



## Full wwPDB EM Validation Report ⓘ

Nov 14, 2022 – 01:57 PM EST

PDB ID : 6X0N  
EMDB ID : EMD-21980  
Title : Bridging of double-strand DNA break activates PARP2/HPF1 to modify chromatin  
Authors : Halic, M.; Bilokapic, S.  
Deposited on : 2020-05-16  
Resolution : 10.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

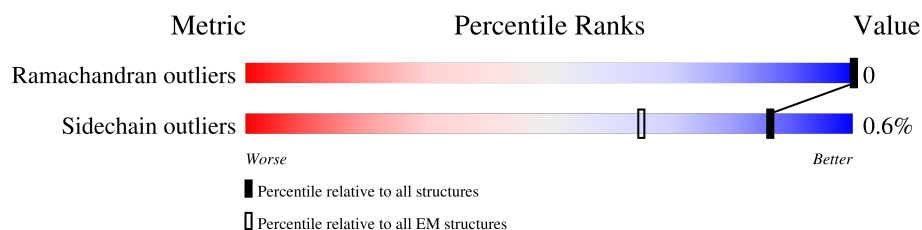
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 10.00 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.







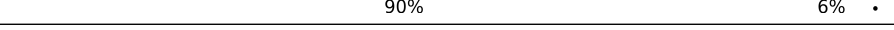
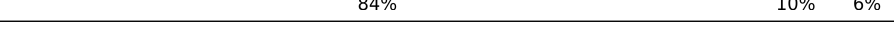
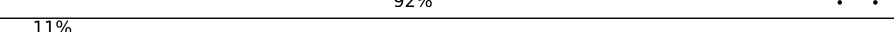
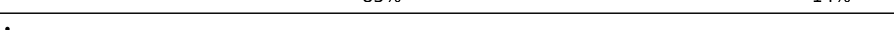
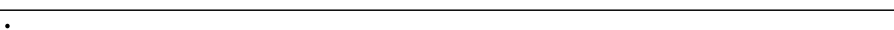
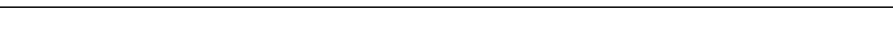
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	73% 27%
1	E	135	73% 27%
1	a	135	11% 71% 29%
1	e	135	17% 70% 30%
2	B	102	78% 21%
2	F	102	78% 21%
2	b	102	21% 76% 24%
2	f	102	14% 75% 24%
3	C	129	84% 15%

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Mol	Chain	Length	Quality of chain
3	G	129	 85%15%
3	c	129	 78%21%
3	g	129	 82%18%
4	D	122	 80%20%
4	H	122	 80%20%
4	d	122	 75%25%
4	h	122	 75%25%
5	I	167	 78%16%6%
5	i	167	 90%6%
6	J	167	 84%10%6%
6	j	167	 92%
7	O	356	 11%85%14%
8	P	590	 80%20%
8	R	590	 19%81%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 32248 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 H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	98	Total	C	N	O	S	0	0
			811	512	157	139	3		
1	E	98	Total	C	N	O	S	0	0
			811	512	157	139	3		
1	a	96	Total	C	N	O	S	0	0
			791	500	151	137	3		
1	e	95	Total	C	N	O	S	0	0
			784	495	150	136	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	GLY	variant	UNP P84233
E	102	ALA	GLY	variant	UNP P84233
a	102	ALA	GLY	variant	UNP P84233
e	102	ALA	GLY	variant	UNP P84233

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			648	410	126	111	1		
2	F	81	Total	C	N	O	S	0	0
			648	410	126	111	1		
2	b	78	Total	C	N	O	S	0	0
			622	393	120	108	1		
2	f	78	Total	C	N	O	S	0	0
			622	393	120	108	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	110	Total	C	N	O	0	0
			850	535	168	147		
3	G	110	Total	C	N	O	0	0
			850	535	168	147		
3	c	102	Total	C	N	O	0	0
			786	495	153	138		
3	g	106	Total	C	N	O	0	0
			818	514	162	142		

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	98	Total	C	N	O	S	0	0
			776	487	144	143	2		
4	H	98	Total	C	N	O	S	0	0
			776	487	144	143	2		
4	d	92	Total	C	N	O	S	0	0
			721	454	129	136	2		
4	h	92	Total	C	N	O	S	0	0
			721	454	129	136	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	variant	UNP P02281
H	29	THR	SER	variant	UNP P02281
d	29	THR	SER	variant	UNP P02281
h	29	THR	SER	variant	UNP P02281

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	157	Total	C	N	O	P	0	0
			3234	1531	608	938	157		
5	i	160	Total	C	N	O	P	0	0
			3299	1561	620	958	160		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	157	Total	C	N	O	P	0	0
			3203	1522	578	946	157		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	160	Total	C	N	O	P	0	0
			3262	1549	590	963	160		

- Molecule 7 is a protein called Histone PARylation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	306	Total	C	N	O	S	0	0
			2488	1597	415	465	11		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-9	MET	-	initiating methionine	UNP Q9NWX4
O	-8	GLY	-	expression tag	UNP Q9NWX4
O	-7	HIS	-	expression tag	UNP Q9NWX4
O	-6	HIS	-	expression tag	UNP Q9NWX4
O	-5	HIS	-	expression tag	UNP Q9NWX4
O	-4	HIS	-	expression tag	UNP Q9NWX4
O	-3	HIS	-	expression tag	UNP Q9NWX4
O	-2	HIS	-	expression tag	UNP Q9NWX4
O	-1	GLY	-	expression tag	UNP Q9NWX4
O	0	GLY	-	expression tag	UNP Q9NWX4
O	174	LYS	ARG	variant	UNP Q9NWX4

- Molecule 8 is a protein called Poly [ADP-ribose] polymerase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	474	Total	C	N	O	S	0	0
			3798	2413	654	704	27		
8	R	114	Total	C	N	O	S	0	0
			929	588	161	173	7		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-19	MET	-	initiating methionine	UNP Q9UGN5
P	-18	GLY	-	expression tag	UNP Q9UGN5
P	-17	SER	-	expression tag	UNP Q9UGN5
P	-16	SER	-	expression tag	UNP Q9UGN5
P	-15	HIS	-	expression tag	UNP Q9UGN5
P	-14	HIS	-	expression tag	UNP Q9UGN5
P	-13	HIS	-	expression tag	UNP Q9UGN5

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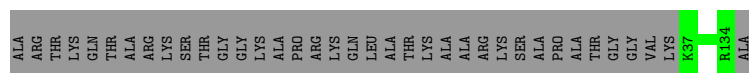
Chain	Residue	Modelled	Actual	Comment	Reference
P	-12	HIS	-	expression tag	UNP Q9UGN5
P	-11	HIS	-	expression tag	UNP Q9UGN5
P	-10	HIS	-	expression tag	UNP Q9UGN5
P	-9	SER	-	expression tag	UNP Q9UGN5
P	-8	SER	-	expression tag	UNP Q9UGN5
P	-7	GLY	-	expression tag	UNP Q9UGN5
P	-6	LEU	-	expression tag	UNP Q9UGN5
P	-5	VAL	-	expression tag	UNP Q9UGN5
P	-4	PRO	-	expression tag	UNP Q9UGN5
P	-3	ARG	-	expression tag	UNP Q9UGN5
P	-2	GLY	-	expression tag	UNP Q9UGN5
P	-1	SER	-	expression tag	UNP Q9UGN5
P	0	HIS	-	expression tag	UNP Q9UGN5
R	-19	MET	-	initiating methionine	UNP Q9UGN5
R	-18	GLY	-	expression tag	UNP Q9UGN5
R	-17	SER	-	expression tag	UNP Q9UGN5
R	-16	SER	-	expression tag	UNP Q9UGN5
R	-15	HIS	-	expression tag	UNP Q9UGN5
R	-14	HIS	-	expression tag	UNP Q9UGN5
R	-13	HIS	-	expression tag	UNP Q9UGN5
R	-12	HIS	-	expression tag	UNP Q9UGN5
R	-11	HIS	-	expression tag	UNP Q9UGN5
R	-10	HIS	-	expression tag	UNP Q9UGN5
R	-9	SER	-	expression tag	UNP Q9UGN5
R	-8	SER	-	expression tag	UNP Q9UGN5
R	-7	GLY	-	expression tag	UNP Q9UGN5
R	-6	LEU	-	expression tag	UNP Q9UGN5
R	-5	VAL	-	expression tag	UNP Q9UGN5
R	-4	PRO	-	expression tag	UNP Q9UGN5
R	-3	ARG	-	expression tag	UNP Q9UGN5
R	-2	GLY	-	expression tag	UNP Q9UGN5
R	-1	SER	-	expression tag	UNP Q9UGN5
R	0	HIS	-	expression tag	UNP Q9UGN5

### 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.

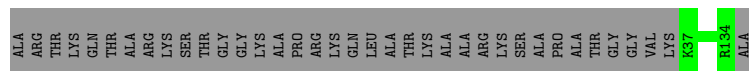
- Molecule 1: Histone H3.2

Chain A:  73% 27%



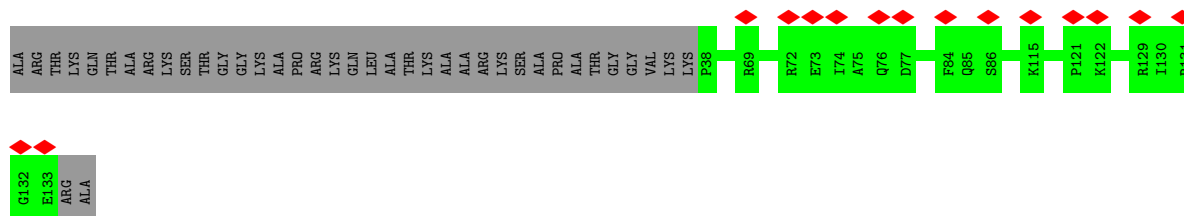
- Molecule 1: Histone H3.2

Chain E:  73% 27%



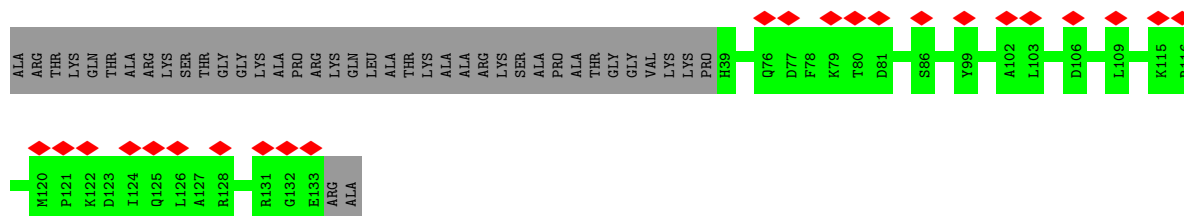
- Molecule 1: Histone H3.2

Chain a:  11% 71% 29%




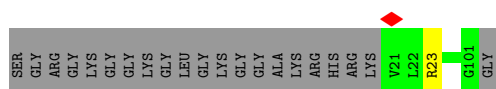
- Molecule 1: Histone H3.2

Chain e:  17% 70% 30%




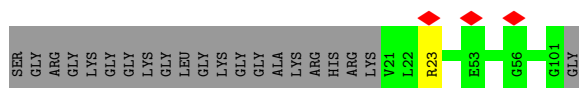
- Molecule 2: Histone H4

Chain B:  78% 21%




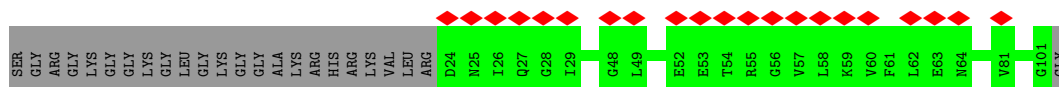
- Molecule 2: Histone H4

Chain F:  78% 21%




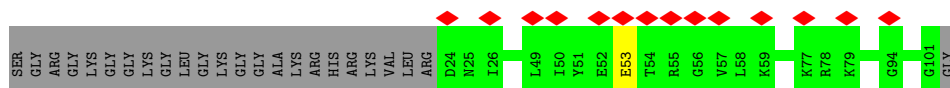
- Molecule 2: Histone H4

Chain b:  21% 76% 24%




- Molecule 2: Histone H4

Chain f:  14% 75% 24%



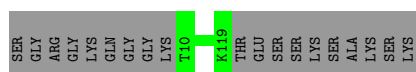
- Molecule 3: Histone H2A

Chain C:  84% 15%




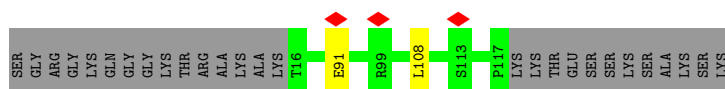
- Molecule 3: Histone H2A

Chain G:  85% 15%

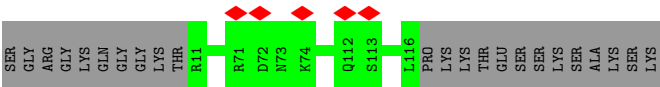
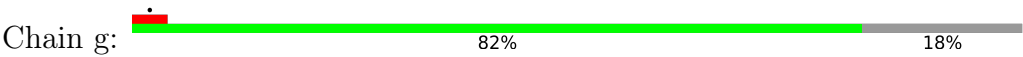


- Molecule 3: Histone H2A

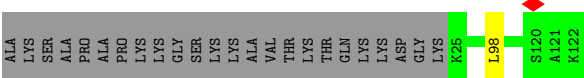
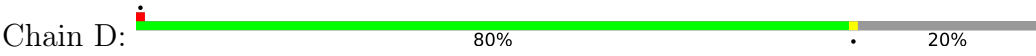
Chain c:  78% 21%



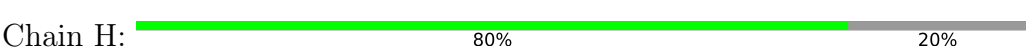
- Molecule 3: Histone H2A



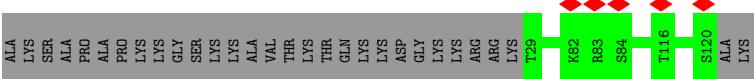
• Molecule 4: Histone H2B 1.1



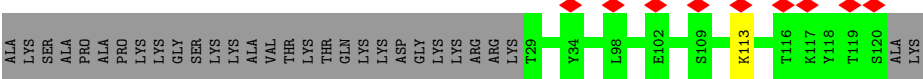
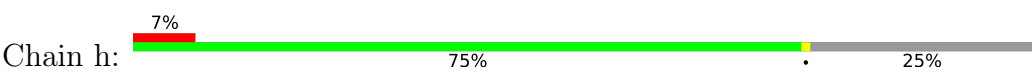
• Molecule 4: Histone H2B 1.1



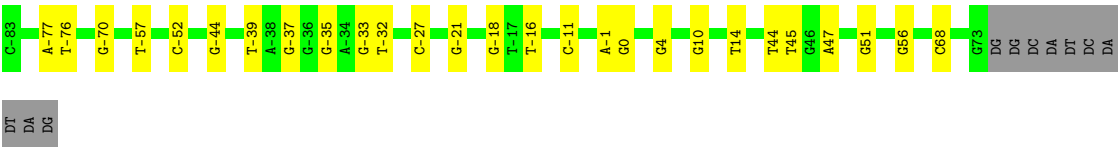
• Molecule 4: Histone H2B 1.1



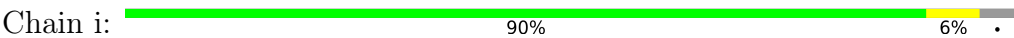
• Molecule 4: Histone H2B 1.1



• Molecule 5: DNA (167-MER)

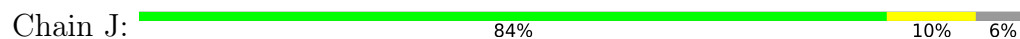


• Molecule 5: DNA (167-MER)





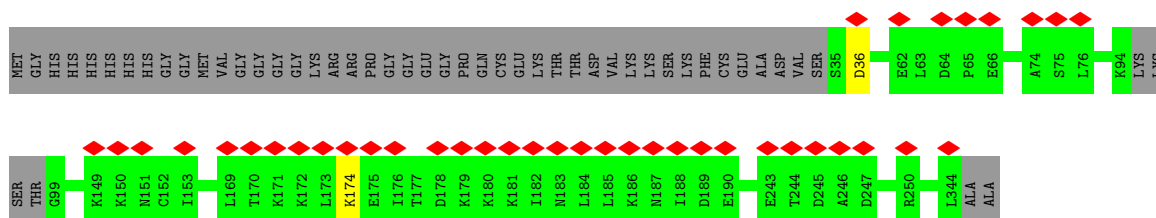
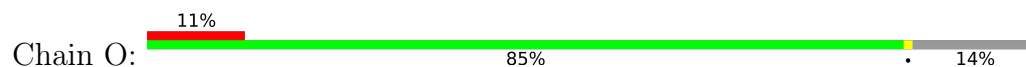
- Molecule 6: DNA (167-MER)



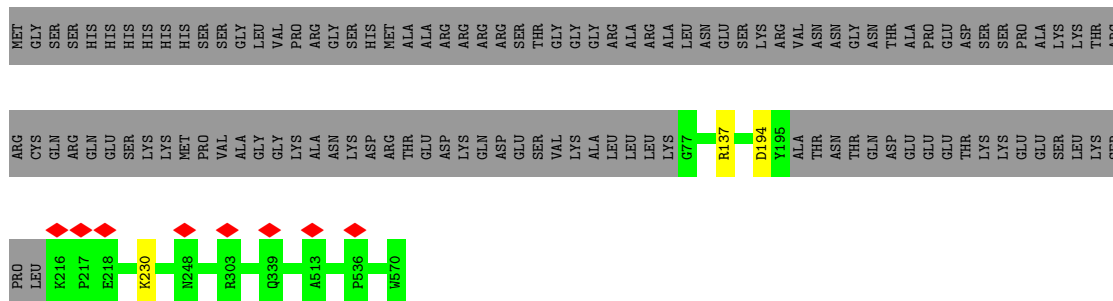
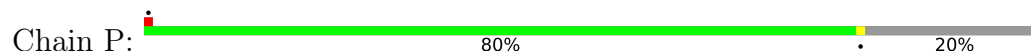
- Molecule 6: DNA (167-MER)



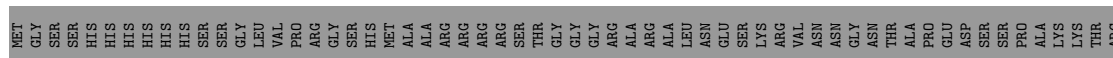
- Molecule 7: Histone PARylation factor 1



- Molecule 8: Poly [ADP-ribose] polymerase 2



- Molecule 8: Poly [ADP-ribose] polymerase 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17000	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 ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	508.8, 508.8, 508.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.35	0/823	0.52	0/1104
1	E	0.36	0/823	0.51	0/1104
1	a	0.34	0/803	0.52	0/1078
1	e	0.32	0/795	0.50	0/1067
2	B	0.31	0/655	0.51	0/878
2	F	0.34	0/655	0.56	0/878
2	b	0.31	0/629	0.52	0/843
2	f	0.36	0/629	0.52	0/843
3	C	0.38	0/860	0.55	0/1159
3	G	0.37	0/860	0.54	0/1159
3	c	0.30	0/796	0.49	0/1077
3	g	0.29	0/827	0.51	0/1115
4	D	0.38	1/787 (0.1%)	0.49	0/1054
4	H	0.37	0/787	0.51	0/1054
4	d	0.28	0/732	0.42	0/986
4	h	0.30	0/732	0.47	0/986
5	I	1.17	22/3632 (0.6%)	1.08	5/5607 (0.1%)
5	i	0.85	6/3705 (0.2%)	1.03	4/5721 (0.1%)
6	J	1.12	12/3588 (0.3%)	1.07	4/5532 (0.1%)
6	j	0.87	6/3654 (0.2%)	1.03	1/5631 (0.0%)
7	O	0.31	0/2543	0.51	1/3428 (0.0%)
8	P	0.30	0/3881	0.53	1/5235 (0.0%)
8	R	0.29	0/949	0.51	0/1277
All	All	0.71	47/34145 (0.1%)	0.81	16/48816 (0.0%)

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	j	-83	DC	OP3-P	-11.26	1.47	1.61
5	I	10	DG	C3'-O3'	-7.82	1.33	1.44
6	J	-44	DA	C3'-O3'	-7.44	1.34	1.44
6	J	46	DA	C3'-O3'	-6.61	1.35	1.44
6	J	10	DC	C3'-O3'	-6.61	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	-52	DC	C3'-O3'	-6.31	1.35	1.44
5	i	80	DA	C1'-N9	-6.26	1.38	1.47
6	J	-27	DC	C3'-O3'	-6.07	1.36	1.44
5	I	-44	DG	C3'-O3'	-5.95	1.36	1.44
6	J	56	DC	C3'-O3'	-5.95	1.36	1.44
5	I	-27	DC	C3'-O3'	-5.88	1.36	1.44
4	D	98	LEU	C-N	-5.87	1.20	1.34
5	i	10	DG	C3'-O3'	-5.87	1.36	1.44
5	I	51	DG	C3'-O3'	-5.83	1.36	1.44
5	I	-39	DT	N1-C2	-5.83	1.33	1.38
6	J	-16	DT	C3'-O3'	-5.80	1.36	1.44
5	I	-37	DG	C3'-O3'	-5.80	1.36	1.44
6	j	10	DC	C3'-O3'	-5.73	1.36	1.44
5	I	-18	DG	N9-C4	-5.69	1.33	1.38
5	I	-16	DT	C3'-O3'	-5.67	1.36	1.44
5	I	-21	DG	C3'-O3'	-5.63	1.36	1.44
5	I	4	DG	C3'-O3'	-5.58	1.36	1.44
5	i	-6	DG	C3'-O3'	-5.53	1.36	1.44
5	I	-11	DC	C3'-O3'	-5.51	1.36	1.44
6	j	4	DC	C3'-O3'	-5.50	1.36	1.44
6	J	-57	DC	C3'-O3'	-5.43	1.36	1.44
6	J	36	DC	C3'-O3'	-5.43	1.36	1.44
5	i	31	DT	C3'-O3'	-5.42	1.36	1.44
5	I	68	DC	C3'-O3'	-5.39	1.36	1.44
6	J	23	DA	N9-C4	-5.37	1.34	1.37
6	J	-37	DG	C3'-O3'	-5.32	1.37	1.44
5	I	56	DG	C3'-O3'	-5.31	1.37	1.44
5	I	-57	DT	C3'-O3'	-5.28	1.37	1.44
5	i	68	DC	C3'-O3'	-5.27	1.37	1.44
5	I	-1	DA	C3'-O3'	-5.21	1.37	1.44
6	j	5	DC	C3'-O3'	-5.21	1.37	1.44
5	i	69	DT	C3'-O3'	-5.13	1.37	1.44
5	I	-76	DT	C3'-O3'	-5.11	1.37	1.44
5	I	45	DT	C3'-O3'	-5.11	1.37	1.44
5	I	0	DG	C3'-O3'	-5.11	1.37	1.44
5	I	-33	DG	C3'-O3'	-5.07	1.37	1.44
6	j	-27	DC	C3'-O3'	-5.07	1.37	1.44
5	I	44	DT	C3'-O3'	-5.06	1.37	1.44
5	I	-32	DT	C3'-O3'	-5.05	1.37	1.44
6	j	-6	DT	C3'-O3'	-5.05	1.37	1.44
6	J	-6	DT	C3'-O3'	-5.04	1.37	1.44
6	J	-67	DA	C3'-O3'	-5.02	1.37	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	j	9	DG	O4'-C1'-N9	-7.90	102.47	108.00
6	J	9	DG	O4'-C1'-N9	-6.90	103.17	108.00
5	I	-77	DA	OP2-P-O3'	6.19	118.81	105.20
6	J	27	DG	O4'-C1'-N9	6.00	112.20	108.00
5	I	-70	DG	O4'-C1'-N9	5.98	112.18	108.00
5	I	-35	DG	O4'-C1'-N9	-5.91	103.86	108.00
5	I	14	DT	O4'-C1'-N1	-5.78	103.95	108.00
6	J	-69	DA	O4'-C1'-N9	-5.74	103.99	108.00
5	I	47	DA	O4'-C1'-N9	-5.47	104.17	108.00
5	i	-72	DC	O4'-C1'-N1	5.46	111.82	108.00
5	i	-74	DC	C3'-C2'-C1'	-5.33	96.11	102.50
6	J	50	DA	O4'-C1'-N9	-5.28	104.30	108.00
8	P	194	ASP	CB-CG-OD2	5.20	122.97	118.30
7	O	36	ASP	CB-CG-OD2	5.19	122.97	118.30
5	i	71	DC	O4'-C1'-N1	5.15	111.60	108.00
5	i	-75	DG	O4'-C4'-C3'	-5.03	102.49	104.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	96/135 (71%)	93 (97%)	3 (3%)	0	100	100
1	E	96/135 (71%)	94 (98%)	2 (2%)	0	100	100
1	a	94/135 (70%)	91 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	93/135 (69%)	91 (98%)	2 (2%)	0	100	100
2	B	79/102 (78%)	79 (100%)	0	0	100	100
2	F	79/102 (78%)	79 (100%)	0	0	100	100
2	b	76/102 (74%)	76 (100%)	0	0	100	100
2	f	76/102 (74%)	76 (100%)	0	0	100	100
3	C	108/129 (84%)	103 (95%)	5 (5%)	0	100	100
3	G	108/129 (84%)	106 (98%)	2 (2%)	0	100	100
3	c	100/129 (78%)	98 (98%)	2 (2%)	0	100	100
3	g	104/129 (81%)	102 (98%)	2 (2%)	0	100	100
4	D	96/122 (79%)	93 (97%)	3 (3%)	0	100	100
4	H	96/122 (79%)	92 (96%)	4 (4%)	0	100	100
4	d	90/122 (74%)	89 (99%)	1 (1%)	0	100	100
4	h	90/122 (74%)	89 (99%)	1 (1%)	0	100	100
7	O	302/356 (85%)	292 (97%)	10 (3%)	0	100	100
8	P	470/590 (80%)	442 (94%)	28 (6%)	0	100	100
8	R	112/590 (19%)	106 (95%)	6 (5%)	0	100	100
All	All	2365/3488 (68%)	2291 (97%)	74 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	86/110 (78%)	86 (100%)	0	100	100
1	E	86/110 (78%)	86 (100%)	0	100	100
1	a	84/110 (76%)	84 (100%)	0	100	100
1	e	83/110 (76%)	83 (100%)	0	100	100
2	B	67/78 (86%)	66 (98%)	1 (2%)	65	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	67/78 (86%)	66 (98%)	1 (2%)	65	80
2	b	64/78 (82%)	64 (100%)	0	100	100
2	f	64/78 (82%)	63 (98%)	1 (2%)	62	79
3	C	87/101 (86%)	85 (98%)	2 (2%)	50	70
3	G	87/101 (86%)	87 (100%)	0	100	100
3	c	81/101 (80%)	79 (98%)	2 (2%)	47	68
3	g	83/101 (82%)	83 (100%)	0	100	100
4	D	84/102 (82%)	84 (100%)	0	100	100
4	H	84/102 (82%)	84 (100%)	0	100	100
4	d	79/102 (78%)	79 (100%)	0	100	100
4	h	79/102 (78%)	78 (99%)	1 (1%)	69	81
7	O	271/308 (88%)	270 (100%)	1 (0%)	91	94
8	P	413/511 (81%)	411 (100%)	2 (0%)	88	93
8	R	100/511 (20%)	99 (99%)	1 (1%)	76	86
All	All	2049/2894 (71%)	2037 (99%)	12 (1%)	86	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	23	ARG
3	C	99	ARG
3	C	108	LEU
2	F	23	ARG
3	c	91	GLU
3	c	108	LEU
2	f	53	GLU
4	h	113	LYS
7	O	174	LYS
8	P	137	ARG
8	P	230	LYS
8	R	91	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	108	ASN
3	C	31	HIS
3	C	104	GLN
3	C	112	GLN
4	D	44	GLN
4	D	64	ASN
4	D	92	GLN
4	D	106	HIS
1	E	108	ASN
3	G	31	HIS
3	G	73	ASN
3	G	104	GLN
4	H	106	HIS
1	a	108	ASN
2	b	25	ASN
4	d	44	GLN
4	d	106	HIS
1	e	39	HIS
1	e	68	GLN
1	e	108	ASN
2	f	93	GLN
3	g	104	GLN
3	g	112	GLN
4	h	81	ASN
4	h	106	HIS
7	O	272	GLN
7	O	311	GLN
8	P	147	HIS
8	P	267	GLN
8	P	290	ASN
8	P	343	HIS
8	P	371	GLN
8	P	381	HIS
8	P	428	HIS
8	P	519	ASN
8	P	553	GLN
8	R	108	GLN
8	R	110	ASN
8	R	122	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 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.

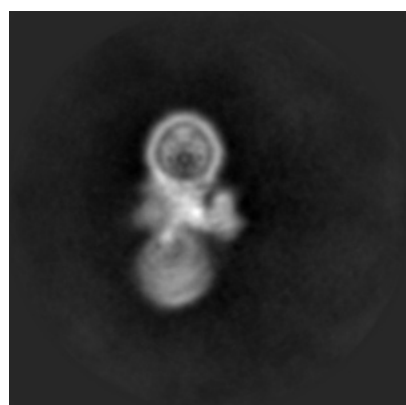
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21980. These allow visual inspection of the internal detail of the map and identification of artifacts.

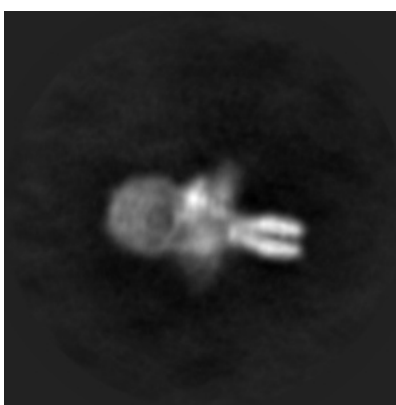
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

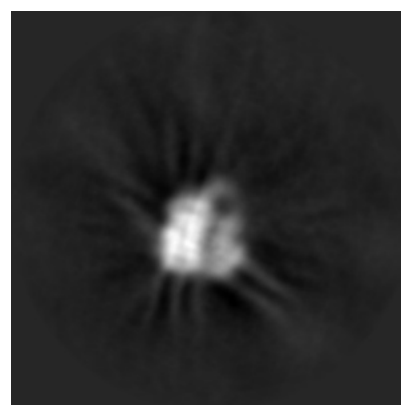
#### 6.1.1 Primary map



X



Y

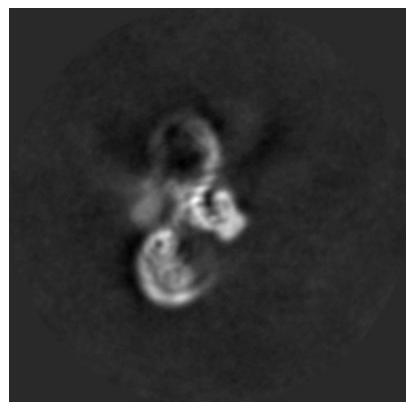


Z

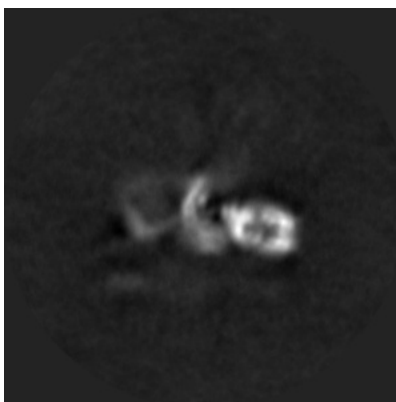
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

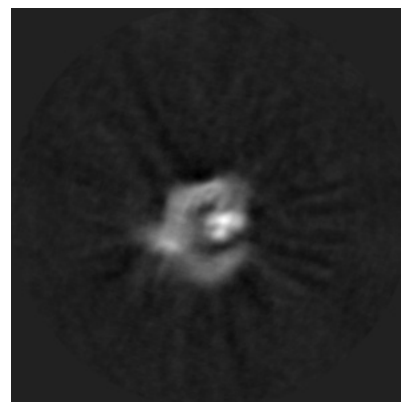
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

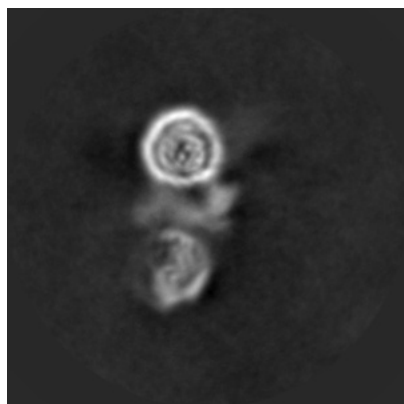


Z Index: 240

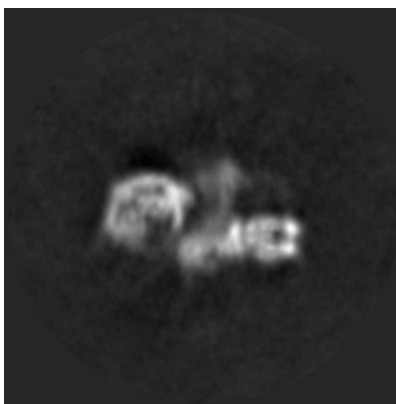
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

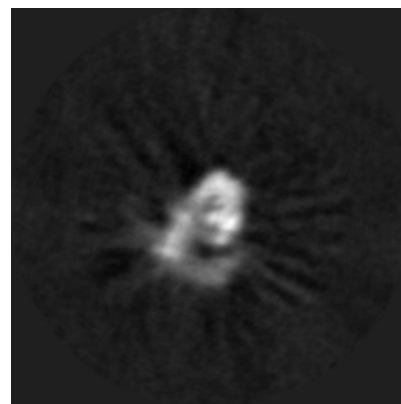
### 6.3.1 Primary map



X Index: 215



Y Index: 188



Z Index: 230

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

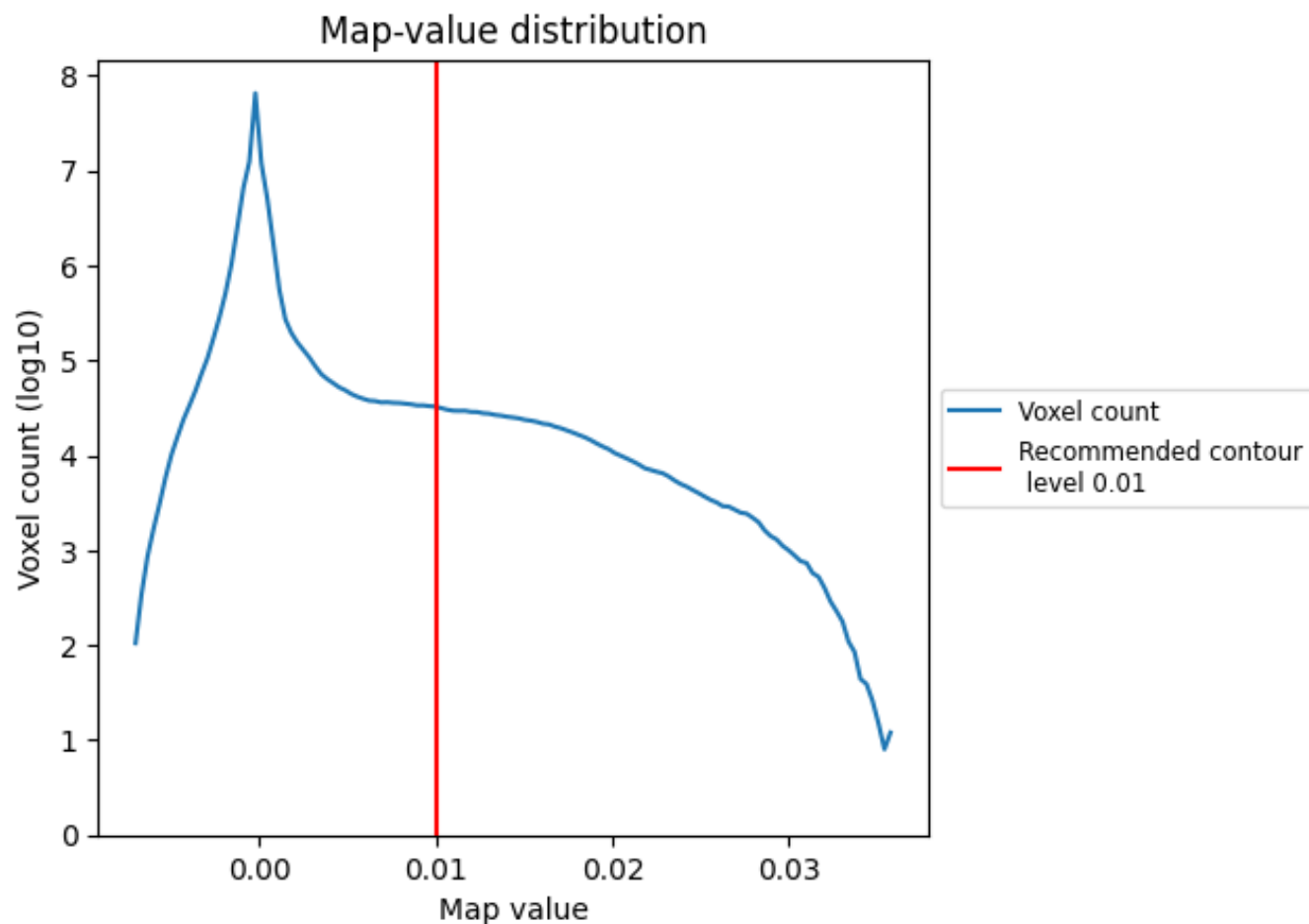
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

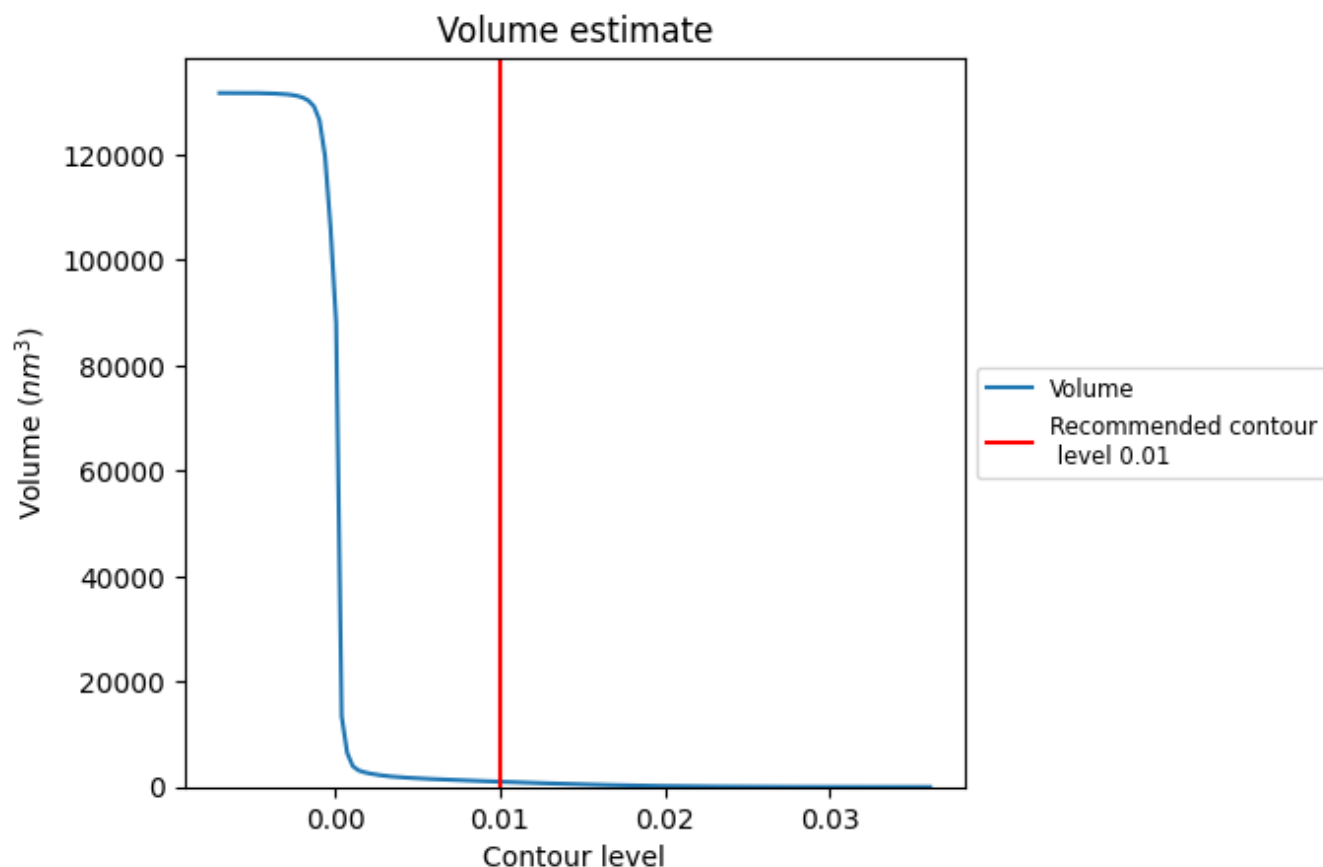
This section contains the results of statistical analysis of the map.

### 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.

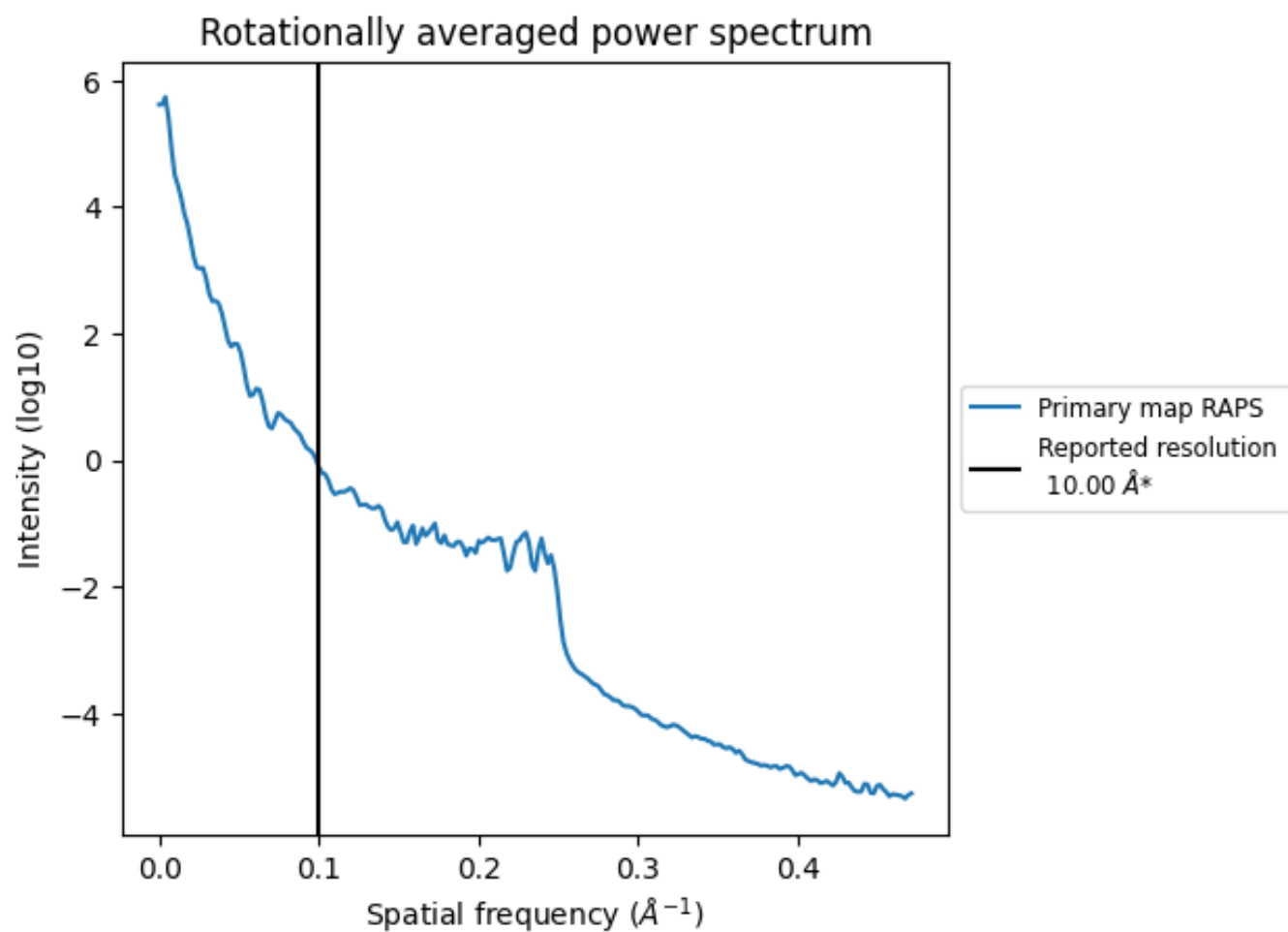
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 990  $\text{nm}^3$ ; this corresponds to an approximate mass of 894 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 0.100 Å<sup>-1</sup>

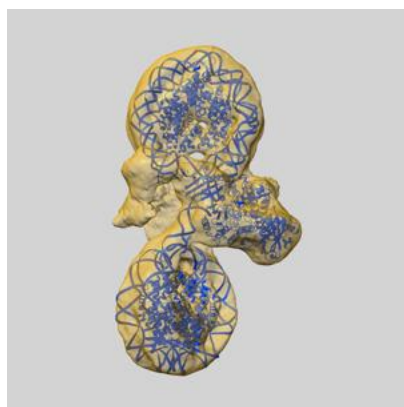
## 8 Fourier-Shell correlation ⓘ

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

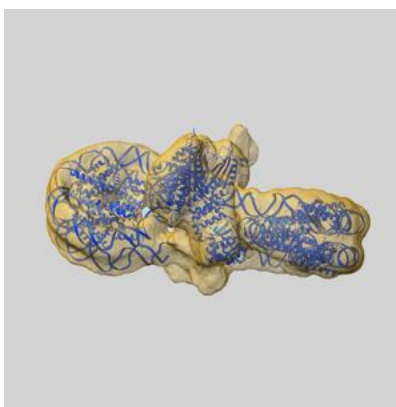
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21980 and PDB model 6X0N. Per-residue inclusion information can be found in section [3](#) on page [8](#).

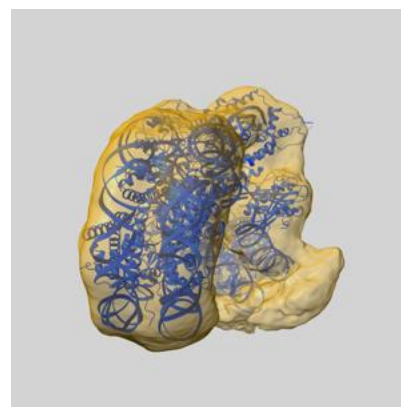
### 9.1 Map-model overlay [i](#)



X



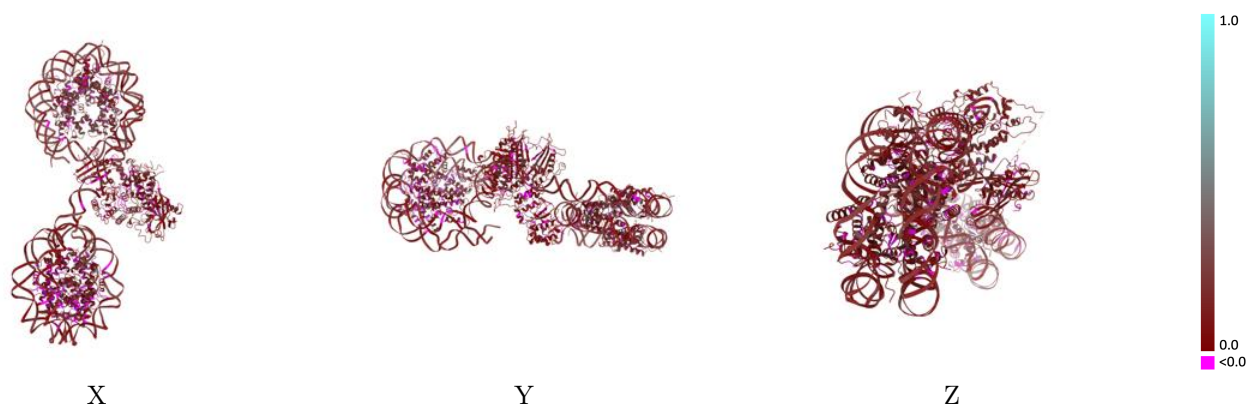
Y



Z

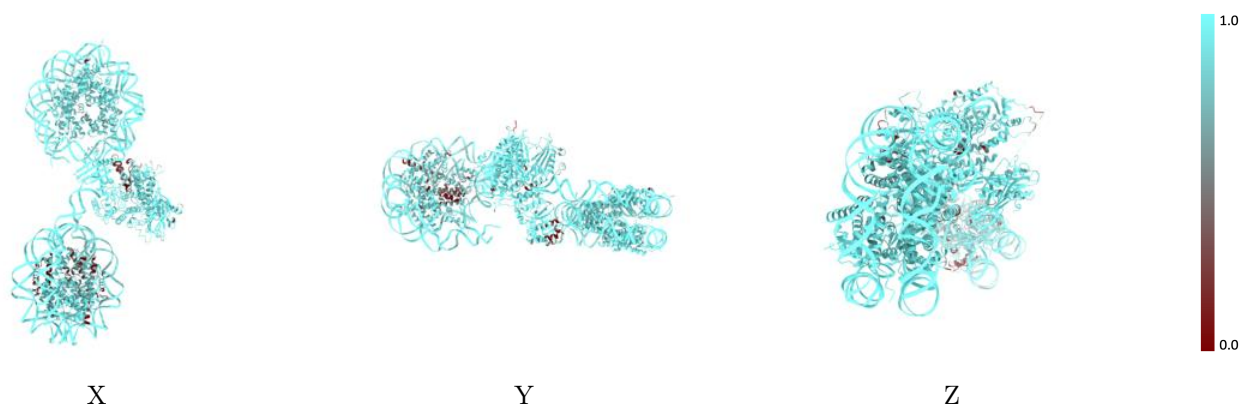
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



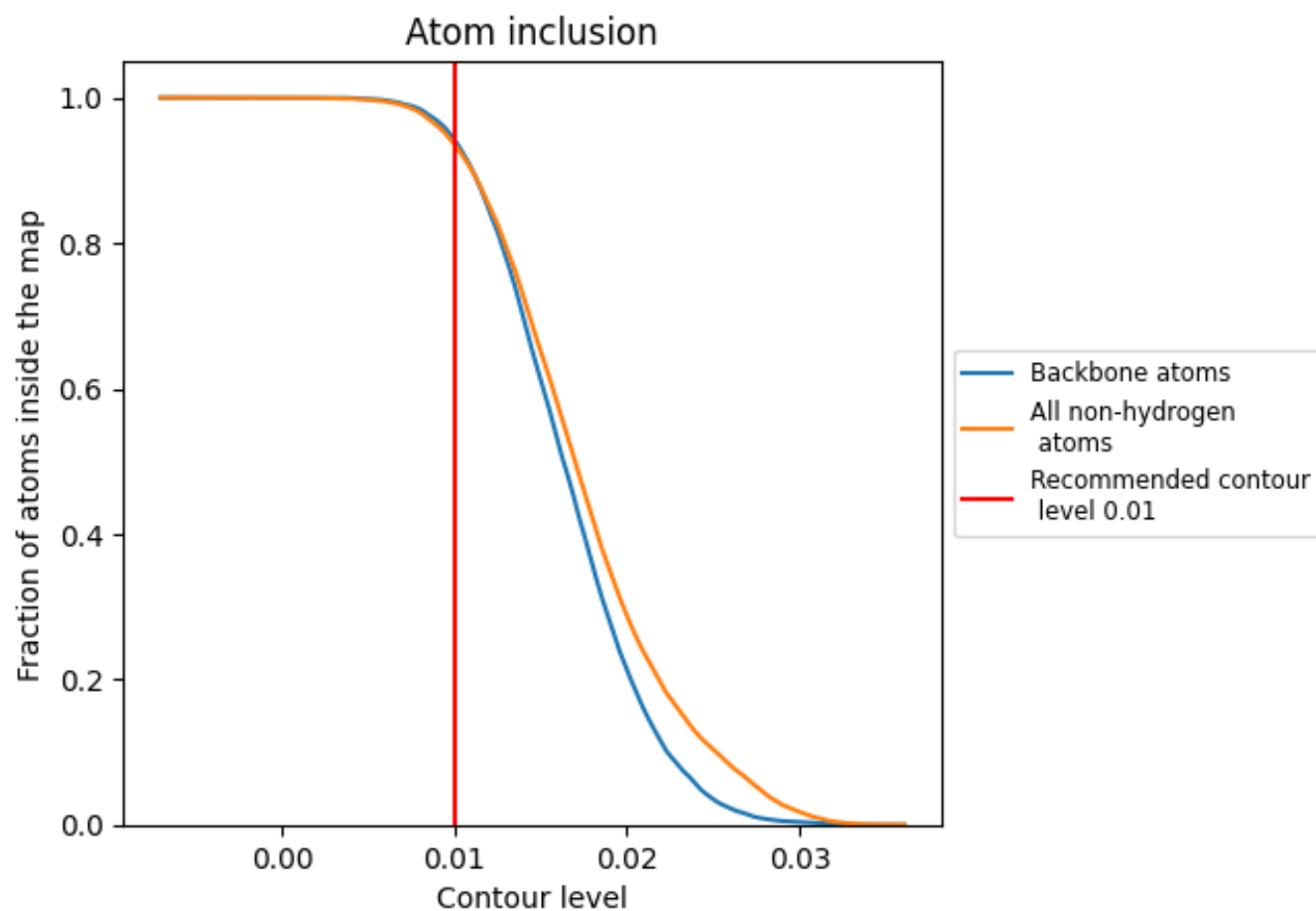
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.1130
A	 0.9718	 0.1180
B	 0.9646	 0.1330
C	 0.9757	 0.1150
D	 0.9735	 0.1100
E	 0.9731	 0.1390
F	 0.9389	 0.1330
G	 0.9830	 0.0960
H	 0.9841	 0.1080
I	 0.9960	 0.1450
J	 0.9959	 0.1450
O	 0.8290	 0.0900
P	 0.9652	 0.1010
R	 0.9563	 0.0970
a	 0.7913	 0.0780
b	 0.6739	 0.0660
c	 0.9251	 0.0840
d	 0.8991	 0.0910
e	 0.7510	 0.0750
f	 0.7943	 0.0920
g	 0.9102	 0.0850
h	 0.8665	 0.0620
i	 0.9615	 0.1260
j	 0.9500	 0.1190

