



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 10:42 AM GMT

PDB ID : 4ILG
Title : Crystal structure of Aar2p in complex with the Prp8p RNaseH and Jab1/MPN domains
Authors : Weber, G.; Herooven, A.C.; Santos, K.F.; Wahl, M.C.
Deposited on : 2012-12-31
Resolution : 2.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

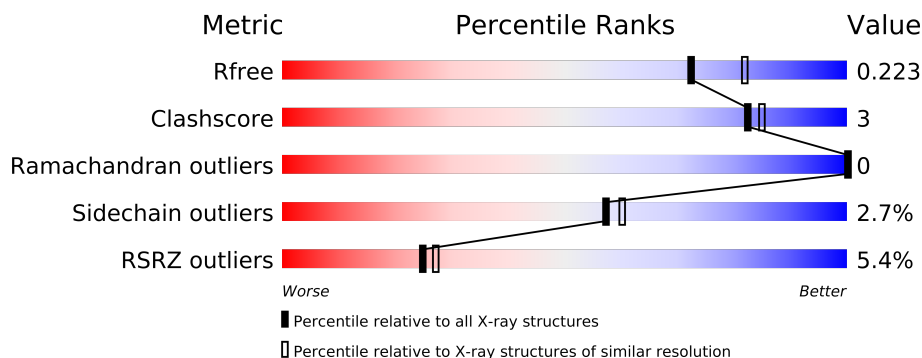
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	342	
2	B	258	
3	C	270	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7524 atoms, of which 0 are hydrogen and 0 are deuterium.

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 A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	7	0
			2710	1731	444	514	21			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	SER	LEU	ENGINEERED MUTATION	UNP P32357
A	154	SER	LYS	ENGINEERED MUTATION	UNP P32357
A	?	-	LEU	DELETION	UNP P32357
A	?	-	GLN	DELETION	UNP P32357
A	?	-	LYS	DELETION	UNP P32357
A	?	-	ALA	DELETION	UNP P32357
A	?	-	GLY	DELETION	UNP P32357
A	?	-	LYS	DELETION	UNP P32357
A	?	-	MET	DELETION	UNP P32357
A	?	-	GLU	DELETION	UNP P32357
A	?	-	ALA	DELETION	UNP P32357
A	?	-	LYS	DELETION	UNP P32357
A	?	-	ASN	DELETION	UNP P32357
A	?	-	GLU	DELETION	UNP P32357
A	?	-	ASP	DELETION	UNP P32357

- Molecule 2 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	14	0
			2129	1364	359	396	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1833	GLY	-	EXPRESSION TAG	UNP P33334

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1834	ALA	-	EXPRESSION TAG	UNP P33334
B	1835	MET	-	EXPRESSION TAG	UNP P33334

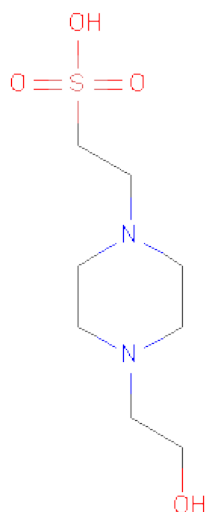
- Molecule 3 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	245	Total	C	N	O	S	0	4	0
			1981	1279	320	376	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2144	GLY	-	EXPRESSION TAG	UNP P33334
C	2145	ALA	-	EXPRESSION TAG	UNP P33334
C	2146	MET	-	EXPRESSION TAG	UNP P33334

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	245	Total 245	O 245	0	0
5	B	241	Total 241	O 241	0	0
5	C	203	Total 203	O 203	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.77Å 63.74Å 110.52Å 90.00° 95.39° 90.00°	Depositor
Resolution (Å)	31.87 – 2.10 31.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (31.87-2.10) 99.7 (31.87-2.10)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.180 , 0.228 0.177 , 0.223	Depositor DCC
R_{free} test set	3062 reflections (4.46%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 68677 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7524	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE

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	0.49	0/2791	0.57	0/3768
2	B	0.54	0/2186	0.61	0/2961
3	C	0.45	0/2038	0.57	0/2763
All	All	0.49	0/7015	0.58	0/9492

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2710	0	0	10	1
2	B	2129	0	0	5	0
3	C	1981	0	0	5	0
4	C	15	0	17	1	0
5	A	245	0	0	6	1
5	B	241	0	0	2	0
5	C	203	0	0	4	0
All	All	7524	0	17	21	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 21 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:2013[B]:ARG:NH1	2:B:2083:ILE:O	2.05	0.89
2:B:1985[A]:GLN:NE2	5:B:2341:HOH:O	2.20	0.72
1:A:307:LYS:NZ	1:A:311[A]:ASN:OD1	2.28	0.66
1:A:149:GLU:OE1	5:A:638:HOH:O	2.14	0.65
1:A:111:ASP:OD1	1:A:113:THR:OG1	2.16	0.63

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	Distance(Å)	Clash(Å)
1:A:73:PRO:O	5:A:612:HOH:O[2_454]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	323/342 (94%)	312 (97%)	11 (3%)	0	100	100
2	B	263/258 (102%)	251 (95%)	12 (5%)	0	100	100
3	C	247/270 (92%)	242 (98%)	5 (2%)	0	100	100
All	All	833/870 (96%)	805 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	305/316 (96%)	300 (98%)	5 (2%)	75	79
2	B	242/233 (104%)	235 (97%)	7 (3%)	55	57
3	C	221/237 (93%)	213 (96%)	8 (4%)	47	46
All	All	768/786 (98%)	748 (97%)	20 (3%)	57	62

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2077	THR
2	B	2078	GLU
3	C	2332	THR
2	B	2067	TYR
2	B	2074	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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 ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EPE	C	2501	-	15,15,15	1.03	1 (6%)	20,20,20	1.82	5 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EPE	C	2501	-	-	0/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2501	EPE	C10-S	3.62	1.83	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2501	EPE	C5-N4-C3	3.99	118.77	108.86
4	C	2501	EPE	C7-N4-C5	3.44	120.19	111.32
4	C	2501	EPE	O3S-S-C10	3.19	109.97	105.93
4	C	2501	EPE	O2S-S-C10	3.16	109.51	106.81
4	C	2501	EPE	C7-N4-C3	2.95	118.93	111.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	321/342 (93%)	-0.06	12 (3%) 39 44	20, 43, 99, 173	0
2	B	252/258 (97%)	-0.04	11 (4%) 33 37	18, 33, 98, 123	0
3	C	245/270 (90%)	0.14	21 (8%) 11 11	24, 41, 104, 168	0
All	All	818/870 (94%)	0.01	44 (5%) 25 27	18, 39, 101, 173	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	2321	ILE	7.3
3	C	2325	LEU	6.5
1	A	109	ASP	5.3
1	A	279	TYR	4.6
3	C	2323	ASN	4.4

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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EPE	C	2501	15/15	0.12	0.28	43,56,73,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.