wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:19 PM GMT

PDB ID	:	1F2U
Title	:	Crystal Structure of RAD50 ABC-ATPase
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Deposited on	:	2000-05-29
Resolution	:	1.60 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

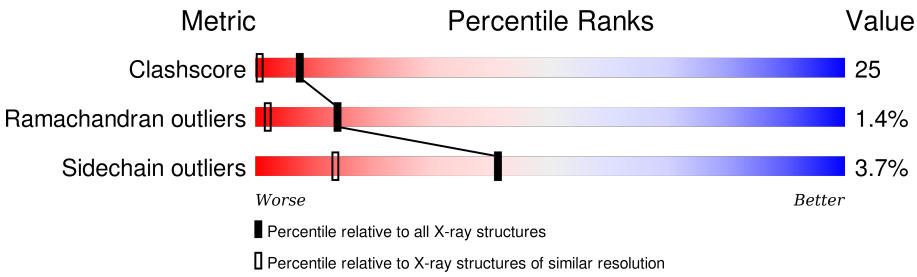
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)

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. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	149	52% 44% •
1	C	149	71% 25% • •
2	B	148	59% 37% • •
2	D	148	57% 37% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5128 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 RAD50 ABC-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	149	1206	776	208	219	3	12	0	0
1	C	148	1199	773	207	216	3	5	0	0

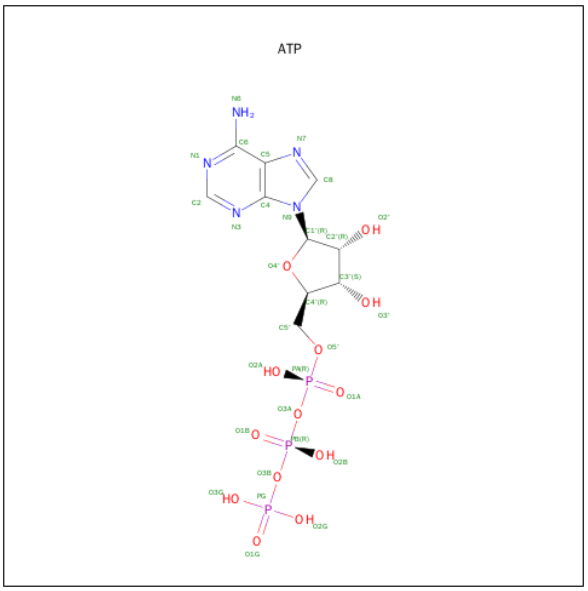
- Molecule 2 is a protein called RAD50 ABC-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	145	1152	737	195	218	2	15	0	0
2	D	142	1134	725	192	215	2	46	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0
			Total	C	N	O	P		
4	C	1	31	10	5	13	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	87	87	87	0	0
			Total	O		
5	B	99	99	99	0	0
			Total	O		
5	C	115	115	115	0	0
			Total	O		
5	D	72	72	72	0	0

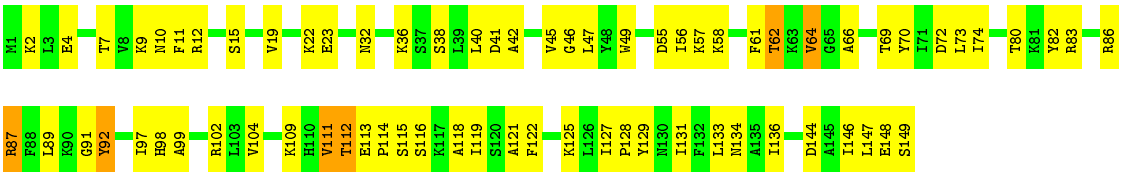
3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: RAD50 ABC-ATPASE

Chain A:

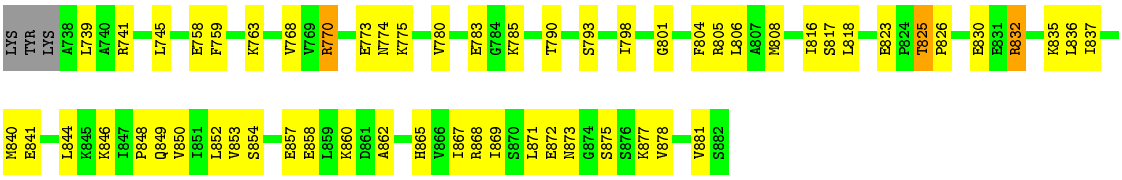


- Molecule 1: RAD50 ABC-ATPASE

Chain C:

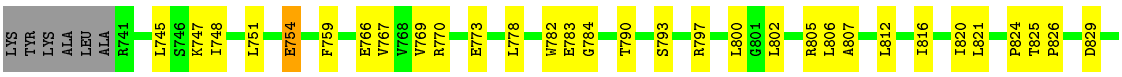
- Molecule 2: RAD50 ABC-ATPASE

Chain B:



- Molecule 2: RAD50 ABC-ATPASE

Chain D:



R832
K835
L836
I837
T838
I839
M840
Y843
L844
I847
V850
I851
L852
V853
S854
H855
D856
E857
E858
L859
K860
H865
V866
I867
R868
I869
E872
N873
G874
S875
S876
K877
S882

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.90Å 82.60Å 106.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.238 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5128	wwPDB-VP
Average B, all atoms ($Å^2$)	64.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.42	0/1228	0.68	0/1647
1	C	0.53	0/1221	0.74	0/1639
2	B	0.49	0/1168	0.75	2/1572 (0.1%)
2	D	0.53	0/1150	0.75	0/1547
All	All	0.49	0/4767	0.73	2/6405 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	798	ILE	CG1-CB-CG2	-5.26	99.82	111.40
2	B	825	THR	N-CA-C	5.25	125.17	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1206	0	1245	80	0
1	C	1199	0	1240	47	1
2	B	1152	0	1191	64	1
2	D	1134	0	1170	74	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	31	0	12	6	0
4	C	31	0	12	7	0
5	A	87	0	0	23	0
5	B	99	0	0	30	0
5	C	115	0	0	18	0
5	D	72	0	0	12	0
All	All	5128	0	4870	240	1

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 25.

The worst 5 of 240 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)
2:D:860:LYS:HE3	2:D:866:VAL:HG11	1.38	1.03
1:A:55:ASP:HB2	5:A:924:HOH:O	1.68	0.93
1:C:57:LYS:HG2	5:C:940:HOH:O	1.73	0.88
2:D:837:ILE:HD11	2:D:858:GLU:HG2	1.55	0.88
1:C:25:ILE:HD11	2:D:844:LEU:HB3	1.56	0.86

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	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:GLU:OE1	1:C:52:ARG:NH2[4_545]	2.08	0.12

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	147/149 (99%)	127 (86%)	18 (12%)	2 (1%)	14 2
1	C	146/149 (98%)	139 (95%)	6 (4%)	1 (1%)	26 8
2	B	143/148 (97%)	127 (89%)	14 (10%)	2 (1%)	14 2
2	D	140/148 (95%)	125 (89%)	12 (9%)	3 (2%)	9 1
All	All	576/594 (97%)	518 (90%)	50 (9%)	8 (1%)	14 2

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	862	ALA
1	A	64	VAL
2	B	881	VAL
2	D	773	GLU
2	D	873	ASN

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	131/131 (100%)	125 (95%)	6 (5%)	33 9
1	C	130/131 (99%)	126 (97%)	4 (3%)	47 19
2	B	124/127 (98%)	120 (97%)	4 (3%)	46 18
2	D	123/127 (97%)	118 (96%)	5 (4%)	37 11
All	All	508/516 (98%)	489 (96%)	19 (4%)	41 13

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	832	ARG
1	C	29	ILE
2	D	754	GLU
2	B	770	ARG
2	D	759	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	C	10	ASN
1	C	110	HIS
2	D	855	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ATP	A	901	3	24,33,33	1.45	6 (25%)	31,52,52	1.17	1 (3%)
4	ATP	C	901	3	24,33,33	1.60	5 (20%)	31,52,52	1.15	3 (9%)

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	ATP	A	901	3	-	0/18/38/38	0/3/3/3
4	ATP	C	901	3	-	0/18/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	ATP	C3'-C4'	-2.82	1.45	1.53
4	C	901	ATP	O5'-C5'	-2.60	1.34	1.44
4	A	901	ATP	C8-N7	-2.19	1.30	1.34
4	A	901	ATP	C3'-C4'	-2.15	1.47	1.53
4	A	901	ATP	PG-O2G	-2.02	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	901	ATP	O3'-C3'-C4'	-2.08	104.82	111.05
4	C	901	ATP	O4'-C4'-C3'	2.36	109.91	105.15
4	A	901	ATP	C4-C5-N7	2.39	111.67	109.48
4	C	901	ATP	C4-C5-N7	2.48	111.76	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	ATP	6	0
4	C	901	ATP	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.