wwPDB EM Validation Summary Report ⓘ

May 12, 2024 – 01:23 am BST

PDB ID	:	6R92
EMDB ID	:	EMD-4766
Title	:	Cryo-EM structure of NCP-THF2(+1)-UV-DDB class B
Authors	:	Matsumoto, S.; Cavadini, S.; Bunker, R.D.; Thoma, N.H.
Deposited on	:	2019-04-02
Resolution	:	4.80 Å(reported)
Based on initial models	:	4ZUX, 3EI4, 4E54, 5Y0C

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:

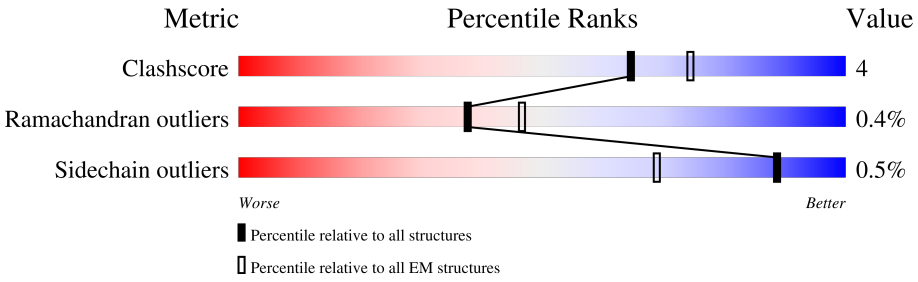
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.80 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 <=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	I	145	86% 14%
2	J	145	86% 14%
3	L	450	63% 18% 19%
4	A	139	54% 16% 29%
4	E	139	59% 12% 29%
5	B	106	7% 71% 7% 23%
5	F	106	5% 71% 7% 23%
6	C	133	6% 80% 7% 12%

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Mol	Chain	Length	Quality of chain
6	G	133	6% 77% 11% 12%
7	D	129	62% 12% 26%
7	H	129	5% 61% 14% 25%
8	K	1163	12% 64% 7% 29%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 40535 atoms, of which 19035 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 DNA chain called Human alpha-satellite DNA (145-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	I	145	4611	1421	1641	535	870	144	0	0

- Molecule 2 is a DNA chain called Human alpha-satellite DNA (145-MER) with abasic sites at positions 93-94.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	J	145	4581	1410	1633	529	865	144	0	0

- Molecule 3 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	L	363	5642	1818	2788	507	513	16	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-22	MET	-	initiating methionine	UNP Q92466
L	-21	ALA	-	expression tag	UNP Q92466
L	-20	SER	-	expression tag	UNP Q92466
L	-19	TRP	-	expression tag	UNP Q92466
L	-18	SER	-	expression tag	UNP Q92466
L	-17	HIS	-	expression tag	UNP Q92466
L	-16	PRO	-	expression tag	UNP Q92466
L	-15	GLN	-	expression tag	UNP Q92466
L	-14	PHE	-	expression tag	UNP Q92466
L	-13	GLU	-	expression tag	UNP Q92466
L	-12	LYS	-	expression tag	UNP Q92466
L	-11	VAL	-	expression tag	UNP Q92466
L	-10	ASP	-	expression tag	UNP Q92466
L	-9	GLU	-	expression tag	UNP Q92466

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-8	ASN	-	expression tag	UNP Q92466
L	-7	LEU	-	expression tag	UNP Q92466
L	-6	TYR	-	expression tag	UNP Q92466
L	-5	PHE	-	expression tag	UNP Q92466
L	-4	GLN	-	expression tag	UNP Q92466
L	-3	GLY	-	expression tag	UNP Q92466
L	-2	GLY	-	expression tag	UNP Q92466
L	-1	GLY	-	expression tag	UNP Q92466
L	0	ARG	-	expression tag	UNP Q92466

- Molecule 4 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	98	Total	C	H	N	O	S	0	0
			1645	508	838	156	139	4		
4	E	98	Total	C	H	N	O	S	0	0
			1646	508	839	156	139	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P68431
A	-1	SER	-	expression tag	UNP P68431
A	0	HIS	-	expression tag	UNP P68431
E	-2	GLY	-	expression tag	UNP P68431
E	-1	SER	-	expression tag	UNP P68431
E	0	HIS	-	expression tag	UNP P68431

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	82	Total	C	H	N	O	S	0	0
			1347	412	694	127	113	1		
5	F	82	Total	C	H	N	O	S	0	0
			1348	412	695	127	113	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62805
B	-1	SER	-	expression tag	UNP P62805
B	0	HIS	-	expression tag	UNP P62805

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P62805
F	-1	SER	-	expression tag	UNP P62805
F	0	HIS	-	expression tag	UNP P62805

- Molecule 6 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	117	Total	C	H	N	O	0	0
			1877	571	968	181	157		
6	G	117	Total	C	H	N	O	0	0
			1878	571	969	181	157		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P04908
C	-1	SER	-	expression tag	UNP P04908
C	0	HIS	-	expression tag	UNP P04908
G	-2	GLY	-	expression tag	UNP P04908
G	-1	SER	-	expression tag	UNP P04908
G	0	HIS	-	expression tag	UNP P04908

- Molecule 7 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	95	Total	C	H	N	O	S	0	0
			1507	468	761	136	140	2		
7	H	97	Total	C	H	N	O	S	0	0
			1555	480	789	142	142	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP P06899
D	-1	SER	-	expression tag	UNP P06899
D	0	HIS	-	expression tag	UNP P06899
H	-2	GLY	-	expression tag	UNP P06899
H	-1	SER	-	expression tag	UNP P06899
H	0	HIS	-	expression tag	UNP P06899

- Molecule 8 is a protein called DNA damage-binding protein 1,DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	825	Total	C	H	N	O	S	0	0
			12898	4100	6420	1092	1250	36		

There are 333 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-22	MET	-	initiating methionine	UNP Q16531
K	-21	ALA	-	expression tag	UNP Q16531
K	-20	SER	-	expression tag	UNP Q16531
K	-19	TRP	-	expression tag	UNP Q16531
K	-18	SER	-	expression tag	UNP Q16531
K	-17	HIS	-	expression tag	UNP Q16531
K	-16	PRO	-	expression tag	UNP Q16531
K	-15	GLN	-	expression tag	UNP Q16531
K	-14	PHE	-	expression tag	UNP Q16531
K	-13	GLU	-	expression tag	UNP Q16531
K	-12	LYS	-	expression tag	UNP Q16531
K	-11	VAL	-	expression tag	UNP Q16531
K	-10	ASP	-	expression tag	UNP Q16531
K	-9	GLU	-	expression tag	UNP Q16531
K	-8	ASN	-	expression tag	UNP Q16531
K	-7	LEU	-	expression tag	UNP Q16531
K	-6	TYR	-	expression tag	UNP Q16531
K	-5	PHE	-	expression tag	UNP Q16531
K	-4	GLN	-	expression tag	UNP Q16531
K	-3	GLY	-	expression tag	UNP Q16531
K	-2	GLY	-	expression tag	UNP Q16531
K	-1	GLY	-	expression tag	UNP Q16531
K	0	ARG	-	expression tag	UNP Q16531
K	396	ILE	-	linker	UNP Q16531
K	397	HIS	-	linker	UNP Q16531
K	398	GLU	-	linker	UNP Q16531
K	399	HIS	-	linker	UNP Q16531
K	400	ALA	-	linker	UNP Q16531
K	401	SER	-	linker	UNP Q16531
K	402	ILE	-	linker	UNP Q16531
K	403	ASP	-	linker	UNP Q16531
K	404	LEU	-	linker	UNP Q16531
K	405	PRO	-	linker	UNP Q16531
K	406	GLY	-	linker	UNP Q16531
K	407	ILE	-	linker	UNP Q16531
K	408	LYS	-	linker	UNP Q16531
K	409	GLY	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
K	410	LEU	-	linker	UNP Q16531
K	411	TRP	-	linker	UNP Q16531
K	412	PRO	-	linker	UNP Q16531
K	413	LEU	-	linker	UNP Q16531
K	414	ARG	-	linker	UNP Q16531
K	415	SER	-	linker	UNP Q16531
K	416	ASP	-	linker	UNP Q16531
K	417	PRO	-	linker	UNP Q16531
K	418	ASN	-	linker	UNP Q16531
K	419	ARG	-	linker	UNP Q16531
K	420	GLU	-	linker	UNP Q16531
K	421	THR	-	linker	UNP Q16531
K	422	ASP	-	linker	UNP Q16531
K	423	ASP	-	linker	UNP Q16531
K	424	THR	-	linker	UNP Q16531
K	425	LEU	-	linker	UNP Q16531
K	426	VAL	-	linker	UNP Q16531
K	427	LEU	-	linker	UNP Q16531
K	428	SER	-	linker	UNP Q16531
K	429	PHE	-	linker	UNP Q16531
K	430	VAL	-	linker	UNP Q16531
K	431	GLY	-	linker	UNP Q16531
K	432	GLN	-	linker	UNP Q16531
K	433	THR	-	linker	UNP Q16531
K	434	ARG	-	linker	UNP Q16531
K	435	VAL	-	linker	UNP Q16531
K	436	LEU	-	linker	UNP Q16531
K	437	MET	-	linker	UNP Q16531
K	438	LEU	-	linker	UNP Q16531
K	439	ASN	-	linker	UNP Q16531
K	440	GLY	-	linker	UNP Q16531
K	441	GLU	-	linker	UNP Q16531
K	442	GLU	-	linker	UNP Q16531
K	443	VAL	-	linker	UNP Q16531
K	444	GLU	-	linker	UNP Q16531
K	445	GLU	-	linker	UNP Q16531
K	446	THR	-	linker	UNP Q16531
K	447	GLU	-	linker	UNP Q16531
K	448	LEU	-	linker	UNP Q16531
K	449	MET	-	linker	UNP Q16531
K	450	GLY	-	linker	UNP Q16531
K	451	PHE	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
K	452	VAL	-	linker	UNP Q16531
K	453	ASP	-	linker	UNP Q16531
K	454	ASP	-	linker	UNP Q16531
K	455	GLN	-	linker	UNP Q16531
K	456	GLN	-	linker	UNP Q16531
K	457	THR	-	linker	UNP Q16531
K	458	PHE	-	linker	UNP Q16531
K	459	PHE	-	linker	UNP Q16531
K	460	CYS	-	linker	UNP Q16531
K	461	GLY	-	linker	UNP Q16531
K	462	ASN	-	linker	UNP Q16531
K	463	VAL	-	linker	UNP Q16531
K	464	ALA	-	linker	UNP Q16531
K	465	HIS	-	linker	UNP Q16531
K	466	GLN	-	linker	UNP Q16531
K	467	GLN	-	linker	UNP Q16531
K	468	LEU	-	linker	UNP Q16531
K	469	ILE	-	linker	UNP Q16531
K	470	GLN	-	linker	UNP Q16531
K	471	ILE	-	linker	UNP Q16531
K	472	THR	-	linker	UNP Q16531
K	473	SER	-	linker	UNP Q16531
K	474	ALA	-	linker	UNP Q16531
K	475	SER	-	linker	UNP Q16531
K	476	VAL	-	linker	UNP Q16531
K	477	ARG	-	linker	UNP Q16531
K	478	LEU	-	linker	UNP Q16531
K	479	VAL	-	linker	UNP Q16531
K	480	SER	-	linker	UNP Q16531
K	481	GLN	-	linker	UNP Q16531
K	482	GLU	-	linker	UNP Q16531
K	483	PRO	-	linker	UNP Q16531
K	484	LYS	-	linker	UNP Q16531
K	485	ALA	-	linker	UNP Q16531
K	486	LEU	-	linker	UNP Q16531
K	487	VAL	-	linker	UNP Q16531
K	488	SER	-	linker	UNP Q16531
K	489	GLU	-	linker	UNP Q16531
K	490	TRP	-	linker	UNP Q16531
K	491	LYS	-	linker	UNP Q16531
K	492	GLU	-	linker	UNP Q16531
K	493	PRO	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
K	494	GLN	-	linker	UNP Q16531
K	495	ALA	-	linker	UNP Q16531
K	496	LYS	-	linker	UNP Q16531
K	497	ASN	-	linker	UNP Q16531
K	498	ILE	-	linker	UNP Q16531
K	499	SER	-	linker	UNP Q16531
K	500	VAL	-	linker	UNP Q16531
K	501	ALA	-	linker	UNP Q16531
K	502	SER	-	linker	UNP Q16531
K	503	CYS	-	linker	UNP Q16531
K	504	ASN	-	linker	UNP Q16531
K	505	SER	-	linker	UNP Q16531
K	506	SER	-	linker	UNP Q16531
K	507	GLN	-	linker	UNP Q16531
K	508	VAL	-	linker	UNP Q16531
K	509	VAL	-	linker	UNP Q16531
K	510	VAL	-	linker	UNP Q16531
K	511	ALA	-	linker	UNP Q16531
K	512	VAL	-	linker	UNP Q16531
K	513	GLY	-	linker	UNP Q16531
K	514	ARG	-	linker	UNP Q16531
K	515	ALA	-	linker	UNP Q16531
K	516	LEU	-	linker	UNP Q16531
K	517	TYR	-	linker	UNP Q16531
K	518	TYR	-	linker	UNP Q16531
K	519	LEU	-	linker	UNP Q16531
K	520	GLN	-	linker	UNP Q16531
K	521	ILE	-	linker	UNP Q16531
K	522	HIS	-	linker	UNP Q16531
K	523	PRO	-	linker	UNP Q16531
K	524	GLN	-	linker	UNP Q16531
K	525	GLU	-	linker	UNP Q16531
K	526	LEU	-	linker	UNP Q16531
K	527	ARG	-	linker	UNP Q16531
K	528	GLN	-	linker	UNP Q16531
K	529	ILE	-	linker	UNP Q16531
K	530	SER	-	linker	UNP Q16531
K	531	HIS	-	linker	UNP Q16531
K	532	THR	-	linker	UNP Q16531
K	533	GLU	-	linker	UNP Q16531
K	534	MET	-	linker	UNP Q16531
K	535	GLU	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
K	536	HIS	-	linker	UNP Q16531
K	537	GLU	-	linker	UNP Q16531
K	538	VAL	-	linker	UNP Q16531
K	539	ALA	-	linker	UNP Q16531
K	540	CYS	-	linker	UNP Q16531
K	541	LEU	-	linker	UNP Q16531
K	542	ASP	-	linker	UNP Q16531
K	543	ILE	-	linker	UNP Q16531
K	544	THR	-	linker	UNP Q16531
K	545	PRO	-	linker	UNP Q16531
K	546	LEU	-	linker	UNP Q16531
K	547	GLY	-	linker	UNP Q16531
K	548	ASP	-	linker	UNP Q16531
K	549	SER	-	linker	UNP Q16531
K	550	ASN	-	linker	UNP Q16531
K	551	GLY	-	linker	UNP Q16531
K	552	LEU	-	linker	UNP Q16531
K	553	SER	-	linker	UNP Q16531
K	554	PRO	-	linker	UNP Q16531
K	555	LEU	-	linker	UNP Q16531
K	556	CYS	-	linker	UNP Q16531
K	557	ALA	-	linker	UNP Q16531
K	558	ILE	-	linker	UNP Q16531
K	559	GLY	-	linker	UNP Q16531
K	560	LEU	-	linker	UNP Q16531
K	561	TRP	-	linker	UNP Q16531
K	562	THR	-	linker	UNP Q16531
K	563	ASP	-	linker	UNP Q16531
K	564	ILE	-	linker	UNP Q16531
K	565	SER	-	linker	UNP Q16531
K	566	ALA	-	linker	UNP Q16531
K	567	ARG	-	linker	UNP Q16531
K	568	ILE	-	linker	UNP Q16531
K	569	LEU	-	linker	UNP Q16531
K	570	LYS	-	linker	UNP Q16531
K	571	LEU	-	linker	UNP Q16531
K	572	PRO	-	linker	UNP Q16531
K	573	SER	-	linker	UNP Q16531
K	574	PHE	-	linker	UNP Q16531
K	575	GLU	-	linker	UNP Q16531
K	576	LEU	-	linker	UNP Q16531
K	577	LEU	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
K	578	HIS	-	linker	UNP Q16531
K	579	LYS	-	linker	UNP Q16531
K	580	GLU	-	linker	UNP Q16531
K	581	MET	-	linker	UNP Q16531
K	582	LEU	-	linker	UNP Q16531
K	583	GLY	-	linker	UNP Q16531
K	584	GLY	-	linker	UNP Q16531
K	585	GLU	-	linker	UNP Q16531
K	586	ILE	-	linker	UNP Q16531
K	587	ILE	-	linker	UNP Q16531
K	588	PRO	-	linker	UNP Q16531
K	589	ARG	-	linker	UNP Q16531
K	590	SER	-	linker	UNP Q16531
K	591	ILE	-	linker	UNP Q16531
K	592	LEU	-	linker	UNP Q16531
K	593	MET	-	linker	UNP Q16531
K	594	THR	-	linker	UNP Q16531
K	595	THR	-	linker	UNP Q16531
K	596	PHE	-	linker	UNP Q16531
K	597	GLU	-	linker	UNP Q16531
K	598	SER	-	linker	UNP Q16531
K	599	SER	-	linker	UNP Q16531
K	600	HIS	-	linker	UNP Q16531
K	601	TYR	-	linker	UNP Q16531
K	602	LEU	-	linker	UNP Q16531
K	603	LEU	-	linker	UNP Q16531
K	604	CYS	-	linker	UNP Q16531
K	605	ALA	-	linker	UNP Q16531
K	606	LEU	-	linker	UNP Q16531
K	607	GLY	-	linker	UNP Q16531
K	608	ASP	-	linker	UNP Q16531
K	609	GLY	-	linker	UNP Q16531
K	610	ALA	-	linker	UNP Q16531
K	611	LEU	-	linker	UNP Q16531
K	612	PHE	-	linker	UNP Q16531
K	613	TYR	-	linker	UNP Q16531
K	614	PHE	-	linker	UNP Q16531
K	615	GLY	-	linker	UNP Q16531
K	616	LEU	-	linker	UNP Q16531
K	617	ASN	-	linker	UNP Q16531
K	618	ILE	-	linker	UNP Q16531
K	619	GLU	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
K	620	THR	-	linker	UNP Q16531
K	621	GLY	-	linker	UNP Q16531
K	622	LEU	-	linker	UNP Q16531
K	623	LEU	-	linker	UNP Q16531
K	624	SER	-	linker	UNP Q16531
K	625	ASP	-	linker	UNP Q16531
K	626	ARG	-	linker	UNP Q16531
K	627	LYS	-	linker	UNP Q16531
K	628	LYS	-	linker	UNP Q16531
K	629	VAL	-	linker	UNP Q16531
K	630	THR	-	linker	UNP Q16531
K	631	LEU	-	linker	UNP Q16531
K	632	GLY	-	linker	UNP Q16531
K	633	THR	-	linker	UNP Q16531
K	634	GLN	-	linker	UNP Q16531
K	635	PRO	-	linker	UNP Q16531
K	636	THR	-	linker	UNP Q16531
K	637	VAL	-	linker	UNP Q16531
K	638	LEU	-	linker	UNP Q16531
K	639	ARG	-	linker	UNP Q16531
K	640	THR	-	linker	UNP Q16531
K	641	PHE	-	linker	UNP Q16531
K	642	ARG	-	linker	UNP Q16531
K	643	SER	-	linker	UNP Q16531
K	644	LEU	-	linker	UNP Q16531
K	645	SER	-	linker	UNP Q16531
K	646	THR	-	linker	UNP Q16531
K	647	THR	-	linker	UNP Q16531
K	648	ASN	-	linker	UNP Q16531
K	649	VAL	-	linker	UNP Q16531
K	650	PHE	-	linker	UNP Q16531
K	651	ALA	-	linker	UNP Q16531
K	652	CYS	-	linker	UNP Q16531
K	653	SER	-	linker	UNP Q16531
K	654	ASP	-	linker	UNP Q16531
K	655	ARG	-	linker	UNP Q16531
K	656	PRO	-	linker	UNP Q16531
K	657	THR	-	linker	UNP Q16531
K	658	VAL	-	linker	UNP Q16531
K	659	ILE	-	linker	UNP Q16531
K	660	TYR	-	linker	UNP Q16531
K	661	SER	-	linker	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
K	662	SER	-	linker	UNP Q16531
K	663	ASN	-	linker	UNP Q16531
K	664	HIS	-	linker	UNP Q16531
K	665	LYS	-	linker	UNP Q16531
K	666	LEU	-	linker	UNP Q16531
K	667	VAL	-	linker	UNP Q16531
K	668	PHE	-	linker	UNP Q16531
K	669	SER	-	linker	UNP Q16531
K	670	ASN	-	linker	UNP Q16531
K	671	VAL	-	linker	UNP Q16531
K	672	ASN	-	linker	UNP Q16531
K	673	LEU	-	linker	UNP Q16531
K	674	LYS	-	linker	UNP Q16531
K	675	GLU	-	linker	UNP Q16531
K	676	VAL	-	linker	UNP Q16531
K	677	ASN	-	linker	UNP Q16531
K	678	TYR	-	linker	UNP Q16531
K	679	MET	-	linker	UNP Q16531
K	680	CYS	-	linker	UNP Q16531
K	681	PRO	-	linker	UNP Q16531
K	682	LEU	-	linker	UNP Q16531
K	683	ASN	-	linker	UNP Q16531
K	684	SER	-	linker	UNP Q16531
K	685	ASP	-	linker	UNP Q16531
K	686	GLY	-	linker	UNP Q16531
K	687	TYR	-	linker	UNP Q16531
K	688	PRO	-	linker	UNP Q16531
K	689	ASP	-	linker	UNP Q16531
K	690	SER	-	linker	UNP Q16531
K	691	LEU	-	linker	UNP Q16531
K	692	ALA	-	linker	UNP Q16531
K	693	LEU	-	linker	UNP Q16531
K	694	ALA	-	linker	UNP Q16531
K	695	ASN	-	linker	UNP Q16531
K	696	ASN	-	linker	UNP Q16531
K	697	SER	-	linker	UNP Q16531
K	698	THR	-	linker	UNP Q16531
K	699	LEU	-	linker	UNP Q16531
K	700	THR	-	linker	UNP Q16531
K	701	ILE	-	linker	UNP Q16531
K	702	GLY	-	linker	UNP Q16531
K	703	THR	-	linker	UNP Q16531

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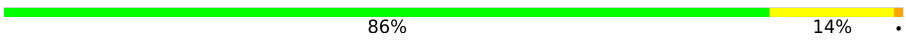
Chain	Residue	Modelled	Actual	Comment	Reference
K	704	ILE	-	linker	UNP Q16531
K	705	ASP	-	linker	UNP Q16531

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.

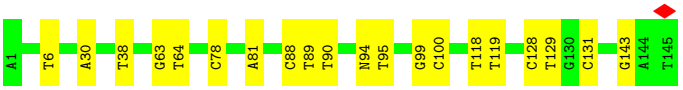
• Molecule 1: Human alpha-satellite DNA (145-MER)

Chain I:



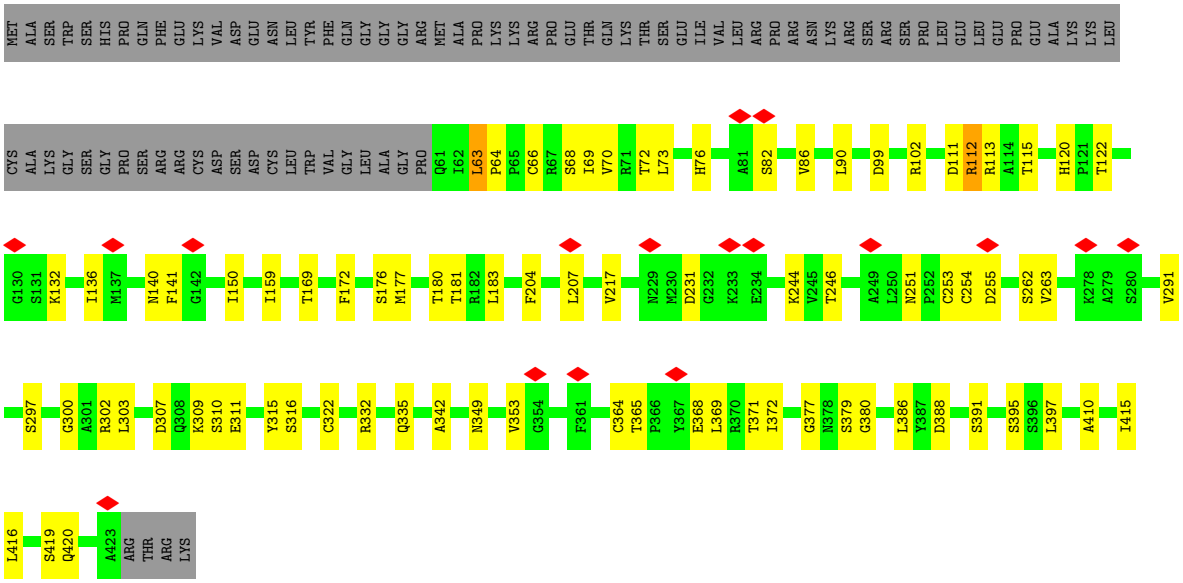
• Molecule 2: Human alpha-satellite DNA (145-MER) with abasic sites at positions 93-94

Chain J:



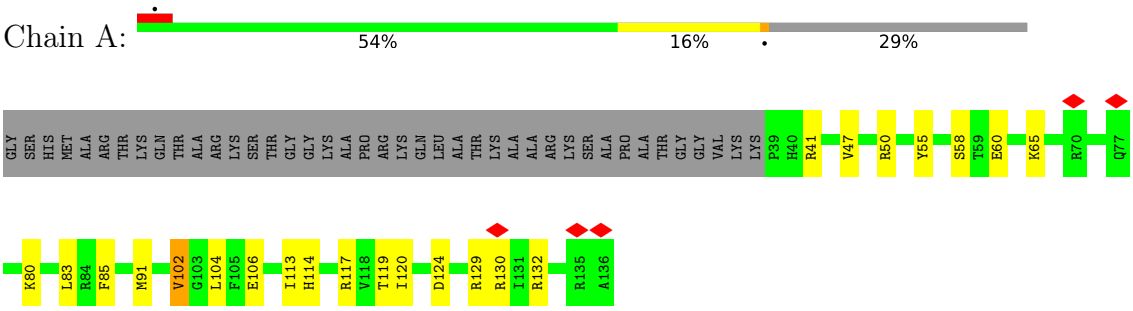
• Molecule 3: DNA damage-binding protein 2

Chain L:



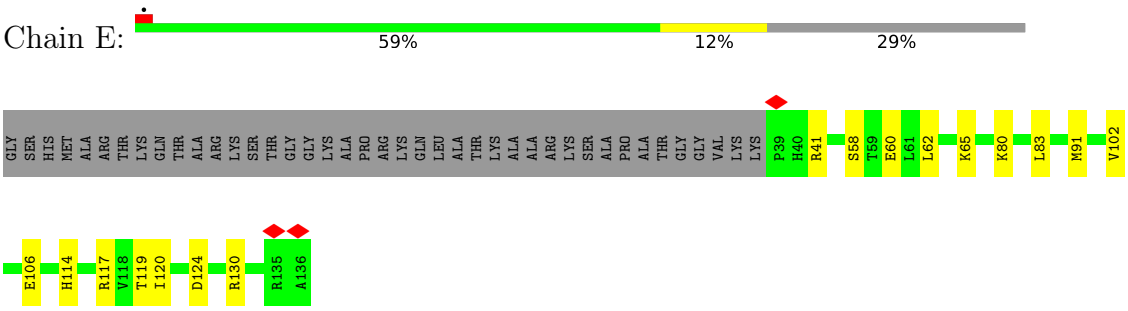
• Molecule 4: Histone H3.1

Chain A:



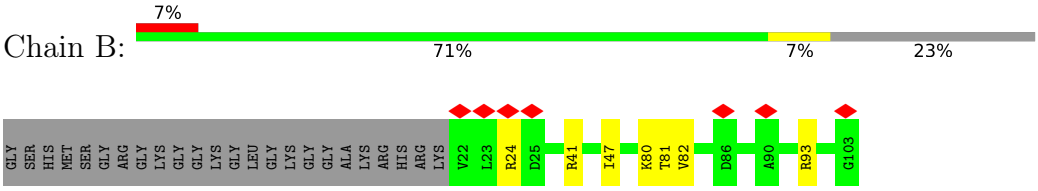
• Molecule 4: Histone H3.1

Chain E:



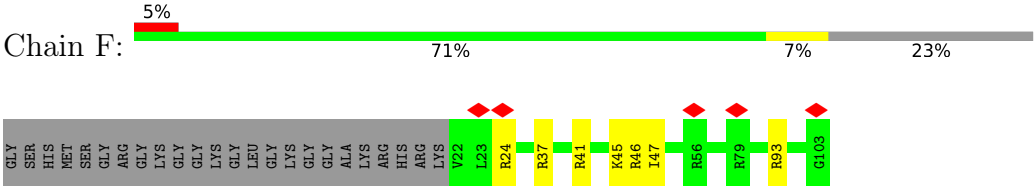
• Molecule 5: Histone H4

Chain B:



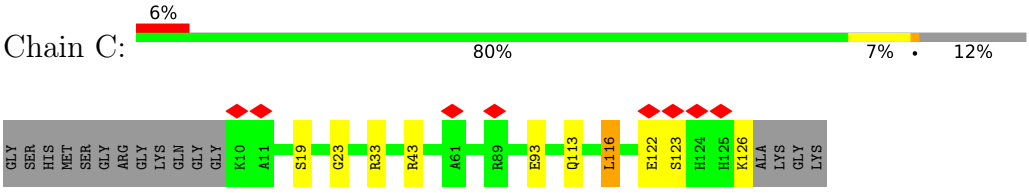
• Molecule 5: Histone H4

Chain F:



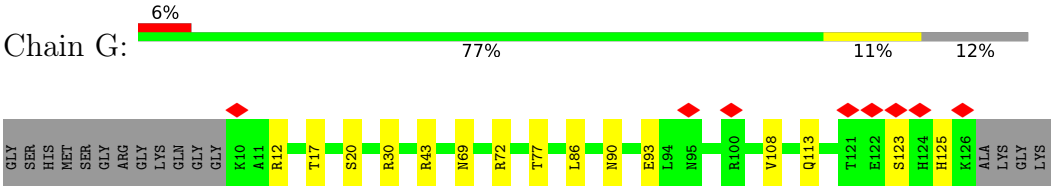
• Molecule 6: Histone H2A type 1-B/E

Chain C:



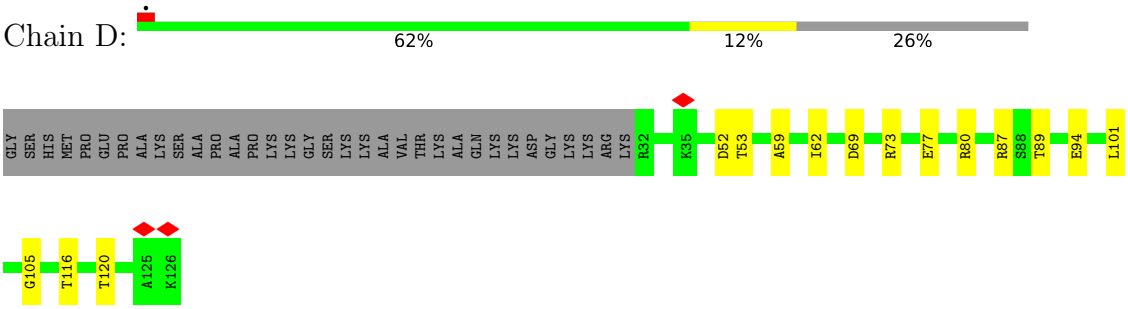
• Molecule 6: Histone H2A type 1-B/E

Chain G:



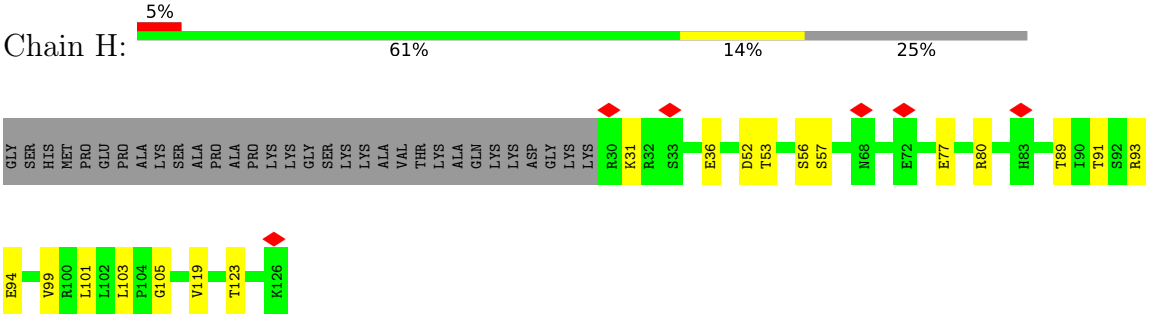
• Molecule 7: Histone H2B type 1-J

Chain D:



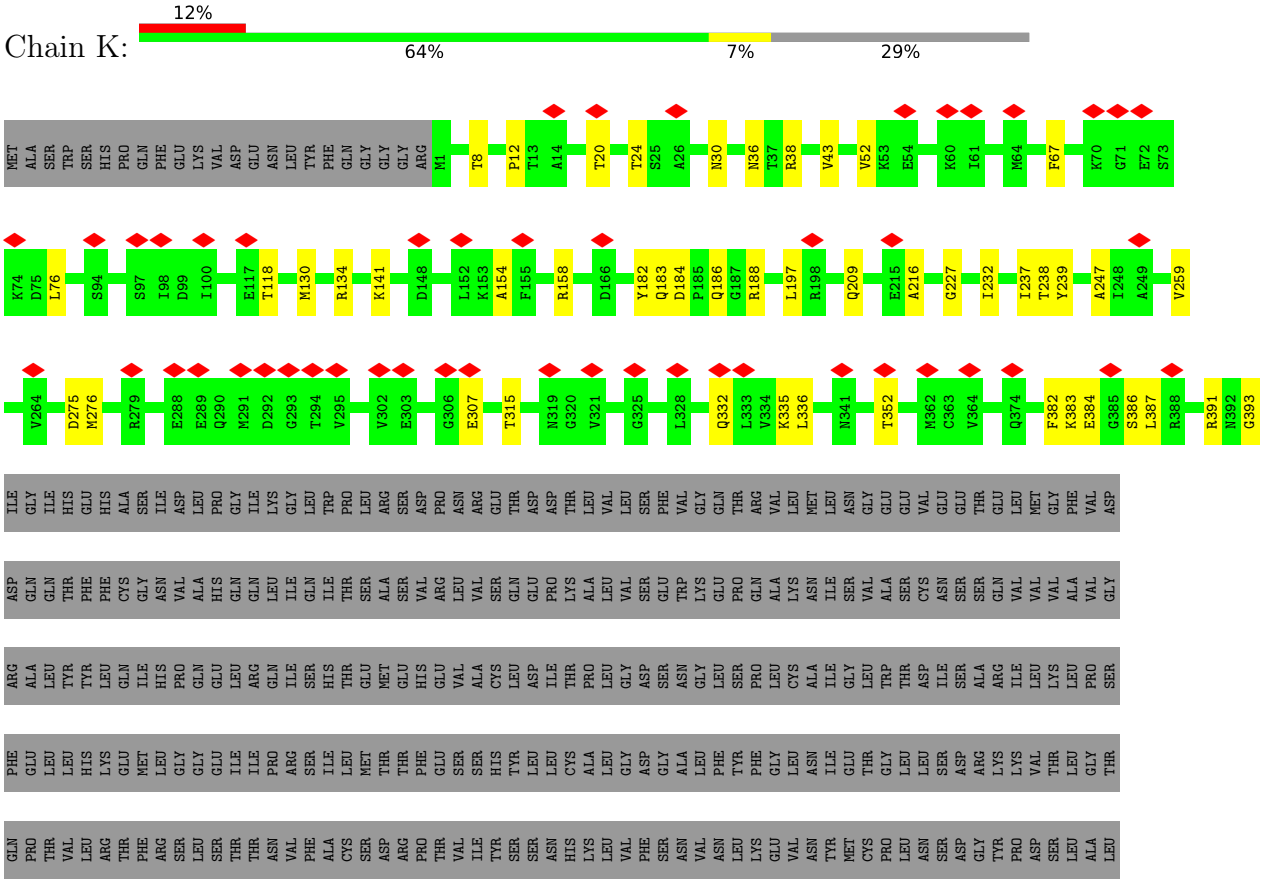
• Molecule 7: Histone H2B type 1-J

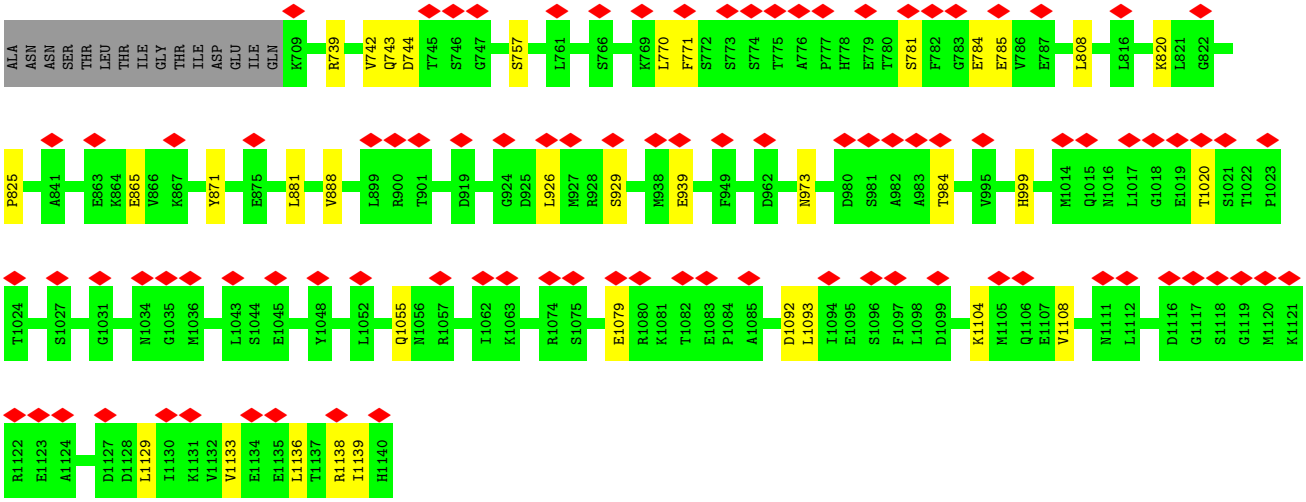
Chain H:



• Molecule 8: DNA damage-binding protein 1,DNA damage-binding protein 1

Chain K:




ALA ASN ASN SER THR LEU THR ILE GLY THR ILE ASP GLU ILE GLN K709 R739 V742 Q743 D744 T745 S746 G747 S757 L761 S766 K769 L770 F771 S772 S773 S774 T775 A776 P777 H778 E779 T780 S781 F782 G783 E784 E785 V786 E787 L808 L816 K820 L821 G822
P825 A841 E863 K864 E865 V866 K867 Y871 E875 L881 V888 L899 R900 T901 D919 G924 D925 L926 M927 R928 S929 M938 E939 F949 D962 N973 D980 S981 A982 A983 T984 V995 H999 M1014 Q1015 N1016 L1017 G1018 E1019 T1020 S1021 T1022 P1023
T1024 S1027 G1031 N1034 G1035 M1036 L1043 S1044 E1045 Y1048 L1052 Q1055 N1056 R1057 I1062 K1063 R1074 S1075 E1079 R1080 K1081 T1082 E1083 P1084 A1085 D1092 L1093 I1094 E1095 S1096 F1097 L1098 D1099 K1104 M1105 Q1106 E1107 V1108 N1111 L1112 D1116 G1117 S1118 G1119 M1120 K1121
R1122 E1123 A1124 D1127 D1128 L1129 I1130 K1131 V1132 V1133 E1134 E1135 L1136 T1137 R1138 I1139 H1140

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48925	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 ($e^-/Å^2$)	40	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	0.049	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0067	Depositor
Map size (Å)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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	I	1.04	1/3331 (0.0%)	1.15	7/5140 (0.1%)
2	J	1.04	1/3281 (0.0%)	1.15	7/5059 (0.1%)
3	L	0.40	0/2935	0.62	2/3991 (0.1%)
4	A	0.47	0/819	0.80	1/1097 (0.1%)
4	E	0.47	0/819	0.80	0/1097
5	B	0.49	0/660	0.82	0/883
5	F	0.49	0/660	0.82	0/883
6	C	0.44	0/921	0.90	4/1239 (0.3%)
6	G	0.42	0/921	0.75	0/1239
7	D	0.49	0/757	0.70	0/1015
7	H	0.45	0/777	0.74	1/1040 (0.1%)
8	K	0.39	0/6595	0.71	3/8919 (0.0%)
All	All	0.67	2/22476 (0.0%)	0.89	25/31602 (0.1%)

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
6	C	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	29	DA	C3'-O3'	-5.86	1.36	1.44
2	J	78	DC	C3'-O3'	-5.57	1.36	1.44

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	116	LEU	CA-CB-CG	10.36	139.13	115.30
3	L	63	LEU	CB-CG-CD2	7.75	124.17	111.00
1	I	95	DT	O4'-C1'-N1	6.07	112.25	108.00
6	C	122	GLU	CB-CA-C	5.96	122.32	110.40
2	J	119	DT	O4'-C1'-N1	5.71	112.00	108.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	126	LYS	CA

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	I	2970	1641	1641	15	0
2	J	2948	1633	1633	18	0
3	L	2854	2788	2805	54	0
4	A	807	838	844	17	0
4	E	807	839	844	12	0
5	B	653	694	696	7	0
5	F	653	695	696	6	0
6	C	909	968	973	6	0
6	G	909	969	973	12	0
7	D	746	761	771	9	0
7	H	766	789	797	11	0
8	K	6478	6420	6445	44	0
All	All	21500	19035	19118	170	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 170 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:J:95:DT:OP2	3:L:244:LYS:NZ	2.14	0.80
8:K:12:PRO:O	8:K:38:ARG:NH1	2.15	0.79
1:I:3:DC:H42	2:J:143:DG:H22	1.30	0.79
3:L:113:ARG:O	3:L:132:LYS:N	2.17	0.78
1:I:3:DC:N4	2:J:143:DG:H22	1.84	0.75

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	
3	L	361/450 (80%)	306 (85%)	54 (15%)	1 (0%)	41	76
4	A	96/139 (69%)	95 (99%)	1 (1%)	0	100	100
4	E	96/139 (69%)	95 (99%)	1 (1%)	0	100	100
5	B	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
5	F	80/106 (76%)	78 (98%)	2 (2%)	0	100	100
6	C	115/133 (86%)	109 (95%)	6 (5%)	0	100	100
6	G	115/133 (86%)	107 (93%)	8 (7%)	0	100	100
7	D	93/129 (72%)	88 (95%)	4 (4%)	1 (1%)	14	51
7	H	95/129 (74%)	92 (97%)	2 (2%)	1 (1%)	14	51
8	K	821/1163 (71%)	800 (97%)	17 (2%)	4 (0%)	29	68
All	All	1952/2627 (74%)	1848 (95%)	97 (5%)	7 (0%)	38	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	K	382	PHE
8	K	929	SER
8	K	1020	THR

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Mol	Chain	Res	Type
7	D	105	GLY
7	H	105	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	312/390 (80%)	312 (100%)	0	100	100
4	A	85/113 (75%)	82 (96%)	3 (4%)	36	60
4	E	85/113 (75%)	82 (96%)	3 (4%)	36	60
5	B	67/81 (83%)	66 (98%)	1 (2%)	65	80
5	F	67/81 (83%)	66 (98%)	1 (2%)	65	80
6	C	93/102 (91%)	93 (100%)	0	100	100
6	G	93/102 (91%)	93 (100%)	0	100	100
7	D	81/107 (76%)	81 (100%)	0	100	100
7	H	83/107 (78%)	82 (99%)	1 (1%)	71	84
8	K	720/1018 (71%)	720 (100%)	0	100	100
All	All	1686/2214 (76%)	1677 (100%)	9 (0%)	89	93

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	24	ARG
7	H	31	LYS
5	B	24	ARG
4	E	102	VAL
4	E	106	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
8	K	93	GLN

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Mol	Chain	Res	Type
8	K	319	ASN
8	K	970	ASN
6	C	32	HIS
7	D	68	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	3DR	J	94	2	8,11,12	0.35	0	9,14,17	0.58	0
2	3DR	J	93	2	8,11,12	0.11	0	9,14,17	0.35	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
2	3DR	J	94	2	-	0/3/15/16	0/1/1/1
2	3DR	J	93	2	-	0/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	94	3DR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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.

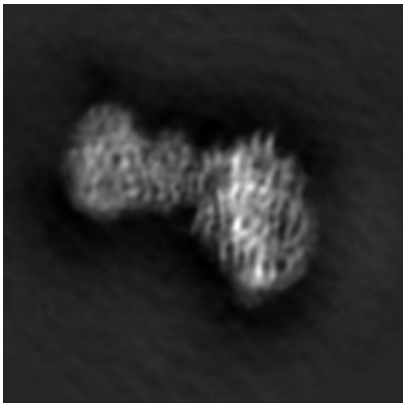
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4766. These allow visual inspection of the internal detail of the map and identification of artifacts.

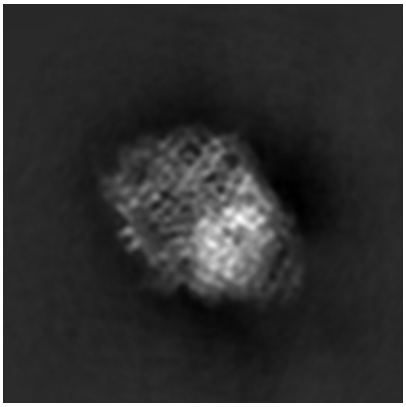
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

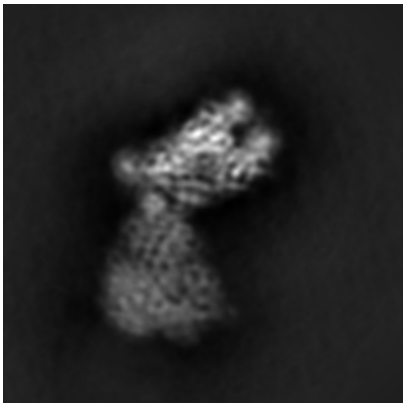
6.1.1 Primary map



X



Y

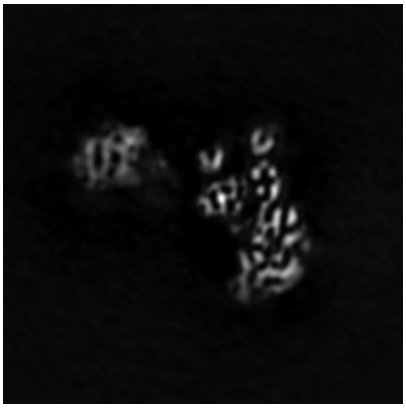


Z

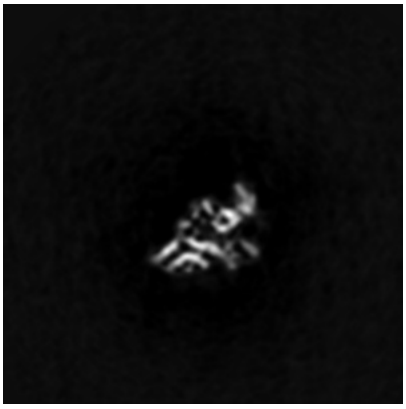
The images above show the map projected in three orthogonal directions.

6.2 Central slices

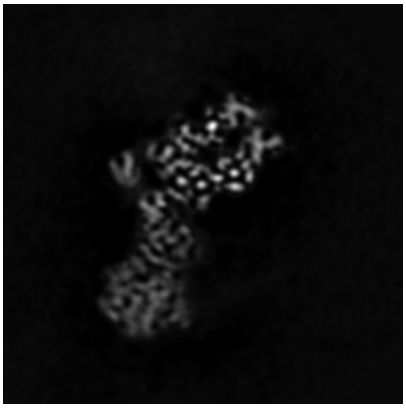
6.2.1 Primary map



X Index: 150



Y Index: 150

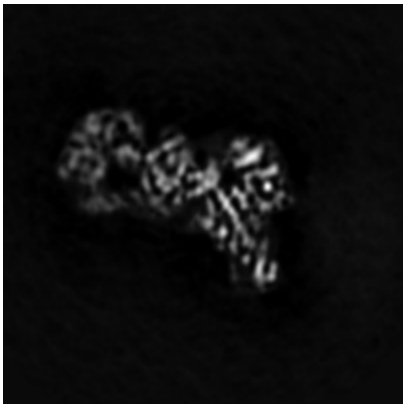


Z Index: 150

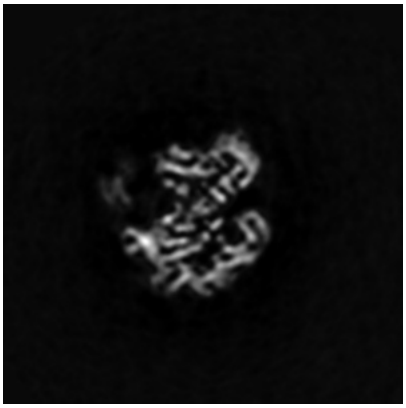
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

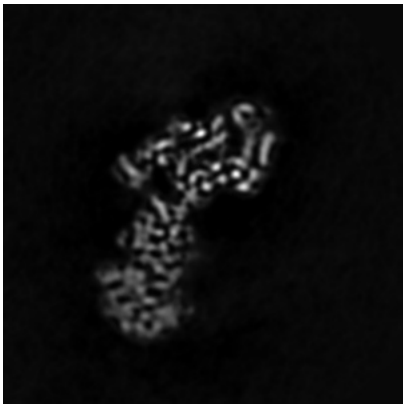
6.3.1 Primary map



X Index: 133



Y Index: 175

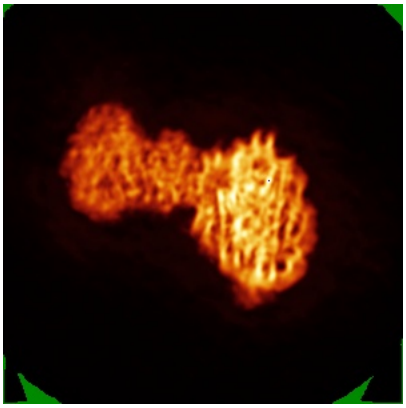


Z Index: 157

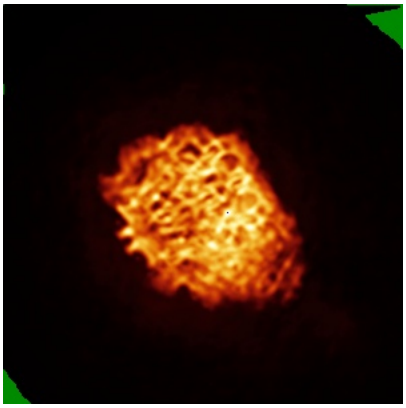
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

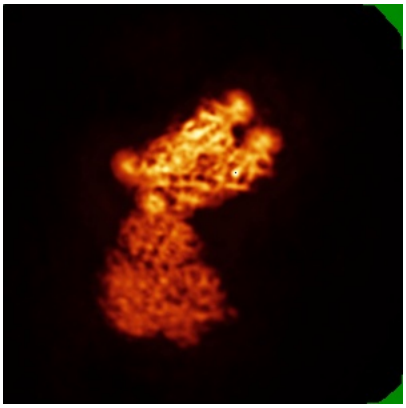
6.4.1 Primary map



X



Y

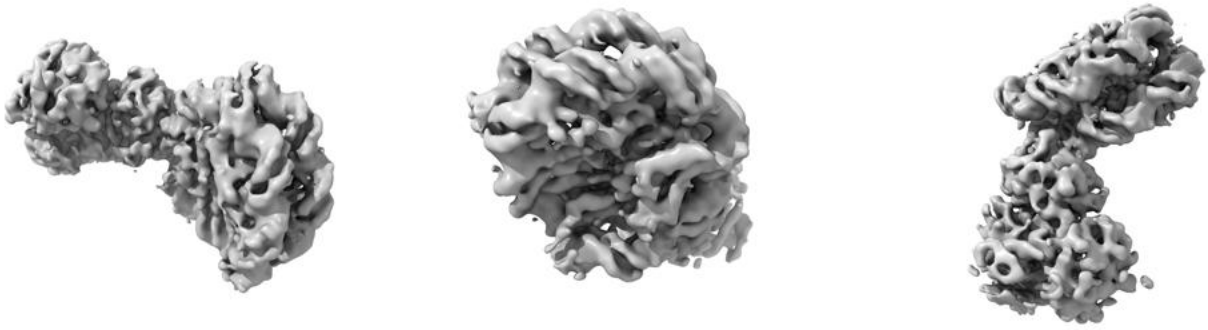


Z

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 0.0067. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

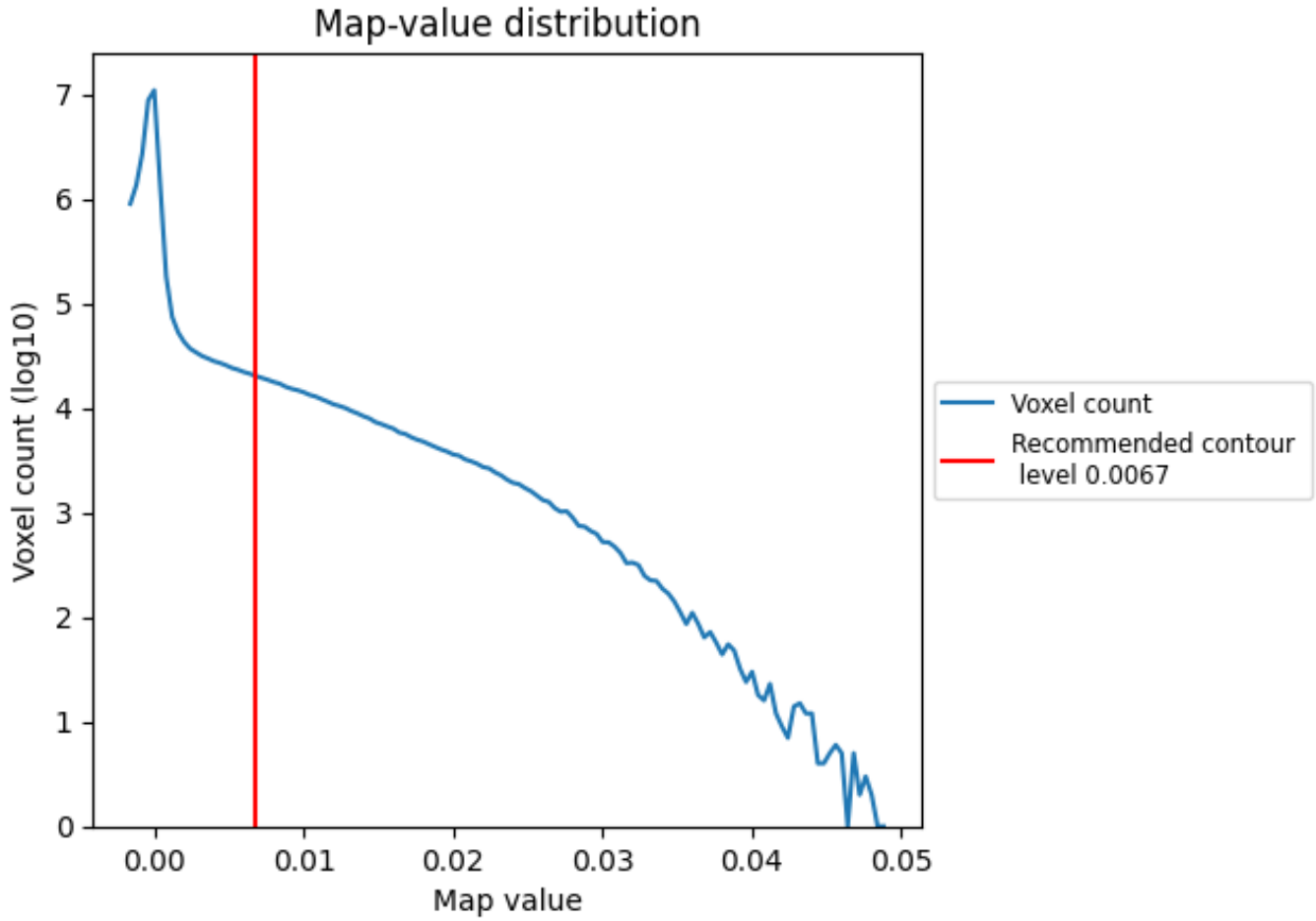
6.6 Mask visualisation (i)

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

7 Map analysis

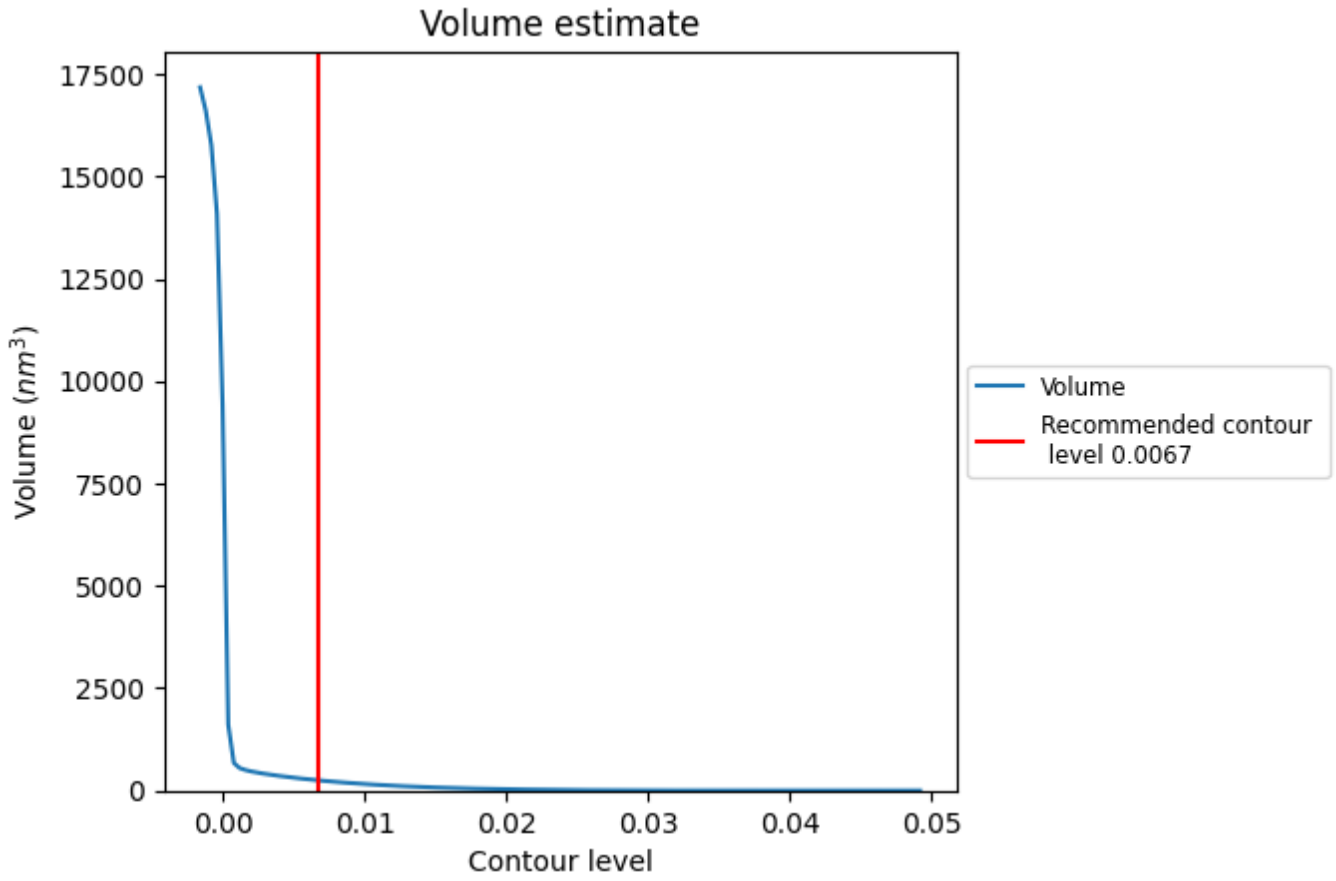
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

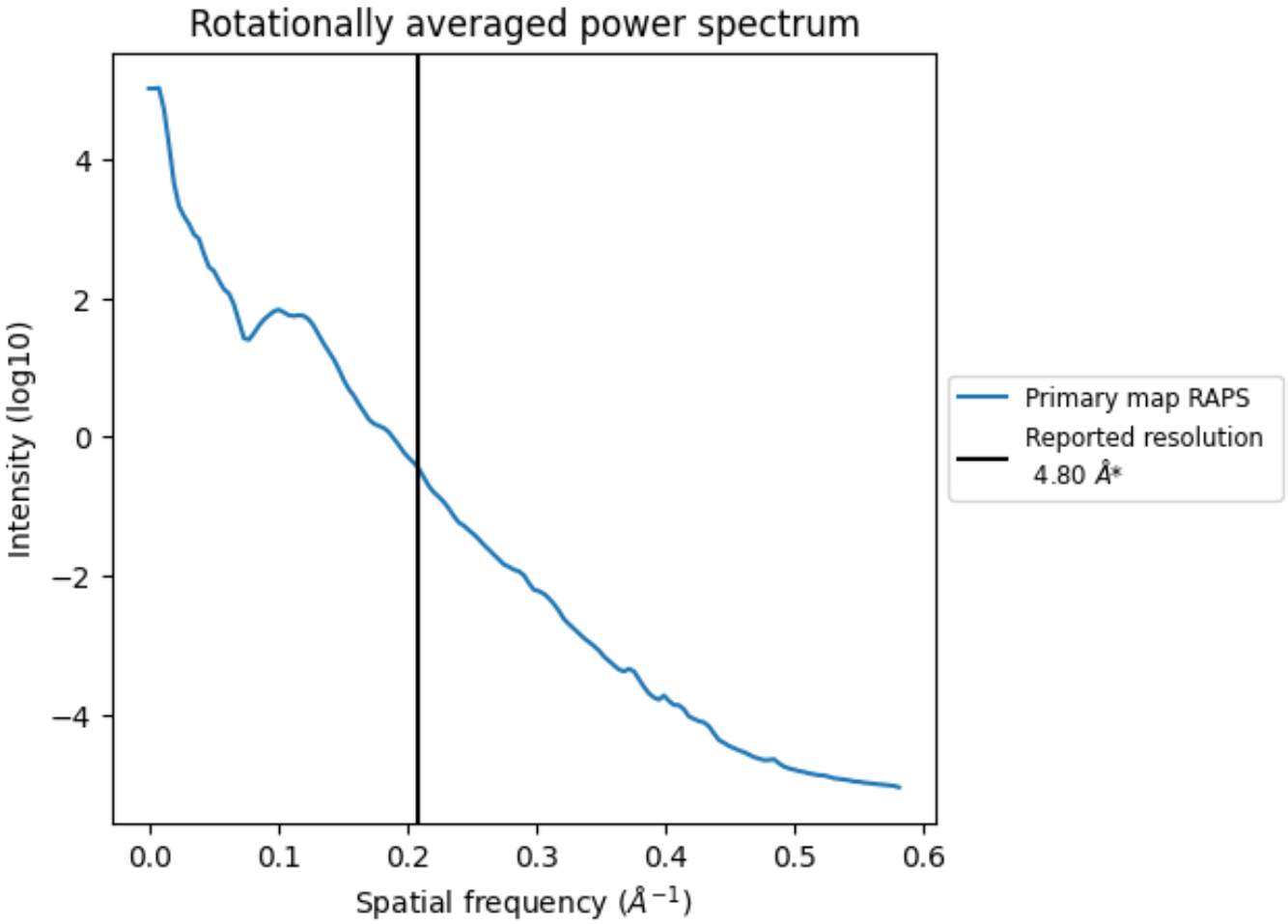
7.2 Volume estimate (i)



The volume at the recommended contour level is 252 nm^3; this corresponds to an approximate mass of 227 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 (i)



*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

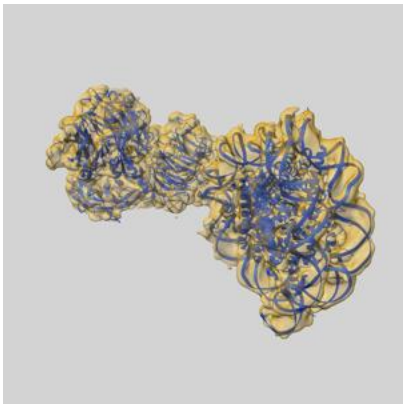
8 Fourier-Shell correlation (i)

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

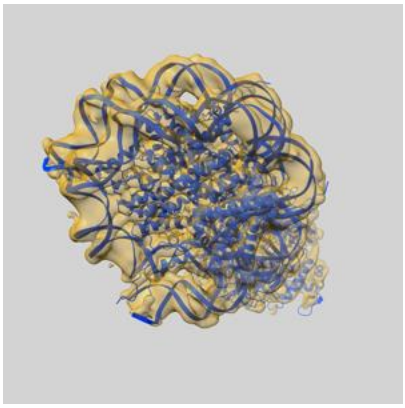
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4766 and PDB model 6R92. Per-residue inclusion information can be found in section 3 on page 16.

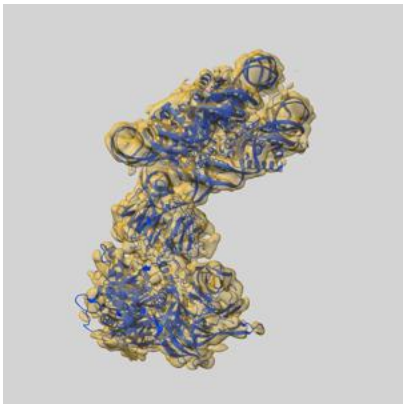
9.1 Map-model overlay



X



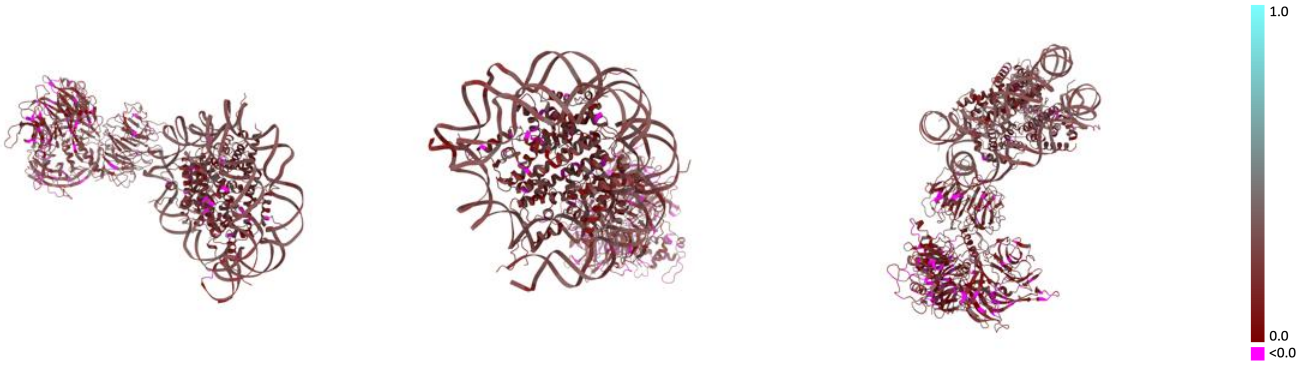
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0067 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.

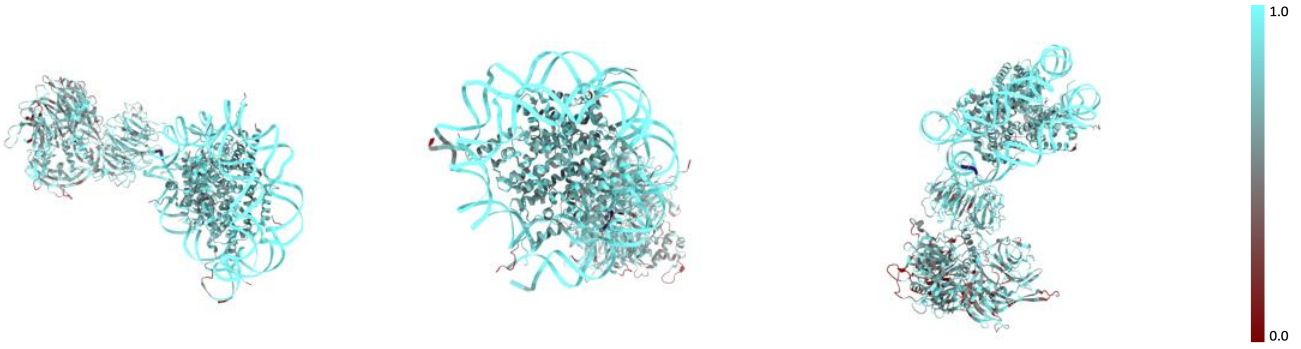
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

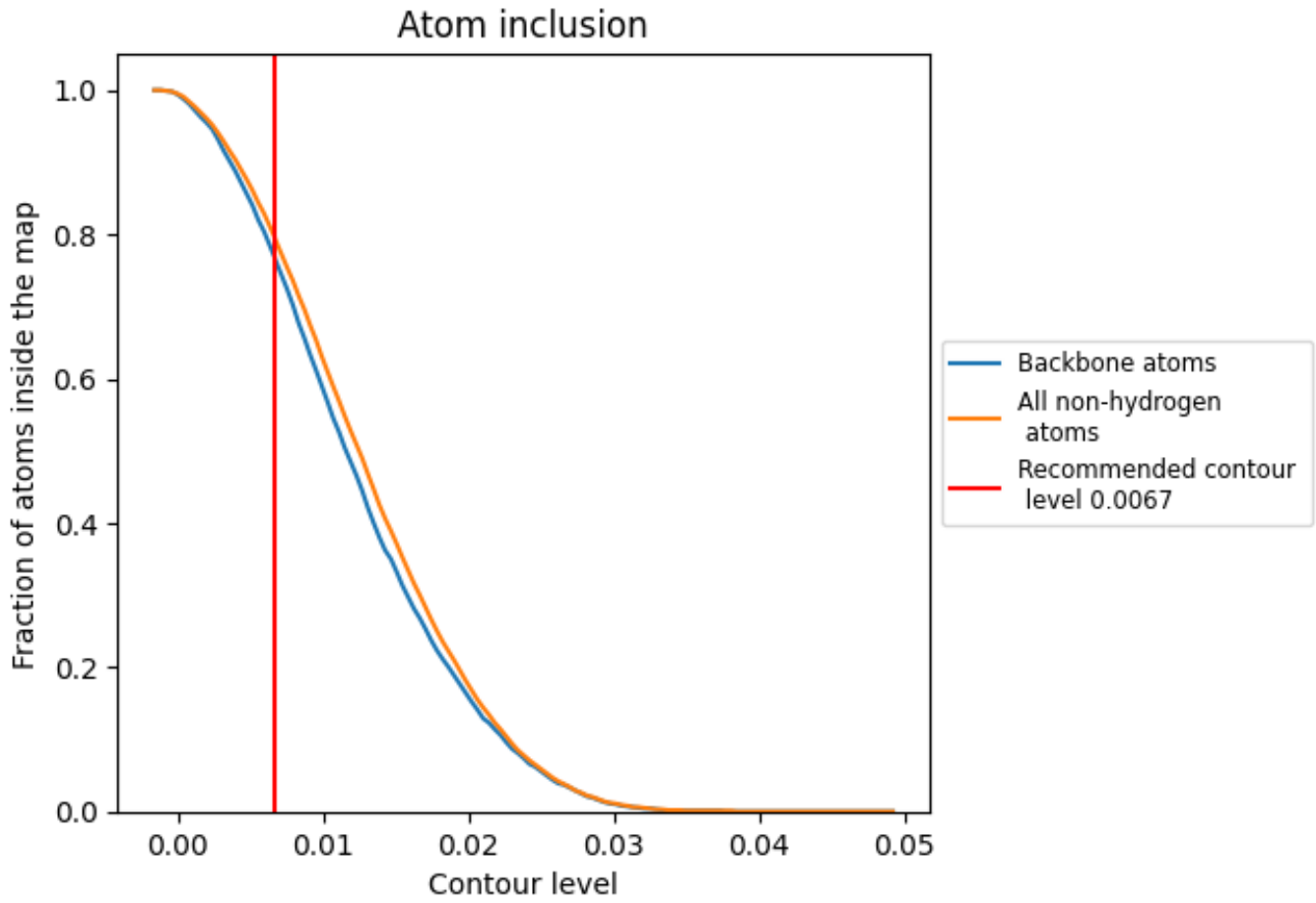
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0067).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 80% 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 (0.0067) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7950	0.2200
A	0.7560	0.2100
B	0.7720	0.2310
C	0.7450	0.2020
D	0.7770	0.2290
E	0.7680	0.1930
F	0.7700	0.2140
G	0.7290	0.2220
H	0.7580	0.2070
I	0.9630	0.2900
J	0.9600	0.2950
K	0.6530	0.1570
L	0.7860	0.2310