



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2026 – 12:13 PM JST

PDB ID : 9L06 / pdb_00009l06
EMDB ID : EMD-62690
Title : The cryo-EM structure of ATRX in complex with the nucleosome in the ADP.BeFx-bound state (composite)
Authors : Zhou, K.; Duan, S.; Liu, Y.
Deposited on : 2024-12-11
Resolution : 3.40 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:

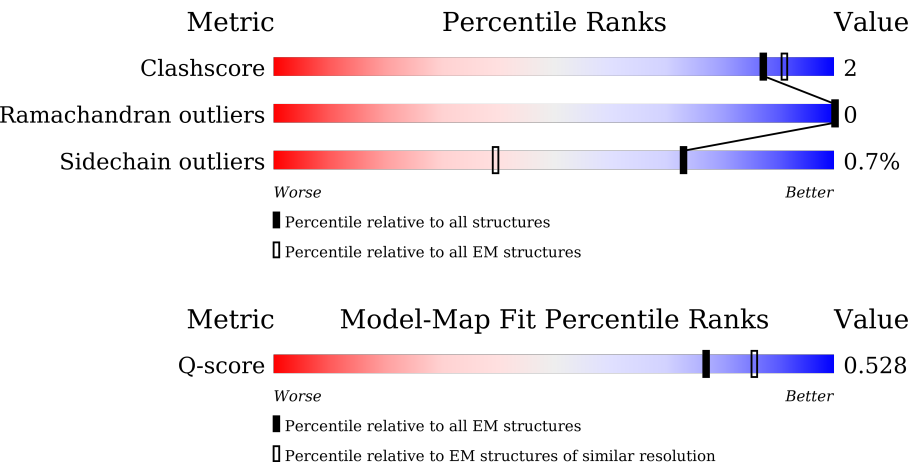
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	136	<div><div></div><div>72%</div><div>28%</div></div>
1	E	136	<div><div></div><div>70%</div><div>30%</div></div>
2	B	87	<div><div>10%</div><div>100%</div></div>
3	C	130	<div><div></div><div>82%</div><div>18%</div></div>

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Mol	Chain	Length	Quality of chain
3	G	130	
4	D	126	
4	H	126	
5	F	86	
6	I	207	
7	J	207	
8	K	1260	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 32845 atoms, of which 15152 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 Histone H3.3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	98	Total	C	H	N	O	S	0	0
			1622	503	826	153	138	2		
1	E	95	Total	C	H	N	O	S	0	0
			1584	489	810	148	135	2		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	87	Total	C	H	N	O	S	0	0
			1464	443	760	142	118	1		

- Molecule 3 is a protein called Histone H2A type 1-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	107	Total	C	H	N	O	0	0
			1660	510	850	158	142		
3	G	107	Total	C	H	N	O	0	0
			1675	513	861	159	142		

- Molecule 4 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	93	Total	C	H	N	O	S	0	0
			1439	449	722	128	138	2		
4	H	93	Total	C	H	N	O	S	0	0
			1469	455	744	130	138	2		

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	86	Total	C	H	N	O	S	0	0
			1373	424	701	130	117	1		

- Molecule 6 is a DNA chain called DNA (207-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	I	147	Total	C	H	N	O	P	0	0
			4648	1424	1650	544	883	147		

- Molecule 7 is a DNA chain called DNA (207-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	147	Total	C	H	N	O	P	0	0
			4678	1434	1649	567	881	147		

- Molecule 8 is a protein called Transcriptional regulator ATRX.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	724	Total	C	H	N	O	S	0	0
			11205	3555	5579	991	1050	30		

There are 107 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1901	UNK	TYR	conflict	UNP P46100
K	1902	UNK	PHE	conflict	UNP P46100
K	1903	UNK	ASP	conflict	UNP P46100
K	1904	UNK	GLU	conflict	UNP P46100
K	1905	UNK	ASP	conflict	UNP P46100
K	1906	UNK	SER	conflict	UNP P46100
K	1907	UNK	MET	conflict	UNP P46100
K	1908	UNK	ASP	conflict	UNP P46100
K	1909	UNK	GLU	conflict	UNP P46100
K	1910	UNK	PHE	conflict	UNP P46100
K	1911	UNK	ILE	conflict	UNP P46100
K	1912	UNK	ALA	conflict	UNP P46100
K	1913	UNK	SER	conflict	UNP P46100
K	1914	UNK	ASP	conflict	UNP P46100
K	1915	UNK	SER	conflict	UNP P46100
K	1916	UNK	ASP	conflict	UNP P46100
K	1917	UNK	GLU	conflict	UNP P46100
K	1918	UNK	THR	conflict	UNP P46100
K	1919	UNK	SER	conflict	UNP P46100
K	1920	UNK	MET	conflict	UNP P46100
K	1921	UNK	SER	conflict	UNP P46100
K	1922	UNK	LEU	conflict	UNP P46100
K	1923	UNK	SER	conflict	UNP P46100

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1924	UNK	SER	conflict	UNP P46100
K	1925	UNK	ASP	conflict	UNP P46100
K	1926	UNK	ASP	conflict	UNP P46100
K	1927	UNK	TYR	conflict	UNP P46100
K	1928	UNK	THR	conflict	UNP P46100
K	1929	UNK	LYS	conflict	UNP P46100
K	1930	UNK	LYS	conflict	UNP P46100
K	1931	UNK	LYS	conflict	UNP P46100
K	1932	UNK	LYS	conflict	UNP P46100
K	1933	UNK	LYS	conflict	UNP P46100
K	1934	UNK	GLY	conflict	UNP P46100
K	1935	UNK	LYS	conflict	UNP P46100
K	1936	UNK	LYS	conflict	UNP P46100
K	1937	UNK	GLY	conflict	UNP P46100
K	1938	UNK	LYS	conflict	UNP P46100
K	1939	UNK	LYS	conflict	UNP P46100
K	1940	UNK	ASP	conflict	UNP P46100
K	1941	UNK	SER	conflict	UNP P46100
K	1942	UNK	SER	conflict	UNP P46100
K	1943	UNK	SER	conflict	UNP P46100
K	1944	UNK	SER	conflict	UNP P46100
K	1945	UNK	GLY	conflict	UNP P46100
K	1946	UNK	SER	conflict	UNP P46100
K	1947	UNK	GLY	conflict	UNP P46100
K	1948	UNK	SER	conflict	UNP P46100
K	1949	UNK	ASP	conflict	UNP P46100
K	1950	UNK	ASN	conflict	UNP P46100
K	1951	UNK	ASP	conflict	UNP P46100
K	1952	UNK	VAL	conflict	UNP P46100
K	1953	UNK	GLU	conflict	UNP P46100
K	1954	UNK	VAL	conflict	UNP P46100
K	1955	UNK	ILE	conflict	UNP P46100
K	1956	UNK	LYS	conflict	UNP P46100
K	1957	UNK	VAL	conflict	UNP P46100
K	1958	UNK	TRP	conflict	UNP P46100
K	1959	UNK	ASN	conflict	UNP P46100
K	1960	UNK	SER	conflict	UNP P46100
K	1961	UNK	ARG	conflict	UNP P46100
K	1962	UNK	SER	conflict	UNP P46100
K	1963	UNK	ARG	conflict	UNP P46100
K	1964	UNK	GLY	conflict	UNP P46100
K	1965	UNK	GLY	conflict	UNP P46100

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1966	UNK	GLY	conflict	UNP P46100
K	1967	UNK	GLU	conflict	UNP P46100
K	1968	UNK	GLY	conflict	UNP P46100
K	1969	UNK	ASN	conflict	UNP P46100
K	1970	UNK	VAL	conflict	UNP P46100
K	1971	UNK	ASP	conflict	UNP P46100
K	1972	UNK	GLU	conflict	UNP P46100
K	1973	UNK	THR	conflict	UNP P46100
K	1974	UNK	GLY	conflict	UNP P46100
K	1975	UNK	ASN	conflict	UNP P46100
K	1976	UNK	ASN	conflict	UNP P46100
K	1977	UNK	PRO	conflict	UNP P46100
K	1978	UNK	SER	conflict	UNP P46100
K	1979	UNK	VAL	conflict	UNP P46100
K	1980	UNK	SER	conflict	UNP P46100
K	1981	UNK	LEU	conflict	UNP P46100
K	1982	UNK	LYS	conflict	UNP P46100
K	1983	UNK	LEU	conflict	UNP P46100
K	1984	UNK	GLU	conflict	UNP P46100
K	1985	UNK	GLU	conflict	UNP P46100
K	1986	UNK	SER	conflict	UNP P46100
K	1987	UNK	LYS	conflict	UNP P46100
K	1988	UNK	ALA	conflict	UNP P46100
K	1989	UNK	THR	conflict	UNP P46100
K	2493	HIS	-	expression tag	UNP P46100
K	2494	HIS	-	expression tag	UNP P46100
K	2495	HIS	-	expression tag	UNP P46100
K	2496	HIS	-	expression tag	UNP P46100
K	2497	HIS	-	expression tag	UNP P46100
K	2498	HIS	-	expression tag	UNP P46100
K	2499	HIS	-	expression tag	UNP P46100
K	2500	HIS	-	expression tag	UNP P46100
K	2501	HIS	-	expression tag	UNP P46100
K	2502	HIS	-	expression tag	UNP P46100
K	2503	ASP	-	expression tag	UNP P46100
K	2504	TYR	-	expression tag	UNP P46100
K	2505	LYS	-	expression tag	UNP P46100
K	2506	ASP	-	expression tag	UNP P46100
K	2507	ASP	-	expression tag	UNP P46100
K	2508	ASP	-	expression tag	UNP P46100
K	2509	ASP	-	expression tag	UNP P46100
K	2510	LYS	-	expression tag	UNP P46100

-
- The chemical structure of ADP (Adenosine Diphosphate) is shown. It consists of an adenine base (a purine ring system with an amino group at N6) attached to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is linked to a diphosphate group (two phosphate groups connected by an oxygen atom). The atoms are labeled with their respective element symbols and coordinates: N6, N7, N1, C6, C5, C8, C4, N3, N9, C2', C3', C4', C5', O4', O3', O2', O3A, O3B, O3C, O4A, O4B, O4C, O5A, O5B, O5C, O6A, O6B, O6C, O7A, O7B, O7C, O8A, O8B, O8C, O9A, O9B, O9C, O10A, O10B, O10C, O11A, O11B, O11C, O12A, O12B, O12C, O13A, O13B, O13C, O14A, O14B, O14C, O15A, O15B, O15C, O16A, O16B, O16C, O17A, O17B, O17C, O18A, O18B, O18C, O19A, O19B, O19C, O20A, O20B, O20C, O21A, O21B, O21C, O22A, O22B, O22C, O23A, O23B, O23C, O24A, O24B, O24C, O25A, O25B, O25C, O26A, O26B, O26C, O27A, O27B, O27C, O28A, O28B, O28C, O29A, O29B, O29C, O30A, O30B, O30C, O31A, O31B, O31C, O32A, O32B, O32C, O33A, O33B, O33C, O34A, O34B, O34C, O35A, O35B, O35C, O36A, O36B, O36C, O37A, O37B, O37C, O38A, O38B, O38C, O39A, O39B, O39C, O40A, O40B, O40C, O41A, O41B, O41C, O42A, O42B, O42C, O43A, O43B, O43C, O44A, O44B, O44C, O45A, O45B, O45C, O46A, O46B, O46C, O47A, O47B, O47C, O48A, O48B, O48C, O49A, O49B, O49C, O50A, O50B, O50C, O51A, O51B, O51C, O52A, O52B, O52C, O53A, O53B, O53C, O54A, O54B, O54C, O55A, O55B, O55C, O56A, O56B, O56C, O57A, O57B, O57C, O58A, O58B, O58C, O59A, O59B, O59C, O60A, O60B, O60C, O61A, O61B, O61C, O62A, O62B, O62C, O63A, O63B, O63C, O64A, O64B, O64C, O65A, O65B, O65C, O66A, O66B, O66C, O67A, O67B, O67C, O68A, O68B, O68C, O69A, O69B, O69C, O70A, O70B, O70C, O71A, O71B, O71C, O72A, O72B, O72C, O73A, O73B, O73C, O74A, O74B, O74C, O75A, O75B, O75C, O76A, O76B, O76C, O77A, O77B, O77C, O78A, O78B, O78C, O79A, O79B, O79C, O80A, O80B, O80C, O81A, O81B, O81C, O82A, O82B, O82C, O83A, O83B, O83C, O84A, O84B, O84C, O85A, O85B, O85C, O86A, O86B, O86C, O87A, O87B, O87C, O88A, O88B, O88C, O89A, O89B, O89C, O90A, O90B, O90C, O91A, O91B, O91C, O92A, O92B, O92C, O93A, O93B, O93C, O94A, O94B, O94C, O95A, O95B, O95C, O96A, O96B, O96C, O97A, O97B, O97C, O98A, O98B, O98C, O99A, O99B, O99C, O100A, O100B, O100C.

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

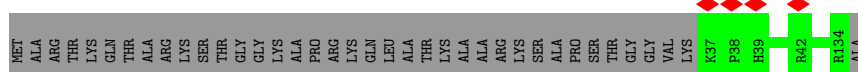
Mol	Chain	Residues	Atoms	AltConf
10	K	1	Total Mg 1 1	0

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

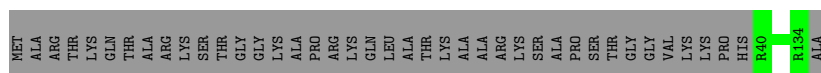
- Molecule 1: Histone H3.3

Chain A: 



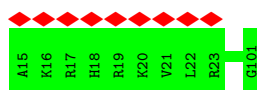
- Molecule 1: Histone H3.3

Chain E: 




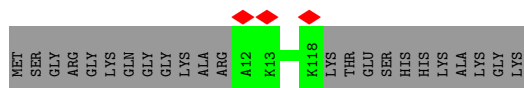
- Molecule 2: Histone H4

Chain B: 




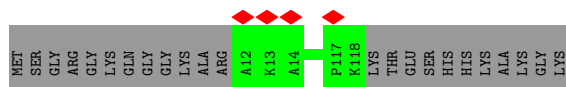
- Molecule 3: Histone H2A type 1-C

Chain C: 

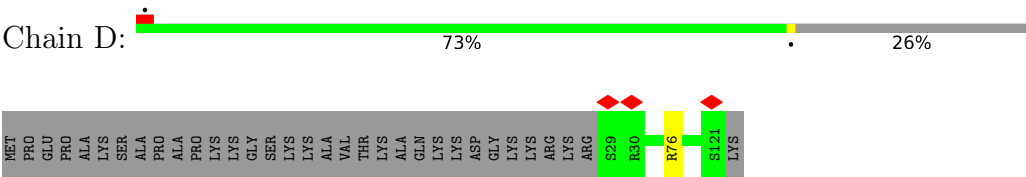


- Molecule 3: Histone H2A type 1-C

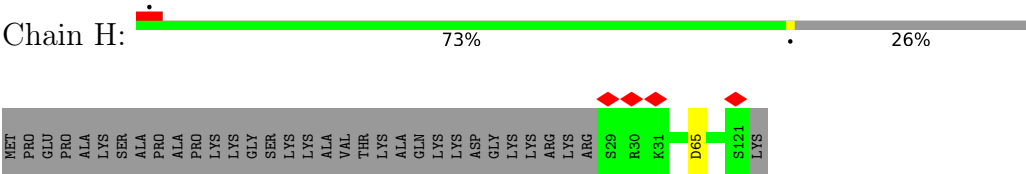
Chain G: 



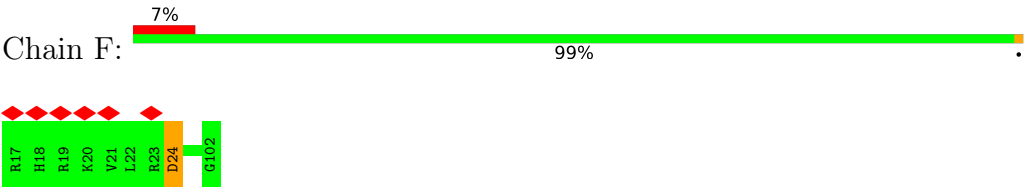
- Molecule 4: Histone H2B type 1-C/E/F/G/I



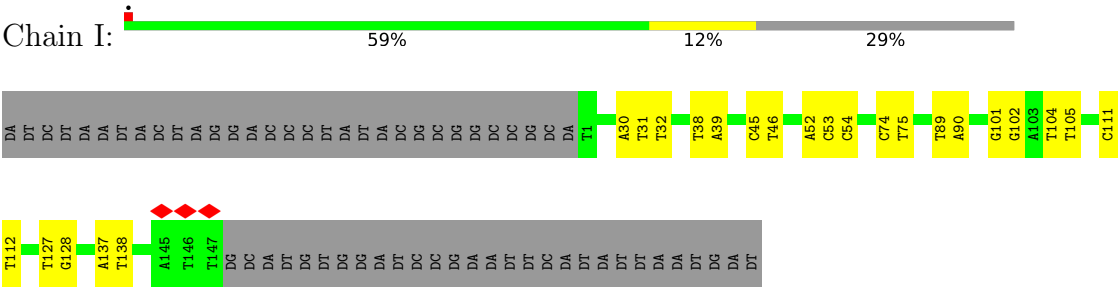
● Molecule 4: Histone H2B type 1-C/E/F/G/I



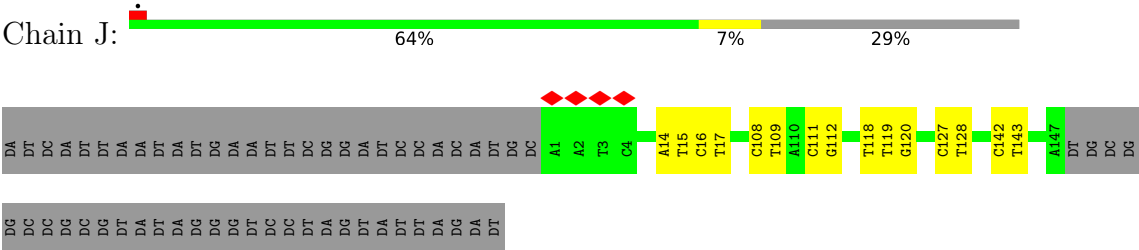
● Molecule 5: Histone H4



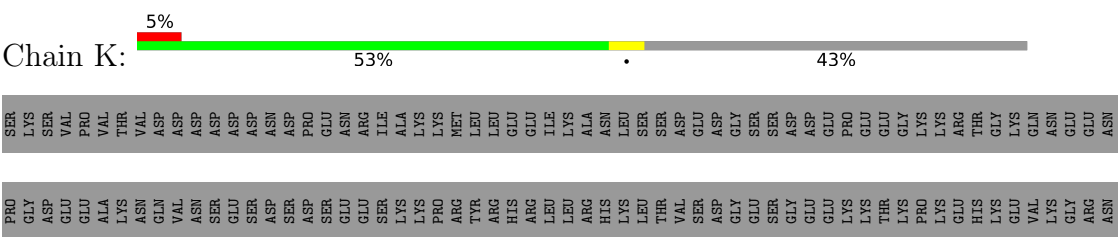
● Molecule 6: DNA (207-MER)



● Molecule 7: DNA (207-MER)



● Molecule 8: Transcriptional regulator ATRX



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	147422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.619	Depositor
Minimum map value	-0.933	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	366.9888, 366.9888, 366.9888	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9557, 0.9557, 0.9557	Depositor

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: ADP, MG

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	0.15	0/808	0.27	0/1086
1	E	0.15	0/784	0.28	0/1052
2	B	0.16	0/712	0.30	0/950
3	C	0.14	0/820	0.28	0/1110
3	G	0.15	0/824	0.27	0/1114
4	D	0.15	0/728	0.28	0/982
4	H	0.15	0/736	0.29	0/990
5	F	0.17	0/680	0.32	0/912
6	I	0.21	0/3359	0.48	0/5178
7	J	0.22	0/3401	0.50	0/5251
8	K	0.16	0/5276	0.27	0/7100
All	All	0.18	0/18128	0.38	0/25725

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 [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	796	826	825	0	0
1	E	774	810	809	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	704	760	757	0	0
3	C	810	850	849	0	0
3	G	814	861	860	0	0
4	D	717	722	721	0	0
4	H	725	744	743	1	0
5	F	672	701	698	1	0
6	I	2998	1650	1651	14	0
7	J	3029	1649	1650	10	0
8	K	5626	5579	5319	38	0
9	K	27	0	12	1	0
10	K	1	0	0	0	0
All	All	17693	15152	14894	64	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 2.

The worst 5 of 64 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)
8:K:2241:LEU:HD23	8:K:2248:ILE:HG21	1.61	0.82
8:K:1483:ILE:HD11	8:K:1803:ARG:NH2	2.00	0.76
8:K:2026:ILE:HG21	8:K:2133:ILE:HD11	1.77	0.66
6:I:104:DT:H2'	6:I:105:DT:H71	1.77	0.65
8:K:1483:ILE:HD11	8:K:1803:ARG:CZ	2.27	0.64

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	96/136 (71%)	96 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	93/136 (68%)	93 (100%)	0	0	100	100
2	B	85/87 (98%)	82 (96%)	3 (4%)	0	100	100
3	C	105/130 (81%)	104 (99%)	1 (1%)	0	100	100
3	G	105/130 (81%)	104 (99%)	1 (1%)	0	100	100
4	D	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
4	H	91/126 (72%)	89 (98%)	2 (2%)	0	100	100
5	F	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
8	K	625/1260 (50%)	592 (95%)	33 (5%)	0	100	100
All	All	1375/2217 (62%)	1332 (97%)	43 (3%)	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 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	82/110 (74%)	82 (100%)	0	100	100
1	E	80/110 (73%)	80 (100%)	0	100	100
2	B	72/72 (100%)	72 (100%)	0	100	100
3	C	80/99 (81%)	80 (100%)	0	100	100
3	G	81/99 (82%)	81 (100%)	0	100	100
4	D	78/106 (74%)	77 (99%)	1 (1%)	61	71
4	H	80/106 (76%)	80 (100%)	0	100	100
5	F	67/71 (94%)	66 (98%)	1 (2%)	57	69
8	K	575/1063 (54%)	569 (99%)	6 (1%)	68	75
All	All	1195/1836 (65%)	1187 (99%)	8 (1%)	73	78

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	K	1814	CYS
8	K	1765	ILE
8	K	1630	THR
8	K	1588	SER
8	K	1694	ASN

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

Mol	Chain	Res	Type
2	B	75	HIS
1	E	85	GLN
5	F	75	HIS
4	H	81	ASN
8	K	1754	ASN

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
9	ADP	K	2601	10	27,29,29	0.46	0	42,45,45	0.46	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
9	ADP	K	2601	10	-	3/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

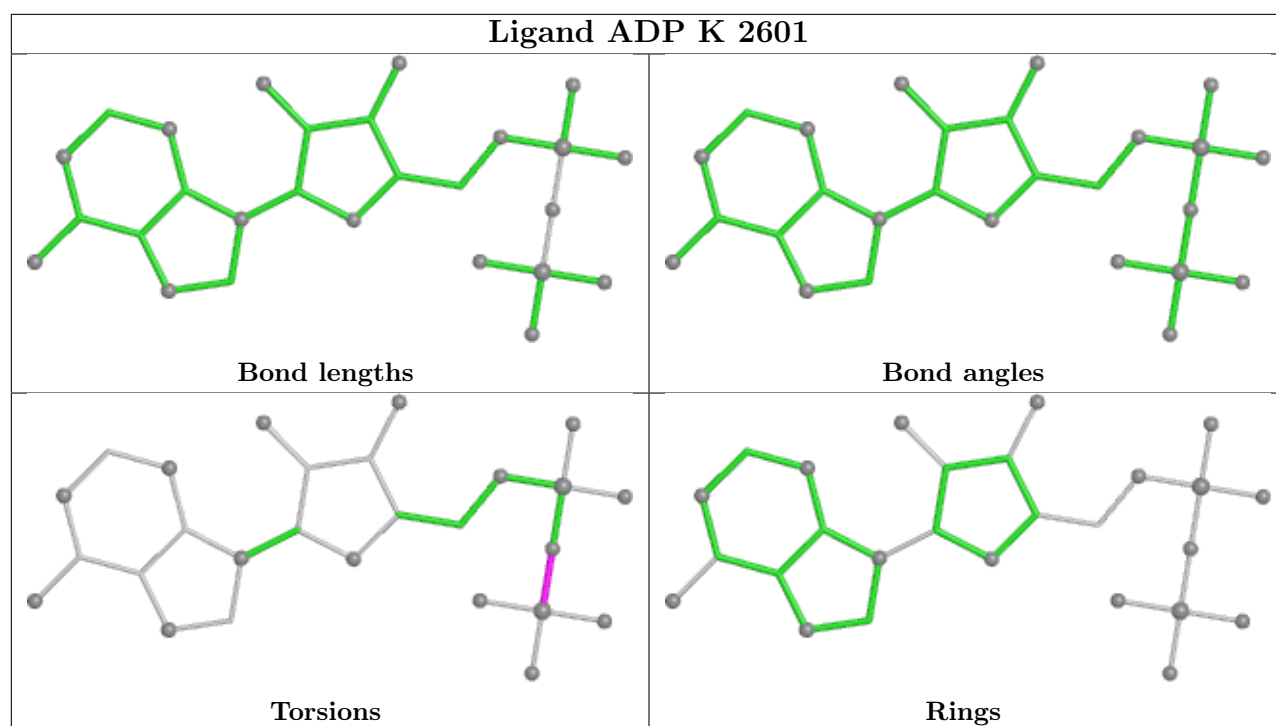
Mol	Chain	Res	Type	Atoms
9	K	2601	ADP	PA-O3A-PB-O2B
9	K	2601	ADP	PA-O3A-PB-O1B
9	K	2601	ADP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	2601	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

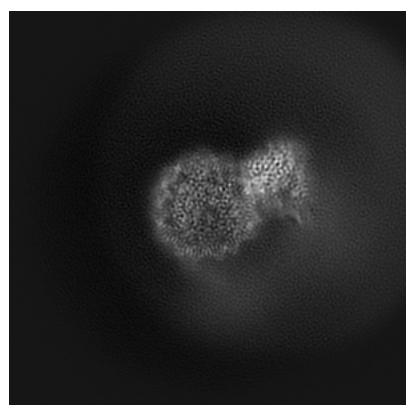
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62690. These allow visual inspection of the internal detail of the map and identification of artifacts.

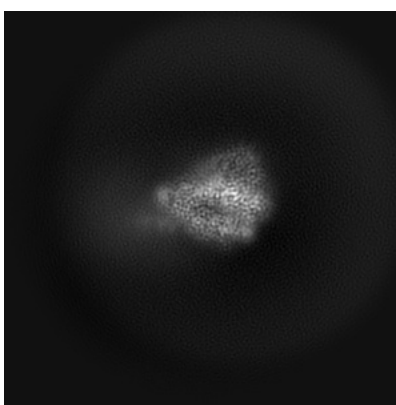
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

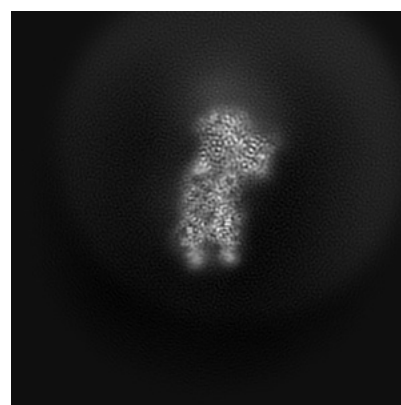
6.1.1 Primary map



X



Y

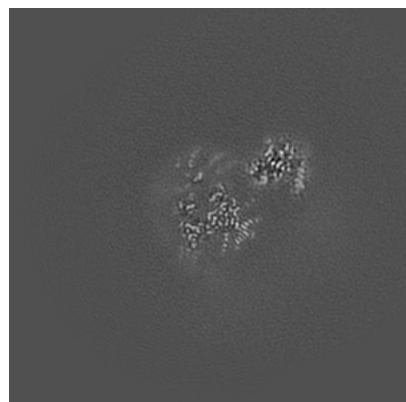


Z

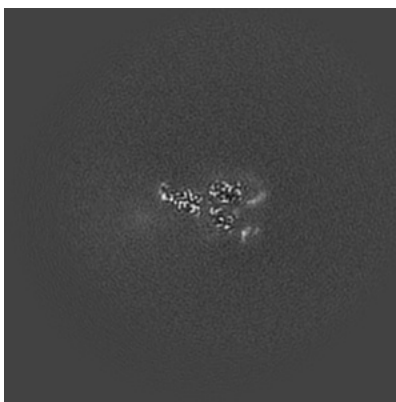
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

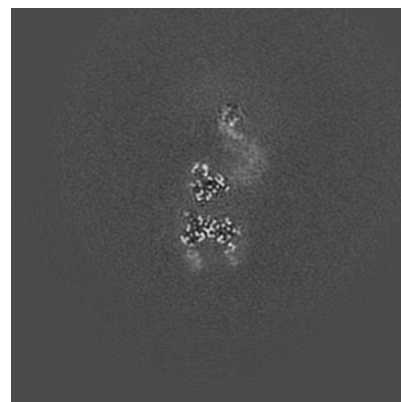
6.2.1 Primary map



X Index: 192



Y Index: 192

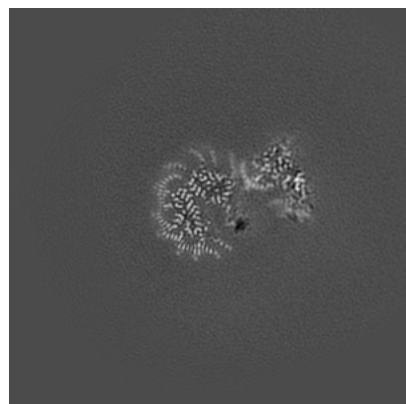


Z Index: 192

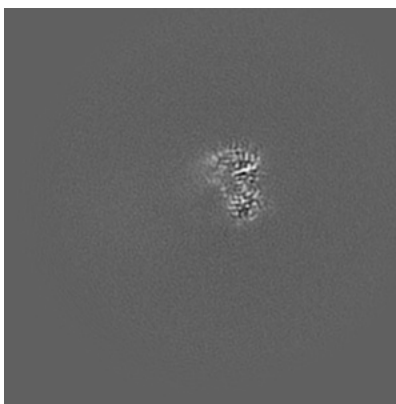
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

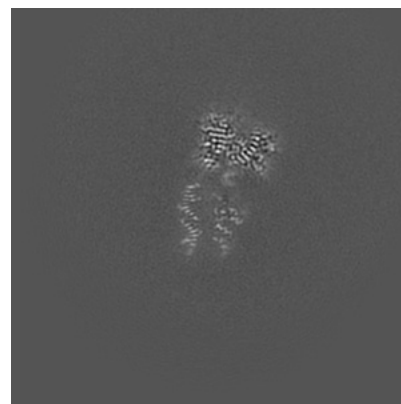
6.3.1 Primary map



X Index: 208



Y Index: 245

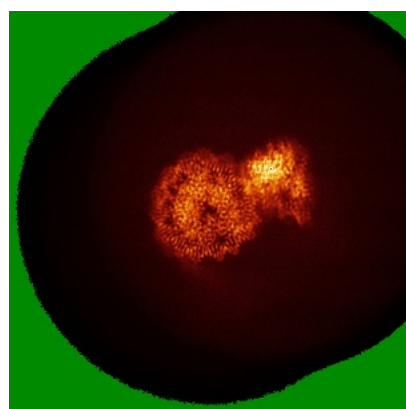


Z Index: 229

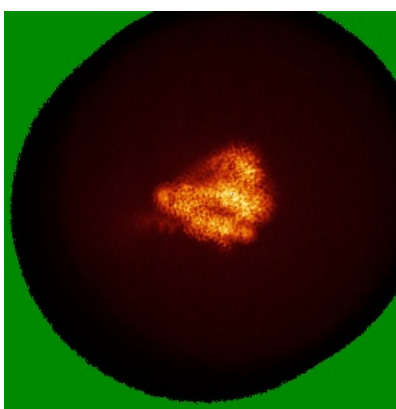
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

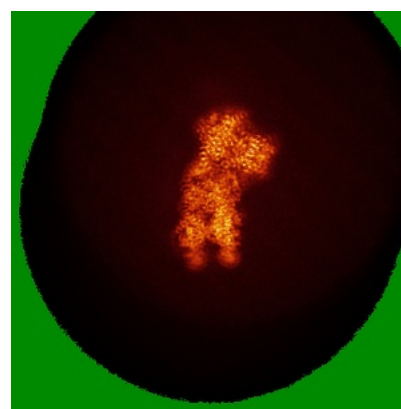
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

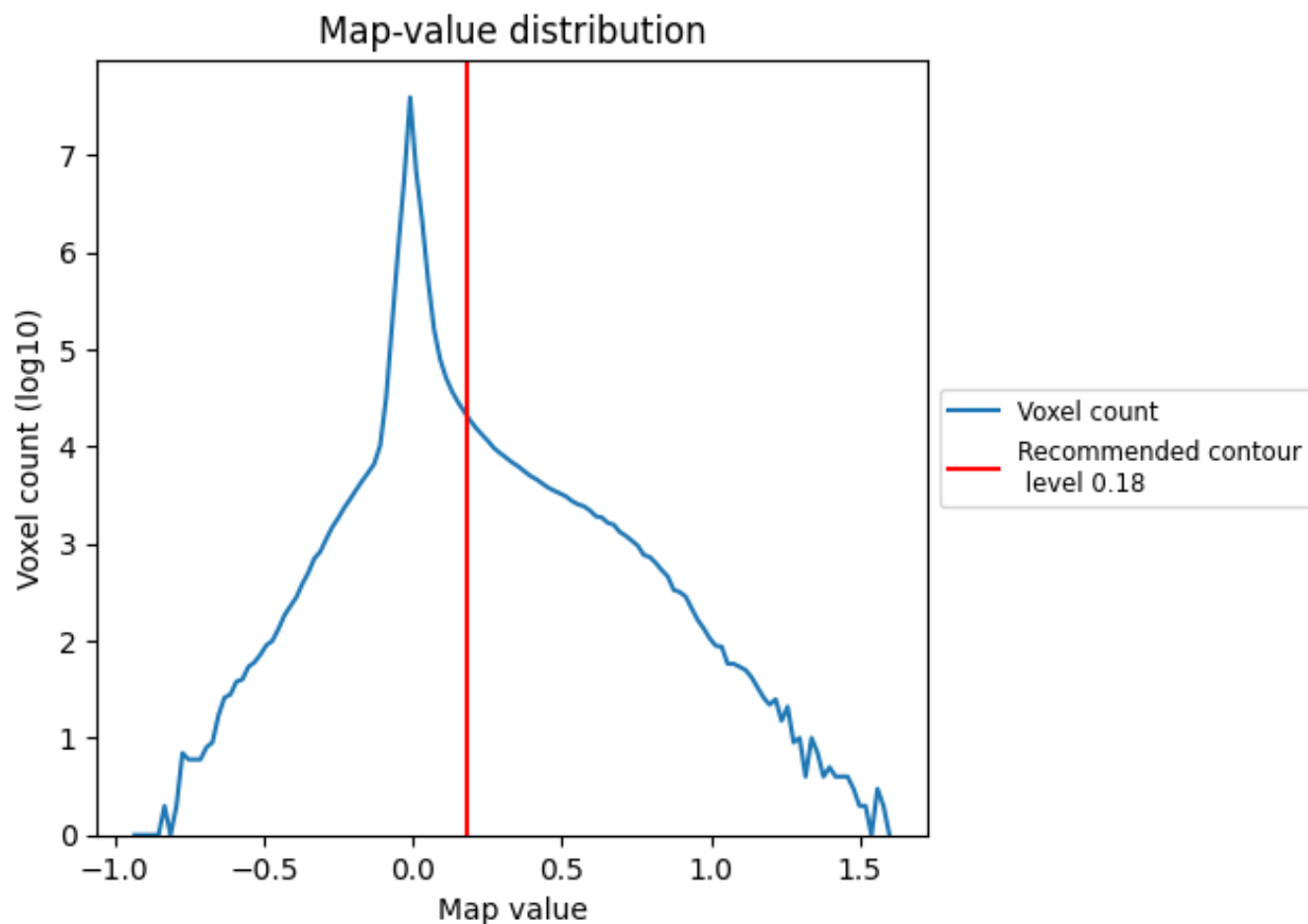
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

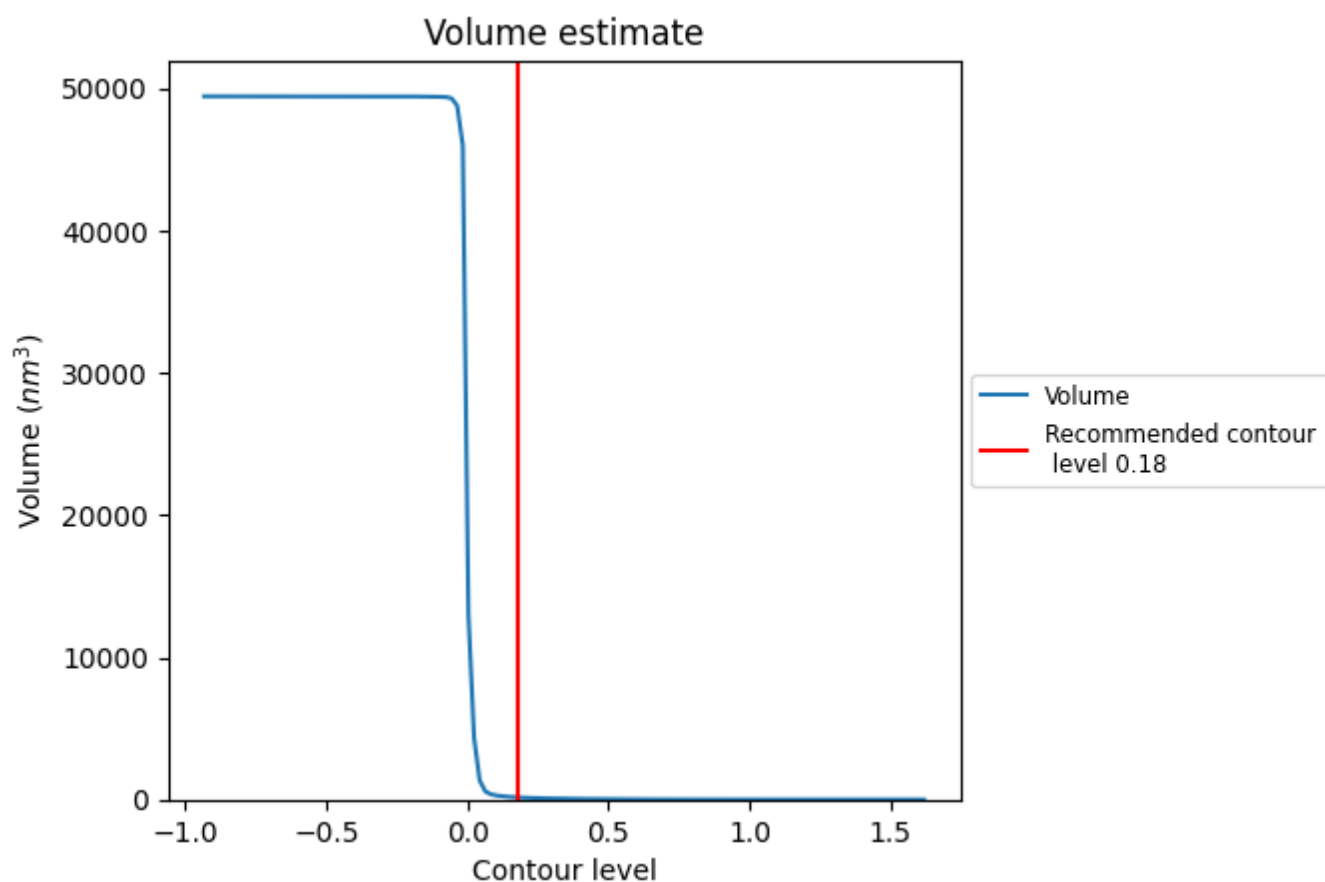
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

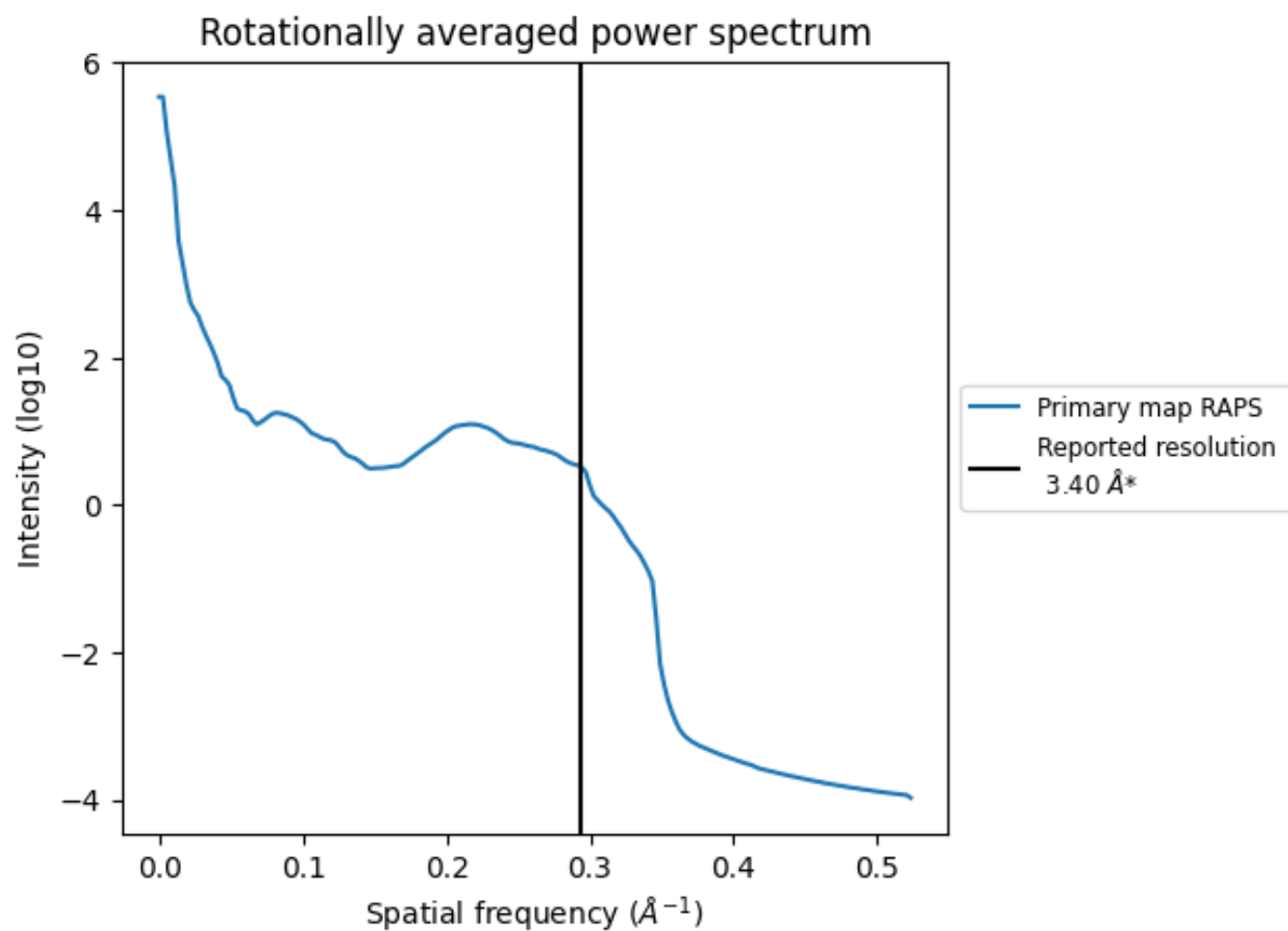
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 135 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

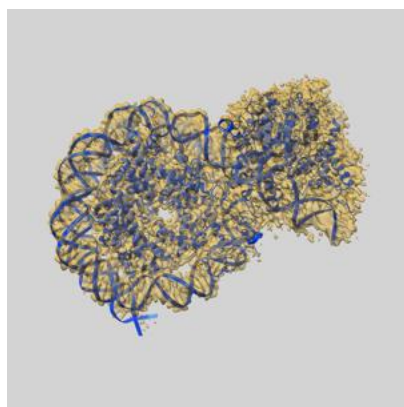
8 Fourier-Shell correlation

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

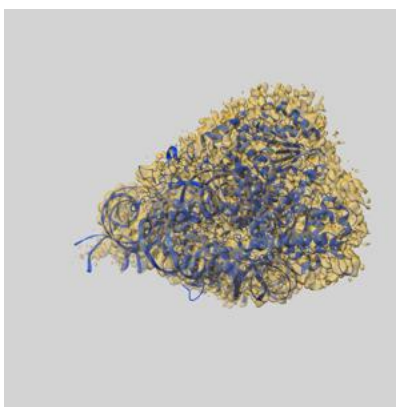
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62690 and PDB model 9L06. Per-residue inclusion information can be found in section [3](#) on page [9](#).

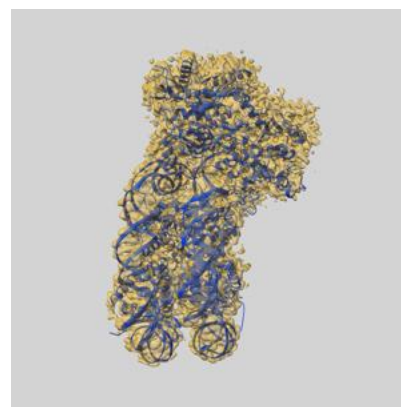
9.1 Map-model overlay [i](#)



X



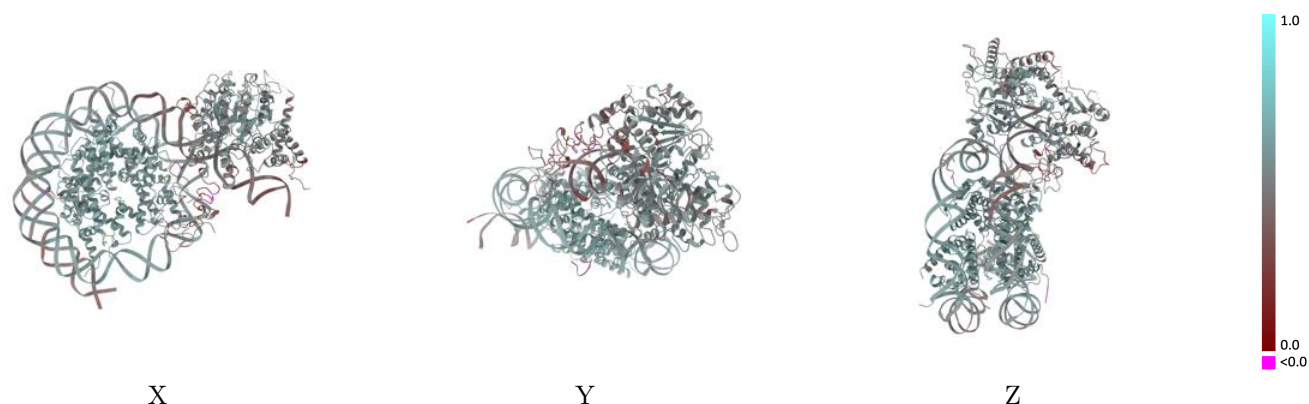
Y



Z

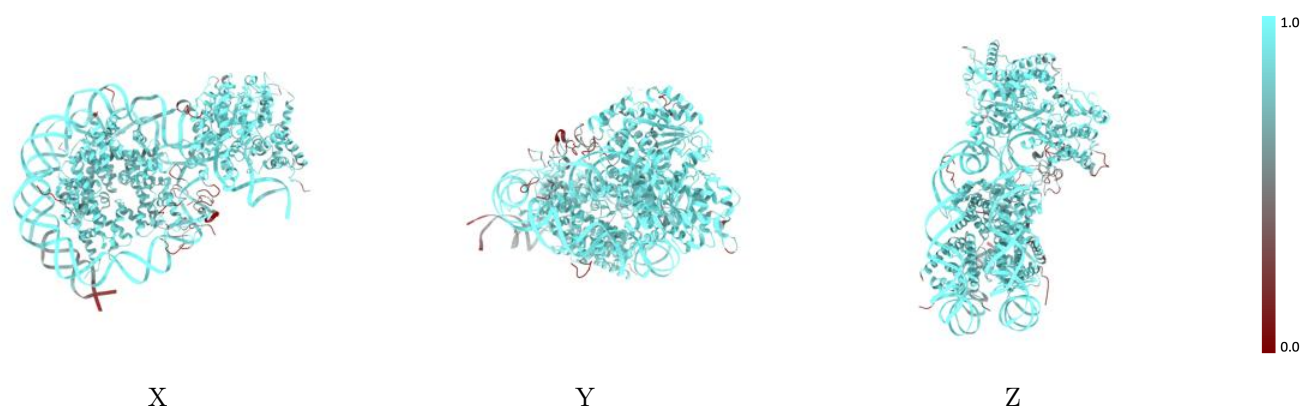
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



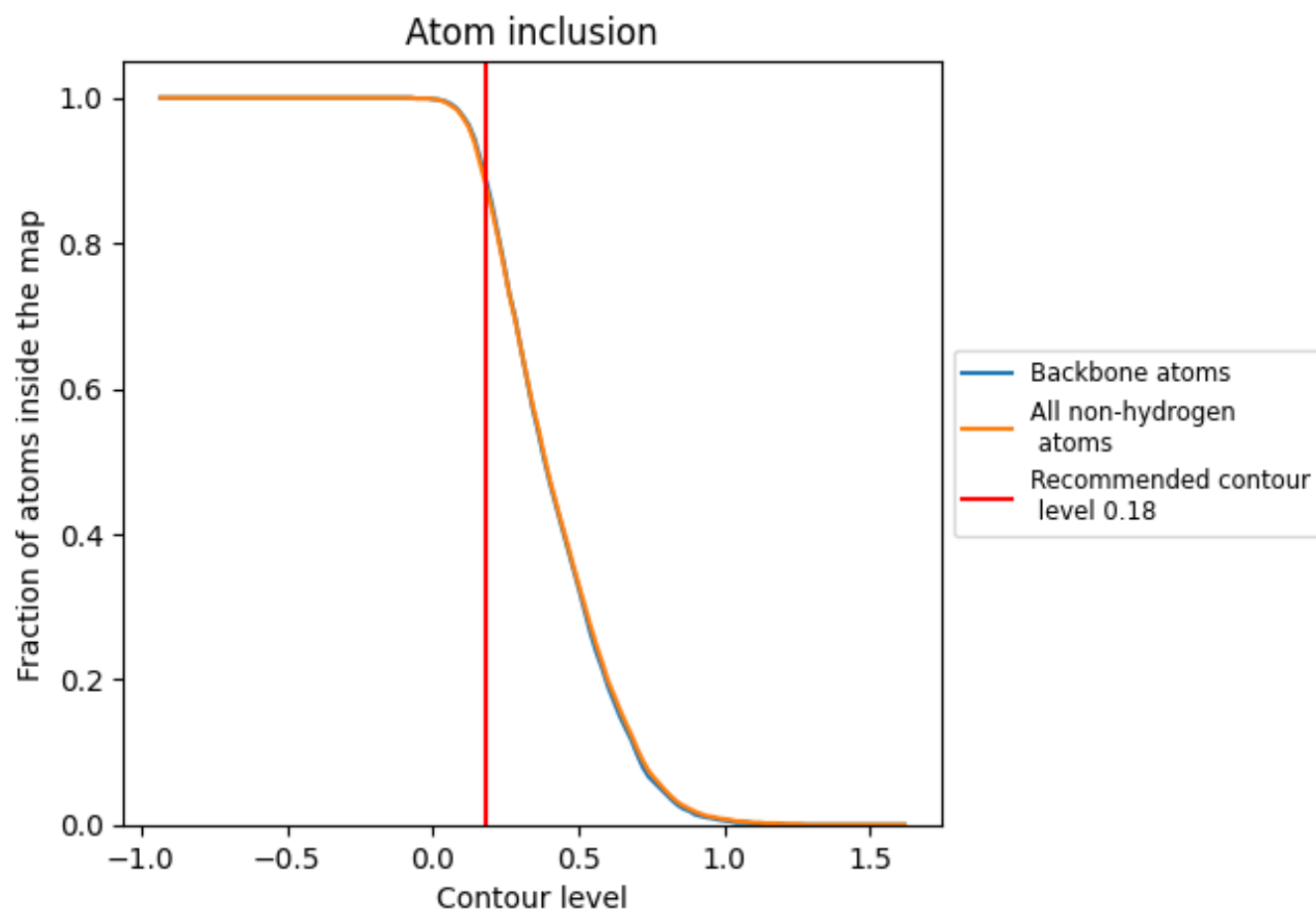
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8840	<div><div></div></div> 0.5280
A	<div><div></div></div> 0.9000	<div><div></div></div> 0.5910
B	<div><div></div></div> 0.8490	<div><div></div></div> 0.5620
C	<div><div></div></div> 0.9040	<div><div></div></div> 0.6000
D	<div><div></div></div> 0.9260	<div><div></div></div> 0.5920
E	<div><div></div></div> 0.9270	<div><div></div></div> 0.6060
F	<div><div></div></div> 0.8920	<div><div></div></div> 0.5810
G	<div><div></div></div> 0.8930	<div><div></div></div> 0.5800
H	<div><div></div></div> 0.8950	<div><div></div></div> 0.5790
I	<div><div></div></div> 0.9050	<div><div></div></div> 0.5050
J	<div><div></div></div> 0.8980	<div><div></div></div> 0.5110
K	<div><div></div></div> 0.8690	<div><div></div></div> 0.4860

1.0

0.0

<0.0