



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Jan 25, 2018 – 04:59 PM EST

PDB ID : 5NP7
EMDB ID: : EMD-8183
Title : CryoEM structure of Human Rad51 on single-stranded DNA to 4.2A resolution.
Authors : Short, J.M.; Venkitaraman, A.
Deposited on : 2017-04-13
Resolution : 4.20 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

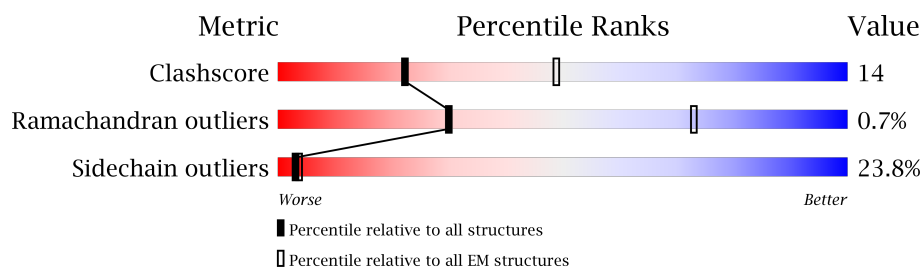
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	339	57% 24% 9% • 8%
1	B	339	56% 24% 10% • 8%
1	C	339	56% 25% 9% • 8%
1	D	339	56% 25% 9% • 8%
1	E	339	55% 25% 9% • 8%
1	F	339	56% 25% 9% • 8%
1	G	339	57% 24% 9% • 8%

2 Entry composition [i](#)

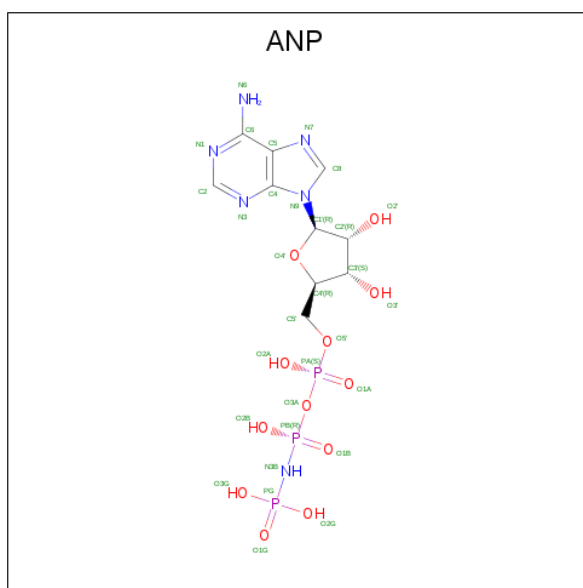
There are 2 unique types of molecules in this entry. The entry contains 16457 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RAD51 homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	B	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	C	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	D	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	E	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	F	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		
1	G	311	Total	C	N	O	S	0	0
			2320	1455	411	441	13		

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

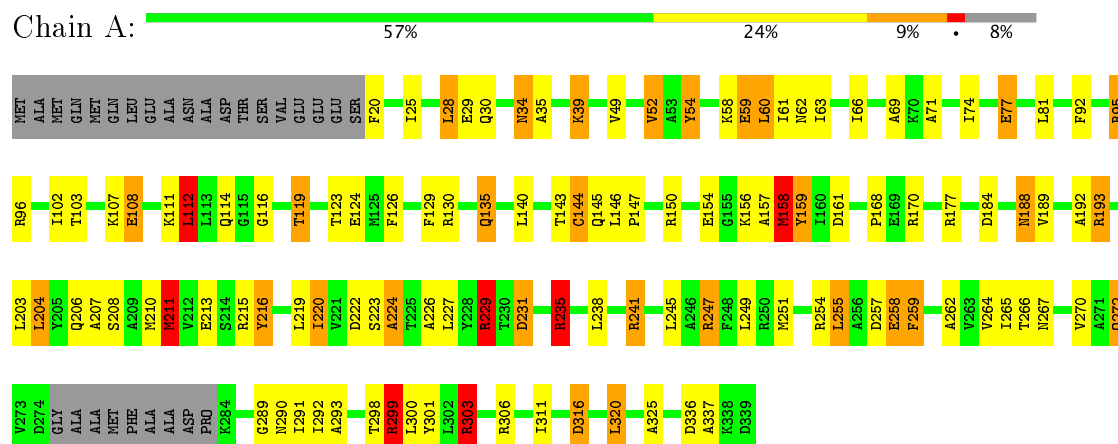


Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	0
2	C	1	Total 31	C 10	N 6	O 12	P 3	0
2	D	1	Total 31	C 10	N 6	O 12	P 3	0
2	E	1	Total 31	C 10	N 6	O 12	P 3	0
2	F	1	Total 31	C 10	N 6	O 12	P 3	0
2	G	1	Total 31	C 10	N 6	O 12	P 3	0

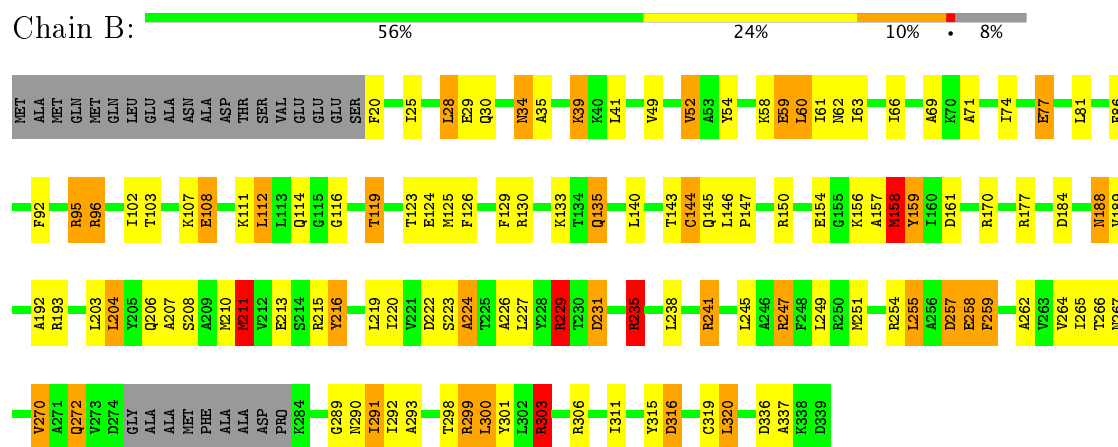
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

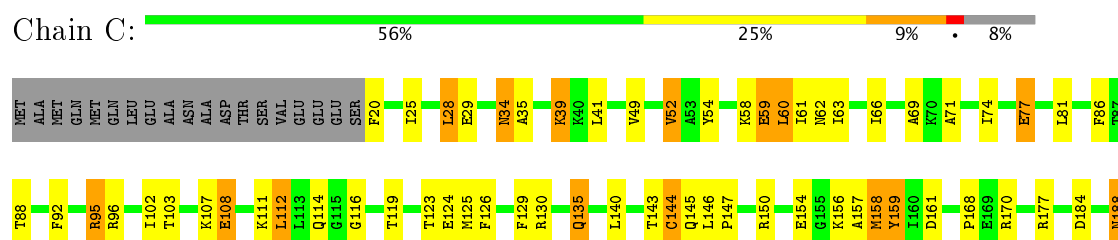
• Molecule 1: DNA repair protein RAD51 homolog 1

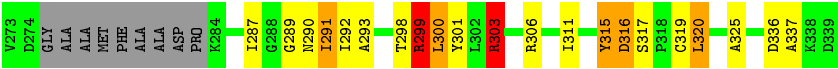


• Molecule 1: DNA repair protein RAD51 homolog 1

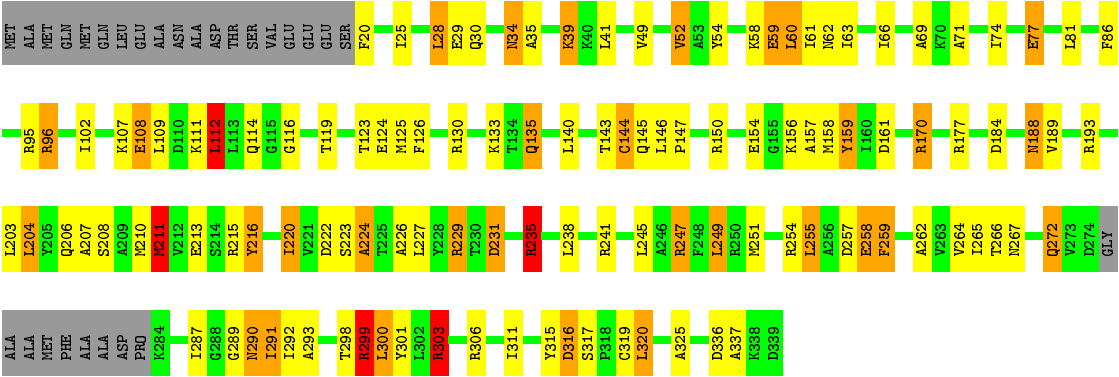


• Molecule 1: DNA repair protein RAD51 homolog 1





● Molecule 1: DNA repair protein RAD51 homolog 1



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=56.2°, rise=16.0 Å, axial sym=C1	Depositor
Number of segments used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; per segment	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	104477	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.99	3/2354 (0.1%)	1.39	24/3182 (0.8%)
1	B	0.99	5/2354 (0.2%)	1.39	25/3182 (0.8%)
1	C	0.99	5/2354 (0.2%)	1.41	27/3182 (0.8%)
1	D	0.99	5/2354 (0.2%)	1.40	27/3182 (0.8%)
1	E	0.99	4/2354 (0.2%)	1.40	24/3182 (0.8%)
1	F	0.99	5/2354 (0.2%)	1.40	27/3182 (0.8%)
1	G	1.00	5/2354 (0.2%)	1.40	24/3182 (0.8%)
All	All	0.99	32/16478 (0.2%)	1.40	178/22274 (0.8%)

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	54	TYR	CE1-CZ	6.85	1.47	1.38
1	B	54	TYR	CE1-CZ	6.36	1.46	1.38
1	G	54	TYR	CE1-CZ	5.98	1.46	1.38
1	E	54	TYR	CG-CD2	5.91	1.46	1.39
1	A	258	GLU	CG-CD	-5.83	1.43	1.51

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	231	ASP	CB-CG-OD2	11.79	128.91	118.30
1	A	231	ASP	CB-CG-OD2	11.42	128.58	118.30
1	B	231	ASP	CB-CG-OD2	11.37	128.53	118.30
1	D	231	ASP	CB-CG-OD2	11.12	128.31	118.30
1	F	231	ASP	CB-CG-OD2	11.10	128.29	118.30

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	2320	0	2268	68	0
1	B	2320	0	2268	70	0
1	C	2320	0	2268	72	0
1	D	2320	0	2268	73	0
1	E	2320	0	2268	74	0
1	F	2320	0	2268	65	0
1	G	2320	0	2268	70	0
2	A	31	0	13	0	0
2	B	31	0	13	1	0
2	C	31	0	13	1	0
2	D	31	0	13	1	0
2	E	31	0	13	1	0
2	F	31	0	13	1	0
2	G	31	0	13	0	0
All	All	16457	0	15967	467	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 14.

The worst 5 of 467 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:D:207:ALA:O	1:D:211:MET:SD	2.06	1.13
1:C:207:ALA:O	1:C:211:MET:SD	2.06	1.13
1:F:207:ALA:O	1:F:211:MET:SD	2.06	1.13
1:B:207:ALA:O	1:B:211:MET:SD	2.06	1.12
1:A:207:ALA:O	1:A:211:MET:SD	2.06	1.12

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 PDB entries followed by that with respect to all EM entries.

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	307/339 (91%)	263 (86%)	42 (14%)	2 (1%)	25	68
1	B	307/339 (91%)	263 (86%)	42 (14%)	2 (1%)	25	68
1	C	307/339 (91%)	265 (86%)	39 (13%)	3 (1%)	18	61
1	D	307/339 (91%)	264 (86%)	41 (13%)	2 (1%)	25	68
1	E	307/339 (91%)	264 (86%)	41 (13%)	2 (1%)	25	68
1	F	307/339 (91%)	265 (86%)	40 (13%)	2 (1%)	25	68
1	G	307/339 (91%)	266 (87%)	39 (13%)	2 (1%)	25	68
All	All	2149/2373 (91%)	1850 (86%)	284 (13%)	15 (1%)	30	68

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ALA
1	A	337	ALA
1	B	224	ALA
1	B	337	ALA
1	C	224	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 PDB entries followed by that with respect to all EM entries.

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	229/269 (85%)	175 (76%)	54 (24%)	1	7
1	B	229/269 (85%)	174 (76%)	55 (24%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	229/269 (85%)	175 (76%)	54 (24%)	1	7
1	D	229/269 (85%)	175 (76%)	54 (24%)	1	7
1	E	229/269 (85%)	173 (76%)	56 (24%)	1	6
1	F	229/269 (85%)	173 (76%)	56 (24%)	1	6
1	G	229/269 (85%)	177 (77%)	52 (23%)	1	8
All	All	1603/1883 (85%)	1222 (76%)	381 (24%)	3	6

5 of 381 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	60	LEU
1	D	316	ASP
1	G	159	TYR
1	D	107	LYS
1	D	206	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	135	GLN
1	D	294	HIS
1	F	294	HIS
1	C	294	HIS
1	G	135	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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

7 ligands are 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
2	ANP	A	600	-	29,33,33	2.44	12 (41%)	28,52,52	2.53	10 (35%)
2	ANP	B	600	-	29,33,33	2.44	11 (37%)	28,52,52	2.53	9 (32%)
2	ANP	C	600	-	29,33,33	2.45	11 (37%)	28,52,52	2.52	9 (32%)
2	ANP	D	600	-	29,33,33	2.46	11 (37%)	28,52,52	2.52	10 (35%)
2	ANP	E	600	-	29,33,33	2.47	12 (41%)	28,52,52	2.52	9 (32%)
2	ANP	F	600	-	29,33,33	2.42	11 (37%)	28,52,52	2.50	11 (39%)
2	ANP	G	600	-	29,33,33	2.42	12 (41%)	28,52,52	2.76	12 (42%)

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	ANP	A	600	-	-	1/13/38/38	0/3/3/3
2	ANP	B	600	-	-	1/13/38/38	0/3/3/3
2	ANP	C	600	-	-	1/13/38/38	0/3/3/3
2	ANP	D	600	-	-	1/13/38/38	0/3/3/3
2	ANP	E	600	-	-	1/13/38/38	0/3/3/3
2	ANP	F	600	-	-	1/13/38/38	0/3/3/3
2	ANP	G	600	-	-	1/13/38/38	0/3/3/3

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	ANP	PG-O3G	-2.39	1.50	1.56
2	B	600	ANP	PG-O3G	-2.39	1.50	1.56
2	C	600	ANP	PG-O3G	-2.38	1.50	1.56
2	E	600	ANP	PG-O3G	-2.38	1.50	1.56
2	D	600	ANP	PG-O3G	-2.30	1.50	1.56

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	600	ANP	N3-C2-N1	-9.38	120.69	128.86
2	A	600	ANP	N3-C2-N1	-8.34	121.59	128.86
2	E	600	ANP	N3-C2-N1	-8.31	121.62	128.86
2	B	600	ANP	N3-C2-N1	-8.29	121.64	128.86
2	C	600	ANP	N3-C2-N1	-8.27	121.65	128.86

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	ANP	O1B-PB-N3B-PG
2	D	600	ANP	O1B-PB-N3B-PG
2	G	600	ANP	O1B-PB-N3B-PG
2	C	600	ANP	O1B-PB-N3B-PG
2	E	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	ANP	1	0
2	C	600	ANP	1	0
2	D	600	ANP	1	0
2	E	600	ANP	1	0
2	F	600	ANP	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.