



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2024 – 01:57 PM JST

PDB ID : 7Y8R
EMDB ID : EMD-33684
Title : The nucleosome-bound human PBAF complex
Authors : Wang, L.; Yu, J.; Yu, Z.; Wang, Q.; He, S.; Xu, Y.
Deposited on : 2022-06-24
Resolution : 4.40 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

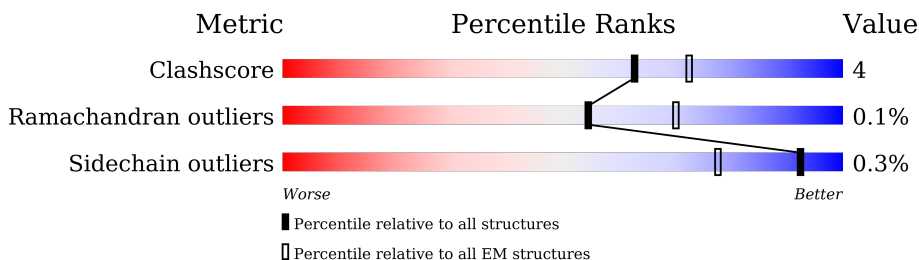
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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.



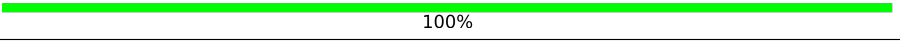







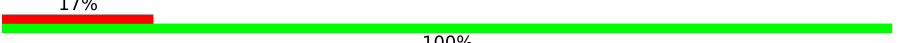






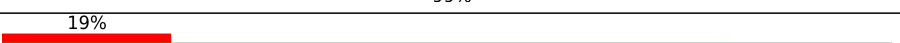
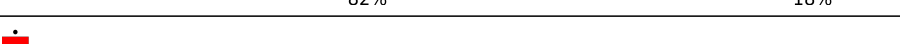
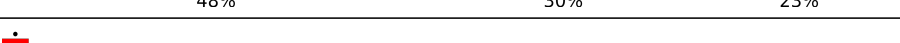

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	135	
1	E	135	
2	B	102	
2	F	102	
3	C	129	
3	G	129	
4	D	125	
4	H	125	

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Mol	Chain	Length	Quality of chain
5	Z	29	
6	I	1647	
7	J	375	
8	K	429	
9	L	1835	
10	M	385	
11	N	1214	
11	O	1214	
12	a	12	
13	P	515	
14	Q	411	
15	R	498	
16	S	651	
17	T	22	
18	U	1597	
19	V	102	
20	X	213	
21	Y	213	
22	W	24	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	ADP	I	1701	-	-	X	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 43109 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 Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	99	Total	C	N	O	S	0	0
			815	514	158	139	4		
1	E	98	Total	C	N	O	S	0	0
			806	508	156	138	4		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	94	Total	C	N	O	S	0	0
			741	465	150	125	1		
2	F	87	Total	C	N	O	S	0	0
			702	442	142	117	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	104	Total	C	N	O	0	0
			799	504	156	139		
3	G	108	Total	C	N	O	0	0
			833	525	165	143		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			755	473	138	142	2		
4	H	94	Total	C	N	O	S	0	0
			736	461	134	139	2		

- Molecule 5 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	Z	29	Total	C	N	O	0	0
			141	83	29	29		

- Molecule 6 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	732	Total	C	N	O	S	0	0
			6051	3831	1104	1087	29		

- Molecule 7 is a protein called ACTB protein (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	360	Total	C	N	O	S	0	0
			2821	1786	474	543	18		

- Molecule 8 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	356	Total	C	N	O	S	0	0
			2787	1767	470	529	21		

- Molecule 9 is a protein called AT-rich interactive domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	521	Total	C	N	O	S	0	0
			4151	2642	708	777	24		

- Molecule 10 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily B member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	362	Total	C	N	O	S	0	0
			2918	1828	511	564	15		

- Molecule 11 is a protein called SWI/SNF complex subunit SMARCC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	255	Total	C	N	O	S	0	0
			2085	1324	366	384	11		
11	O	297	Total	C	N	O	S	0	0
			2354	1489	418	434	13		

- Molecule 12 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	a	12	Total	C	N	O	0	0
			58	34	12	12		

- Molecule 13 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	385	Total	C	N	O	S	0	0
			3174	2006	562	592	14		

- Molecule 14 is a protein called SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	91	Total	C	N	O	S	0	0
			739	456	145	135	3		

- Molecule 15 is a protein called PHD finger protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	44	Total	C	N	O	S	0	0
			366	230	69	66	1		

- Molecule 16 is a protein called Bromodomain-containing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	213	Total	C	N	O	S	0	0
			1738	1102	288	337	11		

- Molecule 17 is a protein called Unkown.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	T	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 18 is a protein called Protein polybromo-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	U	11	Total	C	N	O	0	0
			92	60	14	18		

- Molecule 19 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	V	84	Total	C	N	O	0	0
			420	252	84	84		

- Molecule 20 is a DNA chain called DNA (213-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	165	Total	C	N	O	P	0	0
			3360	1596	606	993	165		

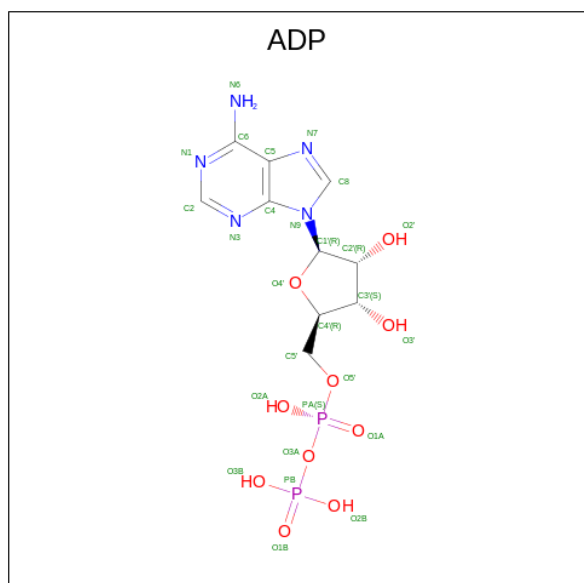
- Molecule 21 is a DNA chain called DNA (213-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	165	Total	C	N	O	P	0	0
			3405	1610	643	987	165		

- Molecule 22 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 23 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

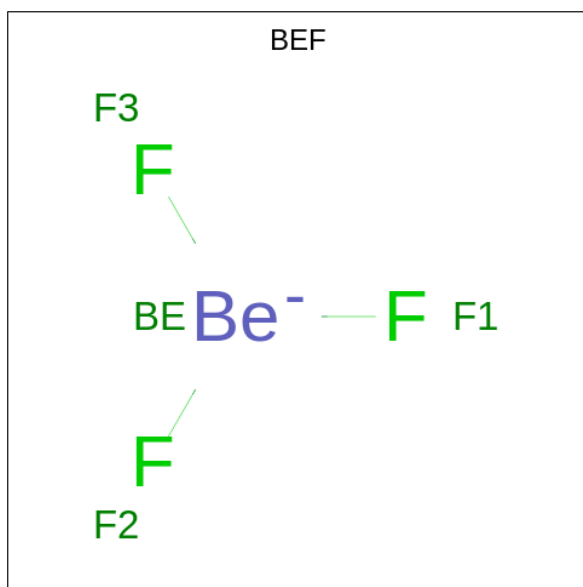


Mol	Chain	Residues	Atoms					AltConf
23	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	I	1	Total	Mg	0
			1	1	

- Molecule 25 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).

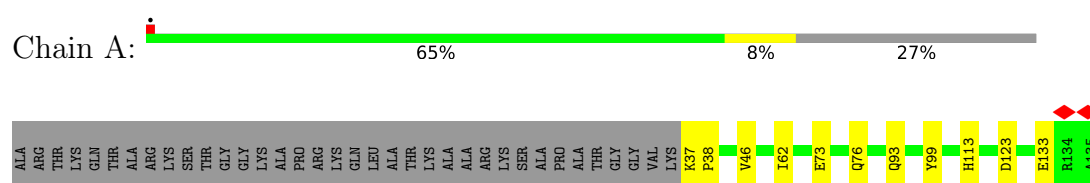


Mol	Chain	Residues	Atoms			AltConf
25	I	1	Total	Be	F	0
			4	1	3	

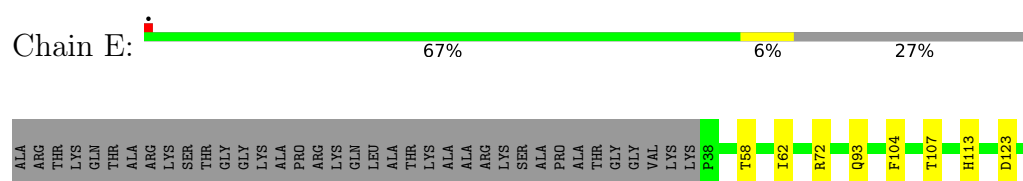
3 Residue-property plots [i](#)

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.

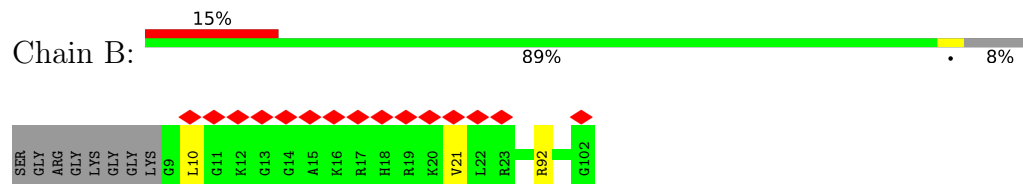
- Molecule 1: Histone H3



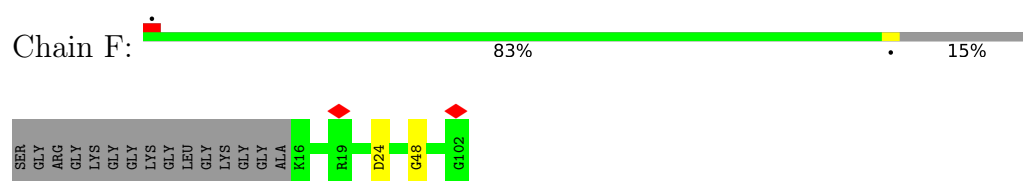
- Molecule 1: Histone H3



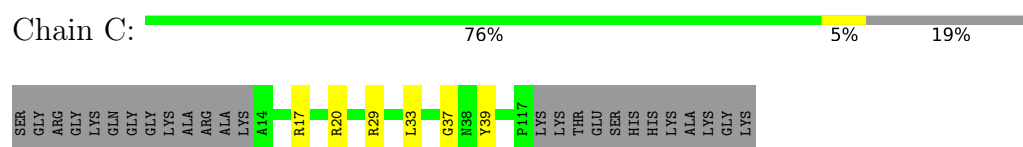
- Molecule 2: Histone H4



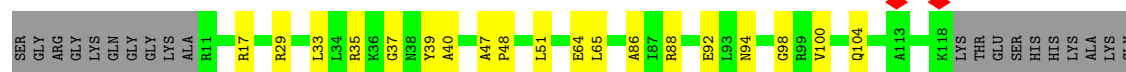
- Molecule 2: Histone H4



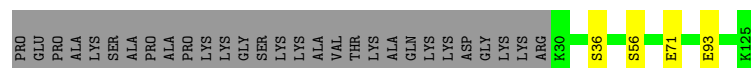
- Molecule 3: Histone H2A type 1-C



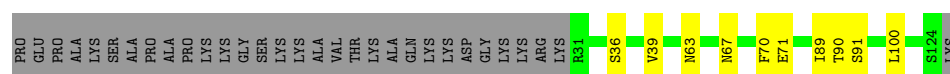
- Molecule 3: Histone H2A type 1-C



- Molecule 4: Histone H2B



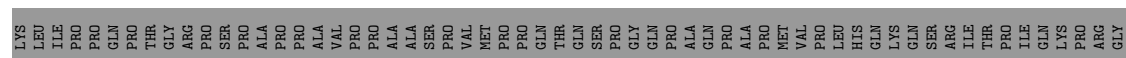
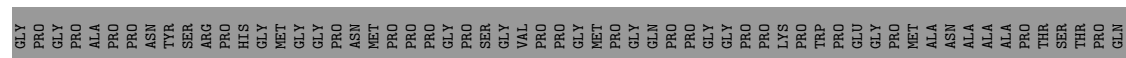
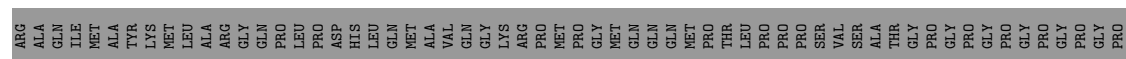
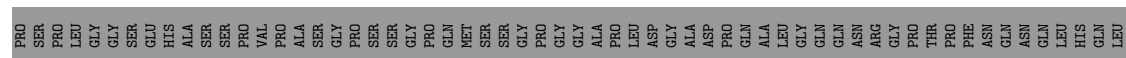
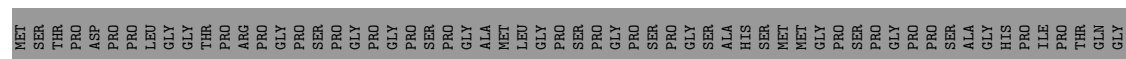
- Molecule 4: Histone H2B

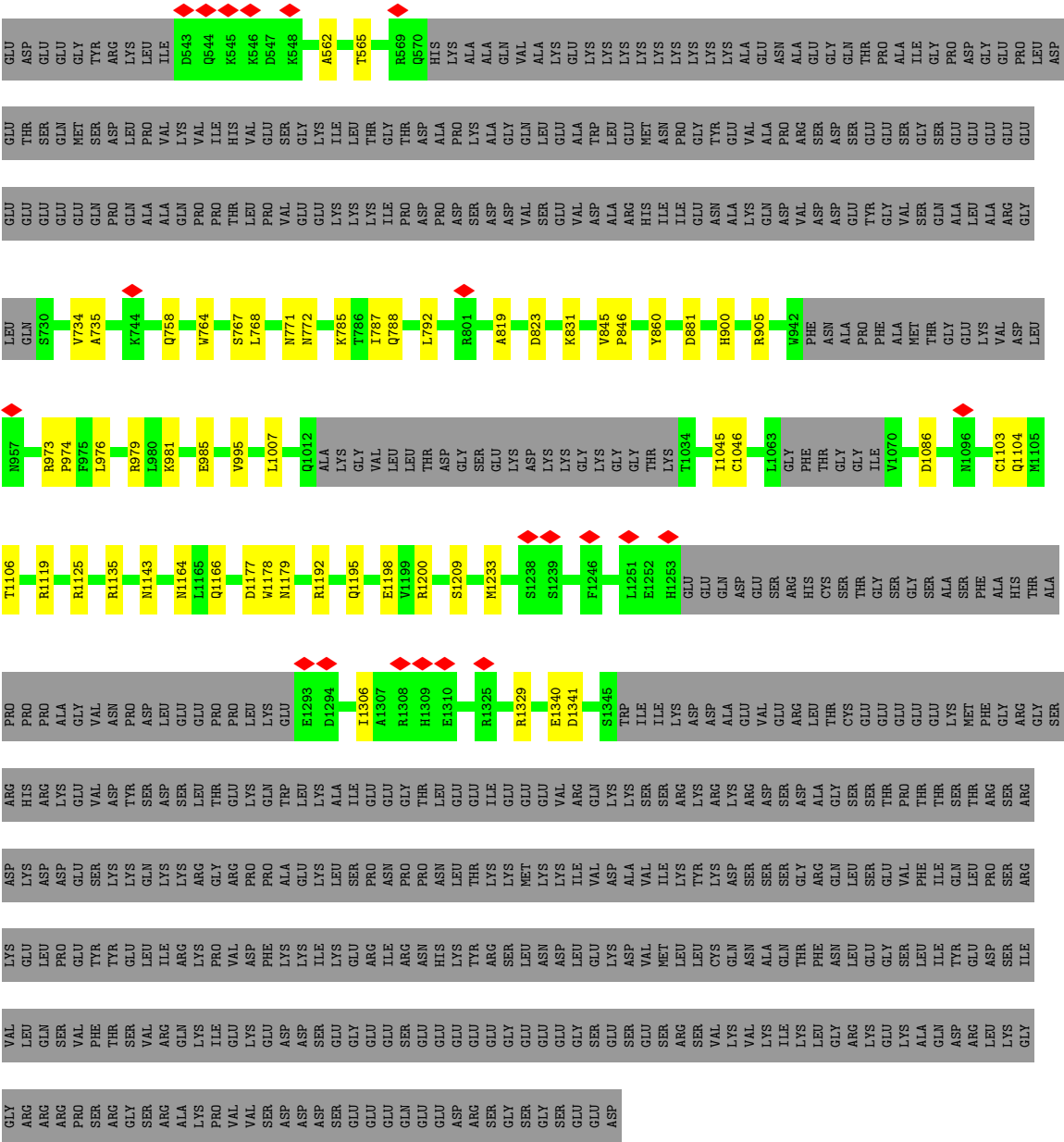


- Molecule 5: Unknown

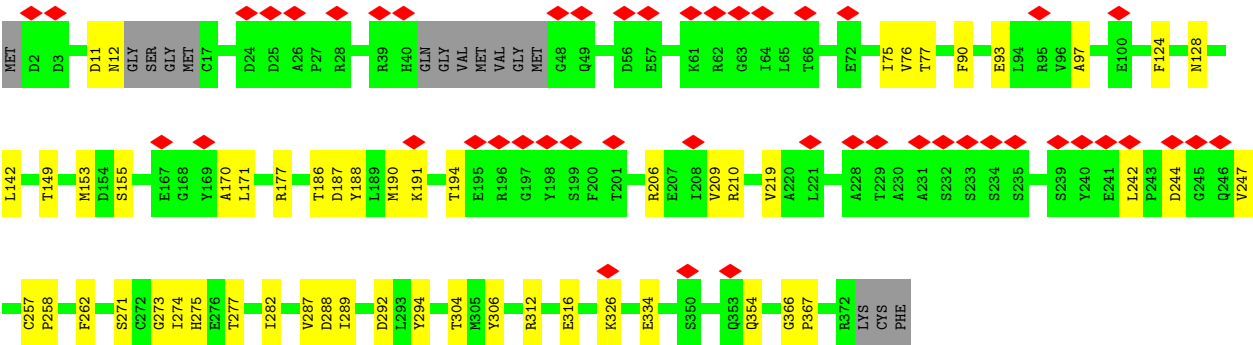
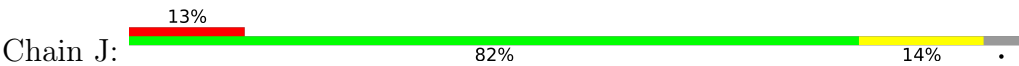


- Molecule 6: Transcription activator BRG1






● Molecule 7: ACTB protein (Fragment)

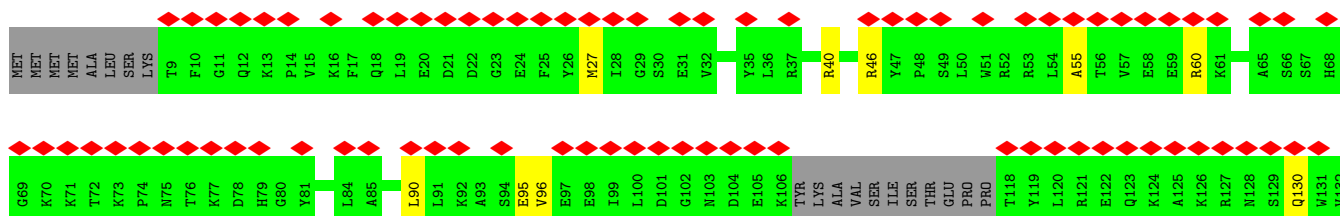


Chain K:



ARG	G1747	R1754	I1764	A1772	L1776	G1786	R1787	L1790	K1791	H1792	H1793	L1797	I1802	L1815	L1818	T1821	VAL	GLN	SER	GLN	SER	LYS	LYS	GLU	GLN	GLU	LYS	ASP	SER	GLU	MET	LEU	GLN
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- Chain M: 





Chain N:



[illegible]

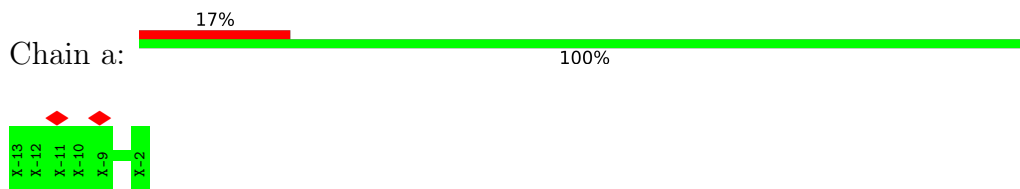
- Molecule 11: SWI/SNF complex subunit SMARCC2



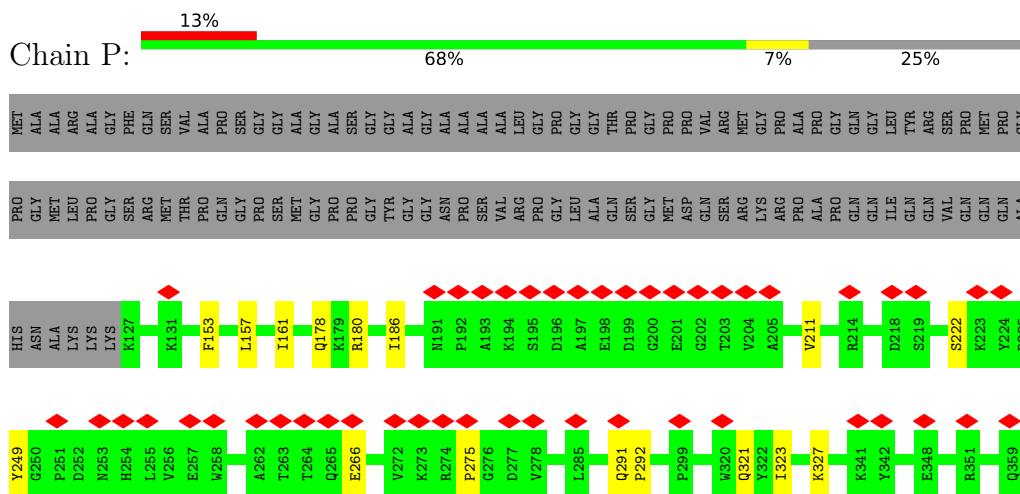
LYS	THR	ALA	THR	SER	PHE	THR	VAL	ARG	TRP	VAL	VAL	GLU	MET
THR	LYS	LYS	GLY	GLU	GLY	HIS	ASN	PRO	ILE	PRO	GLY	GLU	ALA
VAL	LYS	GLU	ALA	SER	LEU	H423	THR	SER	LEU	MET	ASN	PHE	VAL
GLU	THR	THR	ASP	SER	THR	S437	LYS	PRO	THR	MET	GLY	ARG	PHE
ARG	SER	SER	PRO	GLY	ASP	V438	ASP	SER	ASP	GLU	THR	THR	LYS
ASP	ASP	GLU	ALA	PRO	MET	E460	SER	PRO	THR	ILE	GLU	ASP	LYS
ILE	ILE	ALA	PHE	LEU	TYR	F468	GLU	THR	PHE	VAL	GLU	VAL	GLY
GLU	GLU	PRO	GLY	ALA	THR	F468	SER	PRO	ASN	GLY	GLU	SER	GLY
GLY	GLU	LYS	LEU	TYR	LYS	Y473	ALA	GLU	GLU	TRP	TRP	ASN	PRO
ASN	LYS	LYS	GLN	GLN	LYS	VAL	PRO	ALA	TRP	VAL	VAL	ALA	ASN
LEU	SER	GLU	SER	PRO	ASN	VAL	VAL	LYS	MET	ARG	PRO	VAL	VAL
SER	ILE	GLU	SER	ILE	VAL	C486	LYS	LYS	ASN	PRO	PRO	GLN	LYS
THR	GLY	GLU	GLY	PRO	GLY	THR	GLY	ASN	GLU	VAL	VAL	ASN	TYR
THR	ILE	LYS	PHE	THR	PRO	L490	THR	ALA	ASP	LYS	GLY	GLU	GLY
ALA	ALA	LYS	ALA	SER	LYS	THR	MET	LYS	TYR	ARG	GLY	LEU	ALA
ALA	LYS	GLY	GLY	GLN	SER	D515	THR	LYS	GLY	ASP	ILE	SER	ALA
ALA	GLY	THR	THR	SER	ALA	Y473	ASP	GLY	VAL	ASP	ILE	SER	ALA
ALA	ASP	SER	SER	ALA	ALA	L534	LEU	PRO	ASN	LYS	GLN	PRO	ASP
LEU	GLU	GLU	ASP	ALA	SER	A535	LEU	SER	ASN	VAL	GLN	PRO	THR
A867	GLU	GLU	GLU	V683	THR	D536	GLU	THR	ASP	VAL	ASN	PHE	VAL
A868	LYS	GLU	PRO	V684	GLY	T537	GLN	PRO	LYS	LEU	LEU	ILE	THR
A869	SER	SER	ARG	P686	ASP	P538	GLY	TYR	ASN	HIS	PHE	PHE	GLN
A870	LYS	ILE	ILE	R687	GLU	S539	ASP	THR	PRO	TRP	TRP	CYS	LYS
A871	LYS	GLU	GLU	T602	THR	G540	GLU	LYS	VAL	GLY	PRO	ALA	ASN
A872	ASP	SER	SER	V606	GLY	V542	SER	SER	VAL	THR	THR	GLY	VAL
A873	GLY	GLY	GLY	L607	THR	P543	GLU	ARG	ARG	PRO	GLU	GLY	ARG
A874	ASP	ASN	ASN	L608	GLN	L544	THR	GLY	LYS	ASP	LEU	LEU	THR
A875	PRO	PRO	ASP	L609	THR	GLN	THR	HIS	LYS	THR	LYS	CYS	LEU
A876	ILE	VAL	GLU	L610	LYS	THR	LYS	GLU	ILE	SER	ILE	GLY	GLY
A877	VAL	ASP	ALA	L617	THR	THR	GLU	GLU	LYS	ALA	ALA	ASN	TYR
A878	PRO	PRO	VAL	S695	GLY	GLN	ASP	GLN	THR	ILE	LEU	LEU	LYS
A879	GLU	GLU	GLU	GLU	K620	GLN	GLU	GLN	LEU	PRO	LYS	ALA	LYS
A880	LYS	LYS	GLY	F700	H621	THR	ASN	ASN	THR	PRO	GLN	HIS	GLU
A881	LYS	GLU	GLN	S701	K622	SER	SER	LEU	THR	ASP	GLN	GLN	PRO
A882	LYS	PRO	ALA	K702	H623	ALA	THR	THR	GLU	SER	GLU	GLY	THR
A883	PRO	ASP	THR	M703	S624	SER	ASN	ASP	VAL	ASN	ILE	LYS	LYS
A884	LYS	GLU	GLY	E705	E625	GLN	ASN	ASP	GLU	ARG	SER	GLU	GLU
A885	GLY	GLN	LYS	GLU	H626	GLN	GLY	GLY	THR	ILE	GLU	GLY	ALA
A886	GLU	GLN	GLU	VAL	V627	ASN	GLN	PRO	SER	GLY	THR	THR	ASN
A887	GLU	GLU	PRO	PRO	K628	PHE	THR	SER	ASP	VAL	ARG	ARG	LYS
A888	GLY	LYS	LYS	THR	E628	PRO	LYS	PRO	ARG	ALA	THR	THR	SER
A889	VAL	VAL	GLU	ALA	C635	ASP	ASN	VAL	ARG	PRO	PRO	TYR	SER
A890	VAL	VAL	GLU	ALA	L636	LYS	ASN	VAL	ARG	ALA	PRO	LEU	SER
A891	LYS	LYS	ARG	VAL	L637	GLY	PRO	ASP	LYS	THR	THR	PHE	SER
A892	GLU	GLU	GLU	GLY	H638	LYS	LEU	VAL	GLY	GLU	GLU	ASN	GLN
A893	VAL	VAL	GLY	ALA	P639	GLY	HIS	GLY	GLY	LYS	ASN	ASN	VAL
A894	VAL	VAL	GLY	HIS	L640	LYS	GLU	GLY	GLY	PRO	ALA	PRO	VAL
A895	GLU	GLY	GLY	ALA	H641	THR	ASP	VAL	ASN	ARG	SER	SER	GLN
A896	GLU	GLY	ILE	ARG	L642	THR	VAL	VAL	THR	LYS	VAL	MET	GLN
A897	GLY	GLY	GLU	VAL	P643	MET	THR	PRO	GLY	GLN	VAL	ASP	GLN
A898	GLY	GLY	GLU	VAL	K643	GLN	GLY	THR	LYS	THR	TYR	ASN	PHE
A899	GLN	ASP	GLU	GLU	ASN	THR	GLY	THR	LYS	THR	ASN	ASN	ASN

ALA	PRO	ASN	LEU	GLY	PRO
PRO	PRO	PRO	PRO	PRO	PRO
SER	LEU	LEU	PHE	GLN	PRO
PRO	GLY	HIS	PRO	GLN	ALA
THR	ASN	PRO	PRO	GLN	PRO
VAL	LEU	PRO	PRO	PRO	PRO
THR	PRO	PRO	PRO	ALA	GLY
PRO	ALA	THR	PRO	GLY	GLN
PRO	VAL	PRO	PRO	ALA	GLN
PRO	THR	PRO	PRO	PRO	PRO
PRO	THR	THR	PRO	GLN	TLE
PRO	THR	THR	ALA	PRO	PRO
GLN	PRO	SER	PRO	GLY	PRO
		SER	ILE	VAL	THR
		LEU	ILE	PRO	ALA
		PRO	PRO	PRO	ALA
		LEU	PHE	GLY	GLY
		GLY	GLY	VAL	PRO
		PRO	SER	PRO	PRO
		GLY	LEU	PRO	ALA
		LEU	ALA	PRO	VAL
		GLY	ASP	GLY	HIS
		SER	SER	PRO	GLY
		ALA	ILE	HIS	LEU
		ALA	SER	GLY	ALA
		ALA	ILE	PRO	VAL
		GLN	ASN	SER	ALA
		SER	LEU	PRO	PRO
		PRO	PRO	PHE	ALA
		ALA	ALA	PRO	SER
		ILE	PRO	ASN	VAL
		VAL	PRO	GLN	VAL
		ALA	ASN	GLN	PRO
		ALA	LEU	THR	ALA
		VAL	HIS	PRO	PRO
		GLN	GLY	PRO	ALA
		GLY	HIS	SER	GLY
		ASN	HIS	MET	GLY
		LEU	HIS	MET	ALA
		LEU	PRO	PRO	PRO
		PRO	LEU	GLY	PRO
		SER	ALA	VAL	PRO
		ALA	PHE	GLY	SER
		SER	ALA	PRO	LEU
		PRO	PRO	GLY	GLY
		LEU	GLY	SER	PRO
		PRO	THR	GLY	GLY
		ASP	LEU	HIS	SER
		GLY	PRO	PRO	GLN
		THR	PRO	VAL	TLE
		PRO	ASN	ALA	GLY
		LEU	LEU	GLY	GLN
		PRO	VAL	GLY	ALA
		PRO	PRO	ASN	GLY
		PRO	VAL	ALA	GLY
		ASP	SER	PRO	SER
		PRO	THR	LEU	THR
		THR	ALA	GLY	ALA

- Molecule 12: Unknown



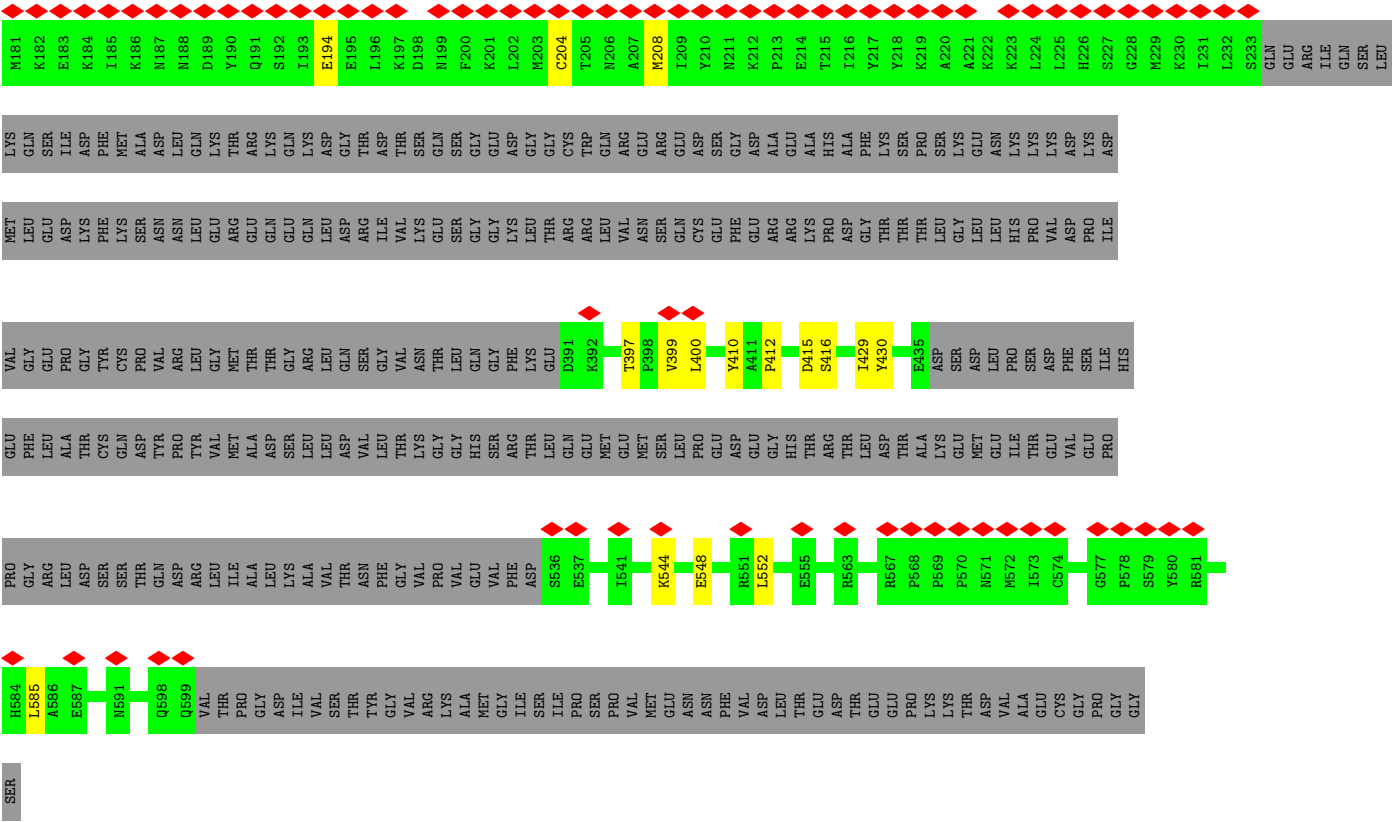
- Molecule 13: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily D member 1



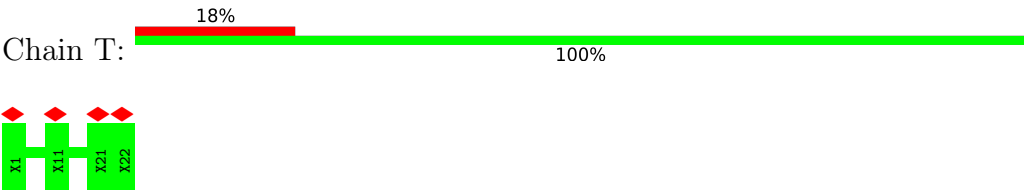
● Molecule 14: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily E member 1

[illegible]





• Molecule 17: Unkown



• Molecule 18: Protein polybromo-1

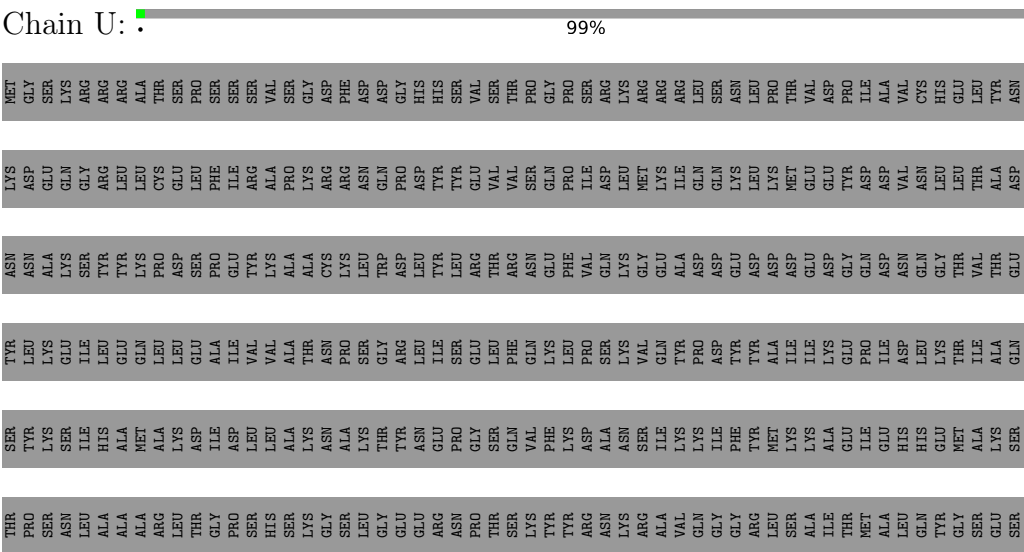




Diagram illustrating a 4x4 grid structure, likely representing a 2D convolution kernel or a small network layer. The grid contains values $x_1, x_2, x_3, x_{14}, x_{15}, x_{16}, x_{19}, x_{20},$ and x_{24} . Red diamonds are placed above the grid cells, indicating connections or weights between the input nodes and the output nodes.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37528	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.472	Depositor
Minimum map value	-0.644	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.28	Depositor
Map size (\AA)	480.24, 480.24, 480.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.334, 1.334, 1.334	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, MG, ADP

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	0.24	0/827	0.36	0/1109
1	E	0.23	0/818	0.36	0/1097
2	B	0.25	0/749	0.41	0/997
2	F	0.23	0/710	0.38	0/948
3	C	0.24	0/809	0.37	0/1093
3	G	0.24	0/843	0.37	0/1136
4	D	0.24	0/766	0.36	0/1026
4	H	0.24	0/747	0.35	0/1004
6	I	0.23	0/6152	0.37	0/8268
7	J	0.23	0/2881	0.41	0/3904
8	K	0.24	0/2849	0.41	0/3866
9	L	0.24	0/4229	0.38	0/5705
10	M	0.24	0/2976	0.41	0/4025
11	N	0.24	0/2125	0.37	0/2870
11	O	0.24	0/2401	0.44	3/3244 (0.1%)
13	P	0.24	0/3237	0.39	0/4369
14	Q	0.23	0/746	0.39	0/999
15	R	0.27	0/372	0.45	0/497
16	S	0.24	0/1773	0.35	0/2390
18	U	0.28	0/94	0.38	0/125
20	X	0.55	0/3763	0.90	0/5800
21	Y	0.54	0/3825	0.88	0/5907
All	All	0.31	0/43692	0.52	3/60379 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	543	PRO	N-CA-CB	6.97	111.67	103.30
11	O	643	PRO	N-CA-CB	6.27	110.82	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	O	647	PRO	N-CA-CB	5.99	110.49	103.30

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	815	0	856	7	0
1	E	806	0	844	7	0
2	B	741	0	796	3	0
2	F	702	0	755	2	0
3	C	799	0	851	5	0
3	G	833	0	895	14	0
4	D	755	0	782	4	0
4	H	736	0	756	8	0
5	Z	141	0	27	0	0
6	I	6051	0	6176	57	0
7	J	2821	0	2780	33	0
8	K	2787	0	2725	34	0
9	L	4151	0	4161	46	0
10	M	2918	0	2870	30	0
11	N	2085	0	2068	25	0
11	O	2354	0	2282	17	0
12	a	58	0	14	0	0
13	P	3174	0	3173	28	0
14	Q	739	0	755	7	0
15	R	366	0	369	6	0
16	S	1738	0	1718	12	0
17	T	110	0	31	0	0
18	U	92	0	84	0	0
19	V	420	0	98	0	0
20	X	3360	0	1853	45	0
21	Y	3405	0	1850	28	0
22	W	120	0	28	0	0
23	I	27	0	12	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	I	1	0	0	0	0
25	I	4	0	0	1	0
All	All	43109	0	39609	366	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 4.

The worst 5 of 366 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)
6:I:1192:ARG:NH1	23:I:1701:ADP:O2A	1.94	0.99
6:I:1192:ARG:HD3	23:I:1701:ADP:H5'1	1.54	0.88
7:J:186:THR:OG1	7:J:206:ARG:O	1.92	0.85
6:I:1166:GLN:OE1	23:I:1701:ADP:H4'	1.78	0.82
6:I:365:GLU:OE1	14:Q:191:THR:OG1	1.97	0.82

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	97/135 (72%)	95 (98%)	2 (2%)	0	100	100
1	E	96/135 (71%)	96 (100%)	0	0	100	100
2	B	92/102 (90%)	87 (95%)	5 (5%)	0	100	100
2	F	85/102 (83%)	84 (99%)	1 (1%)	0	100	100
3	C	102/129 (79%)	101 (99%)	1 (1%)	0	100	100
3	G	106/129 (82%)	102 (96%)	4 (4%)	0	100	100
4	D	94/125 (75%)	94 (100%)	0	0	100	100
4	H	92/125 (74%)	92 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	I	718/1647 (44%)	693 (96%)	25 (4%)	0	100	100
7	J	354/375 (94%)	324 (92%)	30 (8%)	0	100	100
8	K	348/429 (81%)	325 (93%)	23 (7%)	0	100	100
9	L	513/1835 (28%)	474 (92%)	39 (8%)	0	100	100
10	M	358/385 (93%)	325 (91%)	33 (9%)	0	100	100
11	N	247/1214 (20%)	240 (97%)	7 (3%)	0	100	100
11	O	289/1214 (24%)	260 (90%)	26 (9%)	3 (1%)	15	54
13	P	383/515 (74%)	367 (96%)	15 (4%)	1 (0%)	41	76
14	Q	89/411 (22%)	88 (99%)	1 (1%)	0	100	100
15	R	42/498 (8%)	40 (95%)	2 (5%)	0	100	100
16	S	207/651 (32%)	204 (99%)	3 (1%)	0	100	100
18	U	9/1597 (1%)	8 (89%)	1 (11%)	0	100	100
All	All	4321/11753 (37%)	4099 (95%)	218 (5%)	4 (0%)	54	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	O	543	PRO
11	O	643	PRO
13	P	469	VAL
11	O	437	SER

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	86/110 (78%)	86 (100%)	0	100	100
1	E	85/110 (77%)	85 (100%)	0	100	100
2	B	74/78 (95%)	74 (100%)	0	100	100
2	F	72/78 (92%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	81/98 (83%)	81 (100%)	0	100	100
3	G	84/98 (86%)	84 (100%)	0	100	100
4	D	83/105 (79%)	83 (100%)	0	100	100
4	H	81/105 (77%)	81 (100%)	0	100	100
6	I	655/1422 (46%)	654 (100%)	1 (0%)	93	96
7	J	307/318 (96%)	305 (99%)	2 (1%)	84	90
8	K	308/364 (85%)	306 (99%)	2 (1%)	86	92
9	L	465/1587 (29%)	463 (100%)	2 (0%)	91	94
10	M	325/346 (94%)	324 (100%)	1 (0%)	92	95
11	N	221/1030 (22%)	221 (100%)	0	100	100
11	O	241/1030 (23%)	239 (99%)	2 (1%)	81	89
13	P	351/442 (79%)	351 (100%)	0	100	100
14	Q	82/361 (23%)	82 (100%)	0	100	100
15	R	38/437 (9%)	38 (100%)	0	100	100
16	S	196/586 (33%)	196 (100%)	0	100	100
18	U	9/1433 (1%)	9 (100%)	0	100	100
All	All	3844/10138 (38%)	3834 (100%)	10 (0%)	92	95

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	M	193	MET
11	O	437	SER
11	O	438	VAL
8	K	301	ARG
8	K	377	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
9	L	406	HIS
14	Q	199	ASN
9	L	1795	ASN
16	S	206	ASN
10	M	322	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
23	ADP	I	1701	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
25	BEF	I	1703	-	0,3,3	-	-	-	-	-

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
23	ADP	I	1701	-	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	I	1701	ADP	C5-C4	2.51	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	I	1701	ADP	PA-O3A-PB	-3.85	119.63	132.83
23	I	1701	ADP	C3'-C2'-C1'	3.19	105.79	100.98
23	I	1701	ADP	N3-C2-N1	-3.19	123.70	128.68
23	I	1701	ADP	C4-C5-N7	-2.66	106.62	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

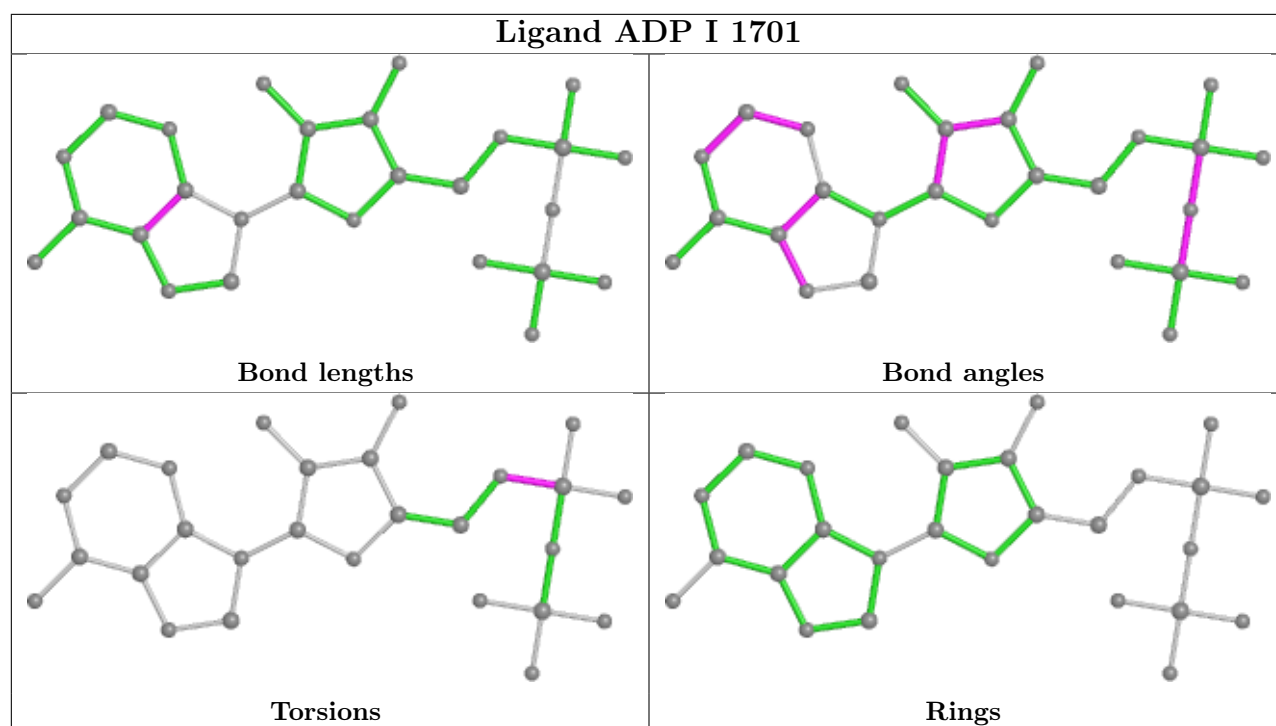
Mol	Chain	Res	Type	Atoms
23	I	1701	ADP	C5'-O5'-PA-O1A
23	I	1701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	I	1701	ADP	11	0
25	I	1703	BEF	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.

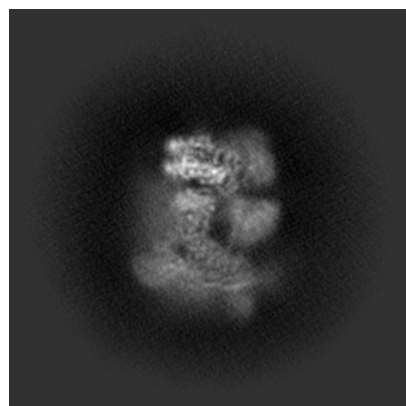
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33684. These allow visual inspection of the internal detail of the map and identification of artifacts.

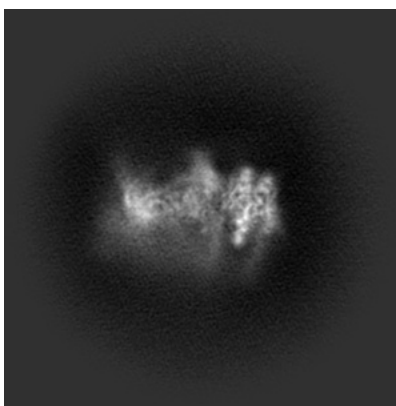
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

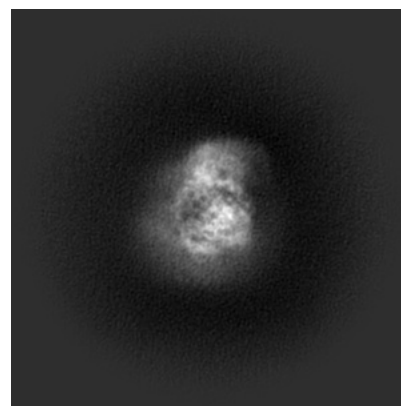
6.1.1 Primary map



X

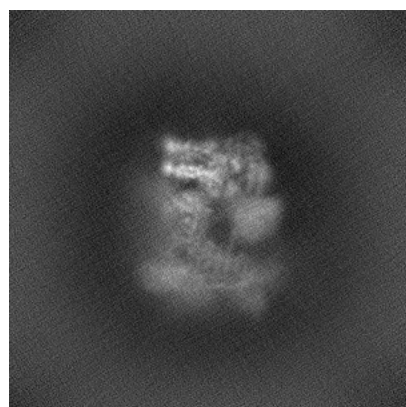


Y

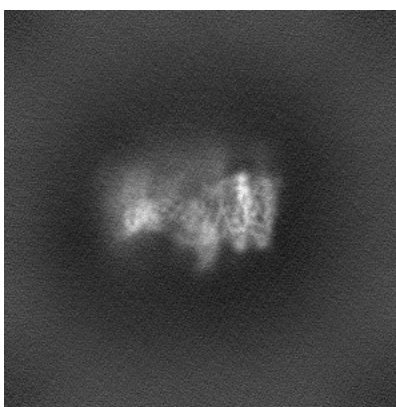


Z

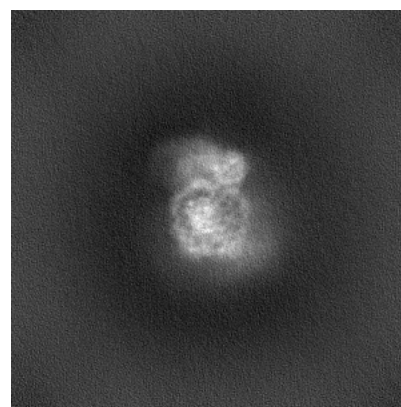
6.1.2 Raw map



X



Y

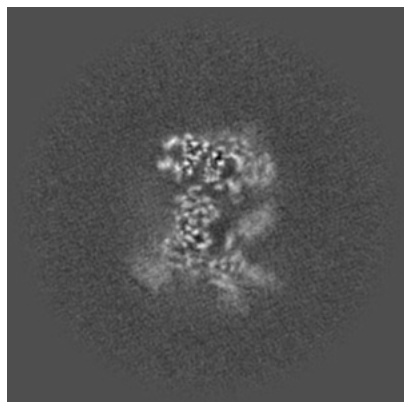


Z

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

6.2 Central slices [i](#)

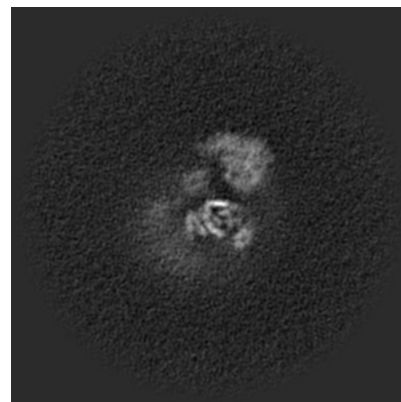
6.2.1 Primary map



X Index: 180

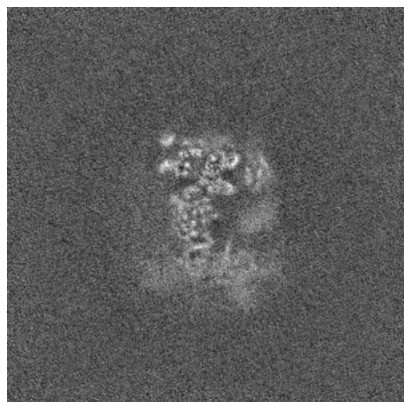


Y Index: 180



Z Index: 180

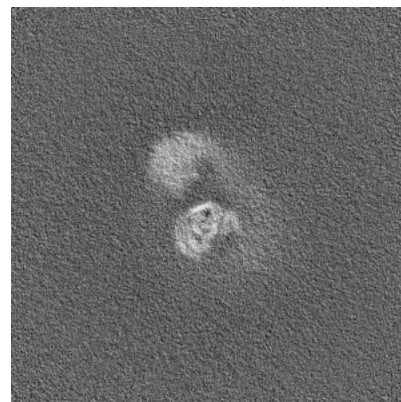
6.2.2 Raw map



X Index: 180



Y Index: 180

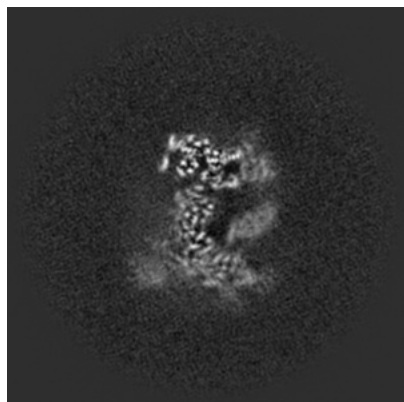


Z Index: 180

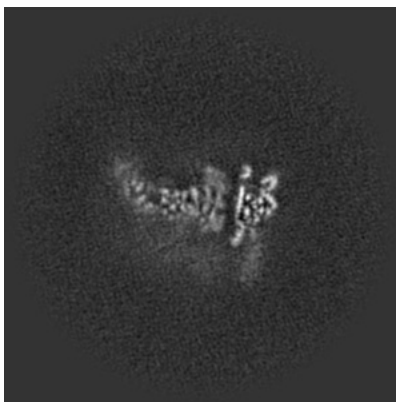
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

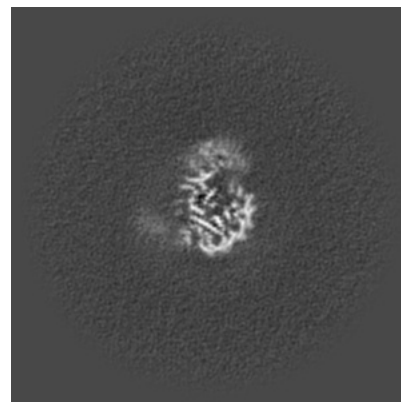
6.3.1 Primary map



X Index: 184

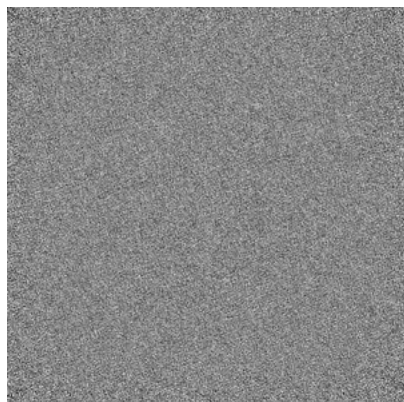


Y Index: 164

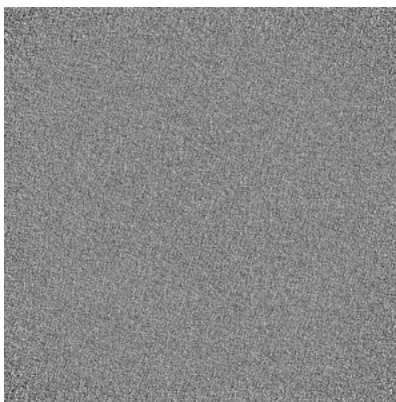


Z Index: 218

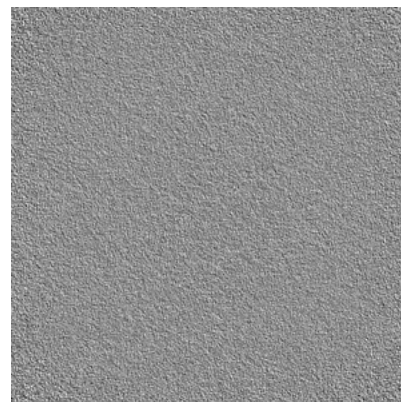
6.3.2 Raw map



X Index: 0



Y Index: 0

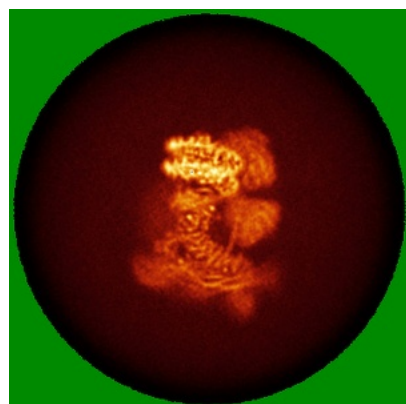


Z Index: 0

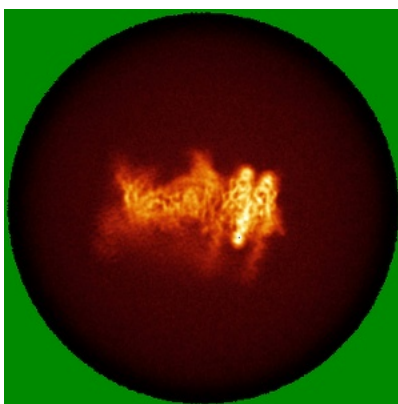
The images above show the largest variance slices of the map in three orthogonal directions.

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

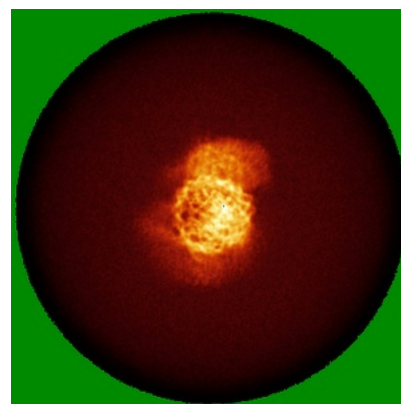
6.4.1 Primary map



X

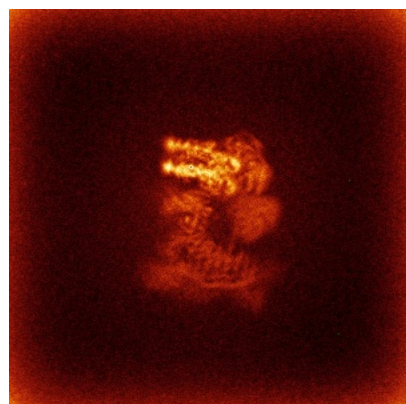


Y

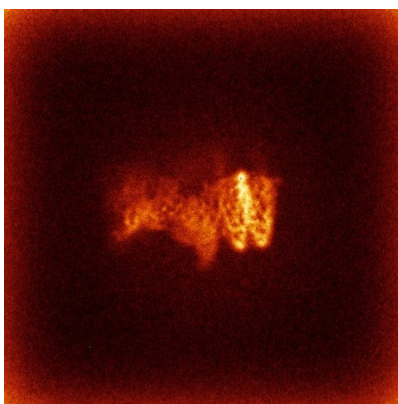


Z

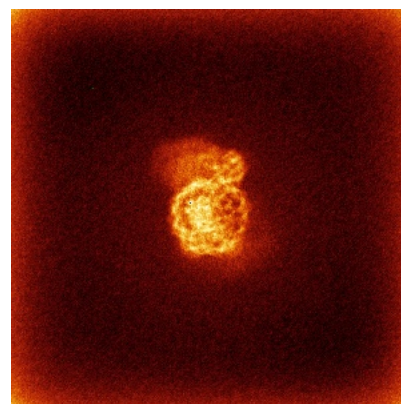
6.4.2 Raw map



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



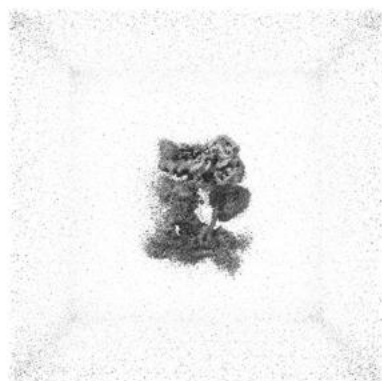
Y



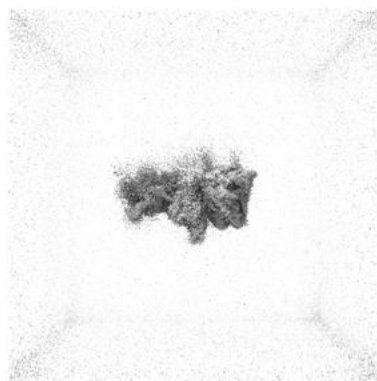
Z

The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

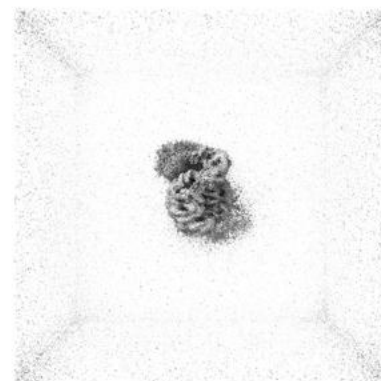
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

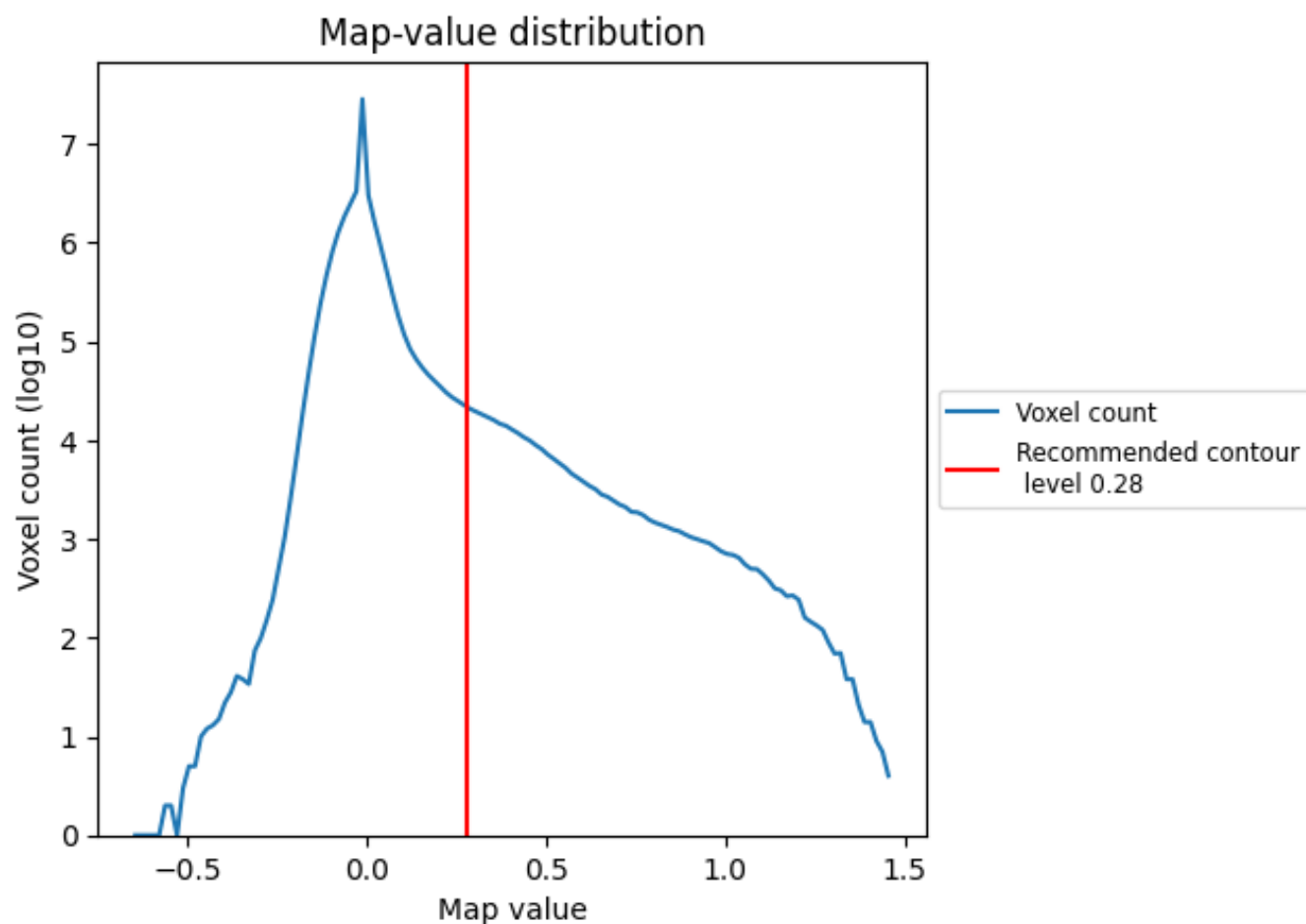
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

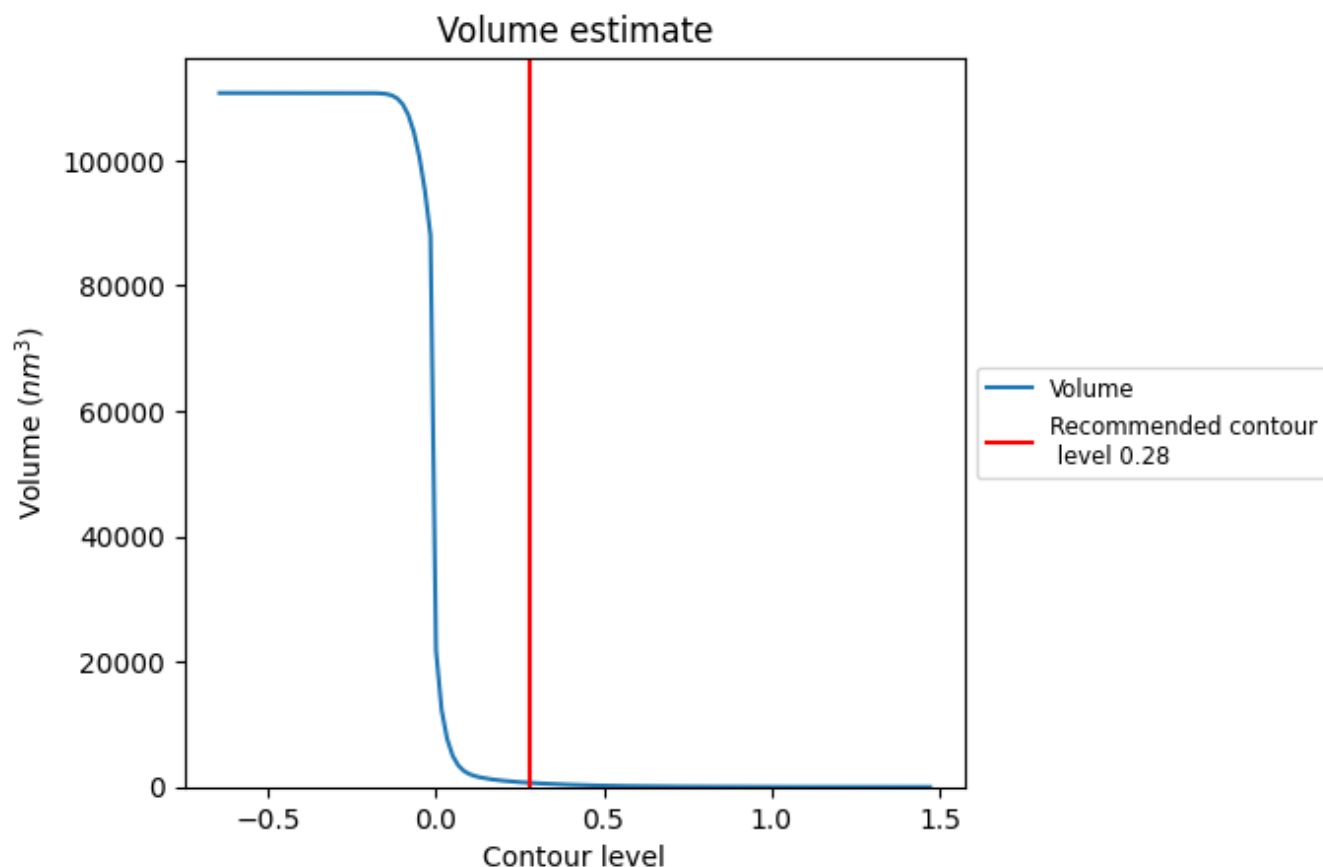
This section contains the results of statistical analysis of the map.

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.

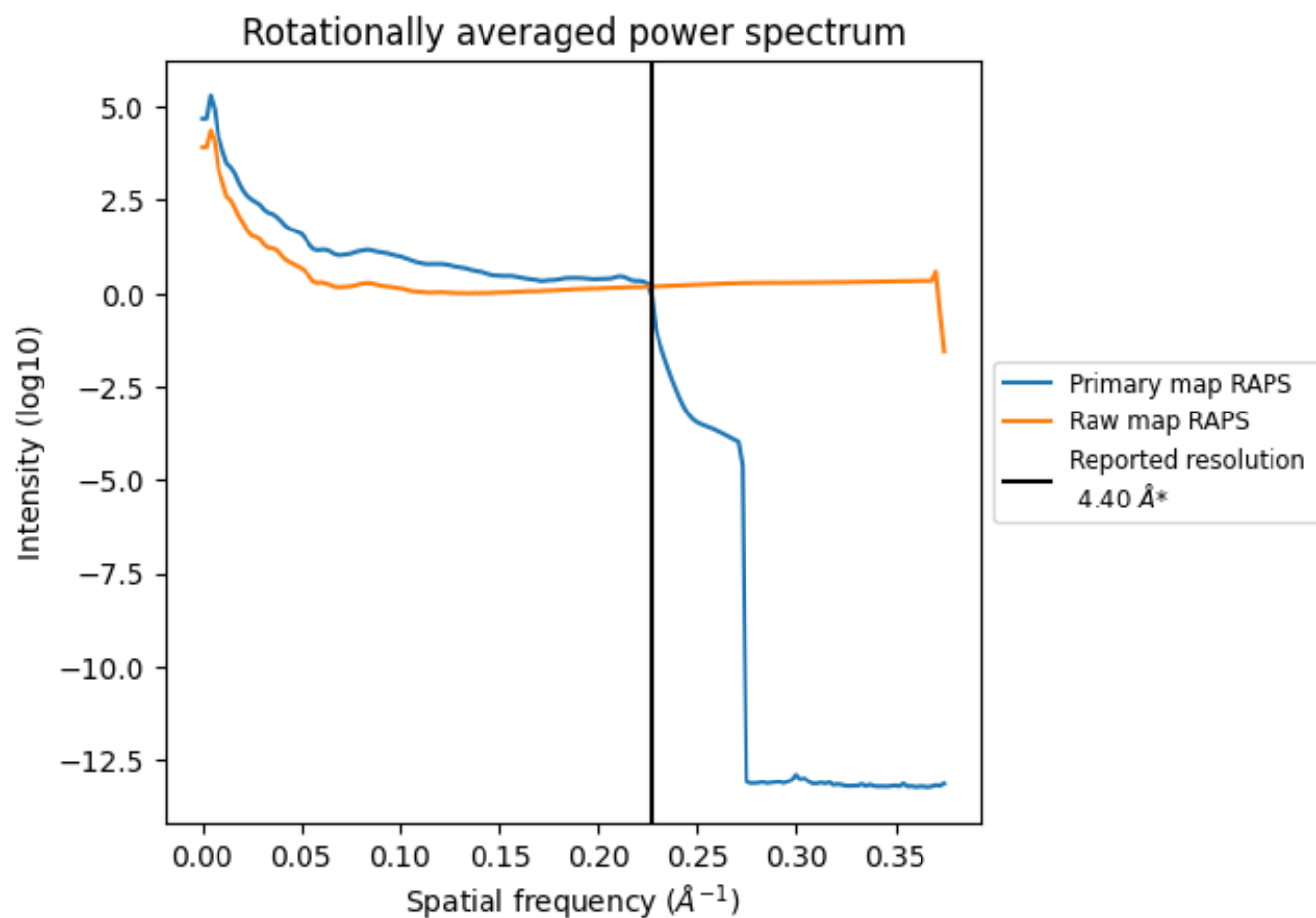
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 660 nm^3 ; this corresponds to an approximate mass of 596 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 ⓘ

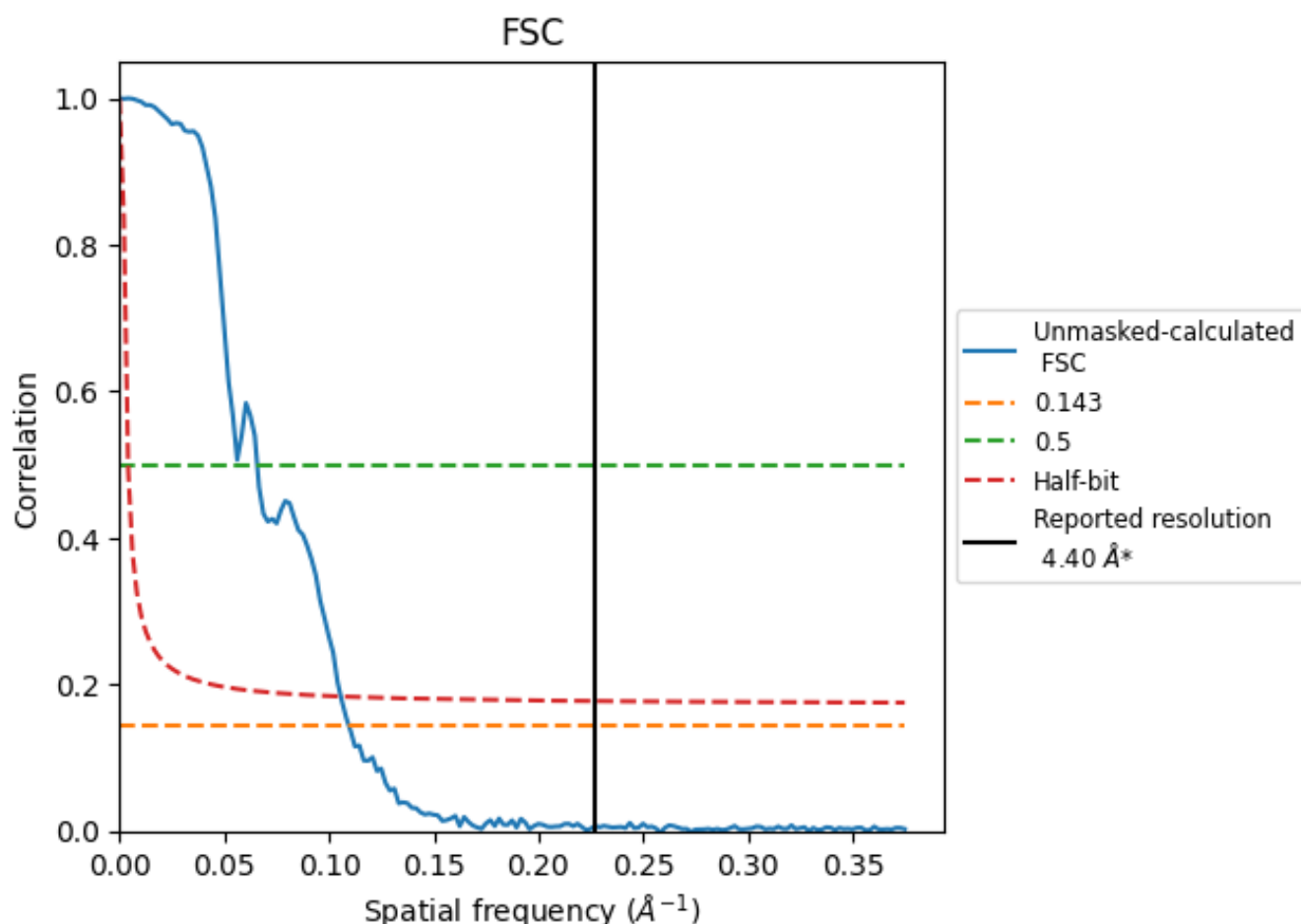


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

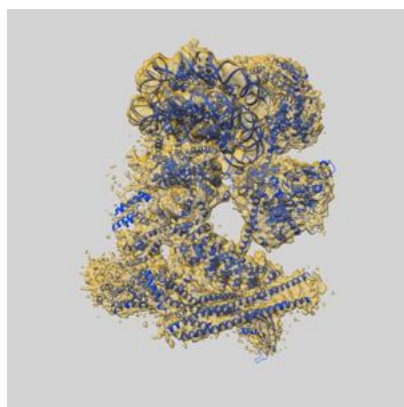
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.13	15.22	9.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.13 differs from the reported value 4.4 by more than 10 %

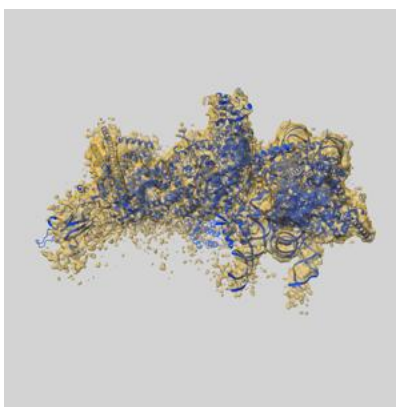
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33684 and PDB model 7Y8R. Per-residue inclusion information can be found in section [3](#) on page [9](#).

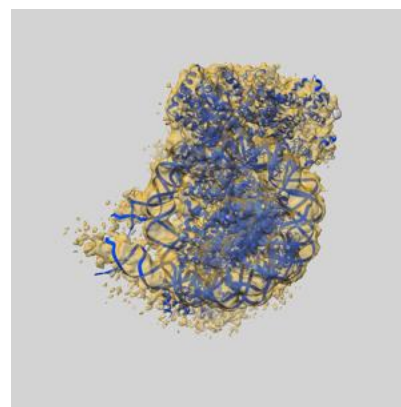
9.1 Map-model overlay [i](#)



X



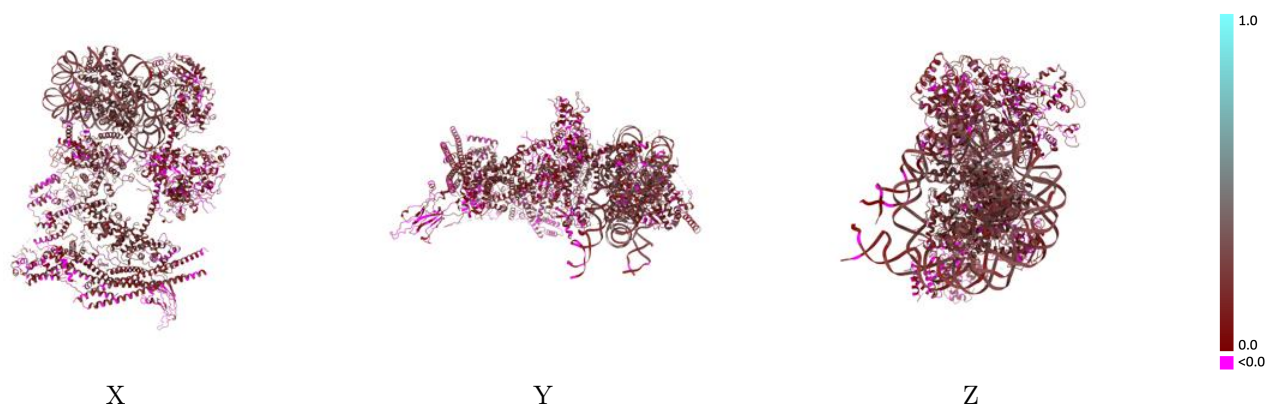
Y



Z

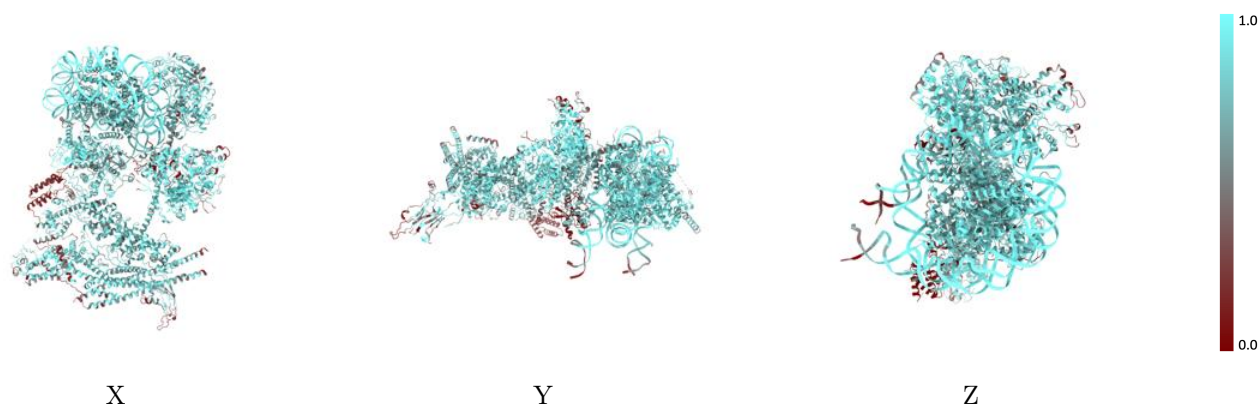
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



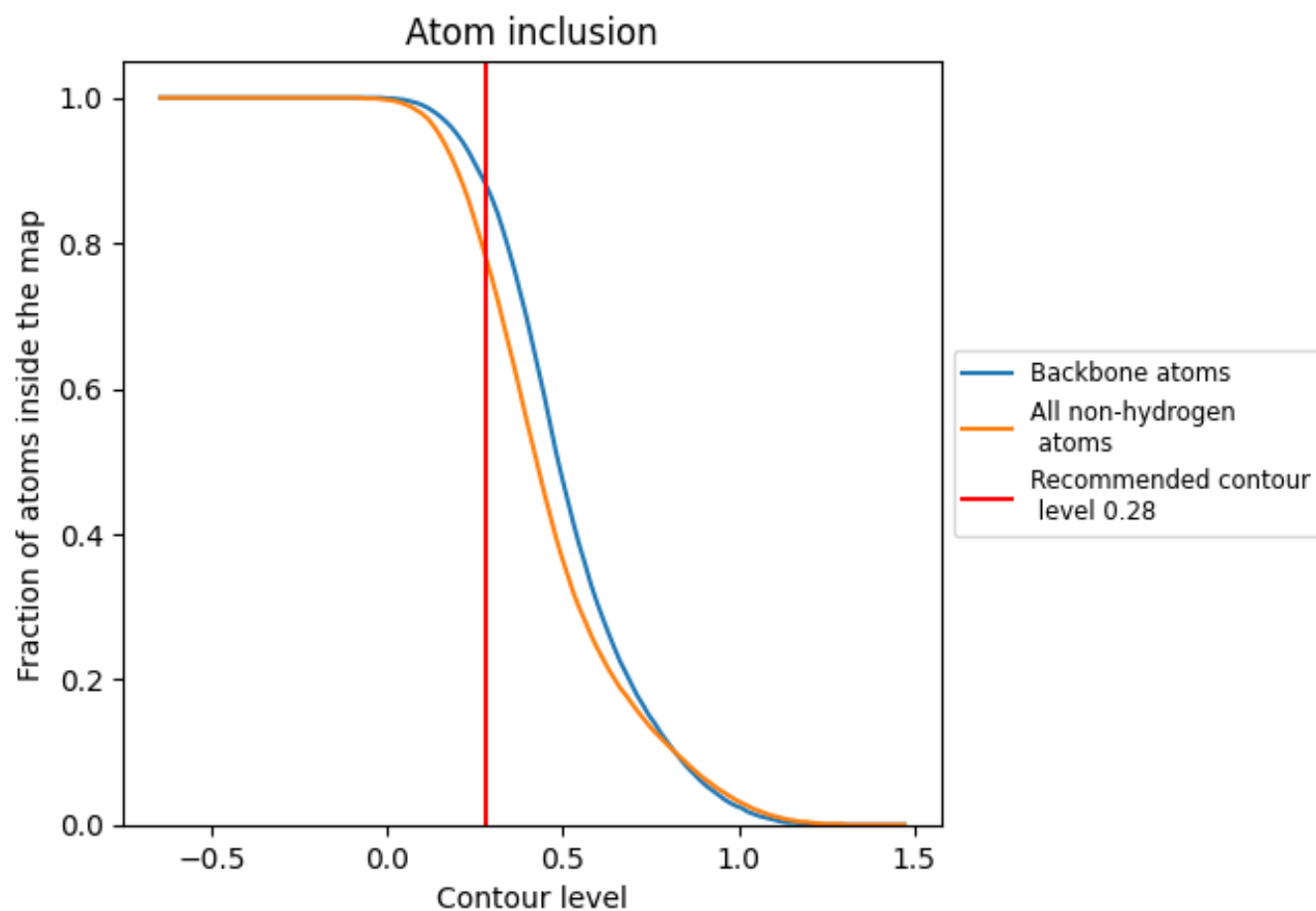
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 78% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7820	 0.1720
A	 0.8330	 0.2410
B	 0.7150	 0.2210
C	 0.8750	 0.2650
D	 0.8860	 0.2630
E	 0.8430	 0.2570
F	 0.8450	 0.2740
G	 0.8160	 0.2600
H	 0.8420	 0.2620
I	 0.8120	 0.1630
J	 0.7990	 0.1100
K	 0.8520	 0.1160
L	 0.7760	 0.1940
M	 0.6240	 0.1630
N	 0.7980	 0.1570
O	 0.7590	 0.1110
P	 0.6950	 0.1030
Q	 0.6720	 0.1420
R	 0.7420	 0.1190
S	 0.3800	 0.0810
T	 0.7910	 0.1600
U	 0.6440	 0.1980
V	 0.7360	 0.1920
W	 0.6670	 0.1900
X	 0.8970	 0.2220
Y	 0.9190	 0.2380
Z	 0.9720	 0.1290
a	 0.7070	 0.1670

