:1961:LEU:HD12	1.88	0.55
2:B:280:SER:HB3	2:B:313:TYR:CE1	2.41	0.55
2:B:54[A]:MET:HE2	3:B:490:HOH:O	2.07	0.54
2:B:203[A]:TYR:CZ	2:B:207:THR:HG21	2.45	0.52
2:B:50:ASP:CB	3:B:483:HOH:O	2.57	0.52
1:A:2066:LYS:HD3	3:A:2105:HOH:O	2.14	0.48
2:B:54[A]:MET:HG3	3:B:474:HOH:O	2.13	0.47
2:B:287:ARG:O	2:B:291:ILE:HD13	2.15	0.47
2:B:1:MET:HB3	2:B:35:ASP:HA	1.98	0.46
2:B:275:LEU:HD22	2:B:283:LEU:HD13	1.99	0.44
2:B:315:GLU:H	2:B:315:GLU:CD	2.25	0.44
2:B:201:LYS:HG3	2:B:252:SER:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:MET:HA	1:A:1969:MET:HE2	2.00	0.44
2:B:70:GLN:HB3	2:B:81:MET:HE1	2.00	0.43
1:A:1907:GLN:HG2	2:B:195:MET:CE	2.48	0.43
2:B:61:ASP:HB2	2:B:123:MET:HG2	2.01	0.42
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.44	0.42
1:A:1859:ARG:HH12	1:A:1979[A]:MET:CE	2.34	0.41
2:B:96:PHE:CB	2:B:102:MET:HE3	2.51	0.41
2:B:275:LEU:HD23	2:B:275:LEU:HA	1.94	0.40
2:B:77:LEU:HD21	2:B:79:LYS:HE3	2.03	0.40
2:B:275:LEU:HD22	2:B:283:LEU:CD1	2.51	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	248/258 (96%)	243 (98%)	5 (2%)	0	100	100
2	B	306/308 (99%)	297 (97%)	9 (3%)	0	100	100
All	All	554/566 (98%)	540 (98%)	14 (2%)	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	226/233 (97%)	224 (99%)	2 (1%)	70	44
2	B	287/284 (101%)	283 (99%)	4 (1%)	59	28
All	All	513/517 (99%)	507 (99%)	6 (1%)	63	32

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1962	ARG
1	A	2060	LEU
2	B	52	SER
2	B	101	MET
2	B	291	ILE
2	B	315	GLU

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

Mol	Chain	Res	Type
1	A	1869	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	237/258 (91%)	0.98	34 (14%) 6 10	9, 25, 49, 79	12 (5%)
2	B	300/308 (97%)	1.21	61 (20%) 3 4	9, 28, 54, 85	9 (3%)
All	All	537/566 (94%)	1.11	95 (17%) 4 6	9, 27, 52, 85	21 (3%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	22	PHE	7.8
1	A	2069	VAL	7.3
2	B	152	LEU	7.1
1	A	1834	ALA	6.3
2	B	173	ALA	6.2
2	B	108	ILE	6.0
2	B	279	TYR	5.7
2	B	1	MET	5.7
1	A	1979[A]	MET	5.6
2	B	54[A]	MET	5.6
2	B	170	SER	5.2
2	B	172	PRO	4.8
2	B	317	LEU	4.8
1	A	1836	ASN	4.7
1	A	2065	ARG	4.5
1	A	1835	MET	4.5
2	B	316	LEU	4.3
1	A	1833	GLY	4.2
2	B	203[A]	TYR	4.1
1	A	1837	SER	4.0
2	B	38	ILE	4.0
2	B	174	HIS	3.9
2	B	2	ASN	3.9
1	A	1838	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	2030	PRO	3.7
2	B	282	ILE	3.7
2	B	313	TYR	3.5
2	B	150	ASN	3.5
2	B	295	SER	3.3
1	A	2028	SER	3.3
2	B	41[A]	VAL	3.3
2	B	87	ALA	3.3
2	B	147	VAL	3.3
2	B	101	MET	3.2
2	B	53	SER	3.2
1	A	1839	ASN	3.2
2	B	275	LEU	3.2
1	A	2017[A]	THR	3.1
1	A	2063	TYR	3.1
1	A	2032	ILE	3.0
2	B	50	ASP	3.0
1	A	1960[A]	GLU	2.9
2	B	92	ILE	2.9
1	A	1962	ARG	2.8
1	A	2027	LEU	2.8
2	B	84	ARG	2.8
2	B	258	LYS	2.8
1	A	1866	PHE	2.8
2	B	291	ILE	2.8
2	B	142	SER	2.7
2	B	25	LYS	2.6
1	A	1862	VAL	2.6
1	A	2060	LEU	2.6
2	B	91	ASN	2.6
2	B	257	PRO	2.6
1	A	1950	ASP	2.5
1	A	2066	LYS	2.5
2	B	110	GLU	2.5
2	B	259	HIS	2.5
2	B	277	GLU	2.5
1	A	2068	ASN	2.5
2	B	49	ALA	2.5
1	A	1840	TYR	2.5
1	A	1846	ASN	2.4
2	B	171	ASP	2.4
2	B	122[A]	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	64[A]	MET	2.4
2	B	109	ASP	2.4
2	B	254	ALA	2.3
1	A	2053[A]	SER	2.3
1	A	1961	LEU	2.3
2	B	27	ASN	2.3
2	B	77	LEU	2.3
2	B	283	LEU	2.3
2	B	106	PRO	2.2
1	A	2021	SER	2.2
1	A	2033	THR	2.2
2	B	131	ARG	2.2
2	B	111	ASP	2.2
2	B	278	GLN	2.2
2	B	81	MET	2.2
1	A	1860	VAL	2.1
2	B	288	VAL	2.1
1	A	1863	HIS	2.1
2	B	96	PHE	2.1
2	B	151	GLU	2.1
2	B	86	GLY	2.1
2	B	315	GLU	2.1
2	B	208	VAL	2.1
1	A	2059	ILE	2.0
2	B	20	TYR	2.0
1	A	1868	GLY	2.0
2	B	93	VAL	2.0
2	B	180	VAL	2.0
2	B	256	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.