Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 06:20 PM JST

PDB ID	:	7EU0
EMDB ID	:	EMD-31305
Title	:	The cryo-EM structure of A. thaliana Pol IV-RDR2 backtracked complex
Authors	:	Fang, C.L.; Wu, X.X.; Huang, K.; Zhang, Y.
Deposited on	:	2021-05-15
Resolution	:	3.16 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*
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:

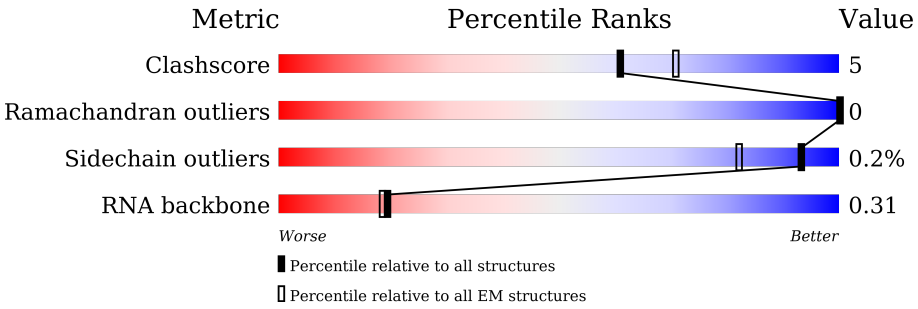
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.16 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
RNA backbone	4643	859

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	A	1510	65% 6% 30%
2	B	1172	81% 9% 10%
3	C	319	82% 9% 9%
4	E	205	89% 7%
5	F	144	51% 47%
6	H	146	79% 7% 14%
7	I	114	11% 90% 9%

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Mol	Chain	Length	Quality of chain
8	J	71	79% 8% 13%
9	K	116	78% 19%
10	L	51	76% 6% 18%
11	M	1133	17% 83% 10% 7%
12	N	20	20% 55% 30% 15%
13	O	39	46% 36% 28% 15% 18%
14	Q	33	12% 52% 33% 15%
15	R	4	25% 75%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32686 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase IV subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1060	7722	4901	1341	1434	46	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerases IV and V subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1054	7861	5020	1418	1379	44	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases II, IV and V subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	291	2148	1367	372	395	14	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases II and IV subunit 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	198	1458	937	265	250	6	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases II, IV and V subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	76	554	355	97	99	3	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases II, IV and V subunit 8B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	126	923	606	147	163	7	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases II, IV and V subunit 9A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	113	Total	C	N	O	S	0	0
			819	502	155	150	12		

- Molecule 8 is a protein called DNA-directed RNA polymerases II, IV and V subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	62	Total	C	N	O	S	0	0
			472	308	83	75	6		

- Molecule 9 is a protein called DNA-directed RNA polymerases II, IV and V subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	94	Total	C	N	O	S	0	0
			711	456	130	124	1		

- Molecule 10 is a protein called DNA-directed RNA polymerases II, IV and V subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	42	Total	C	N	O	S	0	0
			293	182	50	57	4		

- Molecule 11 is a protein called RNA-dependent RNA polymerase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	1052	Total	C	N	O	S	0	0
			8055	5144	1383	1476	52		

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*TP*AP*TP *CP*GP*GP*TP*AP*GP*AP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	17	Total	C	N	O	P	0	0
			353	168	63	105	17		

- Molecule 13 is a RNA chain called RNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	32	Total	C	N	O	P	0	0
			664	297	98	237	32		

- Molecule 14 is a DNA chain called DNA (33-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	28	Total	C	N	O	P	0	0
			561	268	98	167	28		

- Molecule 15 is a RNA chain called RNA (5'-R(*CP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	4	Total	C	N	O	P	0	0
			82	38	16	25	3		

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	C	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

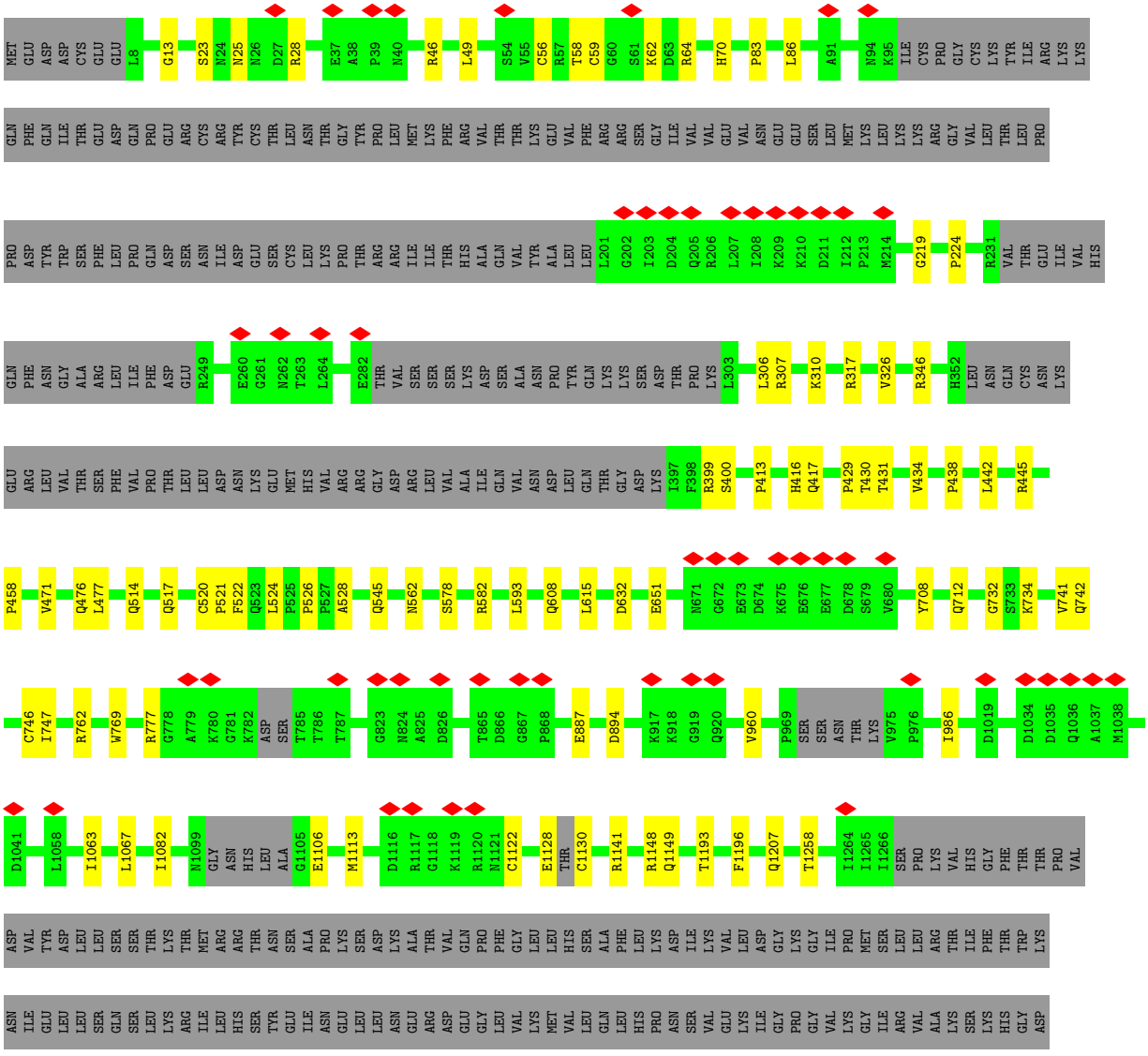
Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	
17	M	1	Total	Mg	0
			1	1	

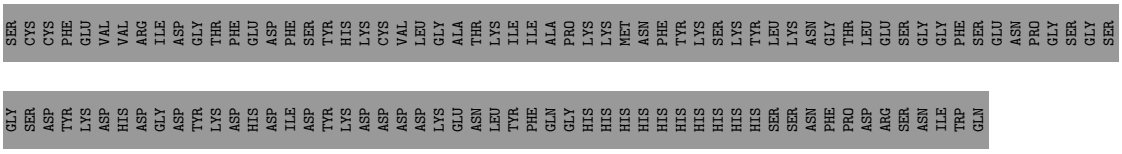
3 Residue-property plots (i)

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: DNA-directed RNA polymerase IV subunit 1

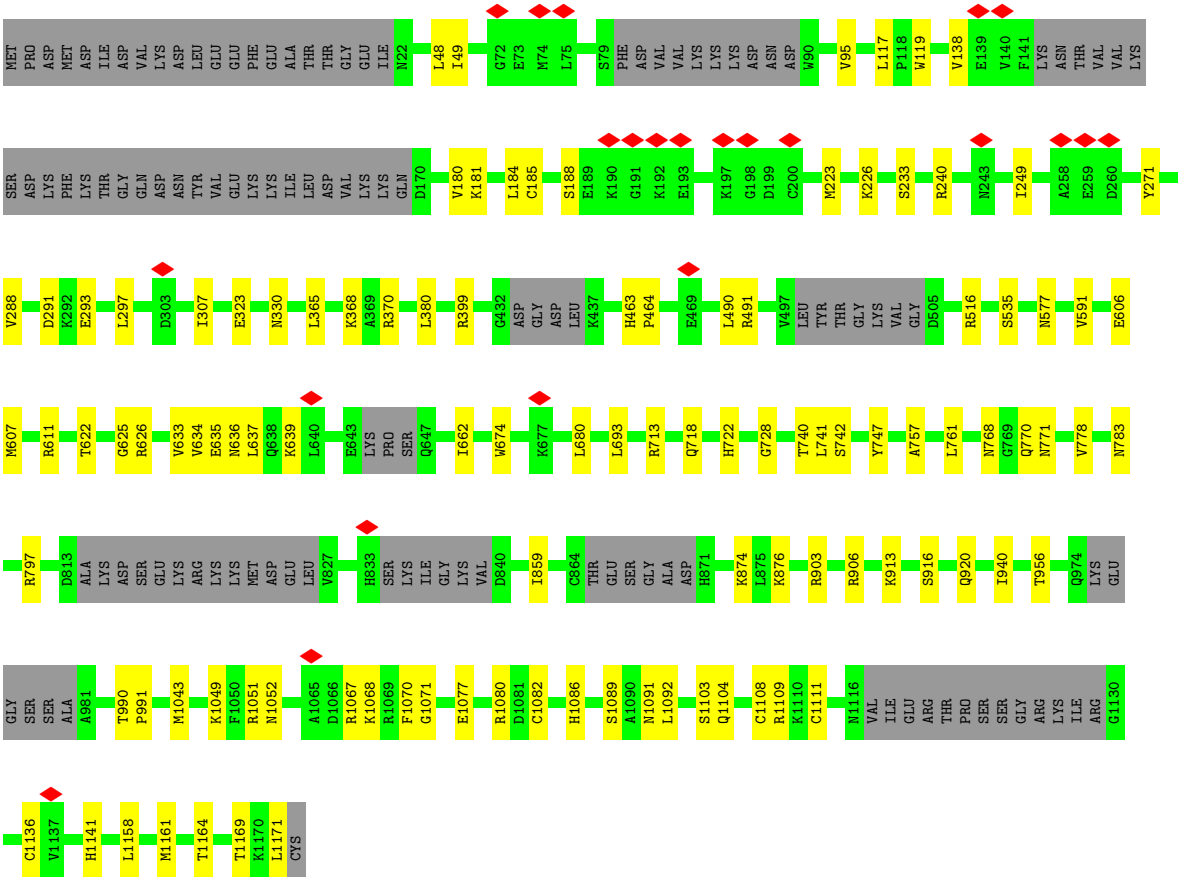
Chain A:





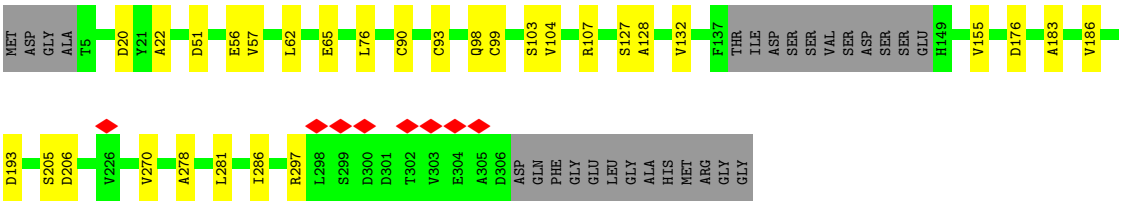
• Molecule 2: DNA-directed RNA polymerases IV and V subunit 2

Chain B:



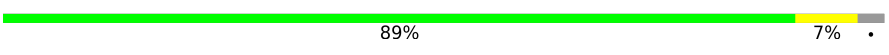
• Molecule 3: DNA-directed RNA polymerases II, IV and V subunit 3

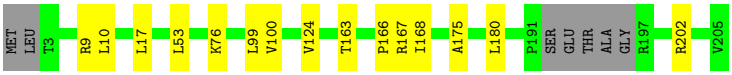
Chain C:



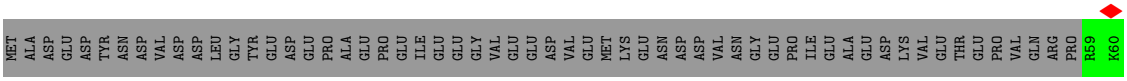
• Molecule 4: DNA-directed RNA polymerases II and IV subunit 5A

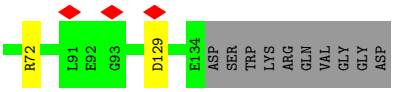
Chain E:



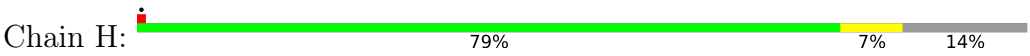


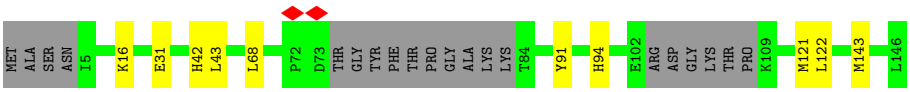
• Molecule 5: DNA-directed RNA polymerases II, IV and V subunit 6A



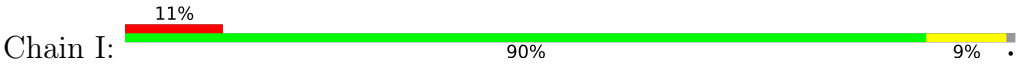


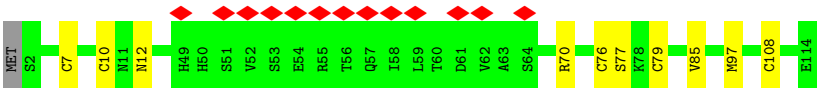
• Molecule 6: DNA-directed RNA polymerases II, IV and V subunit 8B



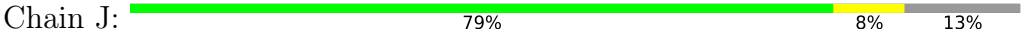


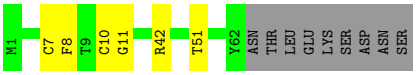
• Molecule 7: DNA-directed RNA polymerases II, IV and V subunit 9A



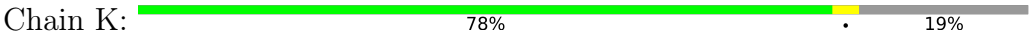


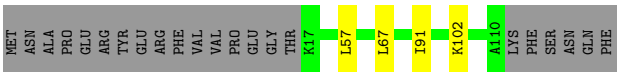
• Molecule 8: DNA-directed RNA polymerases II, IV and V subunit 10



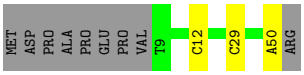


• Molecule 9: DNA-directed RNA polymerases II, IV and V subunit 11



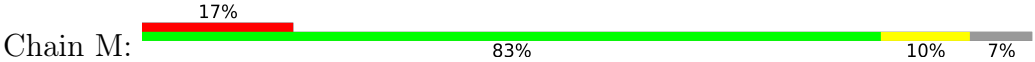


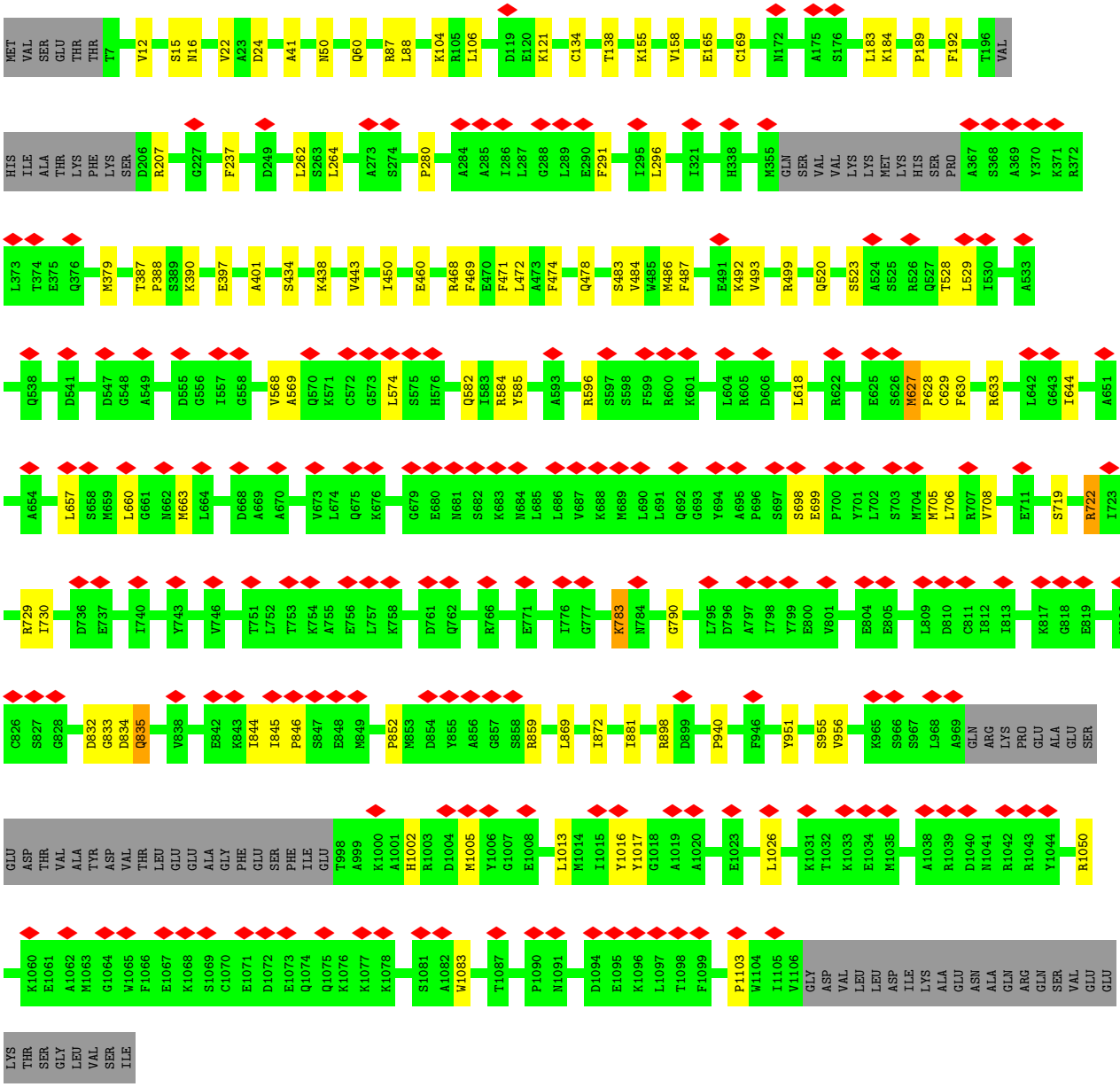
• Molecule 10: DNA-directed RNA polymerases II, IV and V subunit 12



• Molecule 11: RNA-dependent RNA polymerase 2

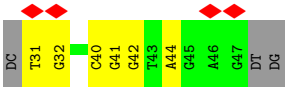
Chain M:



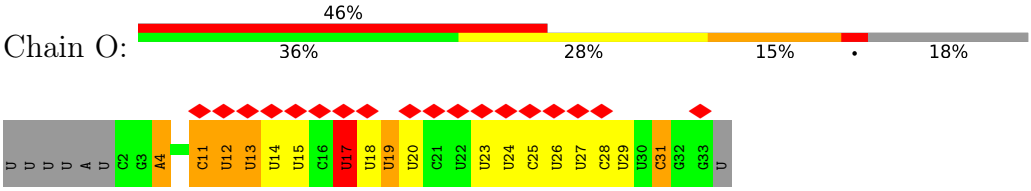


• Molecule 12: DNA (5'-D(*CP*TP*GP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*GP*AP*GP*TP*G)-3')

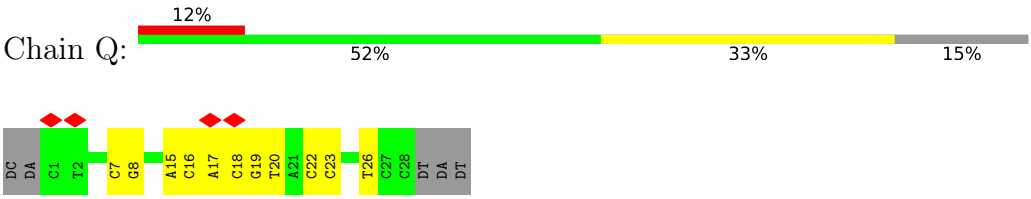
Chain N:



• Molecule 13: RNA (39-MER)



• Molecule 14: DNA (33-MER)



• Molecule 15: RNA (5'-R(*CP*CP*GP*A)-3')

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63253	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.95	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	296.8, 296.8, 296.8	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.25	0/7866	0.46	0/10702
2	B	0.25	0/8026	0.44	1/10875 (0.0%)
3	C	0.25	0/2178	0.47	0/2954
4	E	0.24	0/1479	0.44	0/2011
5	F	0.24	0/564	0.44	0/767
6	H	0.27	0/938	0.55	1/1267 (0.1%)
7	I	0.24	0/835	0.46	0/1135
8	J	0.23	0/479	0.40	0/649
9	K	0.24	0/725	0.43	0/987
10	L	0.24	0/296	0.48	0/401
11	M	0.26	0/8224	0.50	0/11140
12	N	0.46	0/395	0.88	0/609
13	O	0.25	0/736	0.99	2/1141 (0.2%)
14	Q	0.61	1/626 (0.2%)	1.28	3/960 (0.3%)
15	R	0.30	0/91	0.90	0/140
All	All	0.27	1/33458 (0.0%)	0.53	7/45738 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	Q	15	DA	O3'-P	7.00	1.69	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	Q	15	DA	O3'-P-O5'	17.57	137.38	104.00
14	Q	15	DA	P-O3'-C3'	16.42	139.40	119.70
14	Q	15	DA	OP2-P-O3'	-12.83	76.97	105.20
13	O	31	C	N1-C2-O2	6.14	122.58	118.90
6	H	68	LEU	CA-CB-CG	5.52	127.99	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	17	U	P-O3'-C3'	5.34	126.11	119.70
2	B	184	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7722	0	7280	67	0
2	B	7861	0	7490	65	0
3	C	2148	0	2131	22	0
4	E	1458	0	1391	9	0
5	F	554	0	516	2	0
6	H	923	0	860	5	0
7	I	819	0	709	6	0
8	J	472	0	478	6	0
9	K	711	0	675	4	0
10	L	293	0	244	2	0
11	M	8055	0	7752	63	0
12	N	353	0	194	18	0
13	O	664	0	337	10	0
14	Q	561	0	314	42	0
15	R	82	0	45	4	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
17	M	1	0	0	0	0
All	All	32686	0	30416	285	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 5.

All (285) 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)
1:A:56:CYS:HB3	1:A:59:CYS:SG	1.64	1.35
12:N:31:DT:O4	14:Q:17:DA:N6	1.56	1.34
12:N:31:DT:O4	14:Q:17:DA:C6	1.91	1.24
12:N:31:DT:O4	14:Q:17:DA:N1	1.80	1.14
14:Q:19:DG:H2"	14:Q:20:DT:H5'	1.35	1.08
12:N:31:DT:C4	14:Q:17:DA:N1	2.29	1.00
14:Q:19:DG:H2"	14:Q:20:DT:C5'	1.94	0.97
14:Q:19:DG:C2	14:Q:20:DT:C2	2.55	0.94
12:N:31:DT:H2"	12:N:32:DG:O5'	1.68	0.93
12:N:32:DG:N1	14:Q:16:DC:N3	2.19	0.89
12:N:32:DG:N2	14:Q:16:DC:O2	2.05	0.89
1:A:307:ARG:NH2	1:A:310:LYS:HE2	1.90	0.86
1:A:56:CYS:CB	1:A:59:CYS:SG	2.59	0.85
12:N:41:DG:H2"	12:N:42:DG:H8	1.41	0.83
3:C:90:CYS:SG	3:C:93:CYS:HB2	2.20	0.81
14:Q:19:DG:N2	14:Q:20:DT:O2	2.15	0.79
12:N:41:DG:H2"	12:N:42:DG:C8	2.19	0.78
13:O:11:C:H3'	13:O:11:C:O2	1.84	0.77
2:B:1108:CYS:SG	2:B:1111:CYS:HB3	2.26	0.75
1:A:413:PRO:HG3	14:Q:19:DG:N2	2.03	0.73
12:N:32:DG:O6	14:Q:16:DC:N4	2.20	0.71
14:Q:17:DA:H2"	14:Q:18:DC:C5'	2.21	0.71
14:Q:19:DG:C2'	14:Q:20:DT:H5'	2.18	0.71
8:J:7:CYS:SG	8:J:10:CYS:HB3	2.32	0.70
14:Q:19:DG:C2	14:Q:20:DT:N3	2.60	0.70
14:Q:17:DA:H1'	14:Q:18:DC:O4'	1.94	0.68
14:Q:19:DG:N2	14:Q:20:DT:C2	2.64	0.65
14:Q:17:DA:H2"	14:Q:18:DC:O4'	1.95	0.65
2:B:1111:CYS:HB2	2:B:1136:CYS:SG	2.38	0.64
14:Q:19:DG:N3	14:Q:20:DT:C2	2.66	0.64
14:Q:17:DA:H2"	14:Q:18:DC:H5"	1.79	0.64
2:B:771:ASN:HD21	8:J:51:THR:HG21	1.63	0.64
1:A:734:LYS:CD	13:O:13:U:H3	2.10	0.63
13:O:11:C:O2	13:O:11:C:C3'	2.45	0.63
14:Q:17:DA:N9	14:Q:18:DC:C6	2.67	0.62
11:M:280:PRO:HG3	11:M:390:LYS:HB2	1.83	0.61
1:A:734:LYS:HD3	13:O:13:U:H3	1.66	0.61
13:O:11:C:O2	13:O:11:C:C2'	2.46	0.61
12:N:41:DG:H1'	12:N:42:DG:C8	2.37	0.60
14:Q:17:DA:C4	14:Q:18:DC:C6	2.90	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:582:GLN:HE21	11:M:833:GLY:HA3	1.67	0.59
14:Q:17:DA:C4	14:Q:18:DC:C5	2.90	0.59
14:Q:17:DA:C5	14:Q:18:DC:C5	2.90	0.59
12:N:41:DG:C2'	12:N:42:DG:C8	2.85	0.59
1:A:306:LEU:O	1:A:310:LYS:HG2	2.04	0.58
1:A:1082:ILE:HG12	1:A:1113:MET:HG2	1.86	0.57
12:N:41:DG:C1'	12:N:42:DG:C8	2.87	0.56
11:M:106:LEU:HB2	11:M:134:CYS:HB3	1.87	0.56
15:R:17:C:HO5'	15:R:17:C:H6	1.51	0.56
1:A:58:THR:HG21	1:A:70:HIS:CE1	2.41	0.56
1:A:59:CYS:SG	1:A:62:LYS:CB	2.94	0.56
1:A:528:ALA:HA	6:H:94:HIS:HB3	1.86	0.56
2:B:365:LEU:HD12	2:B:368:LYS:HD2	1.86	0.56
13:O:4:A:H61	14:Q:26:DT:H3	1.52	0.56
1:A:56:CYS:HB3	1:A:59:CYS:HG	1.63	0.56
2:B:859:ILE:HG13	2:B:874:LYS:HG2	1.87	0.56
11:M:169:CYS:HB3	11:M:264:LEU:HD22	1.88	0.55
12:N:40:DC:H2"	12:N:41:DG:OP2	2.05	0.55
11:M:835:GLN:OE1	11:M:835:GLN:N	2.40	0.55
1:A:471:VAL:O	1:A:476:GLN:NE2	2.39	0.55
2:B:607:MET:HG3	2:B:622:THR:HB	1.89	0.54
14:Q:19:DG:H2'	14:Q:20:DT:C6	2.42	0.54
1:A:514:GLN:NE2	9:K:57:LEU:O	2.41	0.53
2:B:577:ASN:HD21	2:B:622:THR:H	1.56	0.53
4:E:175:ALA:HA	4:E:180:LEU:HD12	1.91	0.53
1:A:442:LEU:O	1:A:445:ARG:NH2	2.42	0.53
3:C:22:ALA:HB3	3:C:270:VAL:HB	1.90	0.53
1:A:562:ASN:ND2	1:A:578:SER:O	2.41	0.53
14:Q:19:DG:H2"	14:Q:20:DT:O5'	2.09	0.53
1:A:317:ARG:NH1	14:Q:22:DC:OP1	2.41	0.53
8:J:10:CYS:SG	8:J:42:ARG:NH2	2.80	0.53
2:B:718:GLN:NE2	2:B:916:SER:O	2.41	0.53
3:C:127:SER:OG	3:C:128:ALA:N	2.42	0.53
3:C:98:GLN:OE1	3:C:98:GLN:HA	2.08	0.52
11:M:569:ALA:HB1	11:M:574:LEU:HB2	1.91	0.52
2:B:491:ARG:NH2	2:B:535:SER:O	2.42	0.52
11:M:155:LYS:HB3	11:M:192:PHE:HB2	1.92	0.52
2:B:185:CYS:HB3	2:B:188:SER:HB3	1.92	0.52
11:M:183:LEU:HB2	11:M:237:PHE:HB2	1.92	0.52
14:Q:19:DG:H2'	14:Q:20:DT:C7	2.40	0.52
1:A:438:PRO:HD2	1:A:608:GLN:HE22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:GLN:NE2	1:A:522:PHE:O	2.42	0.52
11:M:630:PHE:CE2	11:M:722:ARG:NH1	2.77	0.52
2:B:747:TYR:O	2:B:770:GLN:NE2	2.40	0.52
1:A:651:GLU:OE2	1:A:762:ARG:NH2	2.42	0.51
3:C:186:VAL:HG12	3:C:270:VAL:HA	1.91	0.51
11:M:783:LYS:NZ	11:M:834:ASP:HB2	2.24	0.51
2:B:757:ALA:O	2:B:761:LEU:HB2	2.10	0.51
11:M:790:GLY:HA3	11:M:852:PRO:HA	1.92	0.51
7:I:76:CYS:SG	7:I:77:SER:N	2.84	0.51
14:Q:19:DG:C2'	14:Q:20:DT:C6	2.95	0.51
2:B:1109:ARG:HB2	2:B:1141:HIS:HB2	1.92	0.50
11:M:644:ILE:HG12	11:M:845:ILE:H	1.75	0.50
14:Q:7:DC:H2"	14:Q:8:DG:C8	2.46	0.50
2:B:95:VAL:HG23	2:B:138:VAL:HG22	1.92	0.50
3:C:176:ASP:OD1	3:C:176:ASP:N	2.45	0.50
1:A:417:GLN:O	2:B:1086:HIS:NE2	2.42	0.50
11:M:15:SER:HB2	11:M:87:ARG:HB2	1.93	0.50
11:M:633:ARG:NH1	11:M:719:SER:O	2.44	0.50
11:M:520:GLN:O	11:M:584:ARG:NH1	2.45	0.50
2:B:903:ARG:NH1	3:C:65:GLU:OE1	2.45	0.50
4:E:17:LEU:HD11	4:E:100:VAL:HG21	1.93	0.50
1:A:83:PRO:HA	1:A:86:LEU:HD23	1.92	0.50
1:A:417:GLN:HA	2:B:1082:CYS:HB3	1.94	0.50
4:E:10:LEU:HD21	4:E:53:LEU:HD11	1.94	0.49
1:A:25:ASN:ND2	1:A:219:GLY:O	2.45	0.49
2:B:223:MET:HE3	2:B:240:ARG:HH12	1.77	0.49
5:F:129:ASP:OD1	5:F:129:ASP:N	2.45	0.49
11:M:657:LEU:HA	11:M:660:LEU:HB3	1.94	0.49
15:R:17:C:H6	15:R:17:C:O5'	1.94	0.49
1:A:58:THR:CG2	1:A:70:HIS:CE1	2.95	0.49
2:B:906:ARG:NH1	2:B:1043:MET:SD	2.81	0.49
2:B:1080:ARG:HG3	2:B:1092:LEU:HD11	1.94	0.49
3:C:297:ARG:HB2	9:K:91:ILE:HG21	1.94	0.49
11:M:869:LEU:HD13	11:M:872:ILE:HD12	1.93	0.49
11:M:1013:LEU:HA	11:M:1016:TYR:HB3	1.93	0.49
11:M:50:ASN:O	11:M:207:ARG:NH2	2.46	0.49
1:A:413:PRO:HG3	14:Q:19:DG:H22	1.76	0.49
11:M:698:SER:OG	11:M:699:GLU:N	2.46	0.49
14:Q:17:DA:C2'	14:Q:18:DC:O4'	2.61	0.49
1:A:1128:GLU:O	1:A:1130:CYS:N	2.46	0.49
2:B:591:VAL:HG21	2:B:611:ARG:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:LEU:HD12	3:C:155:VAL:HG23	1.95	0.49
2:B:1051:ARG:HG3	2:B:1070:PHE:HB3	1.93	0.48
1:A:13:GLY:HA2	2:B:1171:LEU:HB3	1.94	0.48
1:A:632:ASP:N	1:A:632:ASP:OD1	2.45	0.48
2:B:634:VAL:HA	2:B:637:LEU:HB2	1.95	0.48
11:M:379:MET:HB2	11:M:401:ALA:HB2	1.94	0.48
1:A:23:SER:O	1:A:28:ARG:NH2	2.47	0.48
7:I:97:MET:O	11:M:859:ARG:NH1	2.45	0.48
1:A:1148:ARG:NH1	1:A:1196:PHE:O	2.46	0.48
2:B:674:TRP:HB3	2:B:693:LEU:HD11	1.94	0.48
2:B:1077:GLU:HG2	2:B:1080:ARG:HH21	1.78	0.48
2:B:1103:SER:OG	2:B:1104:GLN:N	2.46	0.48
2:B:778:VAL:HA	2:B:783:ASN:HD21	1.79	0.48
4:E:76:LYS:HD2	12:N:44:DA:OP1	2.13	0.48
11:M:705:MET:HA	11:M:708:VAL:HG22	1.96	0.48
1:A:416:HIS:HB3	1:A:887:GLU:HB2	1.96	0.48
6:H:91:TYR:HB3	6:H:143:MET:HB2	1.96	0.48
4:E:163:THR:O	4:E:167:ARG:NH1	2.47	0.47
11:M:629:CYS:HB3	11:M:730:ILE:HG13	1.95	0.47
2:B:48:LEU:O	2:B:491:ARG:NH1	2.47	0.47
3:C:286:ILE:HG21	9:K:102:LYS:HB2	1.96	0.47
11:M:471:PHE:O	11:M:499:ARG:NH1	2.47	0.47
7:I:7:CYS:SG	7:I:10:CYS:HB3	2.54	0.47
14:Q:17:DA:C8	14:Q:18:DC:C5	3.03	0.47
1:A:1128:GLU:OE2	4:E:9:ARG:NH2	2.48	0.47
2:B:1049:LYS:HG3	2:B:1067:ARG:HG3	1.96	0.47
3:C:193:ASP:OD1	3:C:193:ASP:N	2.46	0.47
6:H:43:LEU:HD13	6:H:121:MET:HG3	1.97	0.47
14:Q:17:DA:C1'	14:Q:18:DC:O4'	2.63	0.47
1:A:582:ARG:HD3	1:A:732:GLY:HA3	1.97	0.47
2:B:307:ILE:HG23	2:B:380:LEU:HD22	1.96	0.47
2:B:740:THR:HG23	2:B:741:LEU:N	2.29	0.47
2:B:1051:ARG:NH1	2:B:1071:GLY:O	2.47	0.47
4:E:166:PRO:HB2	4:E:202:ARG:HD3	1.96	0.47
4:E:168:ILE:HG23	4:E:202:ARG:HD2	1.96	0.47
7:I:79:CYS:SG	7:I:108:CYS:HB2	2.54	0.47
6:H:42:HIS:HB2	6:H:122:LEU:HB3	1.96	0.47
11:M:460:GLU:O	11:M:468:ARG:NH2	2.48	0.47
11:M:397:GLU:HG2	11:M:1050:ARG:HD2	1.97	0.47
11:M:41:ALA:HB3	11:M:60:GLN:HB3	1.97	0.46
11:M:832:ASP:OD1	11:M:832:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ARG:O	2:B:1052:ASN:ND2	2.42	0.46
1:A:769:TRP:O	1:A:777:ARG:NH2	2.48	0.46
2:B:1109:ARG:NH2	2:B:1169:THR:OG1	2.47	0.46
11:M:474:PHE:HB3	11:M:484:VAL:HG23	1.97	0.46
2:B:920:GLN:NE2	2:B:956:THR:OG1	2.46	0.46
11:M:628:PRO:HA	11:M:729:ARG:HA	1.97	0.46
3:C:98:GLN:OE1	3:C:104:VAL:HA	2.15	0.46
1:A:526:PRO:O	1:A:545:GLN:NE2	2.48	0.46
2:B:606:GLU:O	2:B:626:ARG:NH2	2.41	0.46
1:A:413:PRO:HB3	14:Q:20:DT:O2	2.16	0.46
14:Q:17:DA:H1'	14:Q:18:DC:C1'	2.46	0.46
11:M:12:VAL:HG11	11:M:88:LEU:HD13	1.97	0.46
2:B:713:ARG:NH1	13:O:12:U:OP2	2.48	0.46
14:Q:17:DA:C1'	14:Q:18:DC:C6	2.99	0.46
1:A:23:SER:HB3	2:B:1164:THR:HB	1.98	0.45
1:A:25:ASN:OD1	1:A:28:ARG:NH1	2.49	0.45
1:A:28:ARG:HD3	1:A:224:PRO:HD3	1.99	0.45
2:B:718:GLN:HA	2:B:722:HIS:HB2	1.97	0.45
2:B:876:LYS:HD3	2:B:1068:LYS:HB3	1.97	0.45
3:C:56:GLU:HG3	3:C:57:VAL:HG23	1.96	0.45
1:A:734:LYS:HD2	13:O:13:U:H3	1.79	0.45
1:A:445:ARG:NH1	1:A:887:GLU:OE2	2.50	0.45
11:M:22:VAL:HG13	11:M:24:ASP:H	1.82	0.45
2:B:323:GLU:O	2:B:330:ASN:ND2	2.50	0.45
2:B:633:VAL:HG22	2:B:635:GLU:H	1.82	0.45
3:C:20:ASP:OD1	3:C:20:ASP:N	2.49	0.45
11:M:469:PHE:HB3	11:M:486:MET:HB3	1.99	0.45
1:A:712:GLN:HG2	1:A:741:VAL:HG21	1.98	0.45
11:M:1083:TRP:HB3	11:M:1103:PRO:HB3	1.99	0.45
1:A:517:GLN:HG3	1:A:524:LEU:HD13	1.99	0.44
1:A:1122:CYS:HB2	1:A:1149:GLN:HE22	1.82	0.44
11:M:104:LYS:NZ	11:M:138:THR:OG1	2.45	0.44
11:M:434:SER:HB3	11:M:881:ILE:HG21	1.99	0.44
11:M:596:ARG:HA	11:M:596:ARG:HD3	1.87	0.44
12:N:41:DG:C8	12:N:41:DG:O5'	2.70	0.44
1:A:477:LEU:HD13	1:A:593:LEU:HD11	1.99	0.44
11:M:388:PRO:HB3	11:M:450:ILE:HD12	2.00	0.44
1:A:326:VAL:HG23	1:A:434:VAL:HG23	2.00	0.44
11:M:898:ARG:HH22	11:M:940:PRO:HA	1.83	0.44
14:Q:17:DA:C5	14:Q:18:DC:C4	3.05	0.44
11:M:528:THR:HG21	11:M:568:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:CYS:O	1:A:59:CYS:O	2.35	0.44
1:A:615:LEU:HG	2:B:778:VAL:HG21	1.99	0.44
2:B:233:SER:O	2:B:233:SER:OG	2.32	0.44
2:B:634:VAL:HG11	2:B:680:LEU:HD11	2.00	0.44
11:M:783:LYS:HZ1	11:M:834:ASP:HB2	1.82	0.43
11:M:663:MET:HG2	11:M:706:LEU:HD21	2.00	0.43
11:M:585:TYR:HB3	11:M:618:LEU:HD12	2.00	0.43
1:A:413:PRO:HG3	14:Q:19:DG:H21	1.80	0.43
2:B:297:LEU:HD22	2:B:370:ARG:HG3	1.99	0.43
7:I:70:ARG:HG2	7:I:85:VAL:HG22	2.00	0.43
11:M:898:ARG:HH21	11:M:951:TYR:HB3	1.83	0.43
11:M:158:VAL:HG22	11:M:189:PRO:HB3	2.01	0.43
13:O:11:C:O2	13:O:11:C:H2'	2.18	0.43
12:N:40:DC:C2	12:N:41:DG:C6	3.07	0.43
15:R:18:C:H2'	15:R:19:G:C8	2.53	0.43
1:A:708:TYR:HH	1:A:746:CYS:HG	1.58	0.42
2:B:117:LEU:HD13	2:B:119:TRP:HE1	1.83	0.42
11:M:523:SER:OG	11:M:584:ARG:NH1	2.52	0.42
12:N:40:DC:C4	12:N:41:DG:O6	2.72	0.42
11:M:955:SER:OG	11:M:956:VAL:N	2.52	0.42
2:B:226:LYS:HD3	2:B:577:ASN:HB3	2.01	0.42
3:C:183:ALA:HB2	3:C:281:LEU:HD21	2.00	0.42
11:M:627:MET:HE2	11:M:730:ILE:O	2.19	0.42
14:Q:17:DA:H2"	14:Q:18:DC:C4'	2.49	0.42
2:B:728:GLY:HA3	2:B:768:ASN:HD22	1.85	0.42
8:J:7:CYS:HB3	8:J:11:GLY:H	1.83	0.42
2:B:49:ILE:HG21	2:B:490:LEU:HD13	2.02	0.42
6:H:16:LYS:HB3	6:H:31:GLU:HB2	2.02	0.42
11:M:472:LEU:HD12	11:M:487:PHE:HB2	2.00	0.42
11:M:1013:LEU:HD23	11:M:1017:TYR:HE2	1.85	0.42
1:A:429:PRO:HD2	9:K:67:LEU:HD13	2.02	0.42
2:B:180:VAL:HG12	2:B:181:LYS:HG3	2.02	0.42
11:M:478:GLN:HG2	11:M:483:SER:HB2	2.00	0.42
11:M:844:ILE:HG13	11:M:846:PRO:HD3	2.02	0.42
1:A:894:ASP:OD1	1:A:894:ASP:N	2.45	0.42
2:B:249:ILE:O	2:B:271:TYR:N	2.52	0.42
3:C:76:LEU:HD23	3:C:132:VAL:HG12	2.02	0.42
11:M:438:LYS:HA	11:M:443:VAL:HA	2.01	0.42
1:A:458:PRO:HB3	2:B:1091:ASN:HD21	1.84	0.42
2:B:516:ARG:NH1	2:B:662:ILE:O	2.53	0.41
10:L:12:CYS:SG	10:L:29:CYS:SG	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:GLU:OE2	1:A:1141:ARG:NH2	2.51	0.41
3:C:51:ASP:HA	10:L:50:ALA:HB3	2.02	0.41
1:A:742:GLN:HG2	1:A:747:ILE:HA	2.02	0.41
2:B:940:ILE:HD11	8:J:42:ARG:HB3	2.03	0.41
3:C:205:SER:OG	3:C:206:ASP:N	2.54	0.41
11:M:387:THR:HG1	11:M:390:LYS:H	1.68	0.41
2:B:288:VAL:HG13	2:B:293:GLU:HG3	2.02	0.41
3:C:22:ALA:HB2	3:C:278:ALA:HB1	2.01	0.41
3:C:51:ASP:N	3:C:51:ASP:OD1	2.53	0.41
3:C:107:ARG:HA	3:C:107:ARG:HD2	1.93	0.41
11:M:291:PHE:HD2	11:M:296:LEU:HB2	1.85	0.41
13:O:17:U:O2'	13:O:19:U:OP2	2.38	0.41
1:A:399:ARG:NH1	1:A:400:SER:O	2.54	0.41
1:A:1258:THR:HB	2:B:1089:SER:HB2	2.02	0.41
11:M:1002:HIS:HA	11:M:1005:MET:HG2	2.03	0.41
1:A:960:VAL:HA	1:A:986:ILE:HG12	2.02	0.41
2:B:399:ARG:HB3	2:B:625:GLY:HA3	2.02	0.41
2:B:797:ARG:NH1	8:J:8:PHE:O	2.53	0.41
11:M:1026:LEU:HD23	11:M:1026:LEU:HA	1.92	0.41
1:A:477:LEU:HB3	1:A:593:LEU:HD21	2.03	0.41
2:B:990:THR:HA	2:B:991:PRO:HD3	1.97	0.41
11:M:16:ASN:OD1	11:M:16:ASN:N	2.53	0.41
14:Q:22:DC:H2"	14:Q:23:DC:H5'	2.03	0.41
1:A:520:CYS:HA	1:A:521:PRO:HD3	1.95	0.41
2:B:463:HIS:HA	2:B:464:PRO:HD3	1.95	0.41
3:C:99:CYS:HB2	3:C:103:SER:H	1.86	0.41
4:E:99:LEU:HD21	4:E:124:VAL:HG22	2.03	0.41
15:R:18:C:H2'	15:R:19:G:H8	1.86	0.40
2:B:636:ASN:HB2	2:B:639:LYS:HE3	2.03	0.40
2:B:1158:LEU:HA	2:B:1161:MET:HG2	2.02	0.40
11:M:492:LYS:HG2	11:M:493:VAL:HG13	2.02	0.40
11:M:528:THR:HG22	11:M:529:LEU:H	1.86	0.40
1:A:49:LEU:HB3	1:A:64:ARG:HG3	2.03	0.40
1:A:1063:ILE:HG23	1:A:1067:LEU:HD23	2.03	0.40
1:A:1258:THR:HG23	5:F:72:ARG:HD2	2.04	0.40
11:M:121:LYS:HG3	11:M:262:LEU:HD21	2.02	0.40
11:M:165:GLU:HB3	11:M:184:LYS:HB2	2.04	0.40
1:A:430:THR:OG1	1:A:431:THR:N	2.54	0.40
1:A:1193:THR:HG21	1:A:1207:GLN:HA	2.04	0.40
2:B:291:ASP:HB2	7:I:12:ASN:HA	2.02	0.40

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	1042/1510 (69%)	1008 (97%)	34 (3%)	0	100	100
2	B	1032/1172 (88%)	1005 (97%)	27 (3%)	0	100	100
3	C	287/319 (90%)	270 (94%)	17 (6%)	0	100	100
4	E	194/205 (95%)	191 (98%)	3 (2%)	0	100	100
5	F	74/144 (51%)	69 (93%)	5 (7%)	0	100	100
6	H	120/146 (82%)	113 (94%)	7 (6%)	0	100	100
7	I	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
8	J	60/71 (84%)	57 (95%)	3 (5%)	0	100	100
9	K	92/116 (79%)	89 (97%)	3 (3%)	0	100	100
10	L	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
11	M	1044/1133 (92%)	999 (96%)	45 (4%)	0	100	100
All	All	4096/4981 (82%)	3947 (96%)	149 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	772/1344 (57%)	771 (100%)	1 (0%)	93	98
2	B	773/1029 (75%)	771 (100%)	2 (0%)	92	97
3	C	220/280 (79%)	220 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	E	133/191 (70%)	133 (100%)	0	100 100
5	F	50/128 (39%)	50 (100%)	0	100 100
6	H	84/127 (66%)	84 (100%)	0	100 100
7	I	79/104 (76%)	79 (100%)	0	100 100
8	J	47/66 (71%)	47 (100%)	0	100 100
9	K	67/105 (64%)	67 (100%)	0	100 100
10	L	25/45 (56%)	25 (100%)	0	100 100
11	M	822/1005 (82%)	818 (100%)	4 (0%)	88 95
All	All	3072/4424 (69%)	3065 (100%)	7 (0%)	93 98

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
2	B	742	SER
2	B	913	LYS
11	M	627	MET
11	M	722	ARG
11	M	783	LYS
11	M	835	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	HIS
1	A	563	ASN
1	A	634	GLN
1	A	742	GLN
1	A	910	ASN
1	A	923	GLN
1	A	949	ASN
2	B	220	GLN
2	B	222	GLN
2	B	477	ASN
2	B	577	ASN
2	B	600	GLN
2	B	718	GLN
2	B	749	GLN

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Mol	Chain	Res	Type
2	B	768	ASN
2	B	920	GLN
2	B	955	GLN
2	B	1091	ASN
2	B	1106	HIS
3	C	284	ASN
6	H	124	GLN
7	I	105	ASN
9	K	51	HIS
10	L	47	GLN
11	M	304	HIS
11	M	339	GLN
11	M	788	HIS
11	M	1002	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	O	31/39 (79%)	18 (58%)	2 (6%)
15	R	3/4 (75%)	0	0
All	All	34/43 (79%)	18 (52%)	2 (5%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	O	4	A
13	O	11	C
13	O	12	U
13	O	13	U
13	O	14	U
13	O	15	U
13	O	17	U
13	O	18	U
13	O	19	U
13	O	20	U
13	O	23	U
13	O	24	U
13	O	25	C
13	O	26	U
13	O	27	U
13	O	28	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	O	29	U
13	O	31	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
13	O	17	U
13	O	18	U

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)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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.

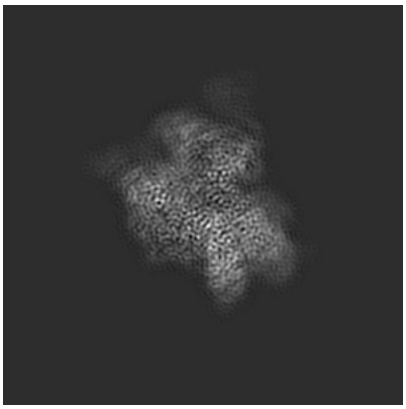
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31305. These allow visual inspection of the internal detail of the map and identification of artifacts.

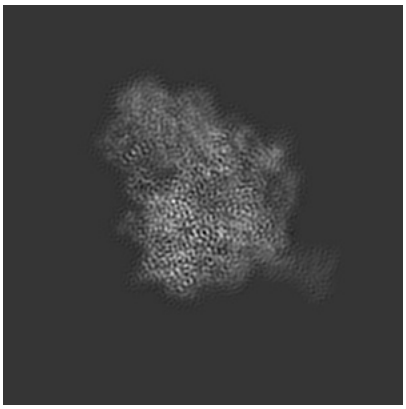
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

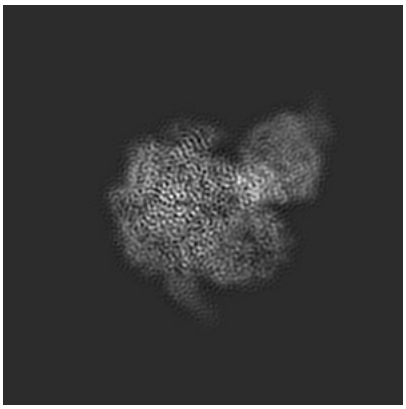
6.1.1 Primary map



X

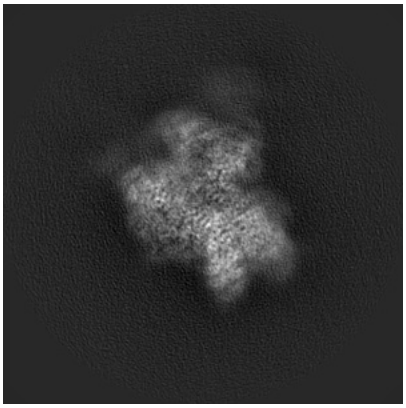


Y

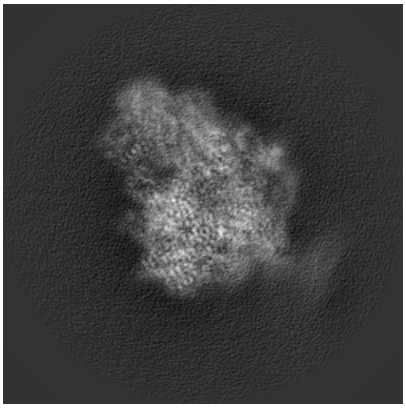


Z

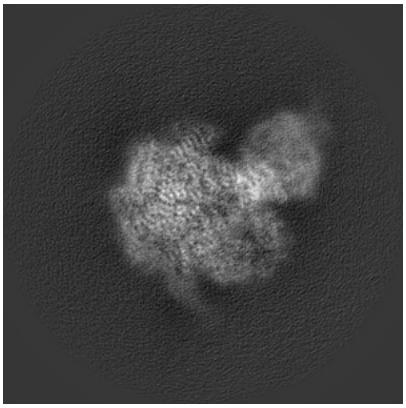
6.1.2 Raw map



X



Y

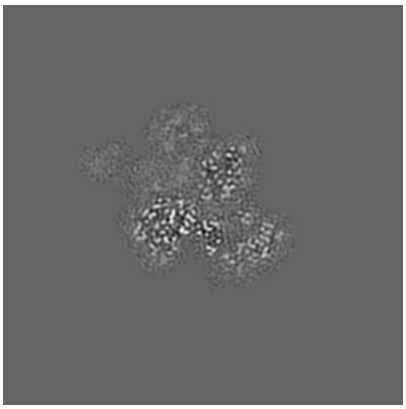


Z

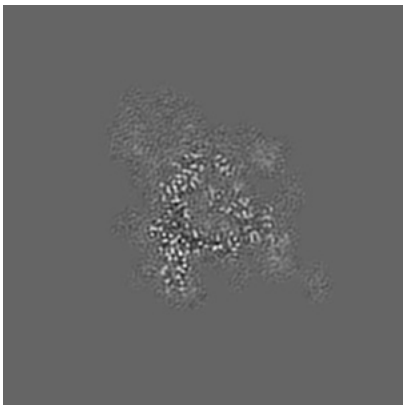
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

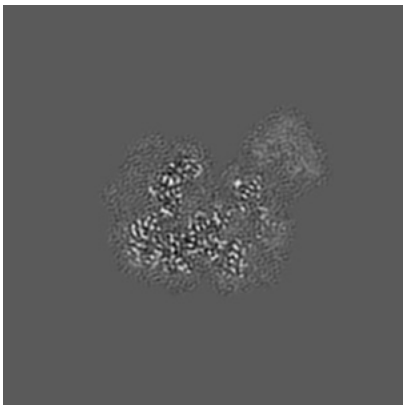
6.2.1 Primary map



X Index: 140

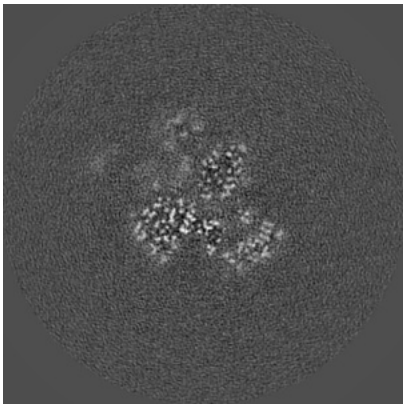


Y Index: 140

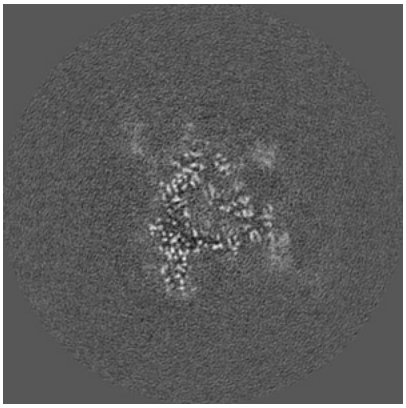


Z Index: 140

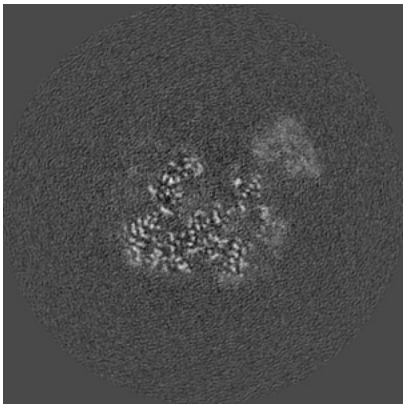
6.2.2 Raw map



X Index: 140



Y Index: 140

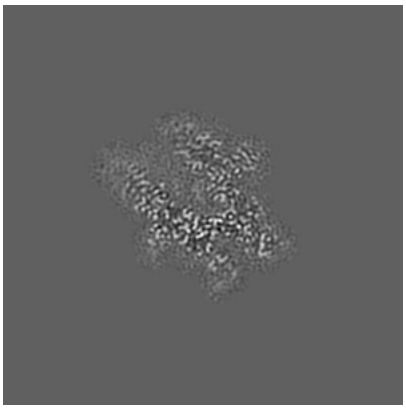


Z Index: 140

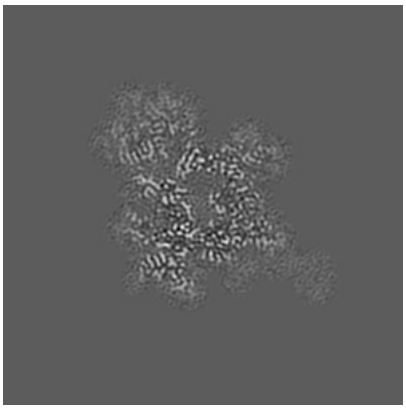
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

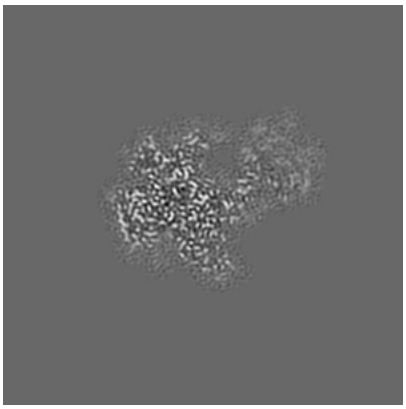
6.3.1 Primary map



X Index: 126

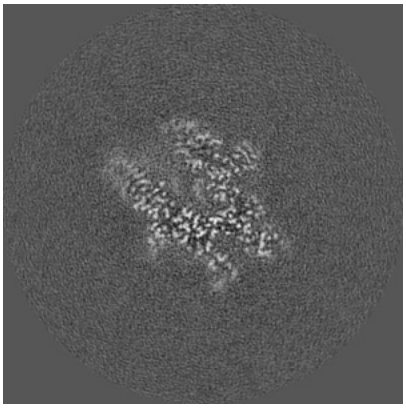


Y Index: 149

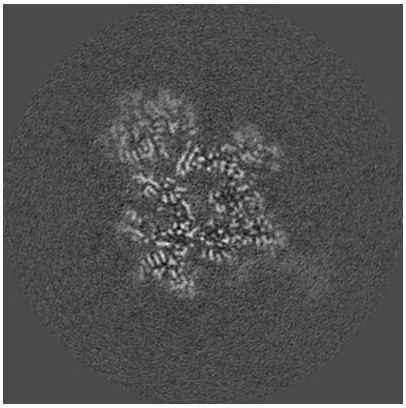


Z Index: 123

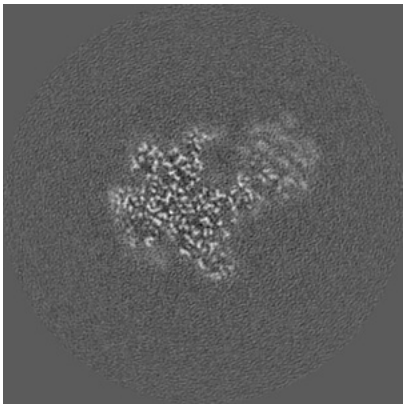
6.3.2 Raw map



X Index: 126



Y Index: 149

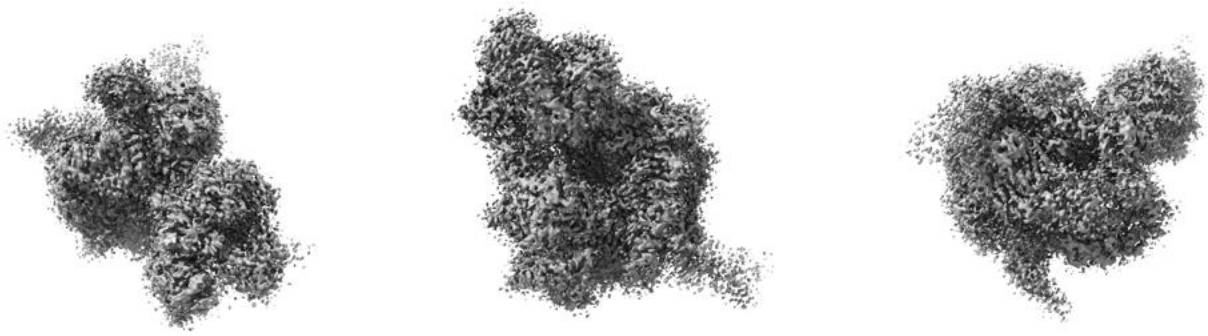


Z Index: 125

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

6.4 Orthogonal surface views (i)

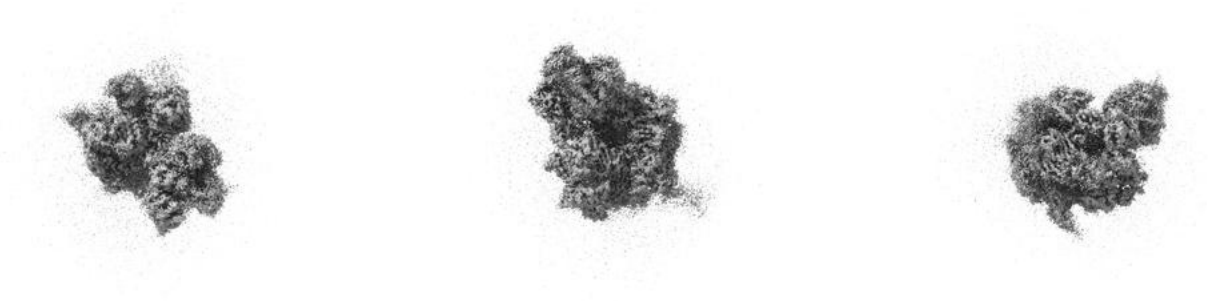
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

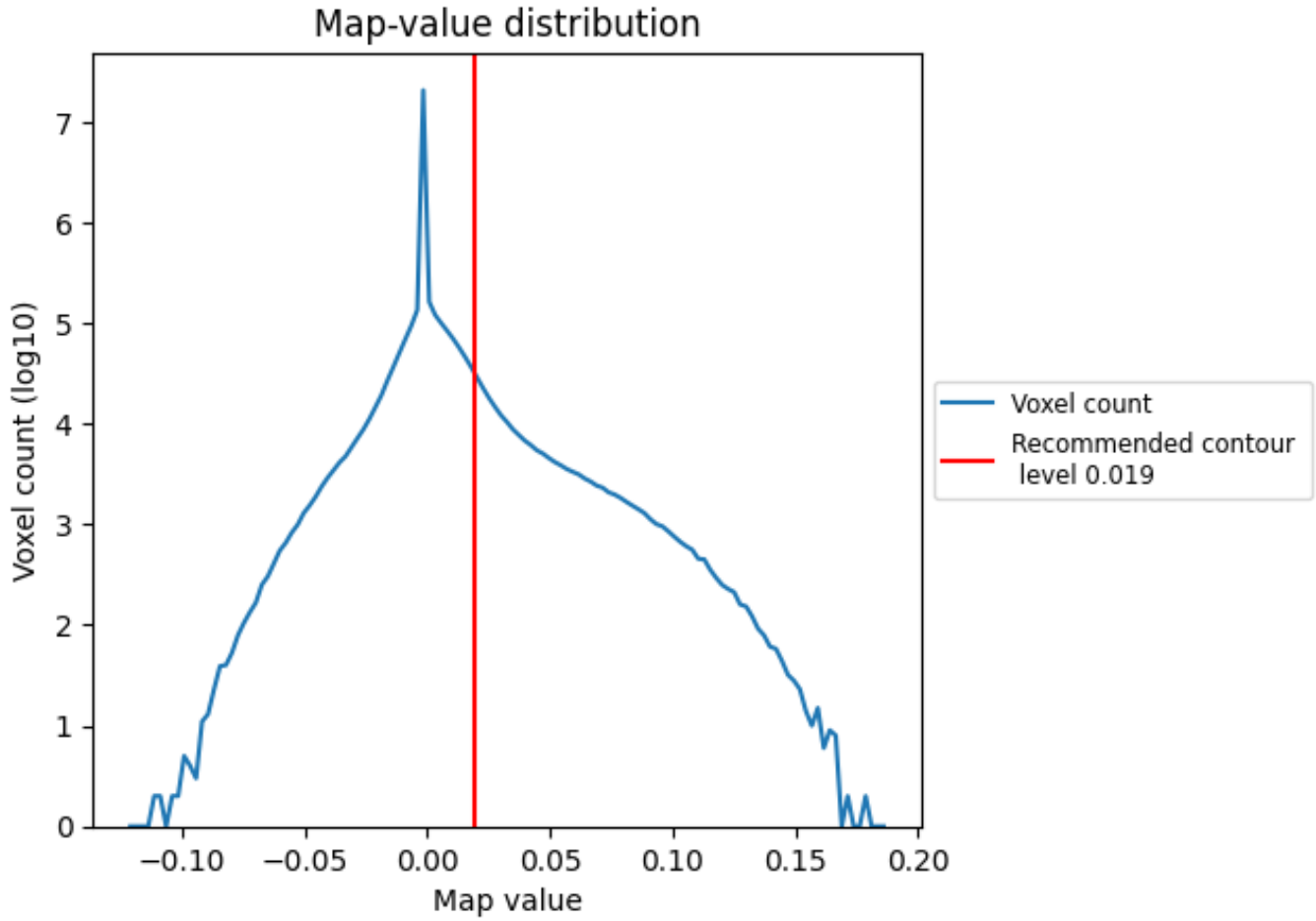
6.5 Mask visualisation (i)

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

7 Map analysis

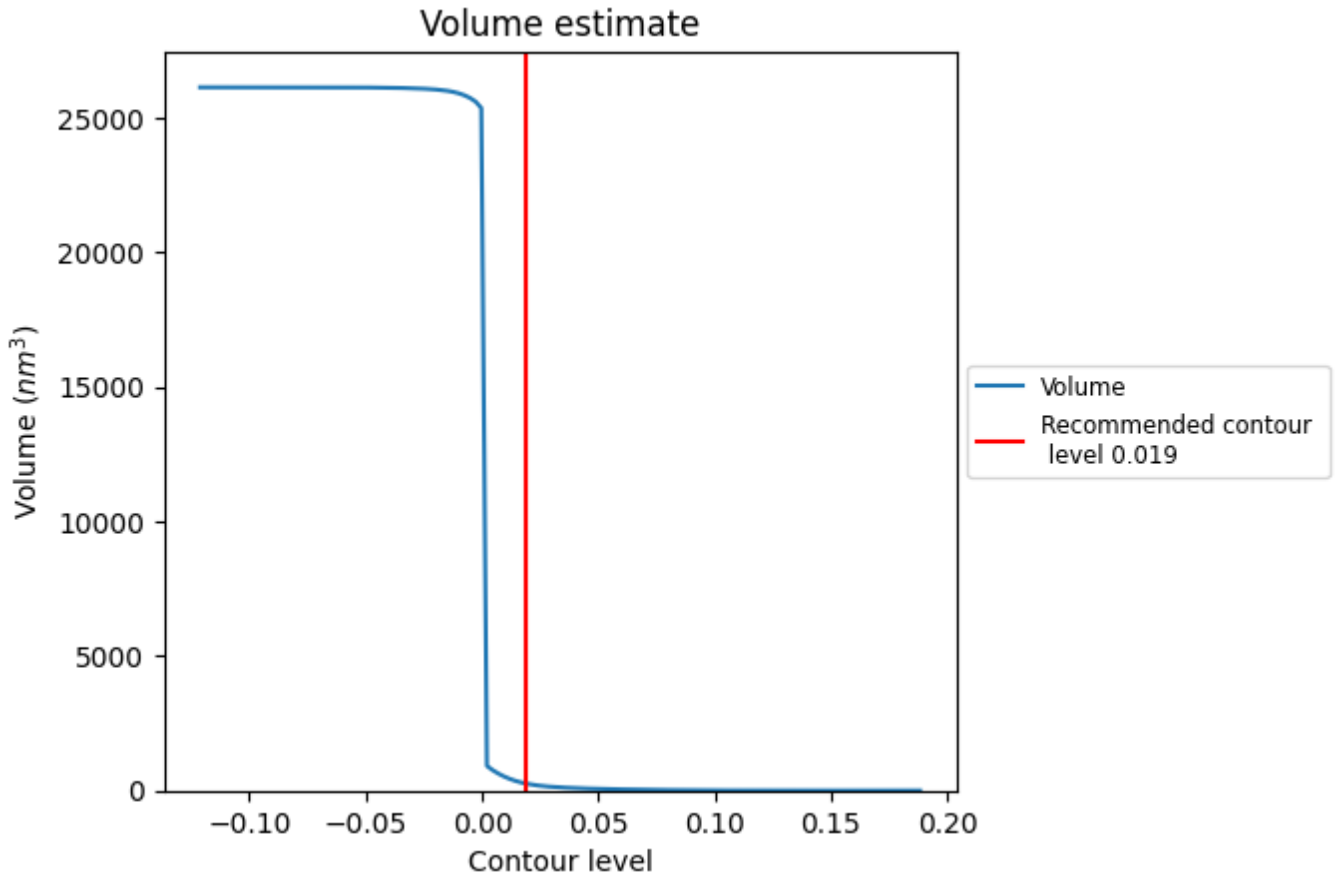
This section contains the results of statistical analysis of the map.

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.

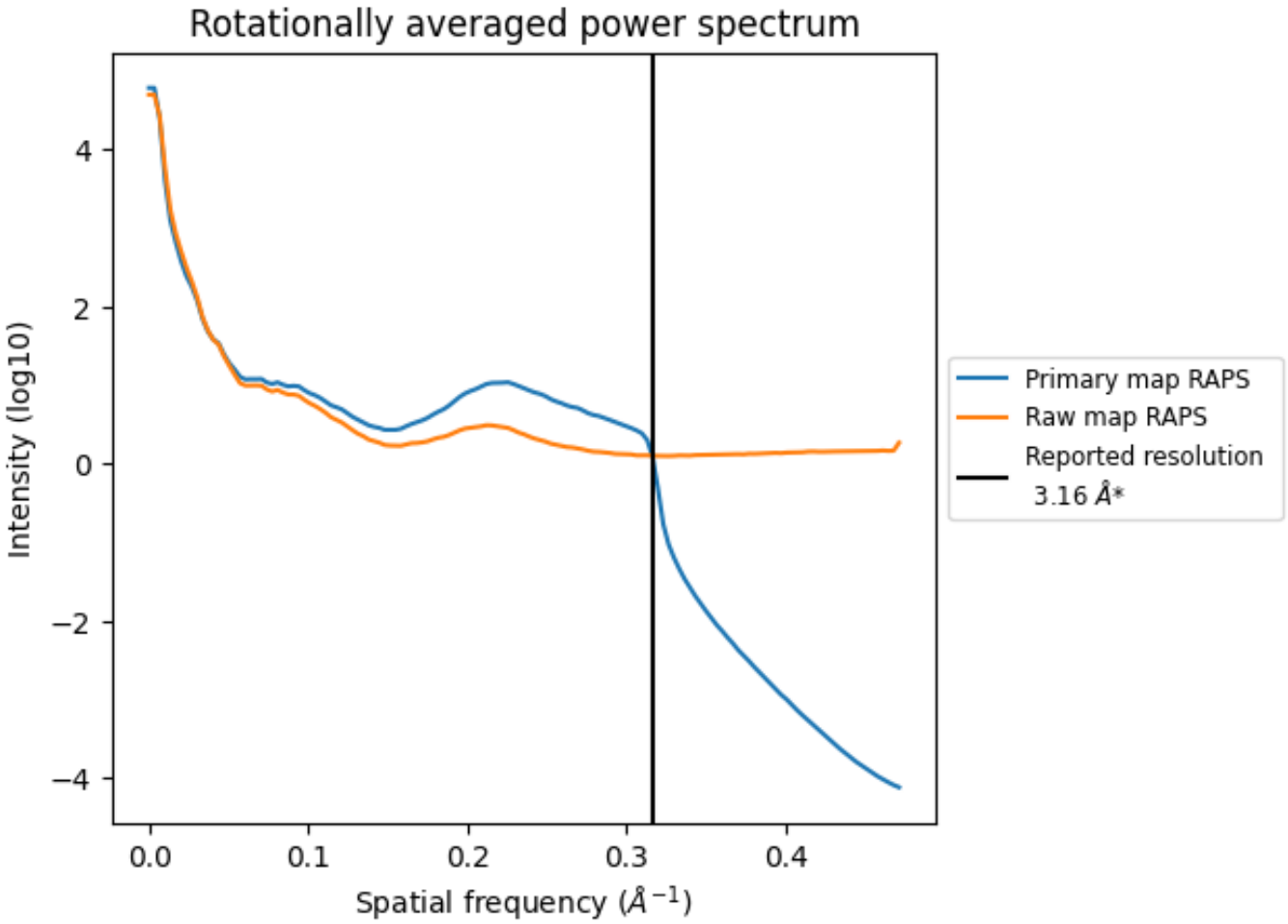
7.2 Volume estimate



The volume at the recommended contour level is 260 nm^3; this corresponds to an approximate mass of 235 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)

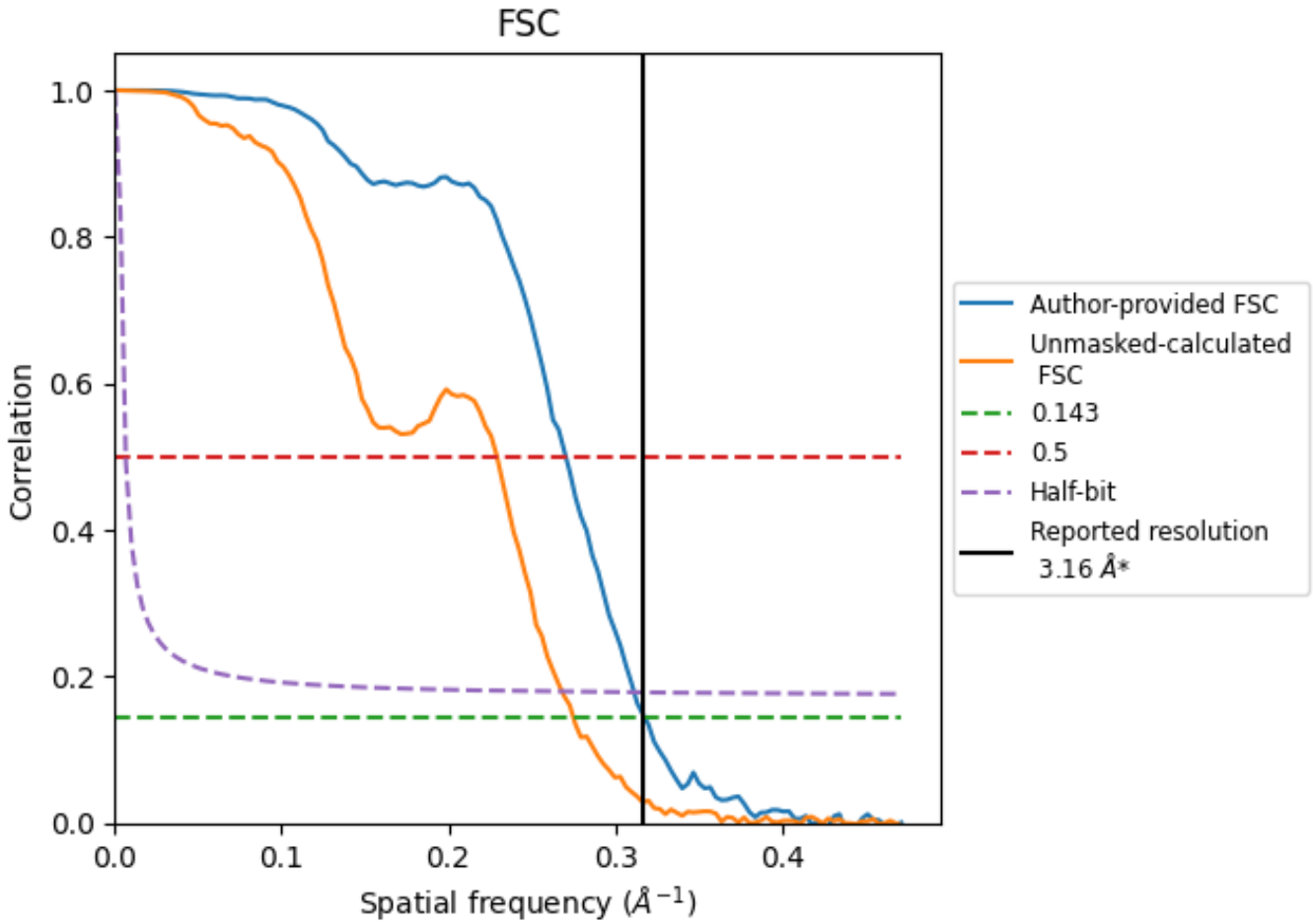


*Reported resolution corresponds to spatial frequency of 0.316 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.316 Å^{-1}

8.2 Resolution estimates (i)

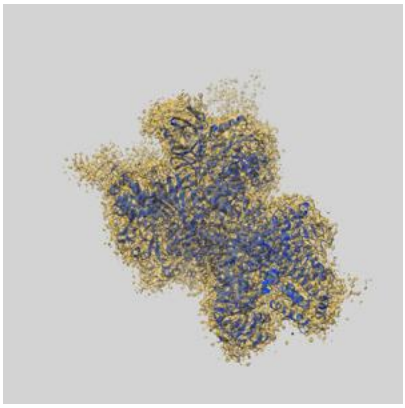
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	3.15	3.70	3.21
Unmasked-calculated*	3.64	4.36	3.73

*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 3.64 differs from the reported value 3.16 by more than 10 %

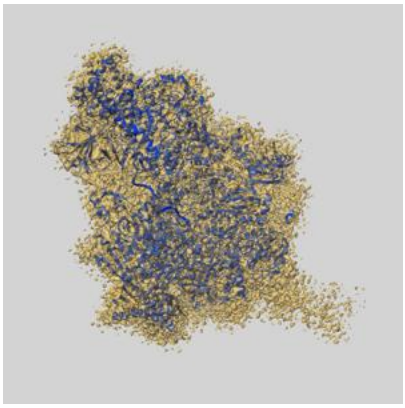
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31305 and PDB model 7EU0. Per-residue inclusion information can be found in section 3 on page 7.

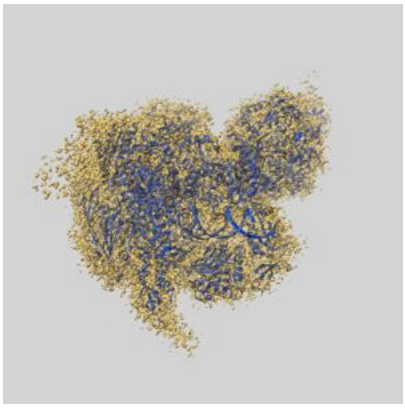
9.1 Map-model overlay



X



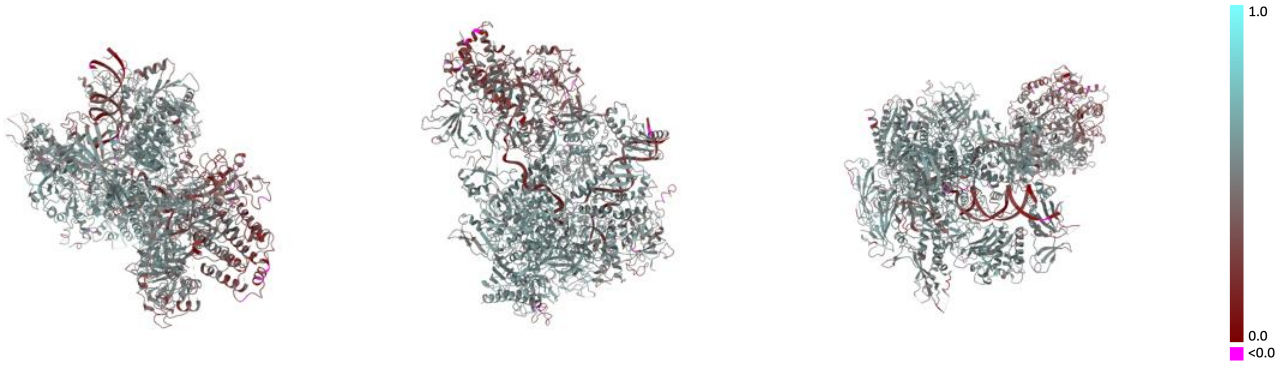
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 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.

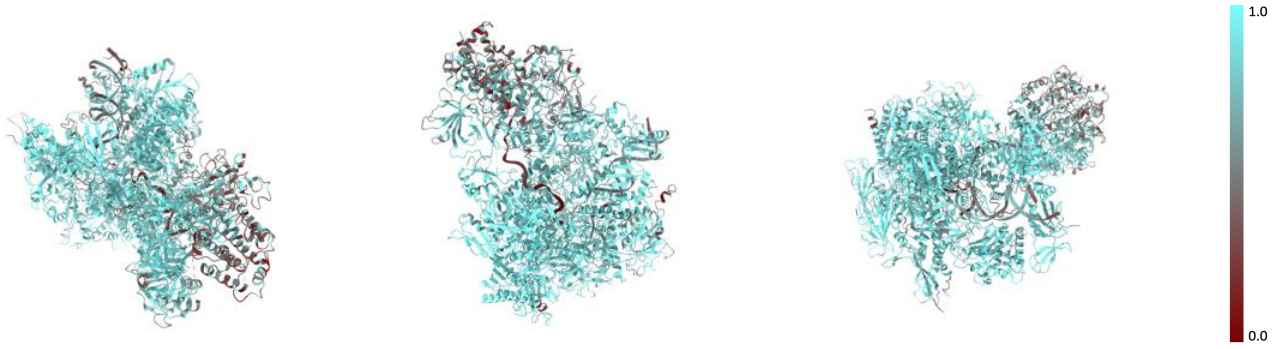
9.2 Q-score mapped to coordinate model (i)



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.

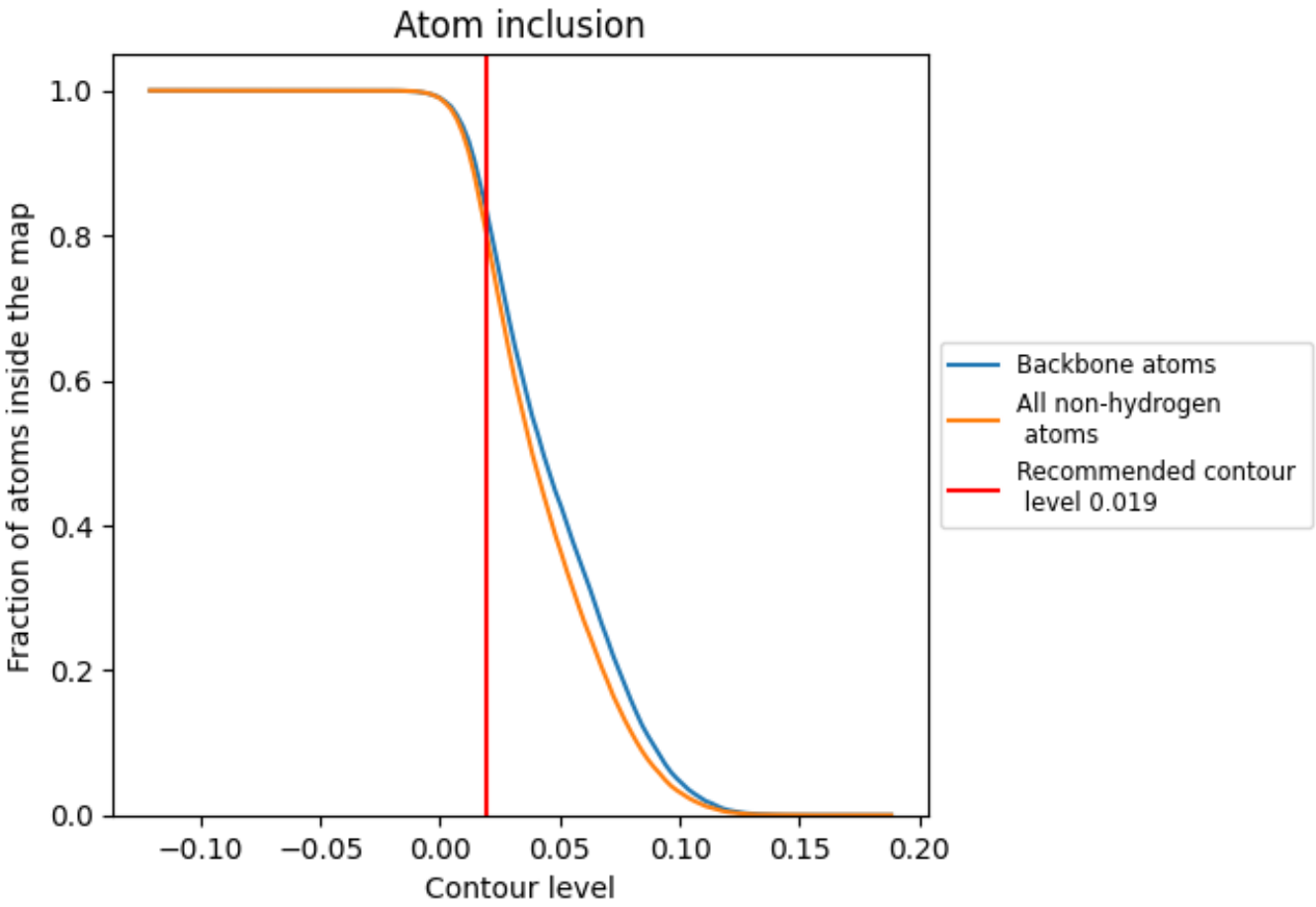
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8077	0.4870
A	0.8538	0.5240
B	0.8951	0.5420
C	0.8815	0.5240
E	0.8713	0.5010
F	0.7837	0.4820
H	0.8840	0.5250
I	0.8296	0.4990
J	0.9328	0.5660
K	0.9255	0.5620
L	0.8958	0.5170
M	0.6770	0.4160
N	0.5269	0.1950
O	0.4322	0.2660
Q	0.5793	0.2560
R	0.8049	0.4250