



wwPDB EM Validation Summary Report ⓘ

May 26, 2025 – 06:37 AM EDT

PDB ID : 7K0Y / pdb_00007k0y
EMDB ID : EMD-22618
Title : Cryo-EM structure of activated-form DNA-PK (complex VI)
Authors : Chen, X.; Gellert, M.; Yang, W.
Deposited on : 2020-09-06
Resolution : 3.70 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

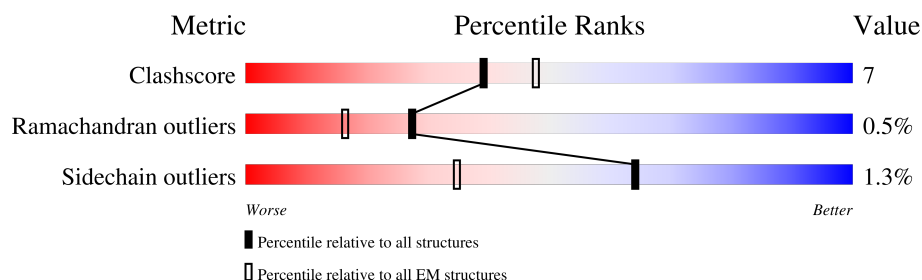
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	4128	
2	B	609	
3	C	732	
4	D	24	
4	F	24	
5	E	16	
5	G	16	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 39835 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3669	Total	C	N	O	S	0	0
			29107	18680	4932	5306	189		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	2	0
			3973	2545	677	733	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	655	Total	C	N	O	S	0	0
			5247	3357	876	988	26		

- Molecule 4 is a DNA chain called DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	24	Total	C	N	O	P	0	0
			484	233	82	146	23		
4	F	21	Total	C	N	O	P	0	0
			425	204	69	131	21		

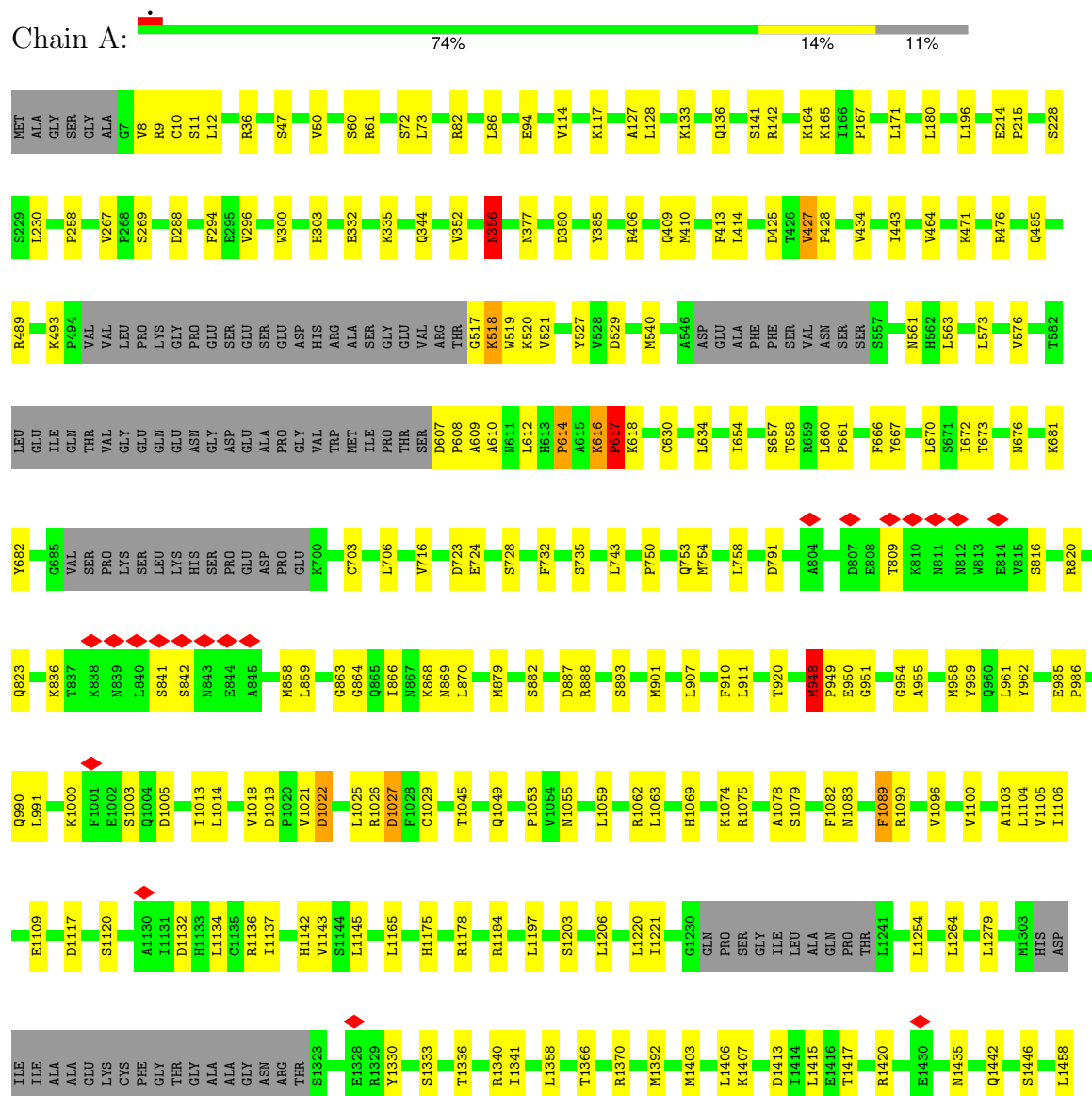
- Molecule 5 is a DNA chain called DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	13	Total	C	N	O	P	0	0
			269	128	58	71	12		
5	G	16	Total	C	N	O	P	0	0
			330	157	68	90	15		

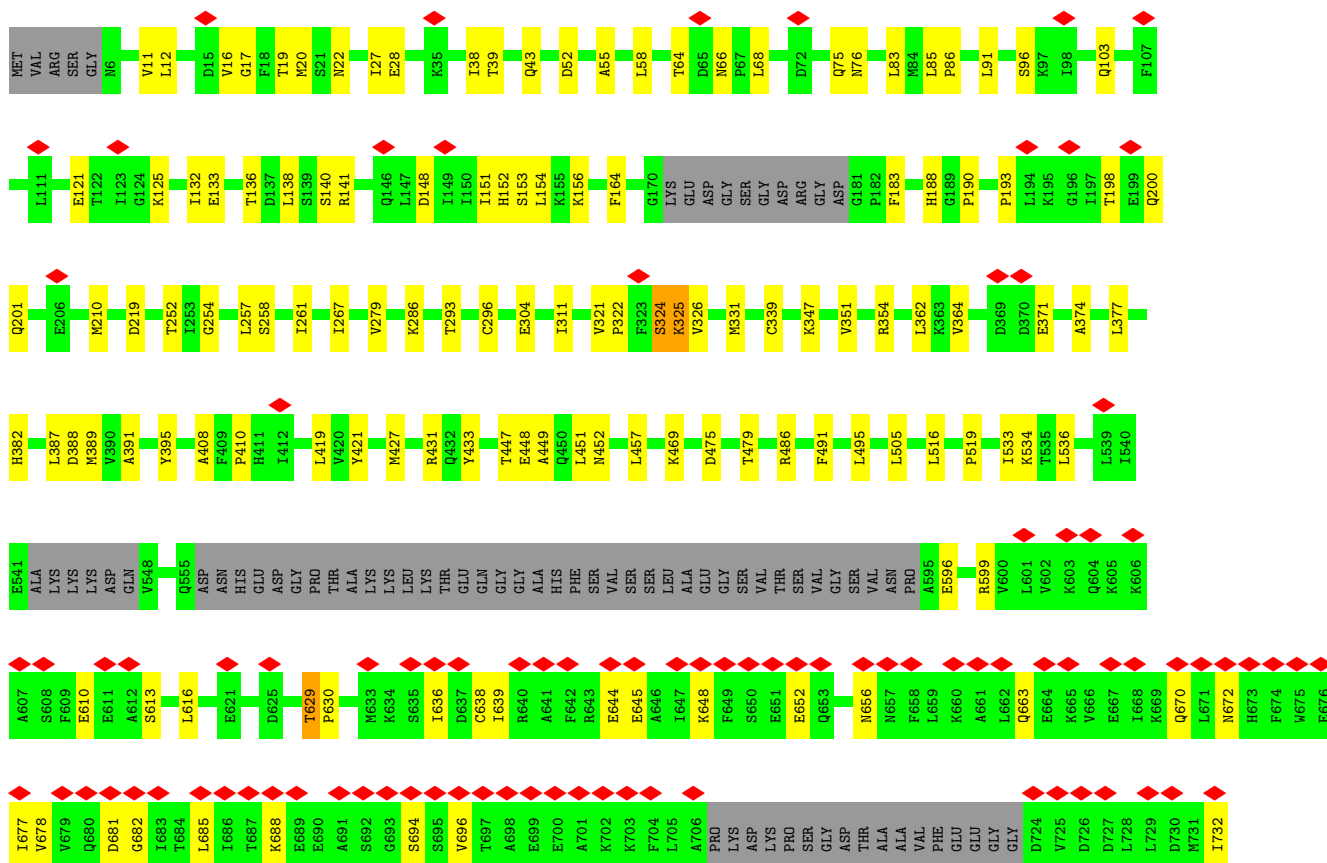
3 Residue-property plots

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: DNA-dependent protein kinase catalytic subunit



N3177	L2976	S2810	GLU	SER	L237	PRO	LEU	H1941	P1810	E1640	H1469
K3192	D2980	F2823	LYS	LEU	I2237	GLN	SER	H1941	R1811	E1640	L1463
I3193	D2980	K2824	LEU	LEU	D2247	GLY	GLU	I1949	R1816	M1643	L1464
L3197	D2983	T2825	SER	PHE	C2248	GLU	MET	I1949	Q1817	L1646	H1465
T3198	E2995	L2826	MET	ALA	L2249	ASP	SER	I1952	S1818	L1646	N1466
P3199	E2995	S2827	TYR	LYS	Q2262	SER	GLN	V1955	F1819	I1467	I1467
LEU	D3000	E2828	ARG	ARG	Q2262	VAL	PHE	F1956	V1820	S1470	S1470
PRO	D3000	K2829	ALA	SER	N2270	P2119	ASP	F1956	D1821	Q1471	Q1471
GLU	S3018	F2848	LYS	GLU	N2270	L2122	PHE	E1958	R1822	T1663	T1663
ASN	S3018	S2849	ALA	ALA	D2284	P2123	THR	E1958	F1668	F1668	F1668
SER	K3029	C2857	TRP	TRP	D2284	S2124	GLY	L1959	V1671	V1671	V1671
MET	Y3040	I2861	VAL	PRO	P2286	F2128	VAL	K1960	T1674	T1674	T1674
VAL	K3048	P2887	GLN	ALA	P2290	L2129	GLN	F1961	L1678	L1678	L1678
ASP	L3051	P2887	GLY	GLY	S2296	H2130	TYR	F1967	L1684	L1684	L1684
GLN	L3051	R2899	LYS	SER	S2296	G2131	SER	F1967	L1833	L1833	L1833
ASP	S3060	LEU	ILE	VAL	S2308	K2142	TYR	F1967	A1835	A1835	A1835
GLY	S3060	LEU	ARG	ARG	S2308	L2133	TYR	F1967	L1836	L1836	L1836
ASP	I3077	LEU	ALA	ALA	Q2348	N2135	SER	I1982	V1850	V1850	V1850
PRO	I3077	LEU	GLN	GLN	Q2348	N2135	SER	I1982	V1850	V1850	V1850
SER	S3083	GLU	GLN	GLN	V2362	L2149	ASP	V1992	R1854	R1854	R1854
ASP	S3083	LEU	HIS	HIS	V2362	V2150	PRO	E1993	T1862	T1862	T1862
ARG	L3091	PRO	ASP	ASP	K2366	T2153	PRO	V1994	F1722	F1722	F1722
MET	L3091	ALA	PHE	PHE	M2379	E2154	THR	GLU	S1726	S1726	S1726
GLU	I3103	LYS	GLY	GLY	E2154	E2155	GLY	VAL	R1729	R1729	R1729
VAL	Q3104	GLN	LEU	LEU	P2387	V2156	ARG	PRO	E1728	E1728	E1728
GLN	Q3104	VAL	THR	THR	P2387	F2157	PHE	GLU	F1729	F1729	F1729
GLU	N3113	ARG	GLN	GLN	R2404	W2164	ARG	R2000	P1730	P1730	P1730
GLN	S3116	GLY	THR	THR	Y2412	W2164	ARG	I2005	T1733	T1733	T1733
GLU	I3117	THR	THR	THR	Y2412	G2179	ARG	I2005	L1760	L1760	L1760
GLU	I3117	ASP	ASP	ASP	L2415	E2180	GLN	R2008	S1753	S1753	S1753
ARG	L3120	LEU	GLY	GLY	L2415	G2181	ASP	K2009	M1762	M1762	M1762
LEU	L3120	LEU	ASP	ASP	H2426	I2182	PRO	E2010	Q1771	Q1771	Q1771
ASP	L3126	TYR	ASN	ASN	R2427	H2183	THR	A2014	H1773	H1773	H1773
TYR	Q3130	ARG	LYS	LYS	E2453	V2186	VAL	A2014	I1785	I1785	I1785
HIS	Q3130	ARG	TRP	TRP	E2453	V2186	HIS	A2015	Q1794	Q1794	Q1794
GLY	E3137	ASP	LEU	LEU	F2461	V2190	ASP	A2016	L1797	L1797	L1797
ASP	L3138	LEU	THR	THR	T2467	I2193	VAL	N2016	V1802	V1802	V1802
PRO	Q3139	VAL	GLY	GLY	T2467	I2193	LEU	GLY	E1803	E1803	E1803
ASP	G3149	ILE	SER	SER	E2471	T2197	ASP	ASP	M1804	M1804	M1804
ILE	G3149	THR	THR	THR	Q2472	G2198	E2082	SER	F1806	F1806	F1806
THR	V3155	THR	THR	THR	M2473	G2198	K2085	GLY	D1806	D1806	D1806
LYS	P3156	LEU	PRO	PRO	Y2474	T2201	R2090	PRO	L1809	L1809	L1809
P3156	P3156	ARG	LEU	LEU	N2475	P2202	P2096	THR			
W3164	W3164	VAL	VAL	VAL	I2476	T2203	H2103	TYR			
Q3278	Q3278	S2788	VAL	VAL	L2480	K2207	H2103	TYR			
R3269	R3269	S2789	ASP	ASP	P2487	V2210	S2107	TYR			
D3270	D3270	K2786	ASP	ASP	P2487	V2210	L2108	TYR			
D3271	D3271	H2787	ARG	ARG	P2487	V2210	GLY	ALA			
Q3278	Q3278	S2789	THR	THR	P2487	V2210	GLY	ASP			
R3269	R3269	T2792	THR	THR	P2487	V2210	GLY	ASP			
D3244	D3244	Q2795	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2795	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
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R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3247	R3247	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
L3259	L3259	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
R3269	R3269	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			
D3244	D3244	Q2799	LEU	LEU	P2487	V2210	GLY	ASP			



- Molecule 4: DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3')

Chain D: 92% 8%



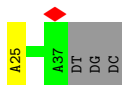
- Molecule 4: DNA (5'-D(*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3')

Chain F: 88% 12%



- Molecule 5: DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*A)-3')

Chain E: 6% 75% 6% 19%



- Molecule 5: DNA (5'-D(*AP*AP*GP*CP*AP*GP*TP*AP*GP*AP*GP*CP*A)-3')

Chain G:



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	254646	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.072	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	408.31998, 408.31998, 408.31998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	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 >5	RMSZ	# Z >5
1	A	0.41	1/29703 (0.0%)	0.69	21/40166 (0.1%)
2	B	0.36	0/4056	0.73	6/5460 (0.1%)
3	C	0.29	0/5347	0.63	0/7208
4	D	0.45	0/540	0.57	0/831
4	F	0.38	0/473	0.54	0/727
5	E	0.27	0/304	0.40	0/468
5	G	0.42	0/372	0.53	0/573
All	All	0.39	1/40795 (0.0%)	0.68	27/55433 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356	ASN	CG-OD1	5.10	1.33	1.23

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2122	LEU	CA-C-N	15.17	138.80	119.84
1	A	2122	LEU	C-N-CA	15.17	138.80	119.84
1	A	3895	GLU	CB-CA-C	10.29	127.15	110.90
2	B	530	TYR	CA-C-N	-10.07	110.00	120.38
2	B	530	TYR	C-N-CA	-10.07	110.00	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1727	ARG	Sidechain

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	29107	0	29371	389	0
2	B	3973	0	4075	89	0
3	C	5247	0	5263	90	0
4	D	484	0	274	3	0
4	F	425	0	240	0	0
5	E	269	0	146	2	0
5	G	330	0	180	0	0
All	All	39835	0	39549	553	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 7.

The worst 5 of 553 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)
2:B:245:LYS:O	2:B:246:VAL:CG2	2.04	1.06
1:A:948:MET:H	1:A:949:PRO:HD2	1.20	1.00
1:A:948:MET:HG3	1:A:949:PRO:HD3	1.40	1.00
1:A:948:MET:H	1:A:949:PRO:CD	1.78	0.96
1:A:630:CYS:O	1:A:634:LEU:HB2	1.69	0.93

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	3635/4128 (88%)	3076 (85%)	543 (15%)	16 (0%)	30	62
2	B	488/609 (80%)	410 (84%)	73 (15%)	5 (1%)	13	44
3	C	645/732 (88%)	547 (85%)	94 (15%)	4 (1%)	22	54
All	All	4768/5469 (87%)	4033 (85%)	710 (15%)	25 (0%)	27	57

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	948	MET
1	A	1772	HIS
1	A	2123	PRO
1	A	2285	LEU
1	A	2573	PRO

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	3207/3671 (87%)	3160 (98%)	47 (2%)	60	75
2	B	447/548 (82%)	444 (99%)	3 (1%)	81	88
3	C	586/649 (90%)	582 (99%)	4 (1%)	81	88
All	All	4240/4868 (87%)	4186 (99%)	54 (1%)	64	77

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1982	ILE
1	A	2827	SER
2	B	530	TYR
1	A	1992	VAL
1	A	2285	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	98	ASN
3	C	627	ASN
2	B	360	HIS
3	C	298	ASN
1	A	1794	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 [i](#)

There are no chain breaks in this entry.

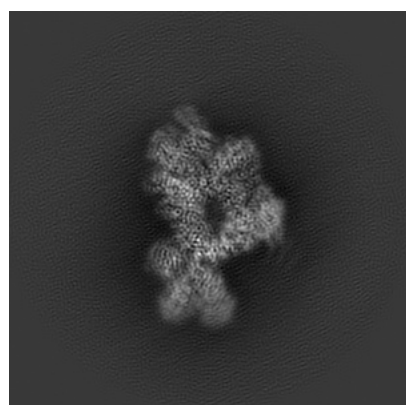
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22618. These allow visual inspection of the internal detail of the map and identification of artifacts.

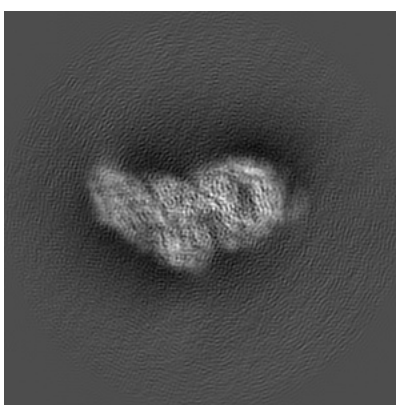
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

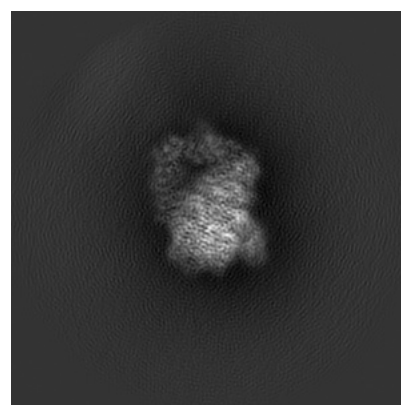
6.1.1 Primary map



X



Y

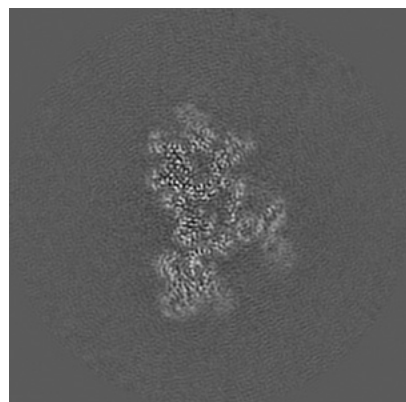


Z

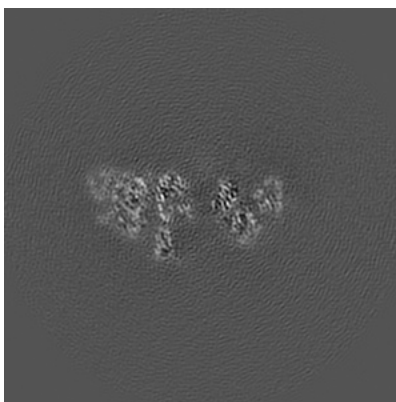
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

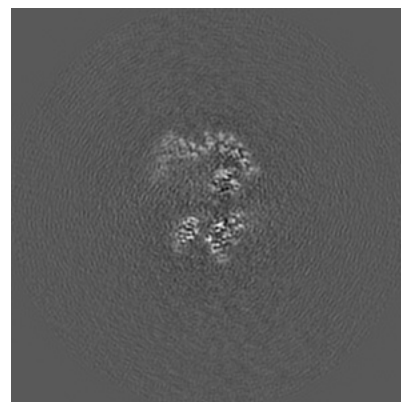
6.2.1 Primary map



X Index: 176



Y Index: 176

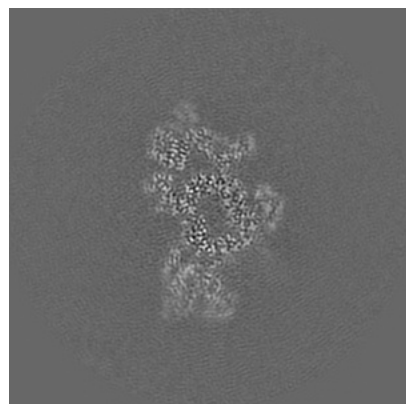


Z Index: 176

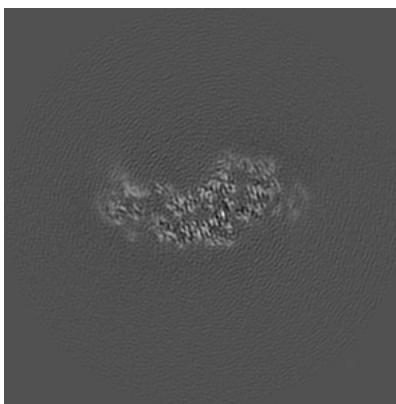
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

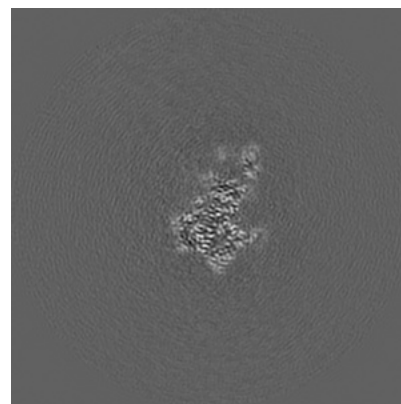
6.3.1 Primary map



X Index: 186



Y Index: 154

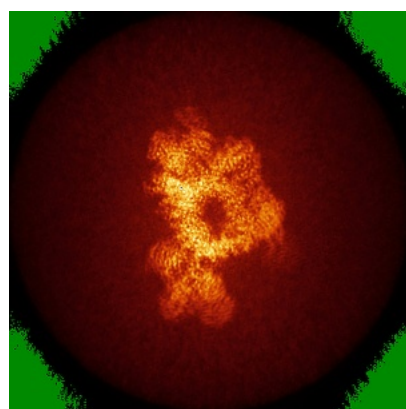


Z Index: 195

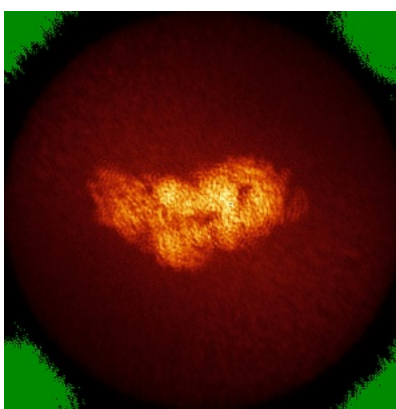
The images above show the largest variance slices of the map in three orthogonal directions.

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

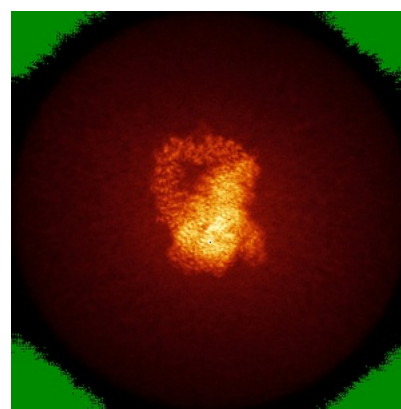
6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

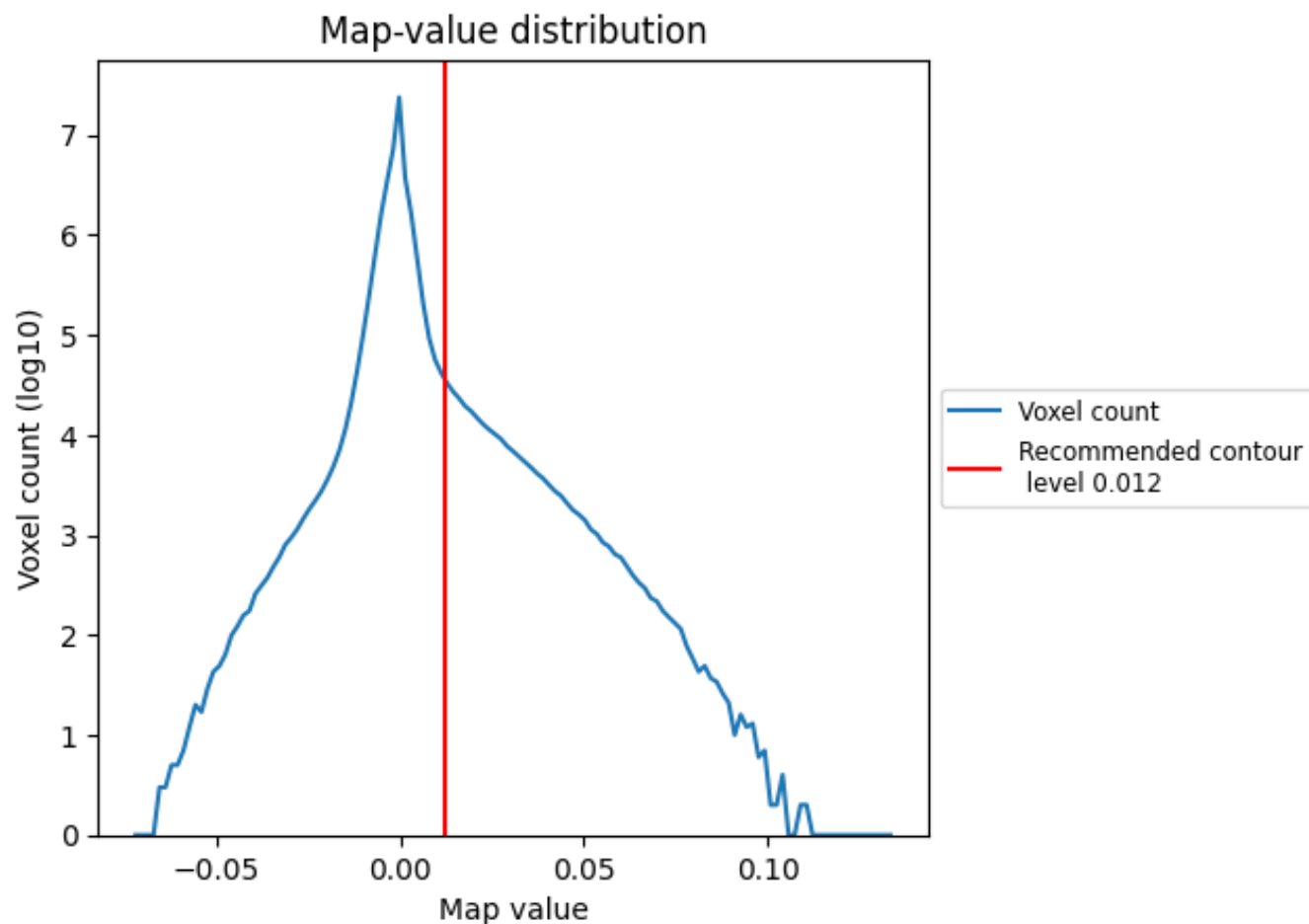
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

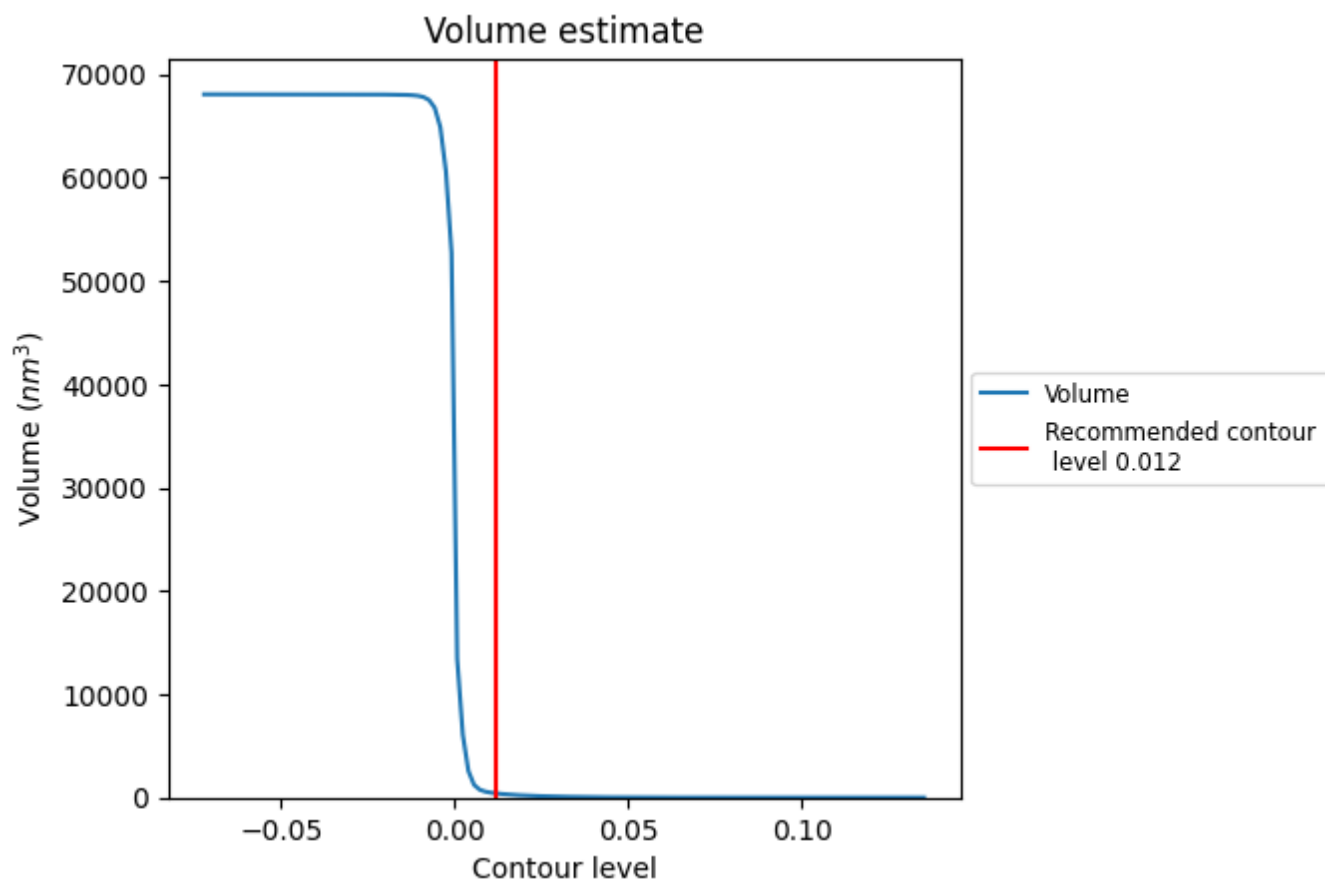
This section contains the results of statistical analysis of the map.

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.

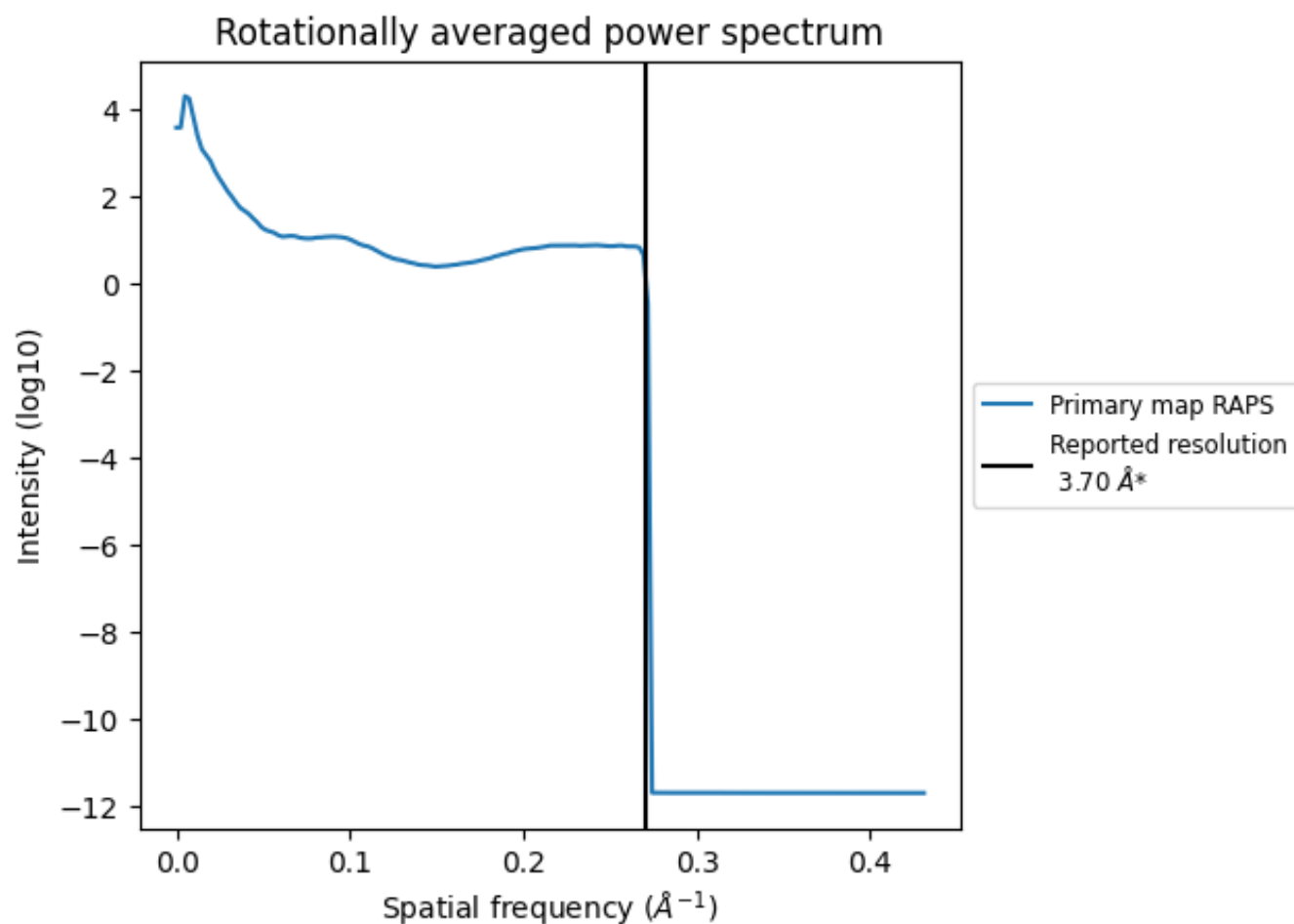
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 405 nm^3 ; this corresponds to an approximate mass of 366 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 0.270 \AA^{-1}

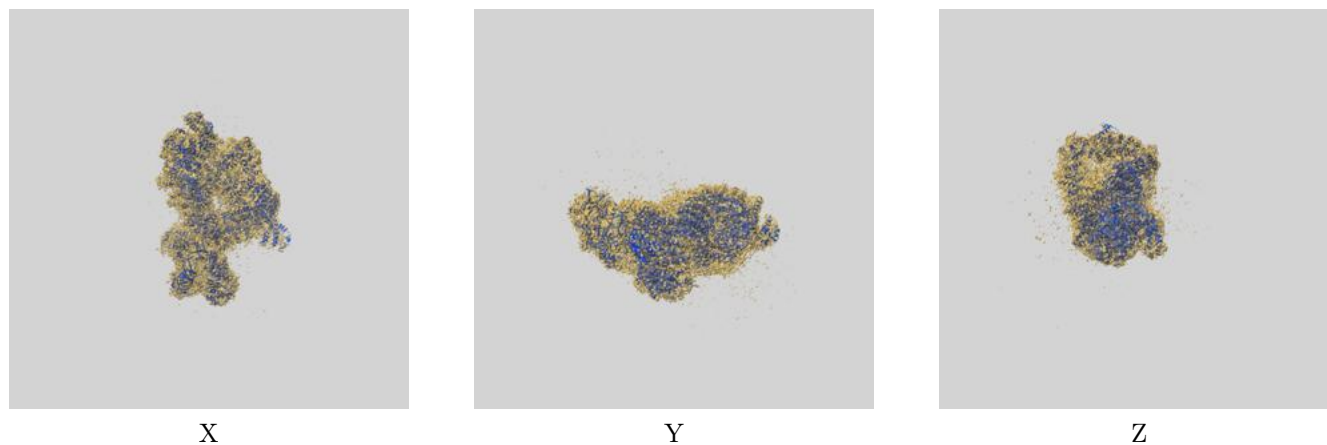
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

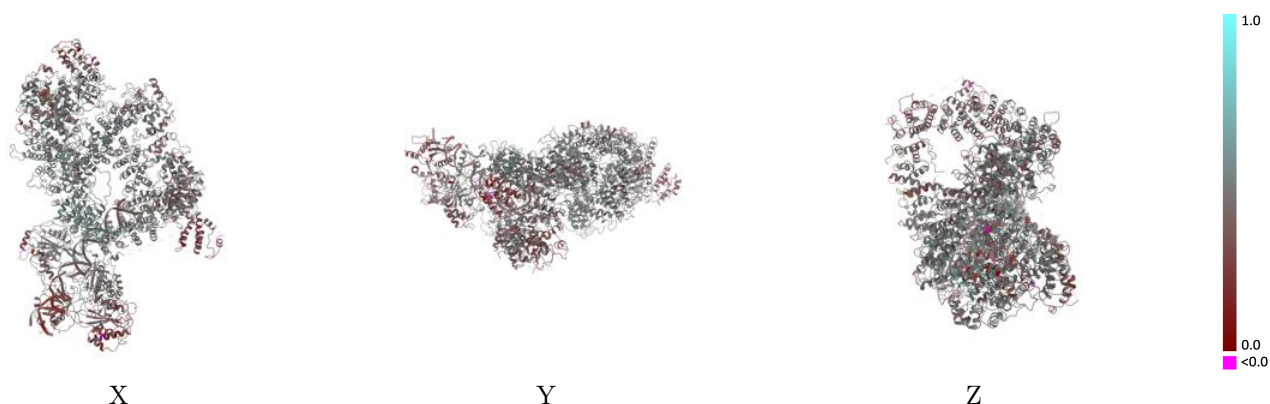
This section contains information regarding the fit between EMDB map EMD-22618 and PDB model 7K0Y. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



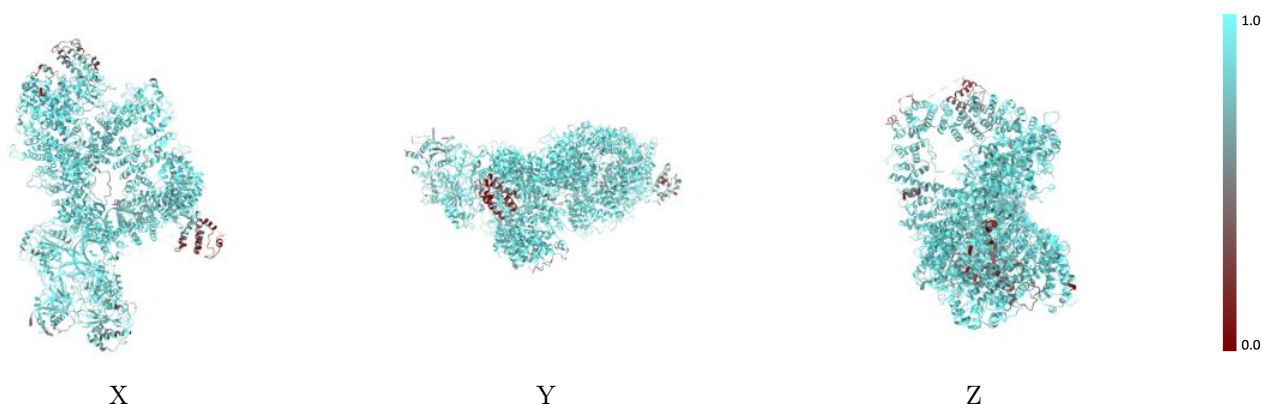
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



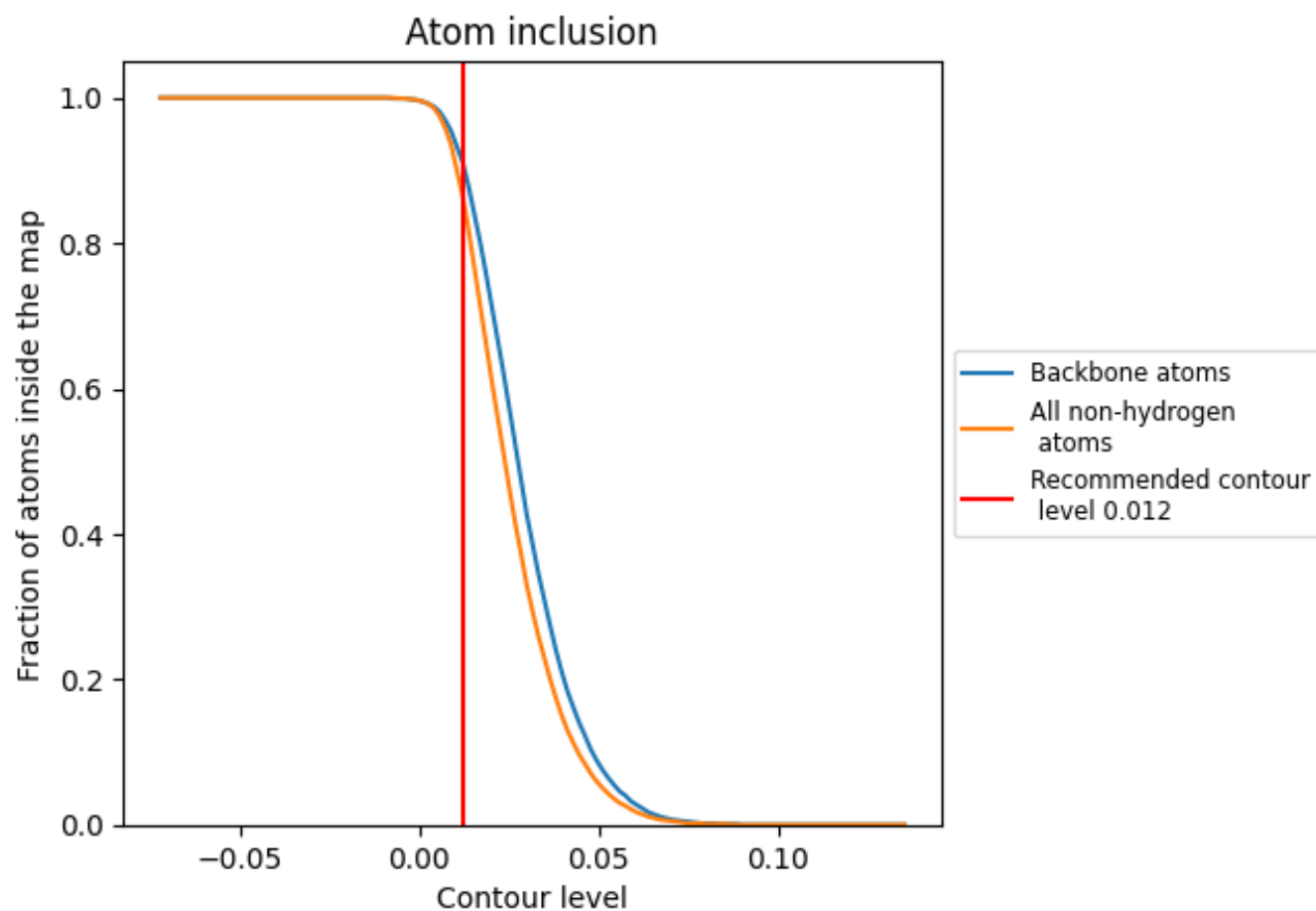
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8680	<div><div></div></div> 0.4410
A	<div><div></div></div> 0.8900	<div><div></div></div> 0.4600
B	<div><div></div></div> 0.8650	<div><div></div></div> 0.4240
C	<div><div></div></div> 0.7390	<div><div></div></div> 0.3700
D	<div><div></div></div> 0.9360	<div><div></div></div> 0.4050
E	<div><div></div></div> 0.7810	<div><div></div></div> 0.2720
F	<div><div></div></div> 0.8960	<div><div></div></div> 0.3270
G	<div><div></div></div> 0.9580	<div><div></div></div> 0.4090

1.0

0.0

<0.0