



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 12:55 am GMT

PDB ID : 5GOX
Title : Eukaryotic Rad50 Functions as A Rod-shaped Dimer
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Deposited on : 2016-07-30
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

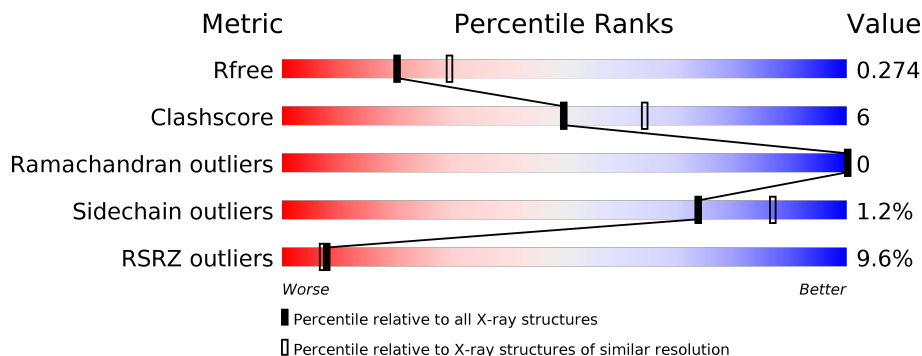
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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 $\leq 5\%$. 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	186	<div> <div>12%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	186	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2980 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 DNA repair protein RAD50.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	Se	0	0	0
			1476	904	268	297	4	3			
1	B	181	Total	C	N	O	S	Se	0	0	0
			1476	904	268	297	4	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	581	GLY	-	expression tag	UNP Q92878
A	582	SER	-	expression tag	UNP Q92878
A	583	HIS	-	expression tag	UNP Q92878
A	584	MSE	-	expression tag	UNP Q92878
B	581	GLY	-	expression tag	UNP Q92878
B	582	SER	-	expression tag	UNP Q92878
B	583	HIS	-	expression tag	UNP Q92878
B	584	MSE	-	expression tag	UNP Q92878

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

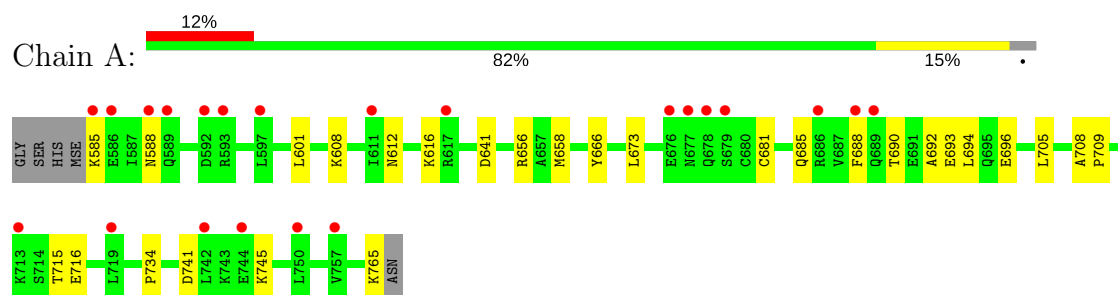
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	5	Total	O	0	0
			5	5		

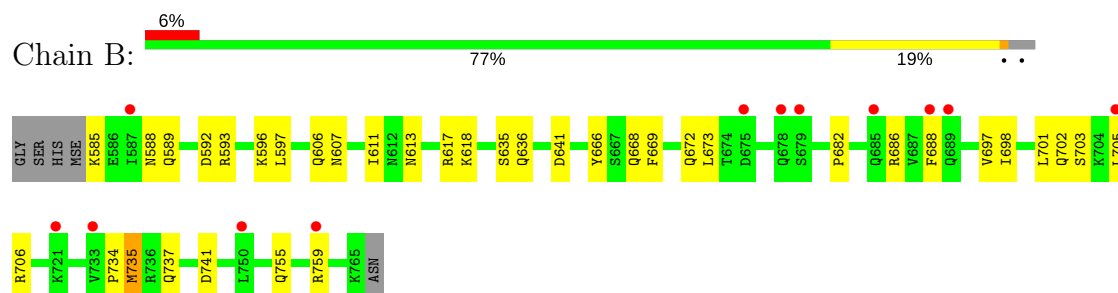
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: DNA repair protein RAD50



• Molecule 1: DNA repair protein RAD50



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.18Å 61.97Å 81.54Å 90.00° 99.75° 90.00°	Depositor
Resolution (Å)	28.22 – 2.40 39.77 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.22-2.40) 99.5 (39.77-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.66 (at 2.39Å)	Xtriage
Refinement program	PHENIX dev_1745	Depositor
R, R_{free}	0.213 , 0.271 0.217 , 0.274	Depositor DCC
R_{free} test set	815 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2980	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.04% 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

5.1 Standard geometry

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

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	0.47	0/1483	0.61	0/1974
1	B	0.45	0/1483	0.63	0/1974
All	All	0.46	0/2966	0.62	0/3948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1476	0	1505	16	0
1	B	1476	0	1505	25	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
3	A	1	0	0	0	0
4	A	4	0	0	0	0
4	B	5	0	0	0	0
All	All	2980	0	3034	38	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 6.

All (38) 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:B:673:LEU:HD21	1:B:682:PRO:HD3	1.77	0.66
1:B:592:ASP:OD2	1:B:596:LYS:NZ	2.31	0.61
1:A:690:THR:HG23	1:A:693:GLU:H	1.68	0.57
1:A:601:LEU:HD21	1:A:765:LYS:HD2	1.86	0.56
1:B:585:LYS:HA	1:B:588:ASN:HD22	1.72	0.54
1:A:734:PRO:HG3	1:B:734:PRO:HG2	1.90	0.54
1:A:681:CYS:O	1:A:685:GLN:HA	2.08	0.54
1:B:585:LYS:O	1:B:589:GLN:HG3	2.07	0.53
1:B:669:PHE:O	1:B:673:LEU:HG	2.09	0.51
1:A:692:ALA:O	1:A:696:GLU:HG3	2.10	0.51
1:B:698:ILE:O	1:B:702:GLN:HG3	2.10	0.51
1:B:755:GLN:NE2	1:B:759:ARG:HH21	2.09	0.50
1:B:666:TYR:HB2	1:B:705:LEU:HD21	1.94	0.49
1:B:635:SER:OG	1:B:636:GLN:N	2.46	0.49
1:B:635:SER:HB3	1:B:641:ASP:OD1	2.13	0.48
1:A:585:LYS:HA	1:A:588:ASN:ND2	2.28	0.48
1:A:673:LEU:HB3	1:A:694:LEU:HD11	1.96	0.48
1:B:735:MSE:HE3	1:B:735:MSE:HB2	1.71	0.48
1:B:666:TYR:CD2	1:B:701:LEU:HD22	2.49	0.47
1:A:612:ASN:ND2	1:A:616:LYS:HE3	2.30	0.47
1:B:688:PHE:CE1	1:B:697:VAL:HG21	2.50	0.47
1:A:641:ASP:OD2	2:A:802:GOL:O1	2.26	0.46
1:A:688:PHE:HA	1:B:686:ARG:HH12	1.82	0.44
1:B:737:GLN:NE2	1:B:741:ASP:OD1	2.51	0.43
1:B:613:ASN:O	1:B:617:ARG:HG3	2.17	0.43
1:A:608:LYS:O	1:A:612:ASN:HB2	2.18	0.43
1:B:666:TYR:HD2	1:B:701:LEU:HD22	1.83	0.43
1:A:741:ASP:O	1:A:745:LYS:HB3	2.19	0.43
1:B:593:ARG:O	1:B:597:LEU:HG	2.19	0.43
1:B:668:GLN:O	1:B:672:GLN:HG3	2.19	0.42
1:B:607:ASN:O	1:B:611:ILE:HG13	2.19	0.42
1:A:708:ALA:N	1:A:709:PRO:HD2	2.35	0.41
1:A:734:PRO:CG	1:B:734:PRO:HG2	2.50	0.41
1:B:618:LYS:HD3	1:B:618:LYS:HA	1.79	0.41
1:B:703:SER:O	1:B:706:ARG:HB3	2.20	0.41
1:A:666:TYR:HB2	1:A:705:LEU:HD21	2.03	0.41
1:B:688:PHE:HE1	1:B:697:VAL:HG21	1.86	0.40
1:A:656:ARG:HB2	1:A:715:THR:HG21	2.03	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	179/186 (96%)	175 (98%)	4 (2%)	0	100	100
1	B	179/186 (96%)	175 (98%)	4 (2%)	0	100	100
All	All	358/372 (96%)	350 (98%)	8 (2%)	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	170/170 (100%)	168 (99%)	2 (1%)	74	87
1	B	170/170 (100%)	168 (99%)	2 (1%)	74	87
All	All	340/340 (100%)	336 (99%)	4 (1%)	74	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	658	MSE
1	A	716	GLU
1	B	606	GLN
1	B	735	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	588	ASN
1	B	588	ASN
1	B	655	GLN
1	B	695	GLN
1	B	755	GLN

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, 1 is monoatomic - leaving 3 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	$\# Z > 2$
2	GOL	A	801	-	5,5,5	0.40	0	5,5,5	0.21	0
2	GOL	A	802	-	5,5,5	0.28	0	5,5,5	0.64	0
2	GOL	B	801	-	5,5,5	0.39	0	5,5,5	0.34	0

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
2	GOL	A	801	-	-	0/4/4/4	0/0/0/0
2	GOL	A	802	-	-	0/4/4/4	0/0/0/0
2	GOL	B	801	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	GOL	1	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

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	178/186 (95%)	0.78	22 (12%) 4 3	55, 88, 131, 169	0
1	B	178/186 (95%)	0.67	12 (6%) 18 16	56, 95, 122, 160	0
All	All	356/372 (95%)	0.72	34 (9%) 8 7	55, 92, 126, 169	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	689	GLN	5.6
1	A	593	ARG	4.2
1	B	678	GLN	4.1
1	A	689	GLN	3.7
1	A	678	GLN	3.5
1	B	587	ILE	3.5
1	A	611	ILE	3.4
1	B	685	GLN	3.3
1	A	744	GLU	3.2
1	B	759	ARG	3.2
1	A	686	ARG	3.1
1	B	688	PHE	3.0
1	B	750	LEU	3.0
1	A	750	LEU	2.9
1	A	592	ASP	2.9
1	A	679	SER	2.8
1	A	597	LEU	2.7
1	A	589	GLN	2.7
1	B	679	SER	2.7
1	A	688	PHE	2.7
1	B	705	LEU	2.6
1	A	757	VAL	2.6
1	B	733	VAL	2.4
1	A	742	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	617	ARG	2.2
1	B	675	ASP	2.2
1	A	677	ASN	2.2
1	A	676	GLU	2.2
1	A	588	ASN	2.1
1	A	713	LYS	2.1
1	A	585	LYS	2.1
1	A	719	LEU	2.1
1	A	586	GLU	2.1
1	B	721	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	801	6/6	0.63	0.29	137,138,141,145	0
2	GOL	A	801	6/6	0.78	0.20	78,85,99,105	0
2	GOL	A	802	6/6	0.80	0.39	95,106,107,109	0
3	ZN	A	803	1/1	0.94	0.17	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.