



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:46 AM GMT

PDB ID : 4HWC
Title : Structure of ATBAG1
Authors : Shen, Y.; Fang, S.
Deposited on : 2012-11-07
Resolution : 1.80 Å(reported)

This is a full wwPDB validation 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>

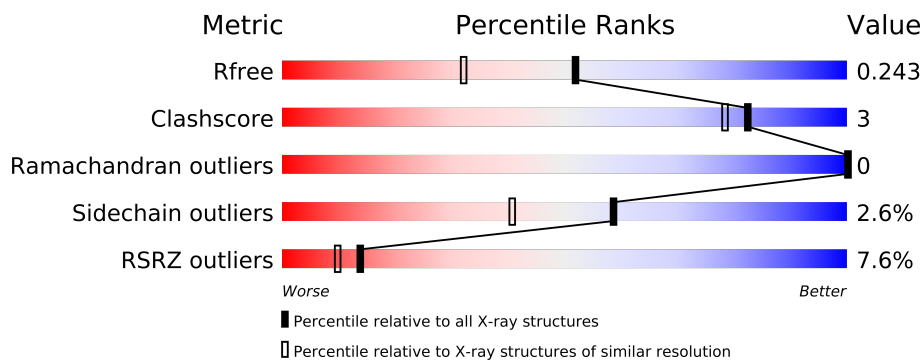
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.80 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	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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. 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	89	
1	B	89	
1	C	89	
1	D	89	
1	E	89	
1	F	89	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4407 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 BAG family molecular chaperone regulator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	0	0
			656	414	113	126	3			
1	B	87	Total	C	N	O	S	0	0	0
			655	414	114	124	3			
1	C	85	Total	C	N	O	S	0	0	0
			651	411	112	125	3			
1	D	81	Total	C	N	O	S	0	0	0
			615	388	106	119	2			
1	E	87	Total	C	N	O	S	0	0	0
			651	410	113	125	3			
1	F	84	Total	C	N	O	S	0	0	0
			634	400	109	122	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
A	154	PRO	-	EXPRESSION TAG	UNP Q0WUQ1
A	155	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
A	156	SER	-	EXPRESSION TAG	UNP Q0WUQ1
B	153	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
B	154	PRO	-	EXPRESSION TAG	UNP Q0WUQ1
B	155	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
B	156	SER	-	EXPRESSION TAG	UNP Q0WUQ1
C	153	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
C	154	PRO	-	EXPRESSION TAG	UNP Q0WUQ1
C	155	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
C	156	SER	-	EXPRESSION TAG	UNP Q0WUQ1
D	153	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
D	154	PRO	-	EXPRESSION TAG	UNP Q0WUQ1
D	155	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
D	156	SER	-	EXPRESSION TAG	UNP Q0WUQ1
E	153	GLY	-	EXPRESSION TAG	UNP Q0WUQ1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	154	PRO	-	EXPRESSION TAG	UNP Q0WUQ1
E	155	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
E	156	SER	-	EXPRESSION TAG	UNP Q0WUQ1
F	153	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
F	154	PRO	-	EXPRESSION TAG	UNP Q0WUQ1
F	155	GLY	-	EXPRESSION TAG	UNP Q0WUQ1
F	156	SER	-	EXPRESSION TAG	UNP Q0WUQ1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

- Molecule 3 is water.

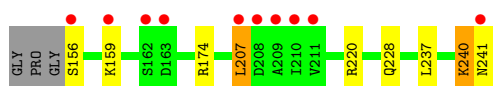
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	92	Total O 92 92	0	0
3	B	78	Total O 78 78	0	0
3	C	123	Total O 123 123	0	0
3	D	78	Total O 78 78	0	0
3	E	99	Total O 99 99	0	0
3	F	73	Total O 73 73	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

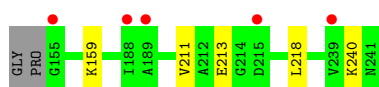
- Molecule 1: BAG family molecular chaperone regulator 1

Chain A: 



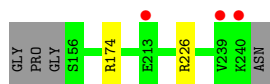
- Molecule 1: BAG family molecular chaperone regulator 1

Chain B: 



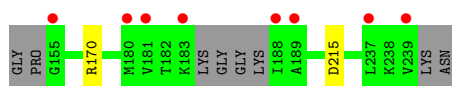
- Molecule 1: BAG family molecular chaperone regulator 1

Chain C: 



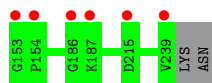
- Molecule 1: BAG family molecular chaperone regulator 1

Chain D: 



- Molecule 1: BAG family molecular chaperone regulator 1

Chain E: 



- Molecule 1: BAG family molecular chaperone regulator 1

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.72Å 96.85Å 103.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.48 – 1.80 35.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (35.48-1.80) 99.2 (35.48-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.238 , 0.251 0.234 , 0.243	Depositor DCC
R_{free} test set	2690 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	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	1 of 53074 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4407	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.50 % 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 3.1349e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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:
CL

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	0.34	0/657	0.61	1/879 (0.1%)
1	B	0.35	0/656	0.54	0/878
1	C	0.29	0/652	0.50	0/872
1	D	0.28	0/615	0.49	0/824
1	E	0.28	0/653	0.48	0/875
1	F	0.27	0/635	0.47	0/852
All	All	0.30	0/3868	0.52	1/5180 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	LEU	CB-CA-C	-5.77	99.23	110.20

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	656	0	0	6	0
1	B	655	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	651	0	0	1	0
1	D	615	0	0	1	0
1	E	651	0	0	0	0
1	F	634	0	0	3	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
3	A	92	0	0	2	0
3	B	78	0	0	0	0
3	C	123	0	0	1	0
3	D	78	0	0	1	0
3	E	99	0	0	0	0
3	F	73	0	0	4	0
All	All	4407	0	0	12	0

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.

All (12) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:228:GLN:NE2	3:A:473:HOH:O	2.45	0.49
1:A:156:SER:O	1:A:156:SER:OG	2.30	0.49
1:F:174:ARG:NH2	3:F:315:HOH:O	2.46	0.48
1:F:228:GLN:NE2	3:F:344:HOH:O	2.46	0.47
1:D:170:ARG:CZ	3:D:377:HOH:O	2.63	0.47
1:F:170:ARG:O	3:F:347:HOH:O	2.20	0.46
1:B:211:VAL:CG2	3:F:347:HOH:O	2.64	0.45
1:A:207:LEU:O	1:A:220:ARG:NH1	2.51	0.44
1:A:237:LEU:O	1:A:241:ASN:N	2.51	0.44
1:A:174:ARG:NH2	3:A:489:HOH:O	2.51	0.43
1:C:226:ARG:CD	3:C:320:HOH:O	2.67	0.42
1:A:240:LYS:O	1:A:241:ASN:C	2.55	0.42

There are no symmetry-related clashes.

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	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
1	B	85/89 (96%)	85 (100%)	0	0	100	100
1	C	83/89 (93%)	83 (100%)	0	0	100	100
1	D	77/89 (86%)	77 (100%)	0	0	100	100
1	E	85/89 (96%)	85 (100%)	0	0	100	100
1	F	82/89 (92%)	82 (100%)	0	0	100	100
All	All	496/534 (93%)	494 (100%)	2 (0%)	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	72/75 (96%)	70 (97%)	2 (3%)	56	38
1	B	70/75 (93%)	66 (94%)	4 (6%)	29	11
1	C	72/75 (96%)	71 (99%)	1 (1%)	78	69
1	D	67/75 (89%)	66 (98%)	1 (2%)	76	66
1	E	70/75 (93%)	70 (100%)	0	100	100
1	F	69/75 (92%)	66 (96%)	3 (4%)	40	19
All	All	420/450 (93%)	409 (97%)	11 (3%)	59	41

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LYS
1	A	240	LYS
1	B	159	LYS
1	B	213	GLU
1	B	218	LEU
1	B	240	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	174	ARG
1	D	215	ASP
1	F	174	ARG
1	F	192	ASP
1	F	226	ARG

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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	86/89 (96%)	0.79	10 (11%) 5 4	12, 24, 56, 98	0
1	B	87/89 (97%)	0.46	5 (5%) 23 17	11, 22, 49, 67	0
1	C	85/89 (95%)	0.27	3 (3%) 42 33	10, 19, 33, 114	0
1	D	81/89 (91%)	0.54	8 (9%) 8 6	15, 24, 54, 95	0
1	E	87/89 (97%)	0.30	6 (6%) 17 12	11, 21, 41, 63	0
1	F	84/89 (94%)	0.83	7 (8%) 11 8	17, 28, 50, 90	0
All	All	510/534 (95%)	0.53	39 (7%) 14 10	10, 24, 51, 114	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	239	VAL	5.7
1	A	156	SER	5.4
1	A	211	VAL	4.2
1	B	189	ALA	4.1
1	D	155	GLY	3.4
1	F	214	GLY	3.4
1	D	188	ILE	3.3
1	A	208	ASP	3.3
1	F	157	ALA	3.2
1	A	162	SER	3.1
1	A	159	LYS	3.0
1	B	155	GLY	2.9
1	E	239	VAL	2.9
1	C	240	LYS	2.8
1	A	210	ILE	2.7
1	E	154	PRO	2.7
1	D	181	VAL	2.7
1	D	189	ALA	2.6
1	A	241	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	153	GLY	2.6
1	F	211	VAL	2.6
1	C	239	VAL	2.5
1	A	209	ALA	2.5
1	D	180	MET	2.5
1	A	163	ASP	2.5
1	E	186	GLY	2.5
1	B	239	VAL	2.4
1	F	162	SER	2.4
1	D	183	LYS	2.3
1	F	212	ALA	2.3
1	E	187	LYS	2.3
1	F	239	VAL	2.2
1	D	237	LEU	2.1
1	E	215	ASP	2.1
1	A	207	LEU	2.1
1	C	213	GLU	2.1
1	B	188	ILE	2.1
1	F	216	VAL	2.1
1	B	215	ASP	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 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(Å ²)	Q<0.9
2	CL	A	301	1/1	0.05	-2.06	27,27,27,27	0
2	CL	E	301	1/1	0.06	-2.88	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.