



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

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PDB ID : 5JZC
EMDB ID: : EMD-8183
Title : helical filament
Authors : Short, J.; Liu, Y.
Deposited on : 2016-05-16
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 : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

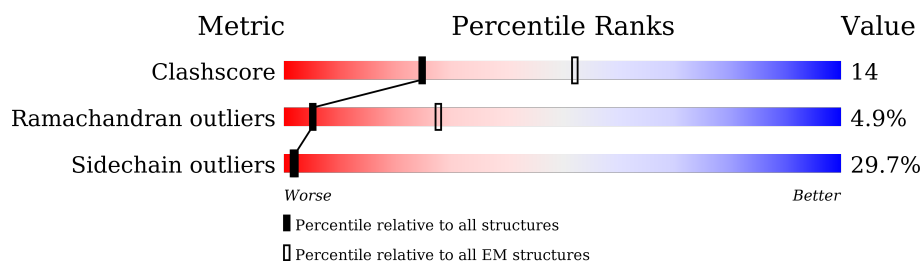
1 Overall quality at a glance

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	
1	B	339	
1	C	339	
1	D	339	
1	E	339	
1	F	339	
1	G	339	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11935 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	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	B	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	C	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	D	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	E	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	F	312	Total	C	N	O	4	0
			1705	1043	332	330		
1	G	312	Total	C	N	O	4	0
			1705	1043	332	330		

T1994	T1995	T1996	T2003	L2018	G2024	G2027	A2029	M2030	Y2031	L2032	D2033	R2039	V2061	A2062	Y2063	A2064	A2069	L2090	L2091	D2094	T2097	Y2100	R2101	Z2104	S2105	G2106	R2107	L2110	F2120	L2125	A2128	A2134	V2135	T2136	Q2140	V2141	V2145	D2146										
MET	ALA	MET	MET	MET	GLN	GLN	LEU	GLU	ALA	ASN	ALA	ASP	THR	SER	VAL	GLU	GLU	SER	G1892	G1893	P1894	G1895	P1896	T1897	N1906	A1907	N1908	F1918	H1919	T1920	A1923	Y1926	L1953	P1954	P1955	A1956	G1957	A1961	T1962	F1963	F1964	R1967	R1968	S1969	E1970	I1974	G1988	T1991

ALA	ALA	MET	PHE	ALA	ALA	ASP	P2147	I2155	T2161	Y2165	L2166	R2167	K2168	T2178	Y2179	P2182	C2183	L2184	P2185	E2186	A2187	E2188	A2189	A2201	K2202	D2203

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	69000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.18	11/1725 (0.6%)	1.39	13/2388 (0.5%)
1	B	1.13	3/1725 (0.2%)	1.41	14/2388 (0.6%)
1	C	1.12	1/1725 (0.1%)	1.35	13/2388 (0.5%)
1	D	1.13	2/1725 (0.1%)	1.32	12/2388 (0.5%)
1	E	1.12	2/1725 (0.1%)	1.34	11/2388 (0.5%)
1	F	1.25	11/1725 (0.6%)	1.36	21/2388 (0.9%)
1	G	1.25	13/1725 (0.8%)	1.39	19/2388 (0.8%)
All	All	1.17	43/12075 (0.4%)	1.36	103/16716 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	4
1	E	0	4
1	F	0	4
1	G	0	4
All	All	0	31

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	2101	ARG	CD-NE	12.95	1.68	1.46
1	F	1789	ARG	CD-NE	11.68	1.66	1.46
1	A	54	TYR	CE1-CZ	10.50	1.52	1.38
1	F	1789	ARG	CZ-NH2	10.34	1.46	1.33
1	G	2101	ARG	NE-CZ	9.97	1.46	1.33

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH2	23.16	131.88	120.30
1	B	541	ARG	NE-CZ-NH2	20.62	130.61	120.30
1	C	853	ARG	NE-CZ-NH2	17.78	129.19	120.30
1	B	541	ARG	NE-CZ-NH1	-16.91	111.84	120.30
1	E	1477	ARG	NE-CZ-NH2	15.01	127.81	120.30

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192	ALA	Peptide
1	A	222	ASP	Peptide
1	A	282	ASN	Peptide
1	A	296	LYS	Peptide
1	A	81	LEU	Peptide

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	1705	0	991	34	0
1	B	1705	0	991	49	0
1	C	1705	0	991	43	0
1	D	1705	0	991	51	0
1	E	1705	0	991	48	0
1	F	1705	0	991	47	0
1	G	1705	0	991	37	0
All	All	11935	0	6937	263	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 263 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:G:2101:ARG:NE	1:G:2101:ARG:CD	1.68	1.54
1:B:541:ARG:HH12	1:B:582:VAL:HG11	1.33	0.94
1:G:1994:ILE:O	1:G:2161:THR:HA	1.70	0.92
1:B:434:ILE:O	1:B:601:THR:HA	1.72	0.88
1:D:1091:GLY:HA3	1:D:1153:ALA:HB2	1.58	0.86

There are no symmetry-related clashes.

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 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	312/339 (92%)	264 (85%)	33 (11%)	15 (5%)	3	32
1	B	312/339 (92%)	259 (83%)	38 (12%)	15 (5%)	3	32
1	C	312/339 (92%)	261 (84%)	35 (11%)	16 (5%)	2	31
1	D	312/339 (92%)	265 (85%)	32 (10%)	15 (5%)	3	32
1	E	312/339 (92%)	263 (84%)	34 (11%)	15 (5%)	3	32
1	F	312/339 (92%)	264 (85%)	33 (11%)	15 (5%)	3	32
1	G	312/339 (92%)	260 (83%)	37 (12%)	15 (5%)	3	32
All	All	2184/2373 (92%)	1836 (84%)	242 (11%)	106 (5%)	5	32

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	PRO
1	A	35	ALA
1	A	82	VAL
1	A	85	GLY

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	37/269 (14%)	26 (70%)	11 (30%)	0	4
1	B	37/269 (14%)	25 (68%)	12 (32%)	0	3
1	C	37/269 (14%)	25 (68%)	12 (32%)	0	3
1	D	37/269 (14%)	26 (70%)	11 (30%)	0	4
1	E	37/269 (14%)	25 (68%)	12 (32%)	0	3
1	F	37/269 (14%)	27 (73%)	10 (27%)	0	5
1	G	37/269 (14%)	28 (76%)	9 (24%)	1	7
All	All	259/1883 (14%)	182 (70%)	77 (30%)	2	4

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	937	PRO
1	D	1243	TYR
1	G	2146	ASP
1	D	983	HIS
1	D	1174	LEU

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 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.