



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 08:19 PM UTC

PDB ID : 6ZFP / pdb_00006zfp
EMDB ID : EMD-11185
Title : Cryo-EM structure of DNA-PKcs (State 2)
Authors : Chaplin, A.K.; Hardwick, S.W.; Chirgadze, D.Y.; Blundell, T.L.
Deposited on : 2020-06-17
Resolution : 3.24 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

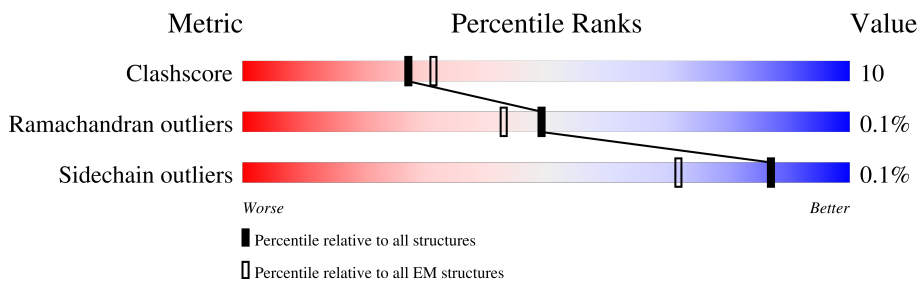
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.24 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	4156	70% 19% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29385 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.

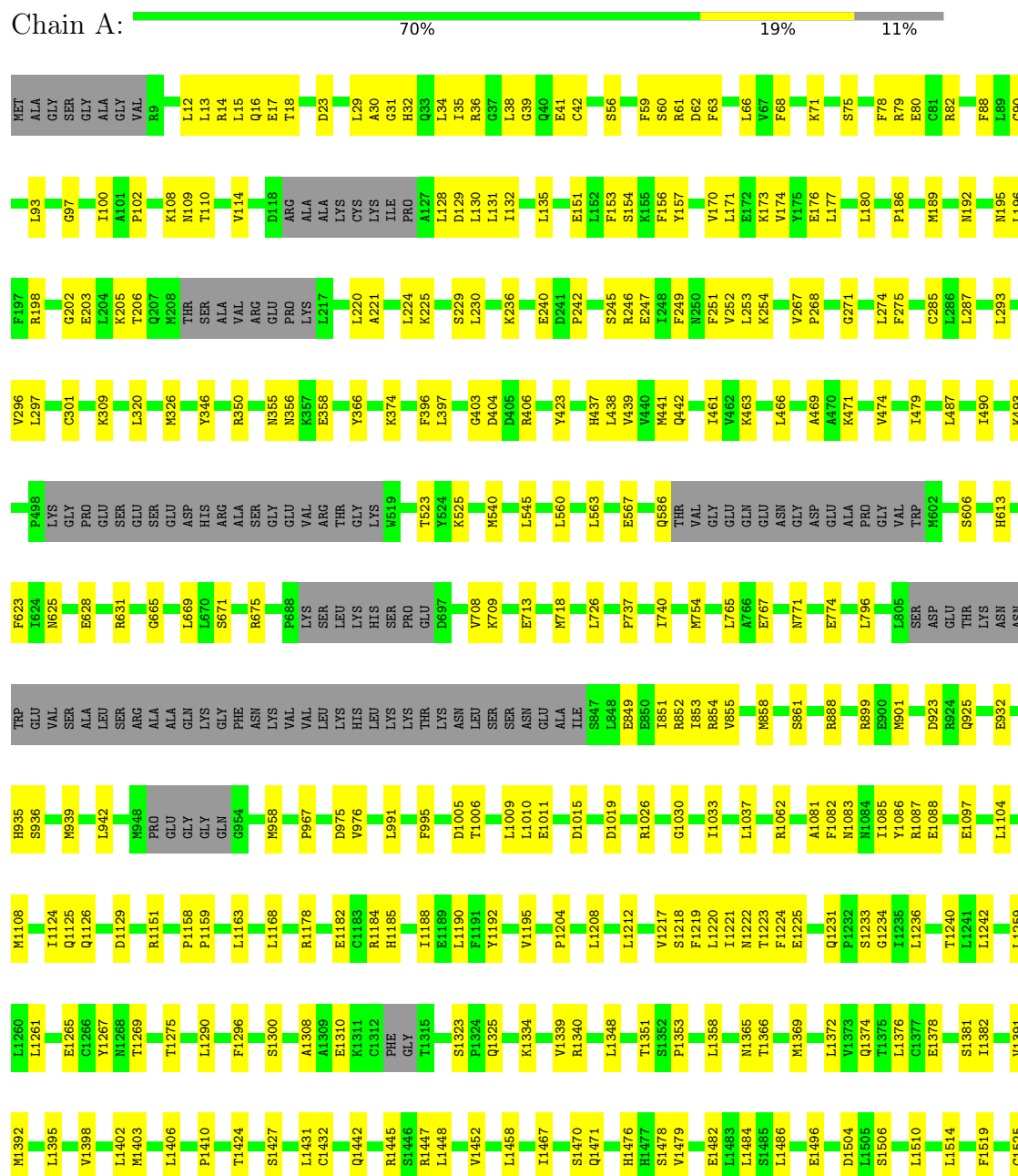
- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit,DNA-PKcs, DNA-PKcs.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3704	29385	18849	4964	5379	193	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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-dependent protein kinase catalytic subunit,DNA-PKCs,DNA-PKCs



R3167	K3009	K2824	GLU	SER	GLN	S2489	D2376	I2256	SER	PHE	K1985	F1814	T1641	E1526
M3176	E3012	E2828	LEU	LEU	THR	D2492	L2385	K2259	VAL	THR	ARG	T1815	K1642	R1527
I3182	E3013	I2832	LEU	PHE	THR	N2493	F2260	F2260	P2119	GLY	ARG	R1816	I1652	L1528
R3186	C3014	D2494	LEU	GLN	GLN	D2494	F2389	G2262	D2121	VAL	ASN	Q1817	D1685	L1532
C3187	S3015	I2498	GLY	HIS	GLY	I2498	V2392	D2269	L2133	GLN	PHE	F1819	K1689	L1538
K3196	E3033	L2517	SER	ARG	SER	L2517	L2396	N2270	L2133	THR	PRO	V1820	G1690	A1541
L3197	P3034	R2522	LEU	LEU	SER	R2522	C2397	S2271	F2145	SER	VAL	D1822	G1690	SER
THR	S3047	ALA	VAL	ALA	ALA	R2522	V2400	V2272	K2148	SER	GLU	L1824	V1693	LEU
PRO	L3053	L2531	ALA	GLN	TRP	L2531	L2277	L2277	I2151	GLN	PRO	L1827	L1710	GLY
LEU	L3062	T2535	GLU	ARG	PRO	T2535	R2404	V2280	I2151	ASP	MET	L1828	R1711	SER
PRO	L3062	E2406	GLN	ALA	VAL	E2406	E2406	M2281	E2155	PRO	GLU	L1836	L1714	GLN
GLU	D3066	L2539	GLY	LEU	ALA	G2407	M2408	C2292	R2158	ARG	ARG	L1837	E1715	GLY
ASP	K3067	L2542	GLN	GLN	GLN	M2408	L2415	S2308	L2169	ARG	LYS	E1838	V1550	S1549
ASN	L3077	L2542	GLN	SER	ILE	L2542	L2411	Q2301	W2164	THR	LYS	I1718	I1718	F1553
SER	L3078	E2551	VAL	VAL	ARG	E2551	Y2412	Q2301	L2165	GLY	TYR	D1864	F1722	F1553
ASN	L3088	T2559	GLY	ALA	ALA	T2559	F2413	V2304	S2166	ARG	ILE	I1867	F1722	E1557
ASP	L3091	F2554	GLY	THR	THR	F2554	Q2414	N2305	P2167	PHE	ILE	S1726	S1726	E1557
GLY	L3092	L2555	GLN	GLN	GLN	L2555	L2415	S2308	L2169	ARG	ARG	M1871	G1732	Y1560
LEU	L3093	L2556	GLN	GLN	GLN	L2556	F2420	S2308	L2169	ARG	GLU	Y1874	T1733	L1562
VAL	L3094	L2557	GLN	GLN	GLN	L2557	F2420	S2308	L2169	ARG	GLU	K1875	R1735	I1567
ARG	L3095	A2568	GLN	GLN	GLN	A2568	M2424	K2313	H2183	GLN	ALA	M1880	G1732	S1561
GLY	L3096	T2567	GLN	GLN	GLN	T2567	M2442	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3097	F2577	GLN	GLN	GLN	F2577	M2444	K2313	M2185	GLN	ALA	K1875	R1735	I1567
GLY	L3098	E2578	GLN	GLN	GLN	E2578	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3099	C2584	GLN	GLN	GLN	C2584	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3100	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
GLY	L3101	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3102	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
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GLY	L3105	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3106	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
GLY	L3107	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3108	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3109	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
GLY	L3110	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3111	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3112	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
GLY	L3113	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3114	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3115	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
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GLY	L3117	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3118	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
GLY	L3119	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3120	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3121	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
GLY	L3122	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3123	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
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GLY	L3126	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
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GLY	L3128	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3129	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
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GLY	L3131	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3132	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
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GLY	L3134	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3135	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
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GLY	L3137	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3138	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
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GLY	L3144	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3145	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
GLY	L3146	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
GLY	L3147	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3148	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
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GLY	L3154	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
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GLY	L3158	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561
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GLY	L3168	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	Y1874	T1733	L1562
GLY	L3169	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	K1875	R1735	I1567
GLY	L3170	E2585	GLN	GLN	GLN	E2585	L2455	K2313	Y2184	GLN	ALA	M1880	G1732	S1561

L4051	V3868	K3665	N3551	D3271
I4059	E3875	L3666	V3555	C3281
L4064	V3878	M3670	K3561	S3284
Y4077	P3879	L3680	L3575	SER
A4081	A3880	K3681	E3582	VAL
R4090	L3882	E3682	L3583	ILE
Q4103	L3883	S3684	K3568	ASP
L4107	A3886	P3685	V3596	SER
M4108	R3889	K3686	L3596	ALA
D4113	E3895	M3687	V3601	GLU
W4127	L3913	E3700	N3602	L3439
M4128	T3917	K3710	K3603	A3444
X5009	D3922	P3711	K3604	L3445
	R3923	E3714	N3605	V3446
	L3924	K3718	E3607	V3447
	L3925	R3718	K3608	E3448
	N3926	F3722	E3611	K3449
	L3938	D3723	K3612	M3450
	R3944	E3724	A3616	L3456
	M3959	L3751	G3617	S3313
	F3960	S3779	G3618	S3314
	K3975	A3780	A3622	Y3315
	Y3981	R3789	L3625	L3316
	A3987	T3790	G3626	S3317
	R3992	S3792	A3627	K3318
	M4000	V3793	F3628	A3322
	M4015	M3796	R3629	E3477
	Q4018	L3602	I3633	E3478
	K4019	L3803	F3636	S3481
	M4020	L3806	E3639	L3482
	K4023	L3816	H3643	M3483
	Q4024	T3819	K3646	T3484
	W4027	L3829	K3650	F3495
		L3843	K3655	I3496
		M3846	L3656	M3502
		M3858	S3657	L3505
		R3864	D3661	L3506
			N3664	D3507
				E3387
				A3396
				GLN
				PRO
				PRD
				SER
				TRP
				TRP
				SER
				CYS
				GLY
				Y3405
				I3410
				K3414
				R3425
				M3430
				ALA
				F3542

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80688	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.95	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/29848	0.40	1/40366 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	3483	MET	N-CA-C	8.44	121.23	111.11

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	29385	0	29509	545	0
All	All	29385	0	29509	545	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 10.

The worst 5 of 545 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ($\text{\AA}$)	Clash overlap ($\text{\AA}$)
1:A:3444:ALA:HA	1:A:3482:LEU:CD2	1.99	0.93
1:A:3618:GLY:H	1:A:3633:ILE:HD12	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3444:ALA:O	1:A:3482:LEU:HD21	1.83	0.79
1:A:899:ARG:HE	1:A:2568:MET:HB2	1.48	0.78
1:A:403:GLY:H	1:A:406:ARG:HH12	1.29	0.78

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	3640/4156 (88%)	3332 (92%)	304 (8%)	4 (0%)	48 77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3481	SER
1	A	2787	HIS
1	A	1968	SER
1	A	1813	SER

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 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	3234/3671 (88%)	3230 (100%)	4 (0%)	88 90

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

Mol	Chain	Res	Type
1	A	2105	HIS
1	A	3477	GLU
1	A	3478	GLU
1	A	3483	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2305	ASN
1	A	3470	GLN
1	A	2422	GLN
1	A	3787	GLN
1	A	3139	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 oligosaccharides 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 ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4128:MET	C	5009:UNK	N	95.34
1	A	5016:UNK	C	6001:UNK	N	49.10

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11185. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.