



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:31 AM GMT

PDB ID : 2Y9Y
Title : Chromatin Remodeling Factor ISW1a(del_ATPase)
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Deposited on : 2011-02-17
Resolution : 3.25 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>

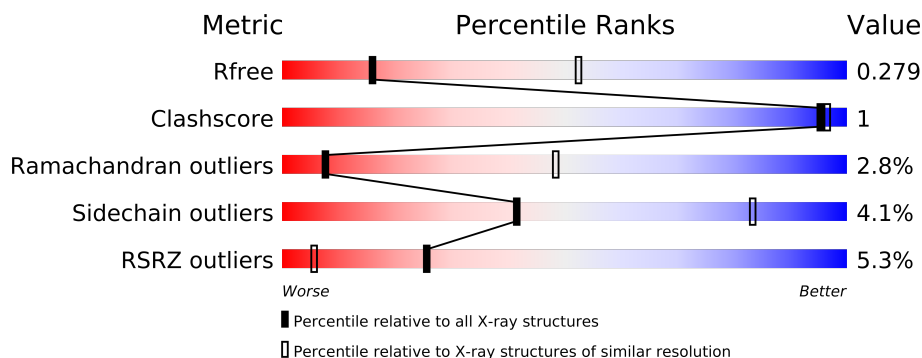
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.25 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	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)

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	374	
2	B	624	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7170 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 IMITATION SWITCH PROTEIN 1 (DEL-ATPASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2317	1473	399	437	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	762	MET	-	EXPRESSION TAG	UNP P38144
A	815	GLN	LYS	ENGINEERED MUTATION	UNP P38144
A	844	LYS	ASP	ENGINEERED MUTATION	UNP P38144
A	848	GLN	GLU	ENGINEERED MUTATION	UNP P38144
A	851	GLN	LYS	ENGINEERED MUTATION	UNP P38144
A	853	GLU	GLN	ENGINEERED MUTATION	UNP P38144
A	1130	HIS	-	EXPRESSION TAG	UNP P38144
A	1131	HIS	-	EXPRESSION TAG	UNP P38144
A	1132	HIS	-	EXPRESSION TAG	UNP P38144
A	1133	HIS	-	EXPRESSION TAG	UNP P38144
A	1134	HIS	-	EXPRESSION TAG	UNP P38144
A	1135	HIS	-	EXPRESSION TAG	UNP P38144

- Molecule 2 is a protein called ISWI ONE COMPLEX PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	592	Total	C	N	O	S	0	0	0
			4853	3123	818	897	15			

There are 2 discrepancies between the modelled and reference sequences:

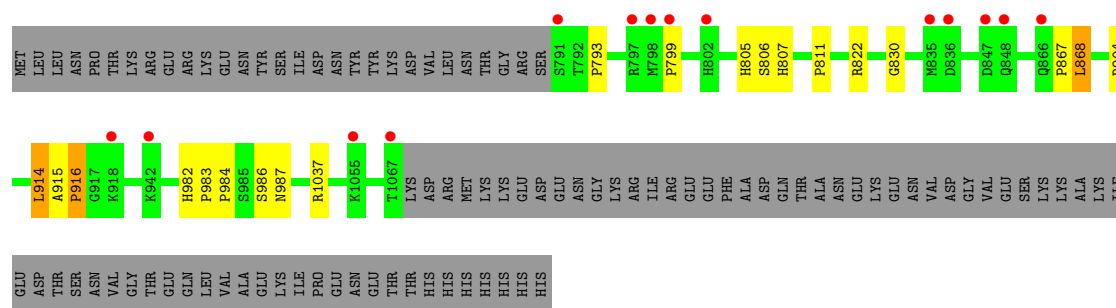
Chain	Residue	Modelled	Actual	Comment	Reference
B	126	MET	-	EXPRESSION TAG	UNP P43596
B	682	LYS	ASN	ENGINEERED MUTATION	UNP P43596

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: IMITATION SWITCH PROTEIN 1 (DEL_ATPASE)

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	206.97Å 206.97Å 215.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.87 – 3.25 29.87 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.87-3.25) 100.0 (29.87-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.283 , 0.296 0.276 , 0.279	Depositor DCC
R_{free} test set	1380 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	120.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 97.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 28010 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.21	0/2368	0.35	0/3186
2	B	0.21	0/4974	0.35	0/6723
All	All	0.21	0/7342	0.35	0/9909

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	2317	0	0	7	0
2	B	4853	0	0	2	0
All	All	7170	0	0	9	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 1.

All (9) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:807:HIS:O	1:A:807:HIS:CG	2.57	0.57
1:A:805:HIS:CG	1:A:806:SER:N	2.77	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:473:LYS:N	2:B:474:PRO:CD	2.71	0.53
1:A:982:HIS:N	1:A:983:PRO:CD	2.74	0.50
2:B:358:ASN:ND2	2:B:358:ASN:N	2.61	0.48
1:A:805:HIS:CD2	1:A:806:SER:N	2.86	0.43
1:A:915:ALA:N	1:A:916:PRO:CD	2.83	0.41
1:A:867:PRO:O	1:A:868:LEU:C	2.58	0.41
1:A:983:PRO:N	1:A:984:PRO:CD	2.84	0.40

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	275/374 (74%)	214 (78%)	52 (19%)	9 (3%)	6	43
2	B	588/624 (94%)	481 (82%)	92 (16%)	15 (3%)	8	51
All	All	863/998 (86%)	695 (80%)	144 (17%)	24 (3%)	8	48

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	799	PRO
1	A	916	PRO
1	A	904	ARG
1	A	793	PRO
2	B	162	TYR
2	B	232	ASP
2	B	331	ALA
2	B	339	THR
2	B	514	GLU
2	B	533	LEU
2	B	622	SER
2	B	690	LEU
2	B	692	LYS

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Mol	Chain	Res	Type
1	A	868	LEU
1	A	914	LEU
2	B	376	ASP
1	A	830	GLY
1	A	986	SER
2	B	278	LYS
2	B	349	ILE
2	B	502	LEU
2	B	688	ASN
1	A	811	PRO
2	B	493	ALA

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	254/343 (74%)	250 (98%)	4 (2%)	75	94
2	B	543/571 (95%)	514 (95%)	29 (5%)	32	76
All	All	797/914 (87%)	764 (96%)	33 (4%)	41	83

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	822	ARG
1	A	914	LEU
1	A	987	ASN
1	A	1037	ARG
2	B	159	LYS
2	B	167	ARG
2	B	228	LYS
2	B	236	LEU
2	B	237	LEU
2	B	255	ASN
2	B	265	THR
2	B	273	LYS
2	B	276	LYS
2	B	284	TRP

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Mol	Chain	Res	Type
2	B	319	LEU
2	B	330	THR
2	B	353	ASN
2	B	358	ASN
2	B	373	ARG
2	B	381	LEU
2	B	413	LEU
2	B	447	LEU
2	B	458	ARG
2	B	520	GLN
2	B	524	ASN
2	B	557	TYR
2	B	605	TYR
2	B	619	ARG
2	B	644	LEU
2	B	685	ILE
2	B	716	ILE
2	B	727	PHE
2	B	739	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 ⓘ

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 ⓘ

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	277/374 (74%)	0.28	14 (5%)	27 6	91, 154, 262, 349	0
2	B	592/624 (94%)	0.31	32 (5%)	25 5	79, 132, 259, 319	0
All	All	869/998 (87%)	0.30	46 (5%)	25 6	79, 138, 261, 349	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	139	GLU	7.7
2	B	469	LYS	7.1
2	B	470	GLU	6.4
2	B	275	ALA	5.4
1	A	798	MET	4.8
2	B	274	SER	4.2
2	B	494	VAL	3.8
2	B	491	LYS	3.7
2	B	495	LYS	3.7
1	A	942	LYS	3.4
2	B	467	GLN	3.3
2	B	472	LYS	3.2
2	B	680	ASP	3.2
2	B	656	LYS	3.2
2	B	468	LEU	3.2
1	A	799	PRO	3.1
2	B	280	PRO	3.1
2	B	661	LYS	3.0
1	A	866	GLN	3.0
2	B	457	ILE	2.8
2	B	471	GLY	2.8
1	A	847	ASP	2.7
2	B	655	LYS	2.7
2	B	493	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	918	LYS	2.6
2	B	681	ASN	2.5
2	B	679	THR	2.5
1	A	791	SER	2.5
2	B	660	GLU	2.5
1	A	1055	LYS	2.5
2	B	498	LYS	2.5
1	A	848	GLN	2.4
2	B	503	PHE	2.3
2	B	659	ASN	2.3
2	B	320	PRO	2.3
2	B	466	LYS	2.2
1	A	797	ARG	2.2
2	B	650	LYS	2.2
2	B	162	TYR	2.2
2	B	658	GLY	2.1
1	A	802	HIS	2.1
2	B	489	GLU	2.1
1	A	835	MET	2.1
1	A	1067	THR	2.1
2	B	273	LYS	2.0
1	A	836	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.