



# wwPDB EM Validation Summary Report ⓘ

Jun 8, 2025 – 01:59 AM JST

PDB ID : 9K3U / pdb\_00009k3u  
EMDB ID : EMD-62029  
Title : Human RNA Polymerase III de novo transcribing complex 5 (TC5)  
Authors : Wang, Q.; Ren, Y.; Jin, Q.; Chen, X.; Xu, Y.  
Deposited on : 2024-10-20  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

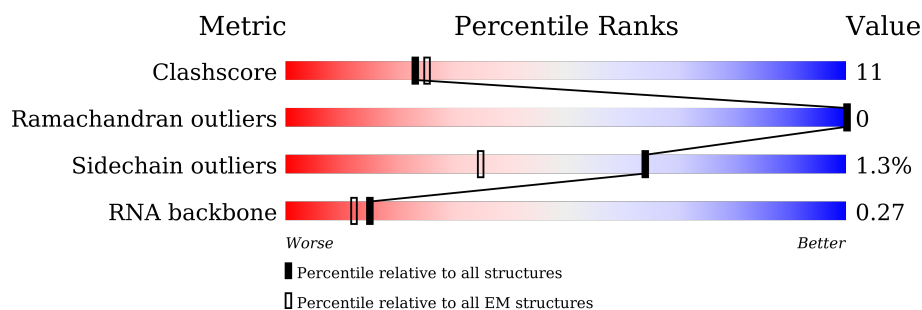
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	368	<div> <div>37%</div> <div>28% 11% 60%</div> </div>
2	3	411	<div> <div>78%</div> <div>74% 14% 9%</div> </div>
3	4	1469	<div> <div>10%</div> <div>14% 83%</div> </div>
4	A	1390	<div> <div>84%</div> <div>15%</div> </div>
5	B	1133	<div> <div>81%</div> <div>15%</div> </div>
6	C	346	<div> <div>82%</div> <div>17%</div> </div>
7	D	148	<div> <div>66%</div> <div>17% 18%</div> </div>

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Mol	Chain	Length	Quality of chain
8	E	210	
9	F	127	
10	G	204	
11	H	150	
12	I	108	
13	J	67	
14	K	133	
15	L	58	
16	M	708	
17	N	398	
18	O	534	
19	P	316	
20	Q	223	
21	U	339	
22	V	419	
23	W	2624	
24	X	97	
25	Y	97	
26	Z	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	SF4	P	401	-	-	X	-
30	GTP	Z	101	-	-	X	-

## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 56785 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 snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	146	Total	C	N	O	S	0	0
			1233	804	212	209	8		

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	374	Total	C	N	O	S	0	0
			3038	1925	521	571	21		

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	247	Total	C	N	O	S	0	0
			2066	1295	378	388	5		

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1378	Total	C	N	O	S	0	0
			10814	6850	1886	2005	73		

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	1097	Total	C	N	O	S	0	0
			8680	5499	1516	1597	68		

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	343	Total	C	N	O	S	0	0
			2736	1723	488	514	11		

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	122	Total	C	N	O	S	0	0
			985	614	172	196	3		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	166	Total	C	N	O	S	0	0
			1337	876	211	245	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	54	Total	C	N	O	S	0	0
			426	267	79	74	6		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	303	Total	C	N	O	S	0	0
			2403	1516	411	460	16		

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	178	Total	C	N	O	S	1	0
			1411	915	246	243	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 23 is a protein called Transcription factor TFIIB component B'' homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (97-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total	C	N	O	P	0	0
			1577	757	275	468	77		

- Molecule 25 is a DNA chain called DNA (97-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	77	Total	C	N	O	P	0	0
			1580	756	291	456	77		

- Molecule 26 is a RNA chain called RNA (5'-R(P\*UP\*GP\*CP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	4	Total	C	N	O	P	0	0
			83	37	12	30	4		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
27	A	2	Total	Zn	0
			2	2	
27	B	1	Total	Zn	0
			1	1	
27	I	1	Total	Zn	0
			1	1	

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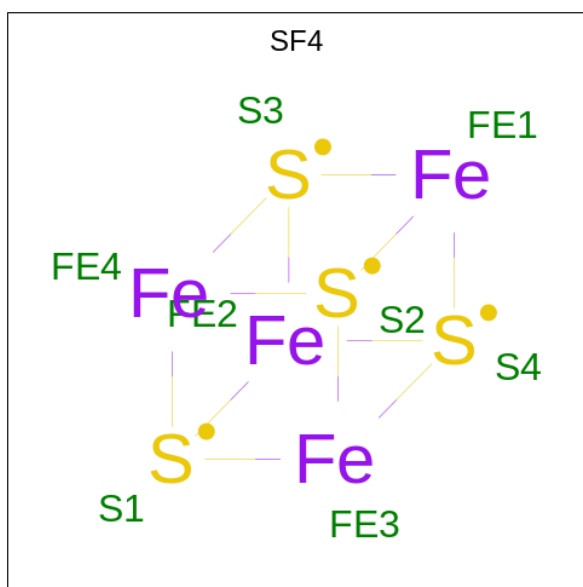
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Mol	Chain	Residues	Atoms		AltConf
27	J	1	Total	Zn	0
			1	1	
27	L	1	Total	Zn	0
			1	1	
27	V	1	Total	Zn	0
			1	1	

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Mg	0
			1	1	

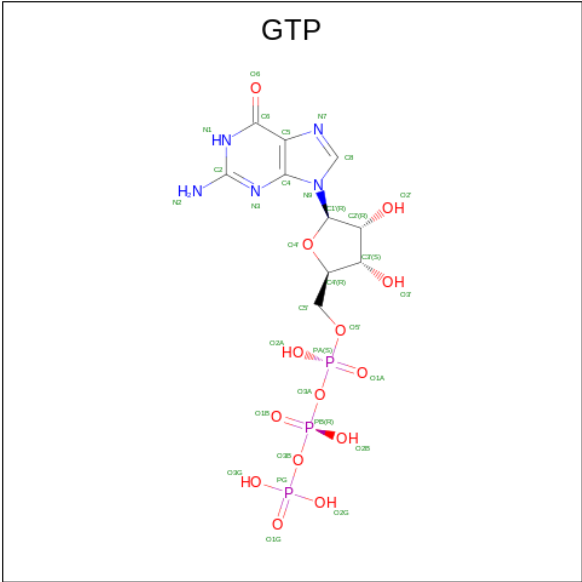
- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
29	P	1	Total	Fe	S	0
			8	4	4	

- Molecule 30 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



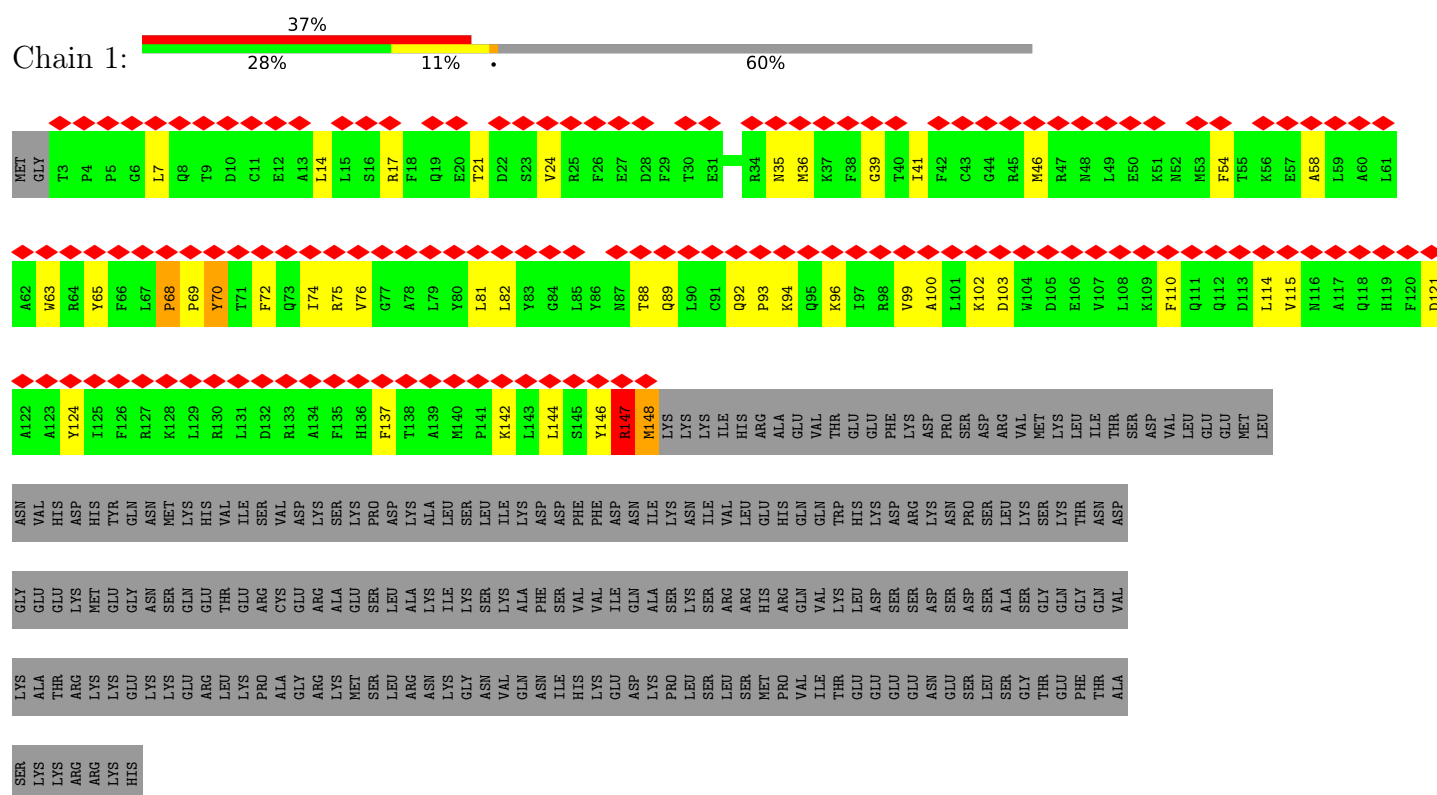


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
30	Z	1	32	10	5	14	3	0

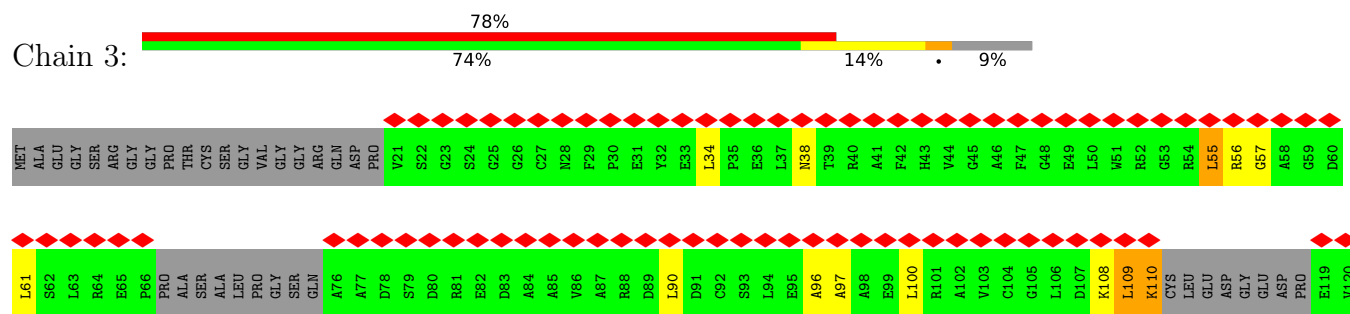
### 3 Residue-property plots [i](#)

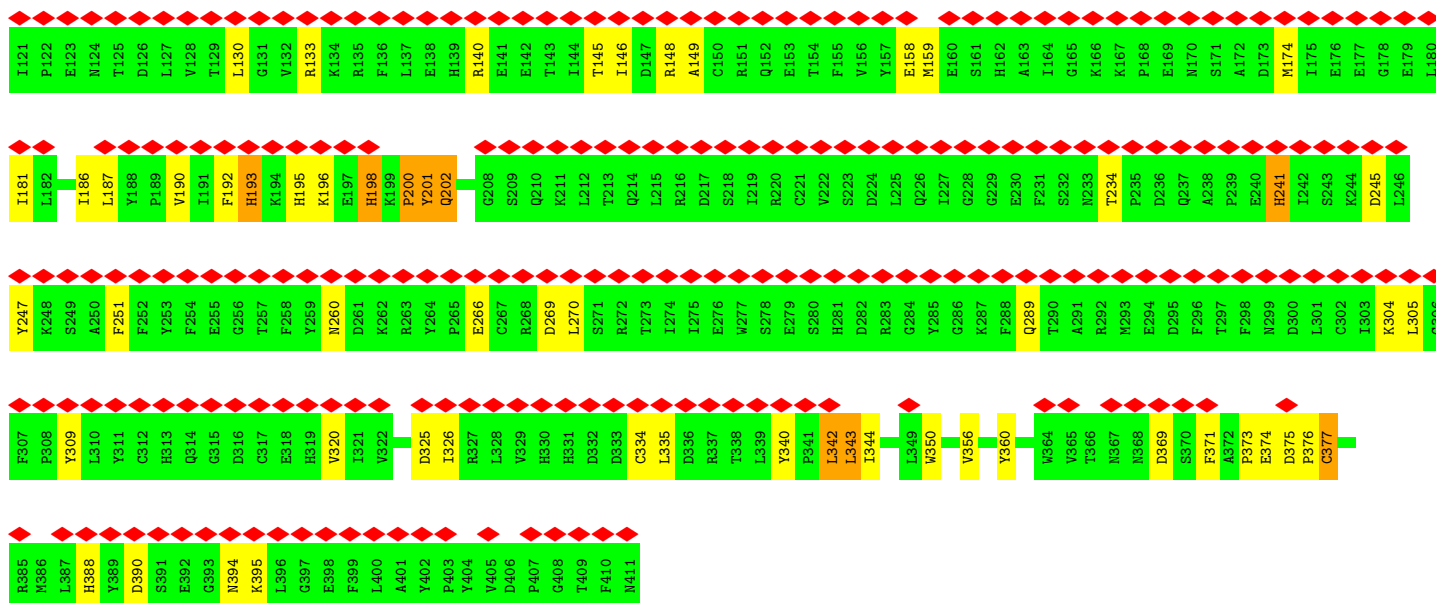
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: snRNA-activating protein complex subunit 1

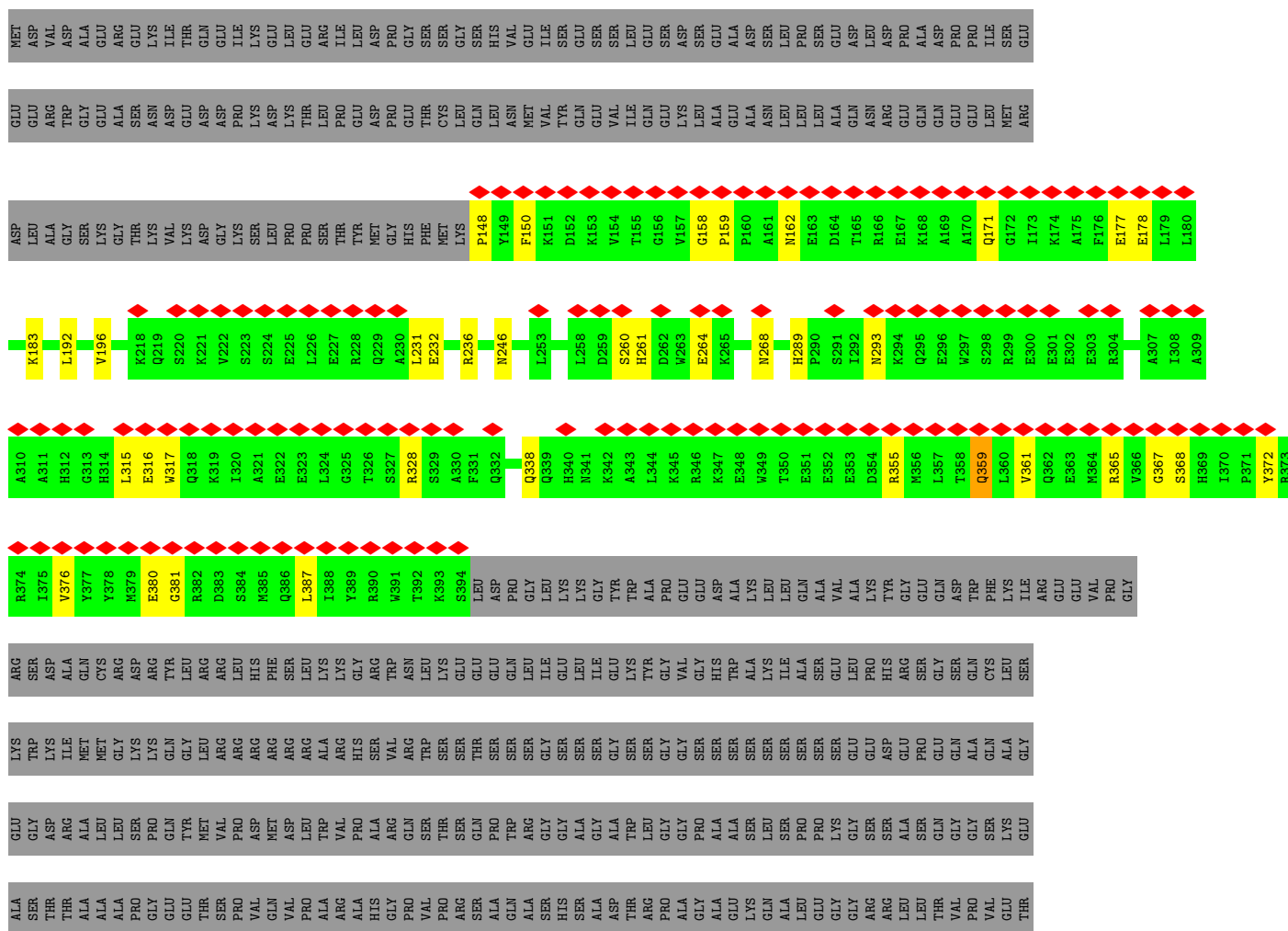


- Molecule 2: snRNA-activating protein complex subunit 3

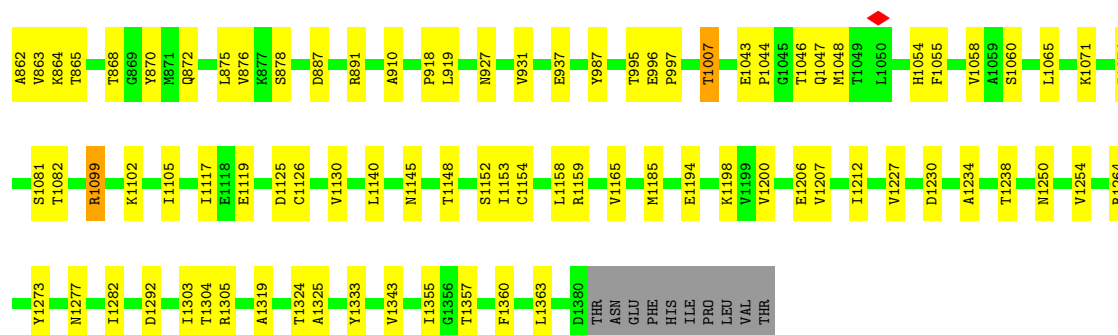




• Molecule 3: snRNA-activating protein complex subunit 4

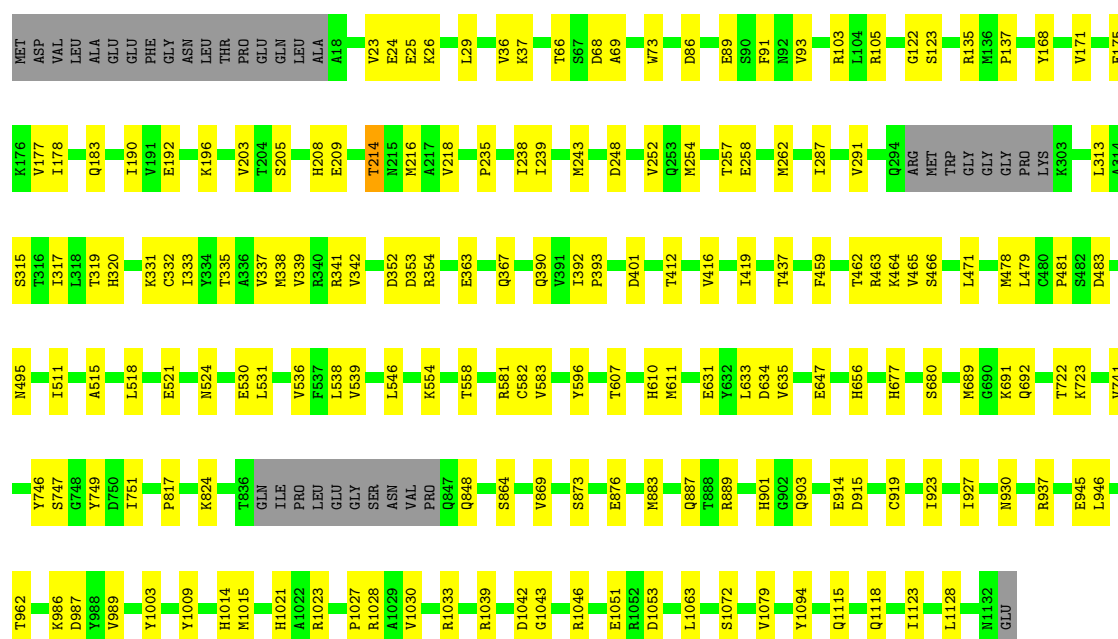






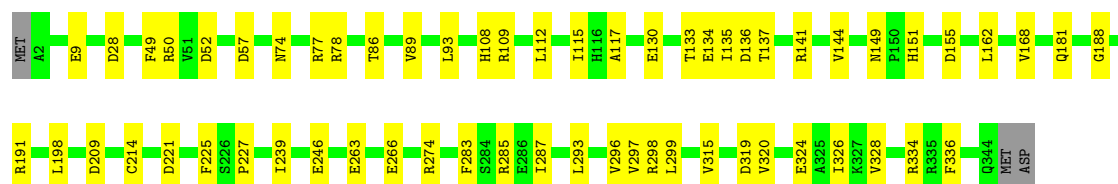
• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

Chain B: 81% 15% .



• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 82% 17% .




• Molecule 7: DNA-directed RNA polymerase III subunit RPC9

Chain D: 66% 17% 18%



ASN  
THR  
ASN  
SER  
ASN  
VAL  
ALA  
MET  
ASP  
GLU  
GLU  
ASP  
PRO  
ALA

- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:  88% 12%

MET D2 E5 L20 T29 E32 T36 E39 Q43 R54 T59 N65 D66 Q71 F75 K85 V89 M94 Q95 A102 L103 I104 V105 L118 M121 Y125 I126 L127 L135 E154 Q210

- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:  54% 6% 40%

MET SER ASN ASP GLU ASP ASN PHE ASP ASP GLY ASP ASP PHE ASP ASP VAL GLU ASP GLU GLY LEU ASP LEU GLU ASN ALA GLU GLY GLY GLN ASN VAL ILE LEU PRO SER GLY ARG PRO GLN ALA ASN GLN LYS R51 R64 R69 E84 G85 E86  
L90 E96 R107 T126 ASP

- Molecule 10: DNA-directed RNA polymerase III subunit RPC8

Chain G:  67% 15% 19%

MET F2 M7 R31 A35 C45 V59 D63 V76 D82 T89 S93 G96 V97 H98 V99 L114 Q115 K119 V128 Y131 Y132 THR GLU GLU GLU ALA HIS ASP LEU TYR MET ASP THR G145 E146 E147 I148 R151 V152 V158 D159  
P162 THR GLY PRO SER SER ASP ALA THR THR SER SER GLU GLU LEU PRO LYS LYS GLU ALA Y184 T185 T186 V187 G188 S189 I190 Q191 E192 L196 W201 THR SER ASN

- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:  79% 20%

MET A2 G3 I4 E7 D8 I9 E18 G19 K20 K21 F22 R27 L28 E33 D42 V50 F66 F67 V59 L70 Q87 F88 K95 V96 D102 E103 R111 L112 Y115 V116 R124 A129 M145 A149 PHE

- Molecule 12: DNA-directed RNA polymerase III subunit RPC10

Chain I:  46% 50%

M1 E16 H21 V49 L53 G54 GLY ALA ALA ALA TRP GLU ASN VAL ASP SER THR ALA GLU SER CYS PRO LYS CYS GLU HIS PRO ARG ALA TYR PHE MET GLN LEU GLN THR ARG SER ALA ASP GLU PRO MET MET THR THR PHE TYR LYS CYS CYS ASN ALA GLN CYS GLY HIS  
ARG TRP ARG ASP

- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

M1	I2	I3	P4		F8	T9	C10	G11		E28	Y29	T30		D36		L40	K41	R42		R46	R47	M48	L49		L65	GLU	LYS
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- Chain K:  68% 9% 23%

MET	GLU	GLU	ASP	GLN	GLU	LEU	GLU	GLU	ARG	LYS	ILE	SER	GLY	LEU	LYS	THR	SER	MET	ALA	GLU	GLY	GLU	ARG	K24	E28	A33	L44	L55	I59	M60	K61	N62	P63	E64	R87	M104	V110	L111	A126	SER	ARG	GLN	ASN	SER	THR
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- Chain L:  72% 7% 21%

MET	ASP	THR	GLN	LYS	ASP	VAL	GLN	PRO	PRO	LYS	GLN	Q13	N26	C36	R42	R58
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- Chain M:  52% 8% 40%

[illegible]

S218	E221	L225	L246	L249	M250	Q254	GLU	GLU	GLU	LYS	ASP	LYS	PRO	VAL	ALA	P264	S265	N266	L276	Q281	V291	M298	G302	S307	V308	A309	V310	L311	R312	Q322	V327	K335	D336	H341	E347	V348	R351	G352	R353	F360
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E370	V374	C378	V382	I394	I395	I396	I401	I409	H412	V415	V416	H421	L436	VAL	LVS	GLU	THR	MET	PRO	PRO	LVS	LVS	PRO	ASP	ALA	ALA	ALA	GLN	SER	SER	GLY	GLY	PRO	ALA	GLY	LEU	VAL	VAL	CYS	CYS	GLY	ASP	GLN	GLN	ARG	ILE	ILE	GLN	VAL	ALA	ALA	LVS	LVS	THR	LVS	LVS	ALA	GLN	GLN	ASN
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ALA LEU LEU LEU ARG GLU GLU LEU GLN ARG ARG LYS GLN LEU ARG VAL PRO PRO ALA VAL PRO PRO GLY GLY VAL ARG ARG LEU LYS GLU GLU PRO PRO VAL SER SER GLU GLU GLY GLY GLU GLU ASP GLU GLU GLN GLU ALA ALA GLU GLU GLU GLU PRO PRO MET ASP THR SER SER PRO PRO SER SER GLY LEU HIS SER LYS LEU ALA

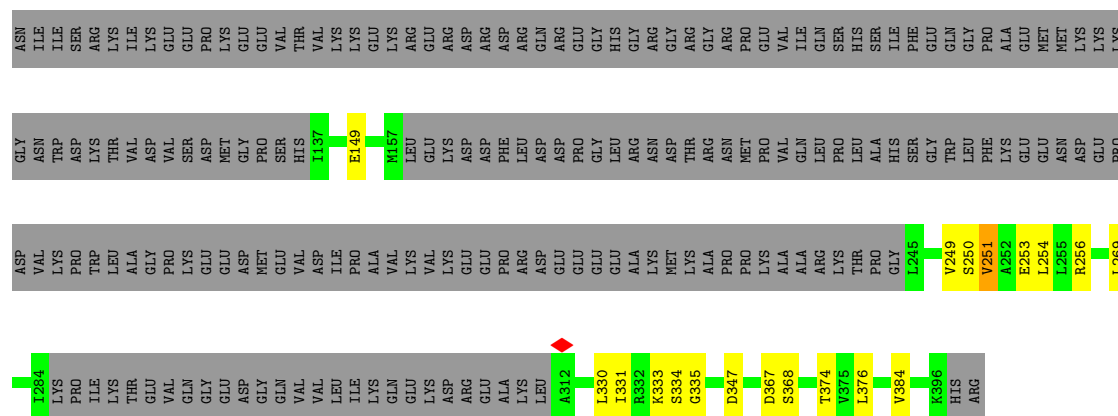
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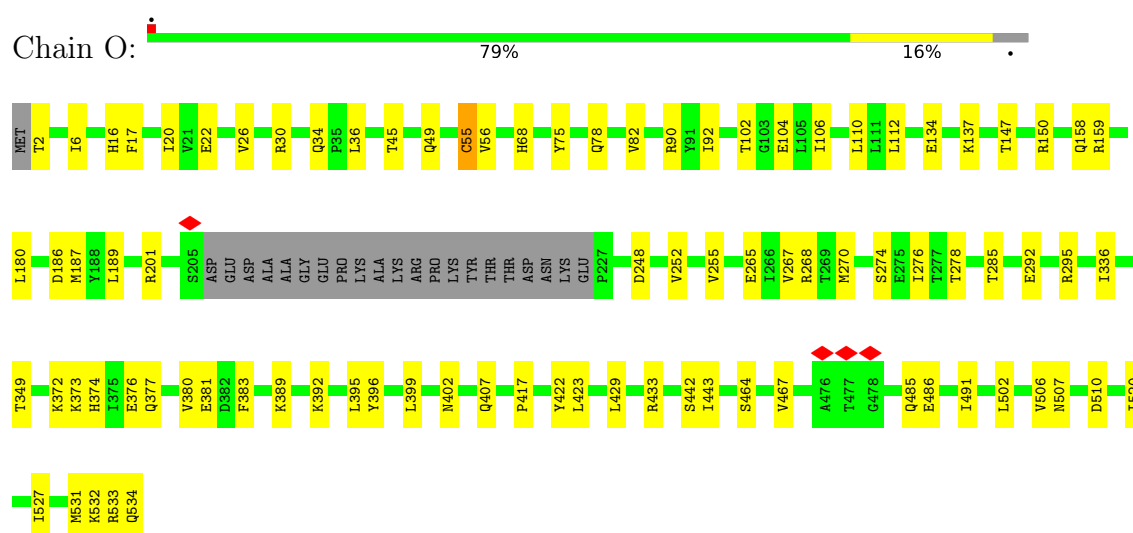
LEU LEU LEU LEU PHE LEU SER SER LYS ASN ASN TYR ARG ARG ARG ARG MET MET LYS LEU THR GLN GLU CYS GLY GLU GLY ASP LEU SER LYS GLN GLN GLU VAL VAL LYS VAL VAL LYS CYS CYS VAL SER SER TYR GLY GLY GLY MET MET TRP TYR LEU LEU LYS GLY THR VAL GLN

- Chain N:  32% 5% 63%

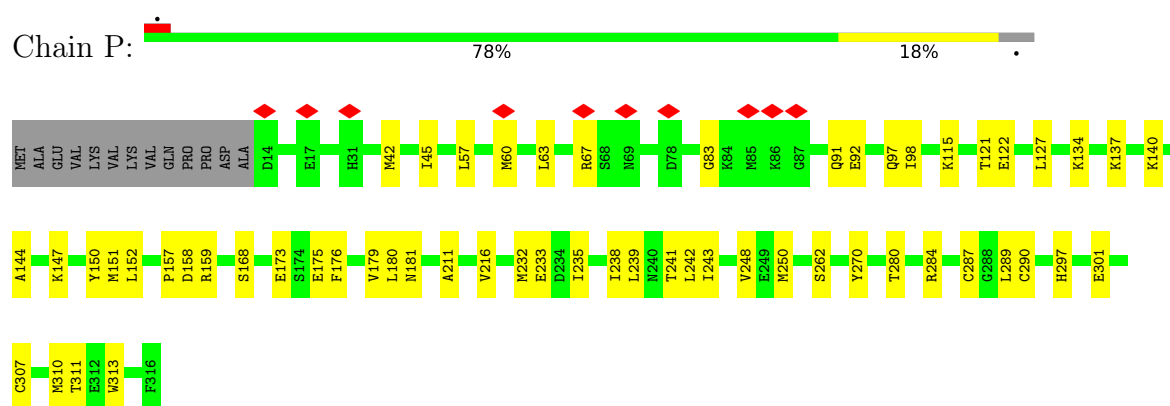
NET	SER	GLU	GLY	ASN	ALA	ALA	GLY	GLU	PRO	SER	THR	PRO	PRO	GLY	GLY	PRO	ARG	PRO	LEU	LEU	THR	THR	ALA	ALA	ARG	GLY	LEU	ILE	GLY	GLY	ARG	ARG	PRO	PRO	ALA	ALA	PRO	PRO	PRO	LEU	THR	THR	PRO	SER	ILE	ARG	SER	SER	ARG	ASP	LEU	THR	LEU	GLY	GLY	VAL	LYS	LYS	LYS	THR	PHE	THR
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• Molecule 18: DNA-directed RNA polymerase III subunit RPC3



• Molecule 19: DNA-directed RNA polymerase III subunit RPC6



• Molecule 20: DNA-directed RNA polymerase III subunit RPC7





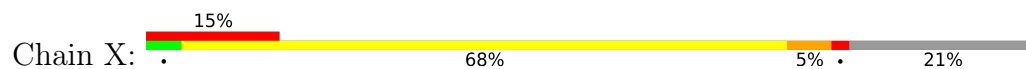






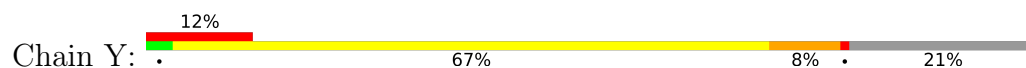
LYS	SER	ALA	GLN	GLY	ARG	ALA	PRO	LEU	ILE	GLU
THR	THR	VAL	SER	GLU	GLY	ASP	ASP	GLN	ASN	THR
GLY	GLN	GLY	LYS	LYS	ARG	LYS	PRO	LYS	ALA	ALA
GLU	GLU	GLY	LYS	ARG	ASN	GLN	SER	ASN	ASN	GLY
ALA	ALA	THR	THR	SER	TYR	SER	GLN	GLY	LEU	THR
THR	PHE	PHE	GLU	GLY	GLY	GLN	GLY	GLY	GLY	GLY
ILE	ILE	GLU	ASP	ASP	ILE	ARG	SER	LEU	ARG	ARG
GLU	PHE	GLU	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY
GLY	GLY	VAL	VAL	ASP	LEU	ARG	ARG	PRO	PRO	PRO
THR	THR	GLU	GLU	GLU	PRO	ARG	ARG	LEU	LEU	LEU
GLU	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG</

- Molecule 24: DNA (97-MER)

[illegible]

DC	DG	DA	DA	DA	DC	DC	DA	DC	C-1	G0	T1	G2	C3	T4	A5	A6	C7	T8	T9	C10	G11	G12	C13	A14	G15	C16	A17	C18	A19	T20	T21	A22	A23	C24	T25	A26	A27
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- Molecule 25: DNA (97-MER)



T-27	T-26	A-25	G-24	T-23	A-22	T-21	A-20	T-19	G-18	T-17	G-16	C-15	T-14	G-13	C-12	C-11	G-10	A-9	A-8	G-7	T-6	T-5	A-4	G-3	C-2	A-1	C0	G0	C1	G1	DG	DG	DG	DG	DT	DT	DT	DT	DC	DC	DG	DG	DC	DC	C12	C13	T14	T15	C16	C17	A18	A18	C19	A20	A21	G22	A23	A23	A24	A25	T26	A27	T28	A29	A30	A31	C32
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C33	C34	A35	A36	C37	A38	A39	A40	T41	C42	C43	A44	A45	A46	T47	A48	C49	T50	T51	T52	C53	A54	A55	G56	T57	T58	A59	DC	DG	DG	DT	DT	DA	DA	DG	DG	DC	DA	DT
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- Molecule 26: RNA (5'-R(P\*UP\*GP\*CP\*U)-3')



U2	G3	C4	U5
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	397000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.367	Depositor
Minimum map value	-5.842	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.172	Depositor
Map size (Å)	429.07724, 429.07724, 429.07724	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332538, 1.332538, 1.332538	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, SF4, 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	1	0.25	0/1266	0.60	3/1708 (0.2%)
2	3	0.23	0/3113	0.55	5/4206 (0.1%)
3	4	0.12	0/2107	0.30	0/2828
4	A	0.12	0/11008	0.25	0/14842
5	B	0.11	0/8845	0.25	0/11930
6	C	0.12	0/2790	0.25	0/3782
7	D	0.12	0/997	0.26	0/1343
8	E	0.12	0/1745	0.24	0/2358
9	F	0.13	0/620	0.24	0/839
10	G	0.12	0/1374	0.27	0/1868
11	H	0.12	0/1207	0.24	0/1628
12	I	0.14	0/434	0.24	0/584
13	J	0.14	0/521	0.25	0/703
14	K	0.12	0/837	0.28	0/1129
15	L	0.15	0/394	0.28	0/524
16	M	0.11	0/3455	0.24	0/4673
17	N	0.12	0/1137	0.25	0/1530
18	O	0.12	0/4141	0.25	0/5592
19	P	0.11	0/2446	0.24	0/3301
20	Q	0.14	0/777	0.25	0/1050
21	U	0.23	0/1439	0.54	3/1938 (0.2%)
22	V	0.38	2/2904 (0.1%)	0.42	6/3941 (0.2%)
23	W	0.14	0/967	0.30	0/1293
24	X	0.44	4/1765 (0.2%)	0.88	13/2720 (0.5%)
25	Y	0.54	6/1773 (0.3%)	0.82	16/2731 (0.6%)
26	Z	1.67	1/91 (1.1%)	2.63	14/139 (10.1%)
All	All	0.21	13/58153 (0.0%)	0.39	60/79180 (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
1	1	0	1
4	A	0	1
24	X	0	2
25	Y	0	1
All	All	0	5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z	5	U	C3'-O3'	10.14	1.57	1.42
24	X	-56	DC	O3'-P	-9.44	1.47	1.61
25	Y	0	DC	O3'-P	-9.33	1.47	1.61
25	Y	15	DT	C4'-O4'	7.90	1.61	1.45
22	V	41	THR	CA-C	-7.80	1.42	1.53

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	193	HIS	CA-CB-CG	-18.84	94.95	113.80
25	Y	54	DA	O3'-P-O5'	-17.59	77.62	104.00
24	X	-47	DA	C5'-C4'-O4'	16.06	133.49	109.40
24	X	-54	DT	O3'-P-O5'	-14.31	82.53	104.00
24	X	-50	DA	C2'-C3'-O3'	-13.85	90.72	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	147	ARG	Sidechain
4	A	1099	ARG	Sidechain
24	X	-47	DA	Sidechain
24	X	-48	DT	Sidechain
25	Y	0	DC	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1233	0	1231	42	0
2	3	3038	0	2911	94	0
3	4	2066	0	2049	31	0
4	A	10814	0	11059	219	0
5	B	8680	0	8805	125	0
6	C	2736	0	2712	43	0
7	D	985	0	1006	18	0
8	E	1715	0	1733	17	0
9	F	610	0	642	7	0
10	G	1337	0	1306	23	0
11	H	1186	0	1147	23	0
12	I	426	0	429	4	0
13	J	512	0	525	8	0
14	K	822	0	810	11	0
15	L	388	0	393	3	0
16	M	3382	0	3376	73	0
17	N	1128	0	1181	17	0
18	O	4075	0	4149	120	0
19	P	2403	0	2408	74	0
20	Q	754	0	759	33	0
21	U	1411	0	1501	58	0
22	V	2853	0	2890	52	0
23	W	943	0	924	20	0
24	X	1577	0	877	214	0
25	Y	1580	0	871	197	0
26	Z	83	0	42	28	0
27	A	2	0	0	0	0
27	B	1	0	0	0	0
27	I	1	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
27	V	1	0	0	0	0
28	A	1	0	0	0	0
29	P	8	0	0	2	0
30	Z	32	0	11	20	0
All	All	56785	0	55747	1222	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 11.

The worst 5 of 1222 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)
24:X:-55:DT:C6	24:X:-54:DT:H71	1.52	1.42
24:X:-49:DG:H22	25:Y:49:DC:N4	1.15	1.42
24:X:-49:DG:N2	25:Y:49:DC:H42	1.09	1.40
26:Z:2:U:OP1	30:Z:101:GTP:C3'	1.82	1.28
26:Z:2:U:P	30:Z:101:GTP:O3'	2.00	1.20

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	1	144/368 (39%)	131 (91%)	13 (9%)	0	100	100
2	3	368/411 (90%)	350 (95%)	18 (5%)	0	100	100
3	4	245/1469 (17%)	234 (96%)	11 (4%)	0	100	100
4	A	1376/1390 (99%)	1348 (98%)	28 (2%)	0	100	100
5	B	1091/1133 (96%)	1058 (97%)	33 (3%)	0	100	100
6	C	341/346 (99%)	335 (98%)	6 (2%)	0	100	100
7	D	120/148 (81%)	117 (98%)	3 (2%)	0	100	100
8	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
9	F	74/127 (58%)	70 (95%)	4 (5%)	0	100	100
10	G	160/204 (78%)	150 (94%)	10 (6%)	0	100	100
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	52/108 (48%)	51 (98%)	1 (2%)	0	100	100
13	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
14	K	101/133 (76%)	98 (97%)	3 (3%)	0	100	100
15	L	44/58 (76%)	41 (93%)	3 (7%)	0	100	100
16	M	418/708 (59%)	404 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	N	140/398 (35%)	140 (100%)	0	0	100	100
18	O	508/534 (95%)	495 (97%)	13 (3%)	0	100	100
19	P	301/316 (95%)	294 (98%)	7 (2%)	0	100	100
20	Q	85/223 (38%)	83 (98%)	2 (2%)	0	100	100
21	U	177/339 (52%)	174 (98%)	3 (2%)	0	100	100
22	V	358/419 (85%)	347 (97%)	11 (3%)	0	100	100
23	W	109/2624 (4%)	101 (93%)	8 (7%)	0	100	100
All	All	6628/11883 (56%)	6430 (97%)	198 (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	1	130/334 (39%)	122 (94%)	8 (6%)	15	45
2	3	330/356 (93%)	313 (95%)	17 (5%)	19	52
3	4	221/1213 (18%)	215 (97%)	6 (3%)	40	71
4	A	1200/1212 (99%)	1192 (99%)	8 (1%)	81	91
5	B	959/988 (97%)	956 (100%)	3 (0%)	91	96
6	C	299/302 (99%)	298 (100%)	1 (0%)	91	96
7	D	114/136 (84%)	114 (100%)	0	100	100
8	E	191/192 (100%)	191 (100%)	0	100	100
9	F	66/111 (60%)	66 (100%)	0	100	100
10	G	149/181 (82%)	148 (99%)	1 (1%)	81	91
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	48/93 (52%)	48 (100%)	0	100	100
13	J	53/56 (95%)	52 (98%)	1 (2%)	52	79
14	K	92/119 (77%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	L	43/55 (78%)	43 (100%)	0	100	100
16	M	377/622 (61%)	377 (100%)	0	100	100
17	N	131/347 (38%)	130 (99%)	1 (1%)	79	90
18	O	458/476 (96%)	457 (100%)	1 (0%)	92	97
19	P	269/280 (96%)	268 (100%)	1 (0%)	89	95
20	Q	84/195 (43%)	83 (99%)	1 (1%)	67	86
21	U	154/293 (53%)	144 (94%)	10 (6%)	14	43
22	V	325/365 (89%)	314 (97%)	11 (3%)	32	66
23	W	102/2381 (4%)	97 (95%)	5 (5%)	21	54
All	All	5924/10438 (57%)	5849 (99%)	75 (1%)	64	85

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	U	299	ARG
23	W	291	TYR
22	V	43	THR
22	V	247	LEU
2	3	377	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
18	O	534	GLN
21	U	166	GLN
4	A	469	HIS
4	A	423	GLN
22	V	49	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	Z	4/4 (100%)	1 (25%)	1 (25%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	Z	5	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	Z	2	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
30	GTP	Z	101	-	26,34,34	1.64	4 (15%)	32,54,54	3.64	16 (50%)
29	SF4	P	401	19	0,12,12	-	-	-		

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
30	GTP	Z	101	-	-	4/18/38/38	0/3/3/3
29	SF4	P	401	19	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Z	101	GTP	C6-N1	-5.48	1.29	1.37
30	Z	101	GTP	C5-C6	-3.22	1.40	1.47
30	Z	101	GTP	C2-N1	-2.63	1.31	1.37
30	Z	101	GTP	C3'-C4'	-2.32	1.47	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Z	101	GTP	C3'-C2'-C1'	9.36	115.08	100.98
30	Z	101	GTP	O4'-C1'-C2'	-8.59	94.38	106.93
30	Z	101	GTP	PB-O3B-PG	-7.19	108.17	132.83
30	Z	101	GTP	PA-O3A-PB	-7.08	108.54	132.83
30	Z	101	GTP	O6-C6-C5	-4.95	114.70	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	Z	101	GTP	C5'-O5'-PA-O3A
30	Z	101	GTP	O4'-C4'-C5'-O5'
30	Z	101	GTP	C3'-C4'-C5'-O5'
30	Z	101	GTP	C5'-O5'-PA-O1A

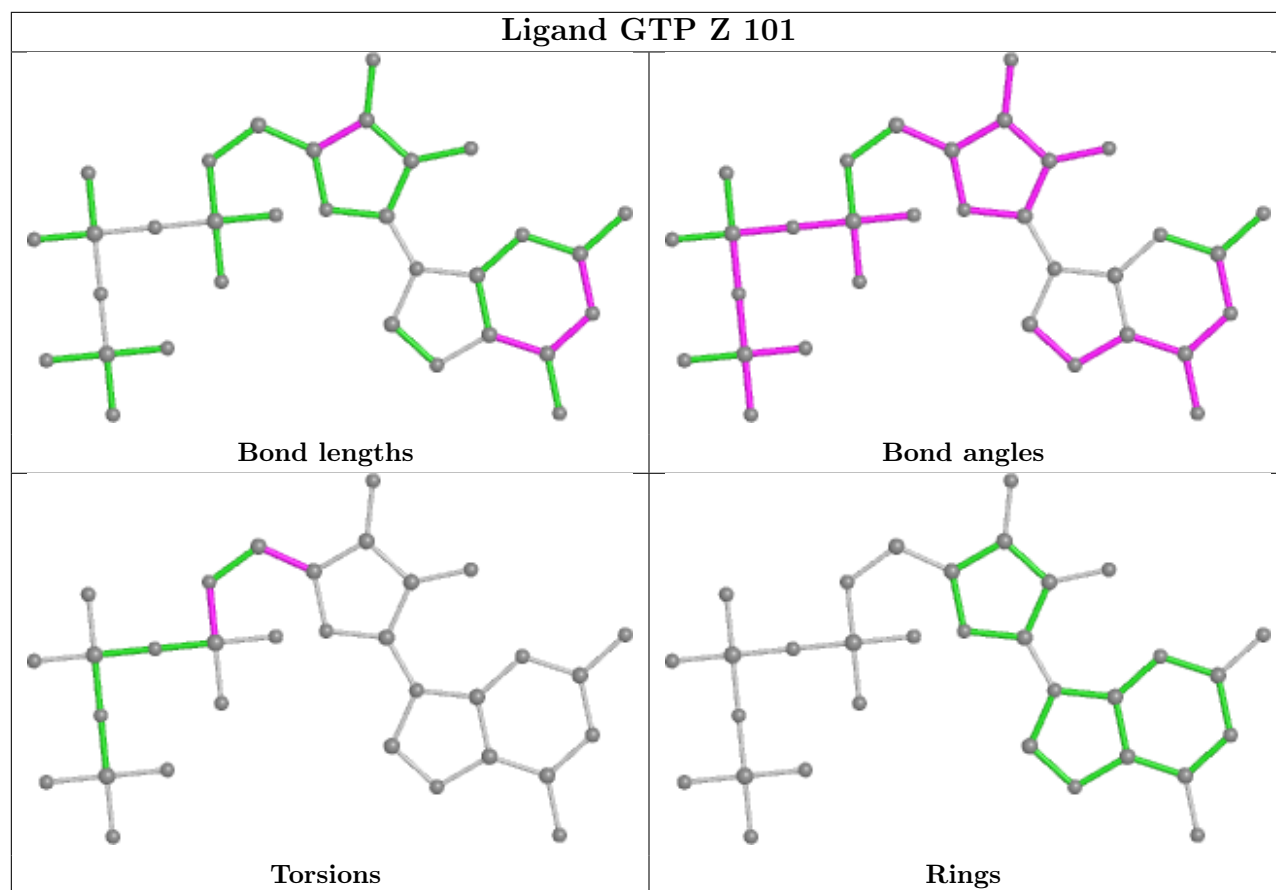
There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	Z	101	GTP	20	0
29	P	401	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

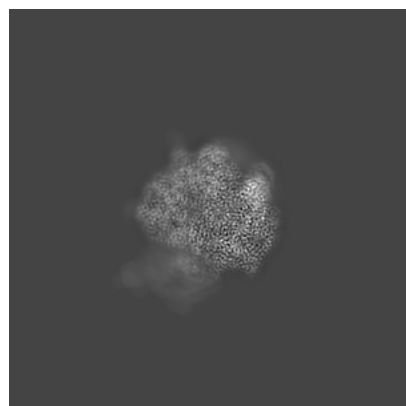
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62029. These allow visual inspection of the internal detail of the map and identification of artifacts.

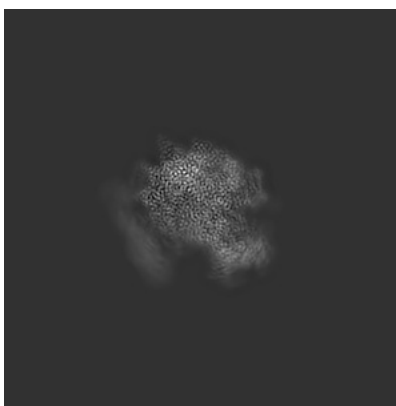
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

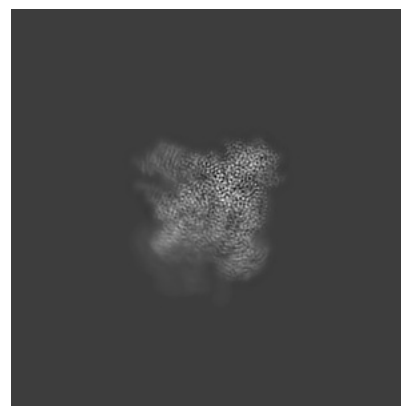
#### 6.1.1 Primary map



X

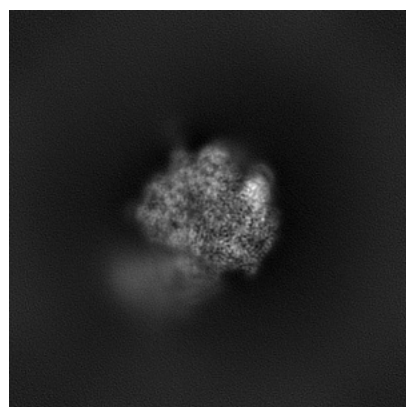


Y

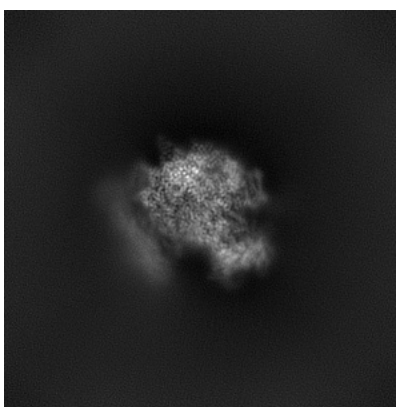


Z

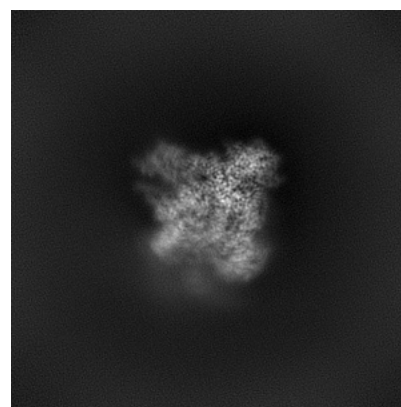
#### 6.1.2 Raw map



X



Y

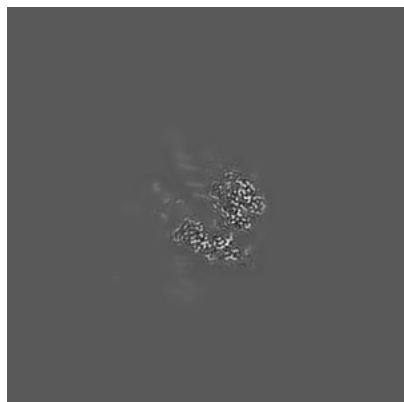


Z

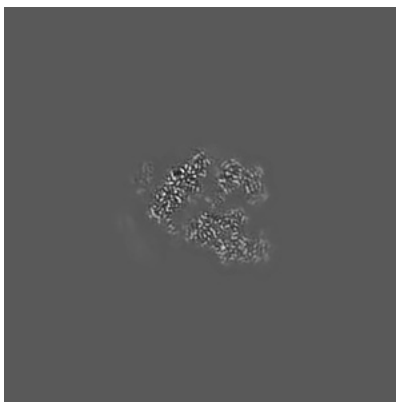
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

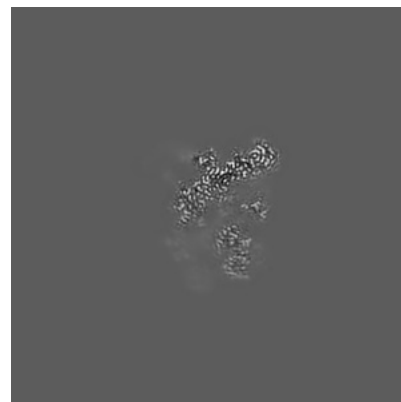
### 6.2.1 Primary map



X Index: 161

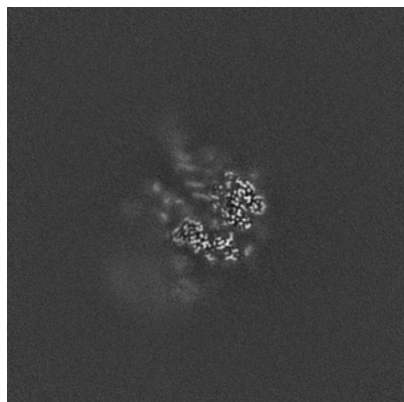


Y Index: 161

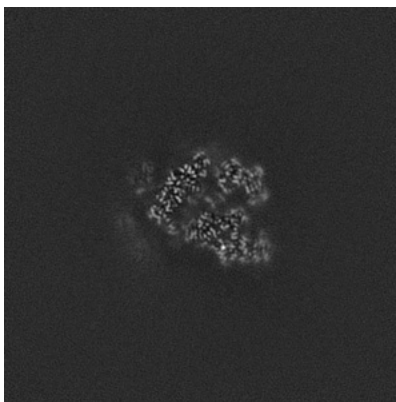


Z Index: 161

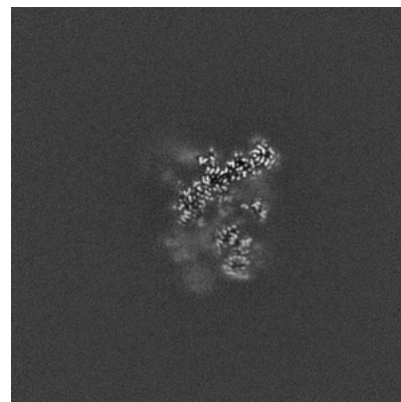
### 6.2.2 Raw map



X Index: 161



Y Index: 161



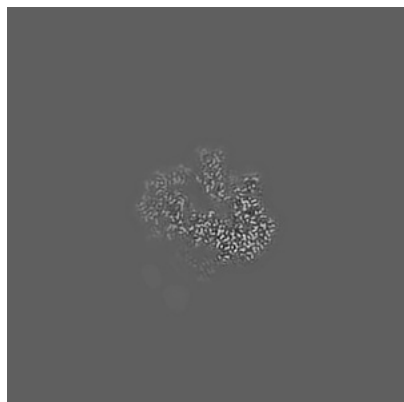
Z Index: 161

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

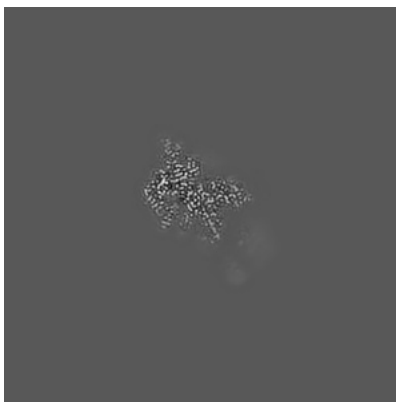


## 6.3 Largest variance slices [i](#)

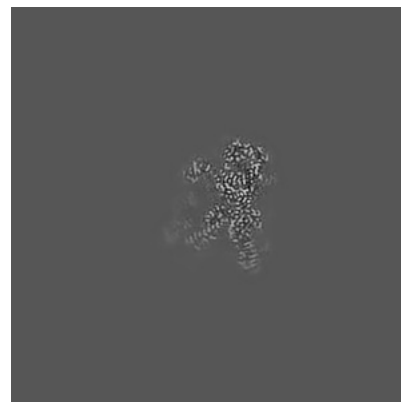
### 6.3.1 Primary map



X Index: 182

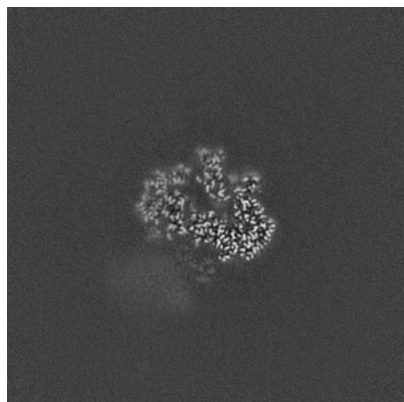


Y Index: 181

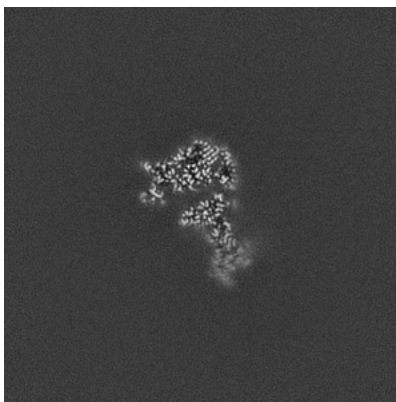


Z Index: 142

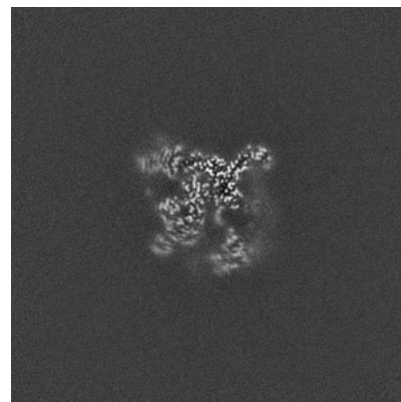
### 6.3.2 Raw map



X Index: 182



Y Index: 198

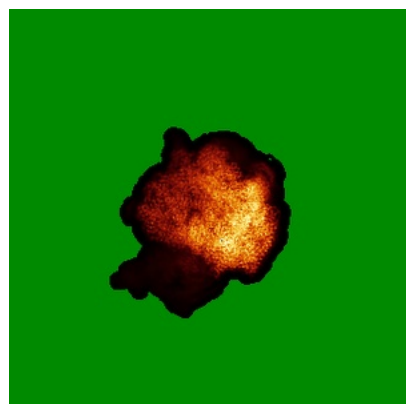


Z Index: 174

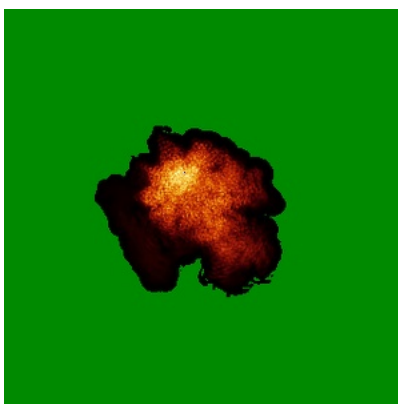
The images above show the largest variance slices of the map in three orthogonal directions.

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

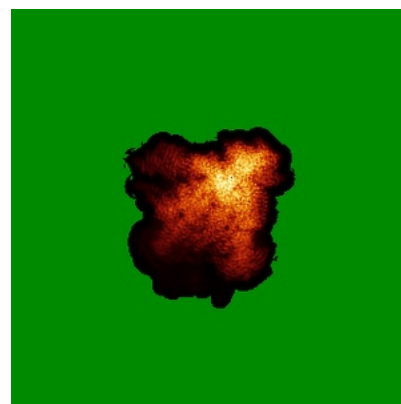
### 6.4.1 Primary map



X

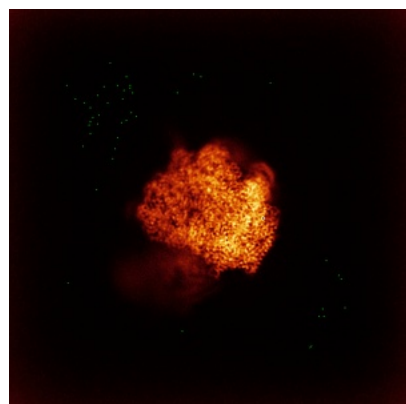


Y

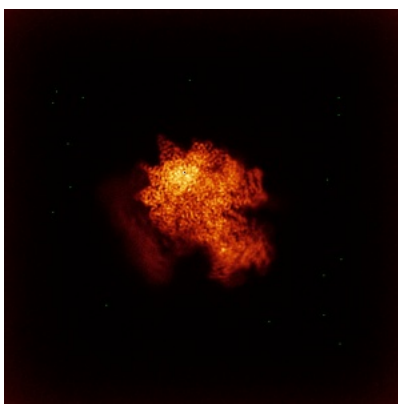


Z

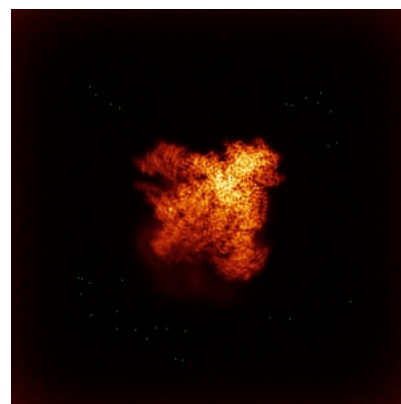
### 6.4.2 Raw map



X



Y

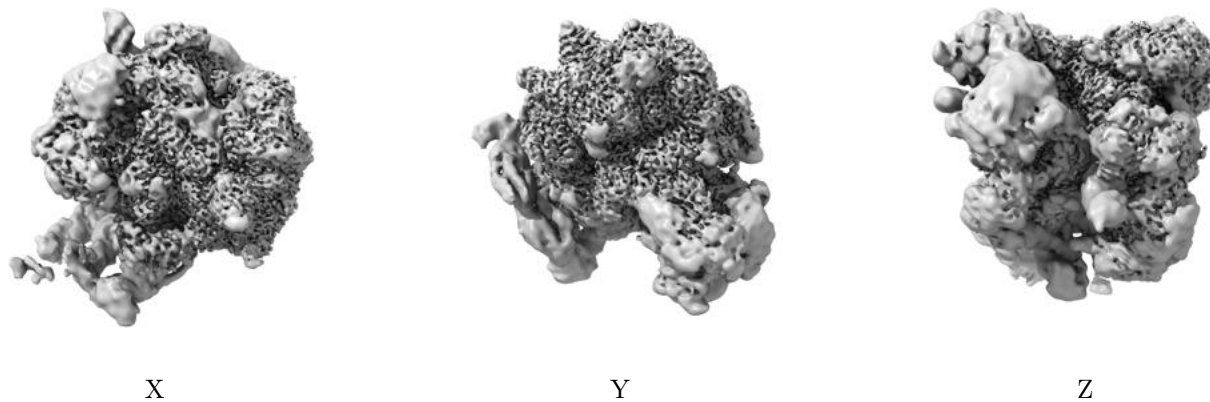


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

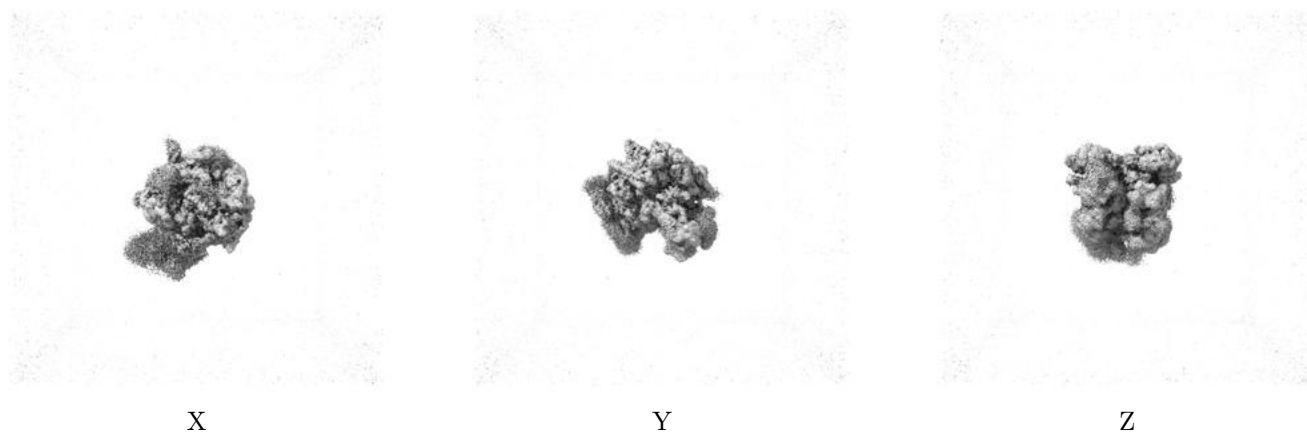
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

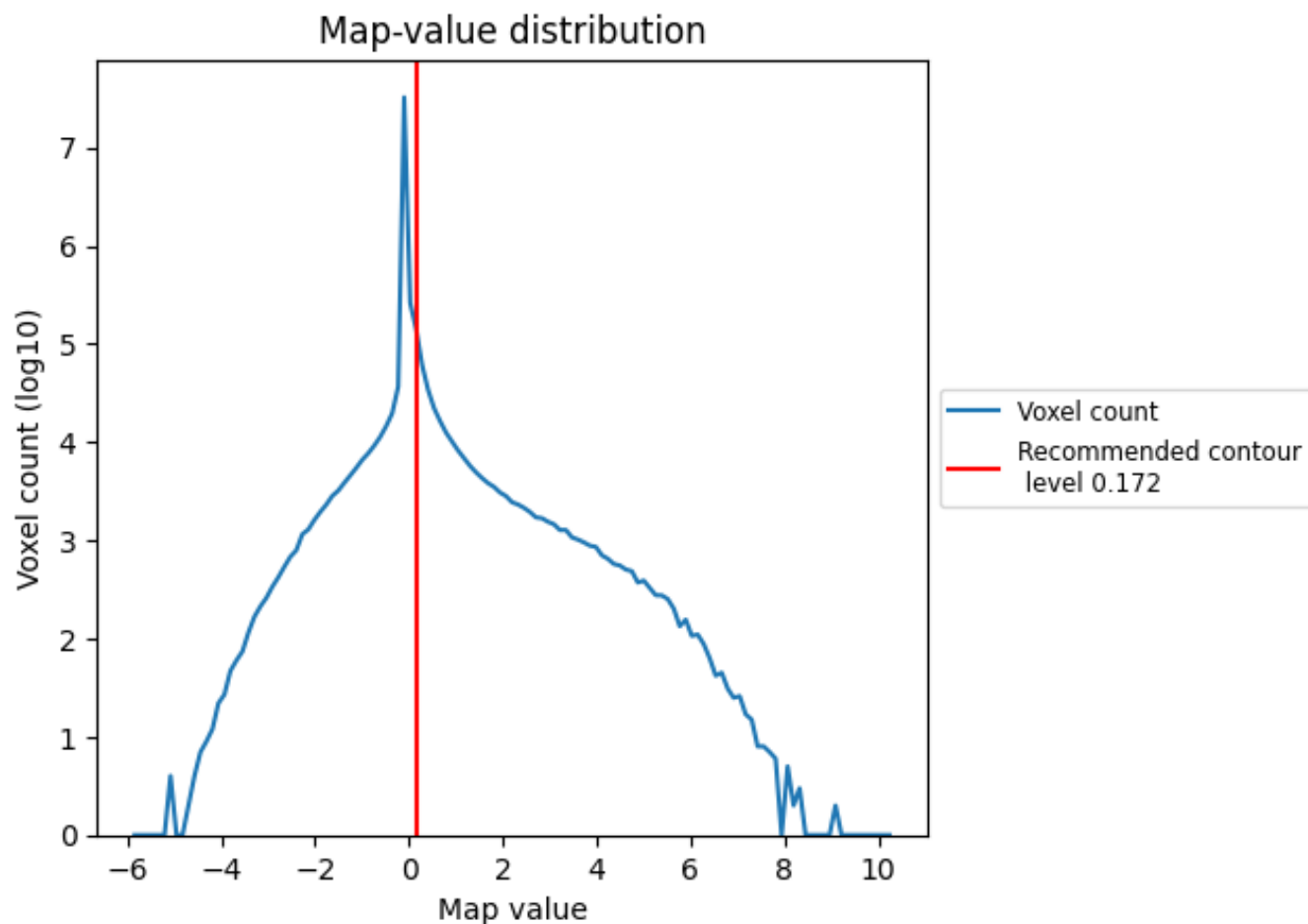
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

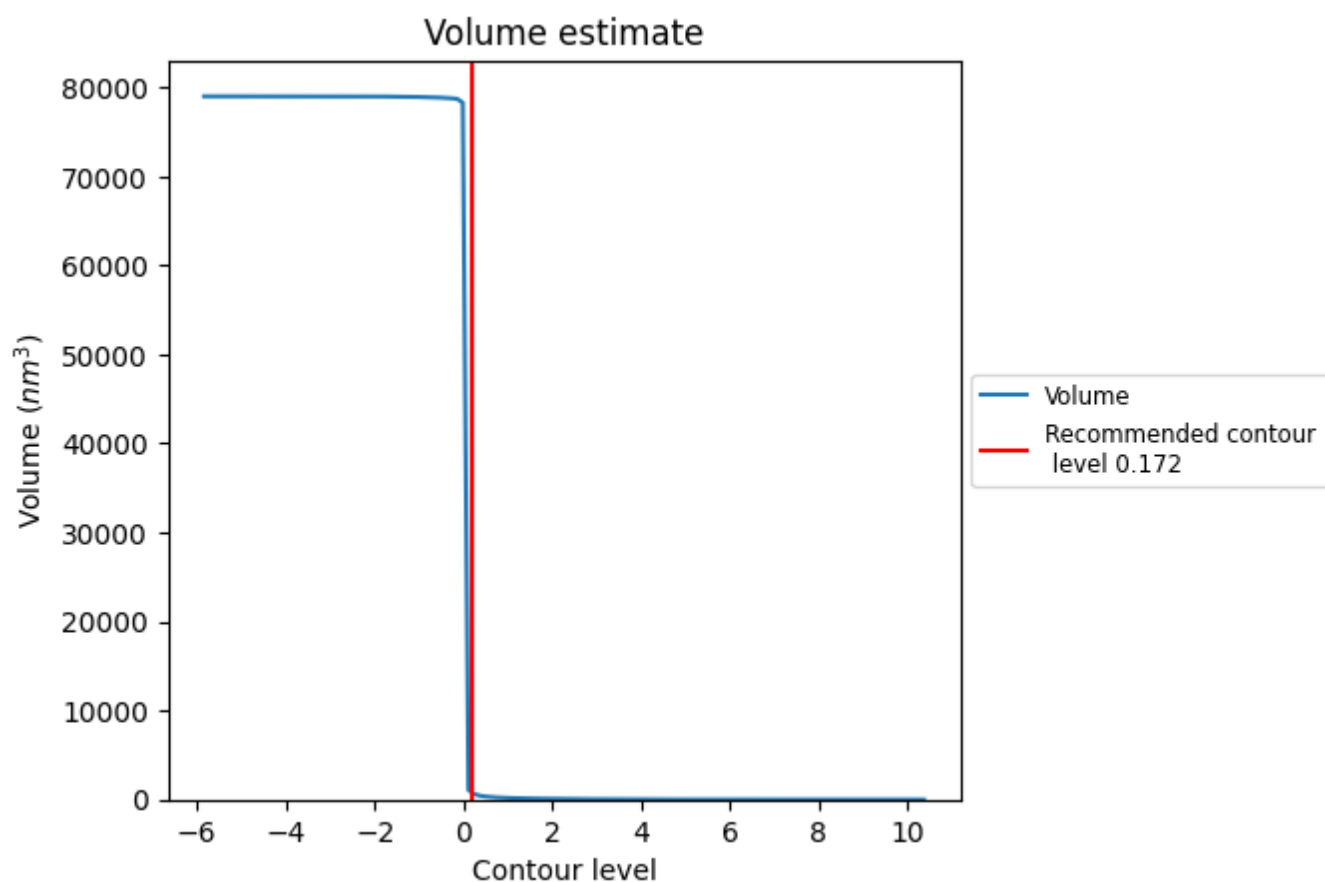
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

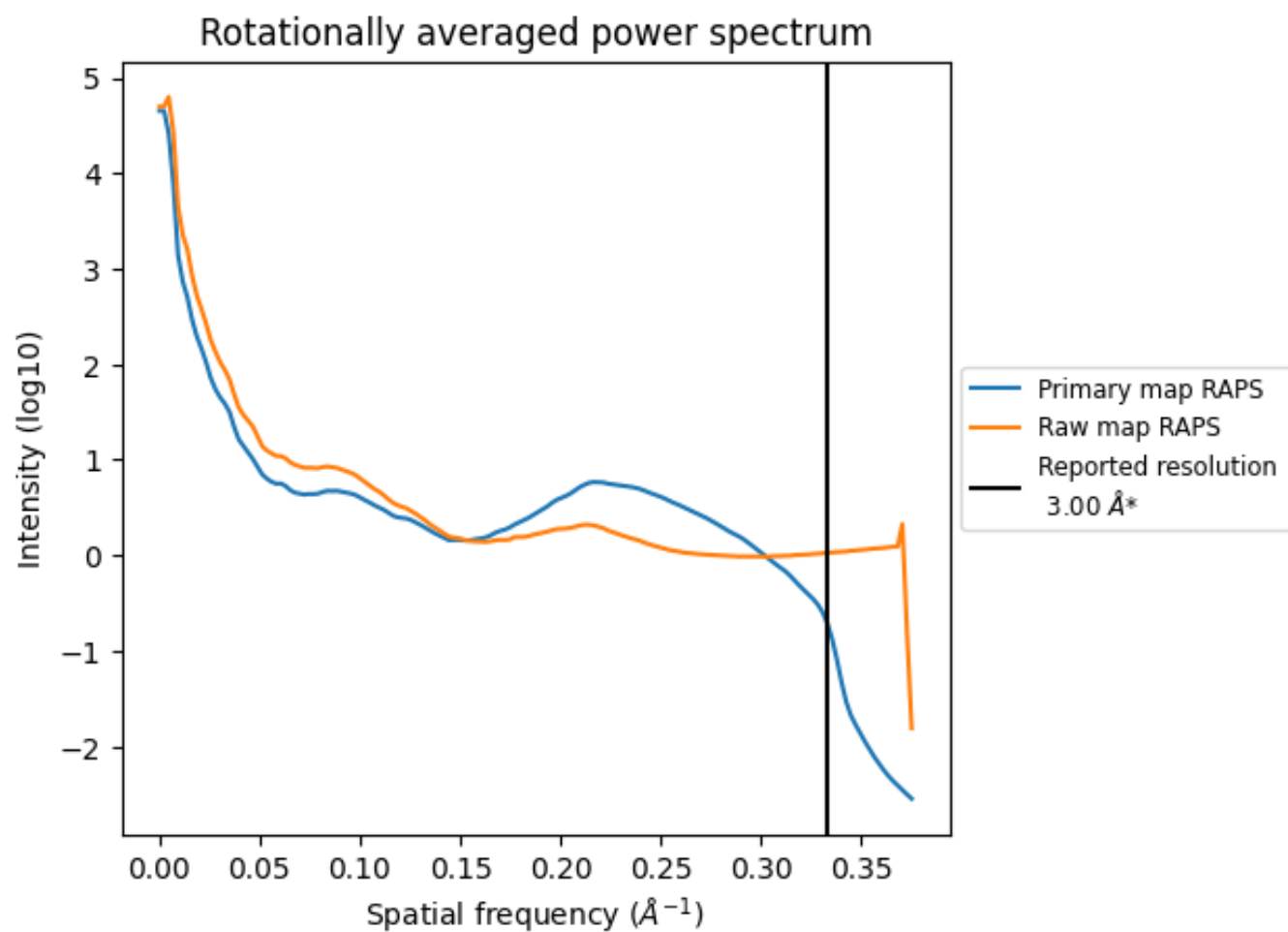
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 857 nm<sup>3</sup>; this corresponds to an approximate mass of 774 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 ⓘ

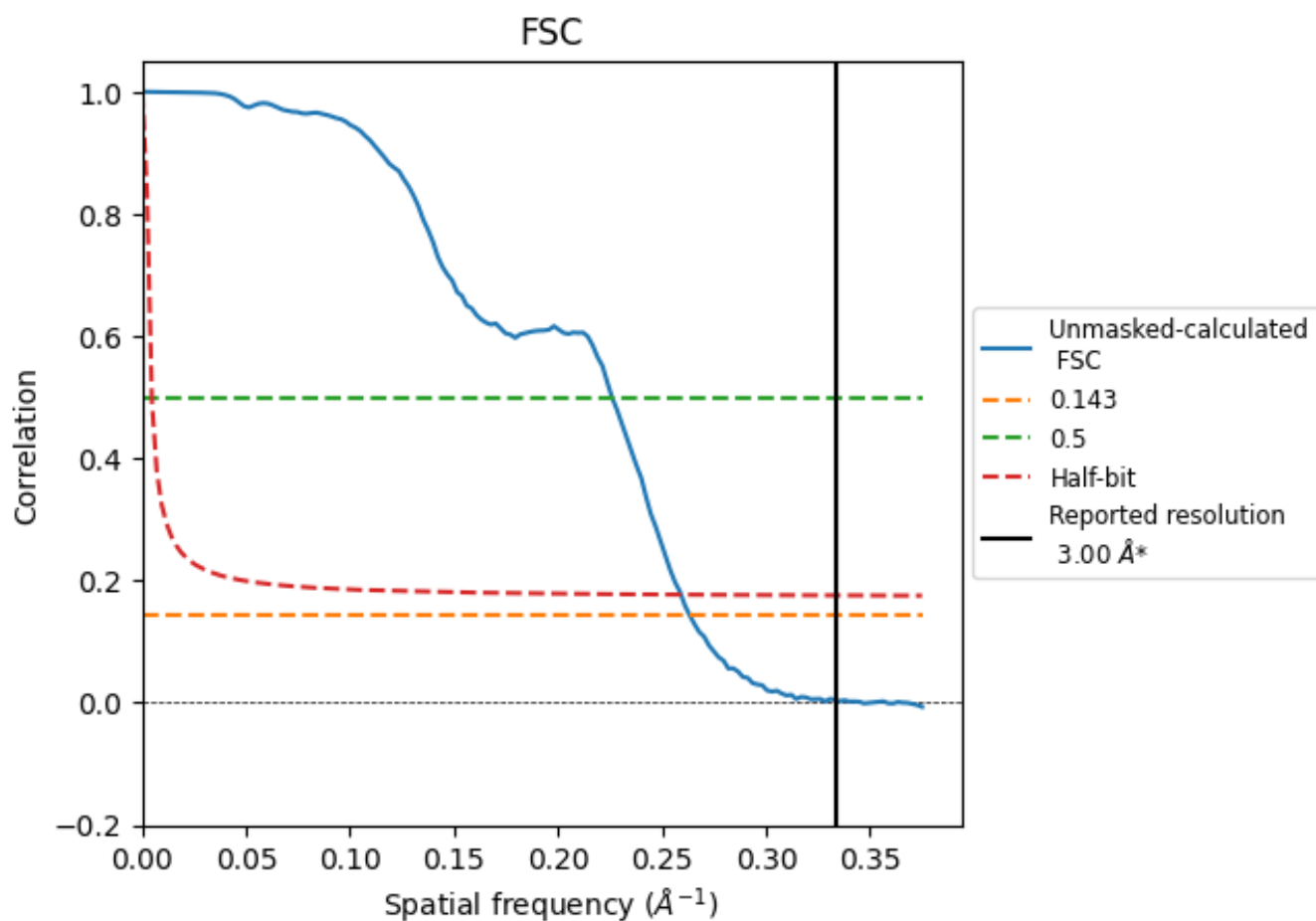


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.42	3.86

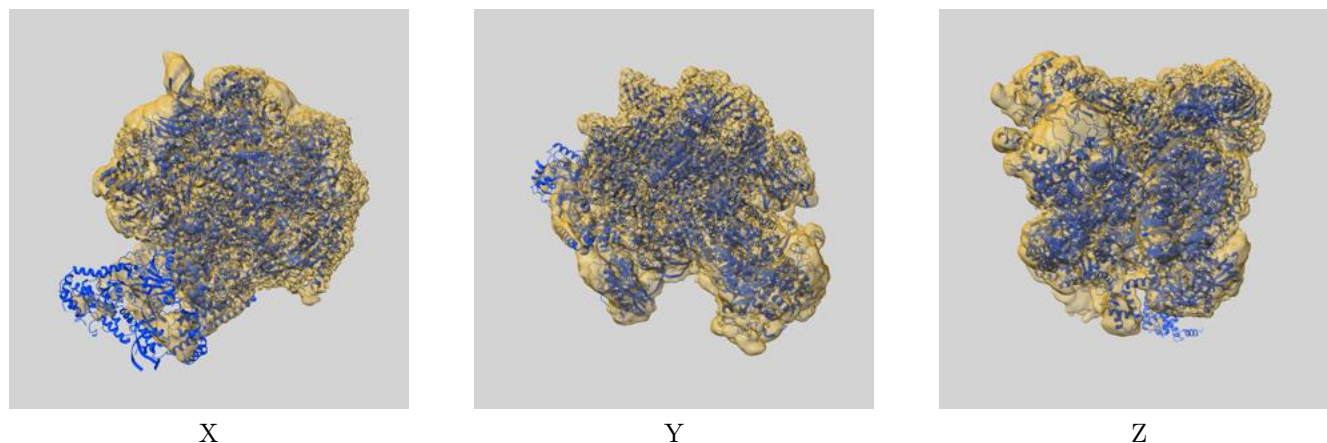
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.80 differs from the reported value 3.0 by more than 10 %



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

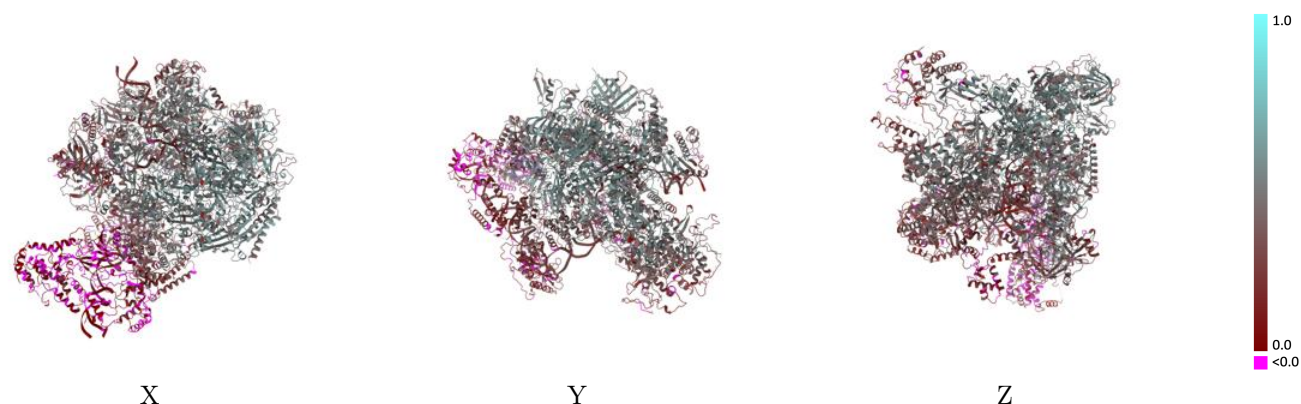
This section contains information regarding the fit between EMDB map EMD-62029 and PDB model 9K3U. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

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



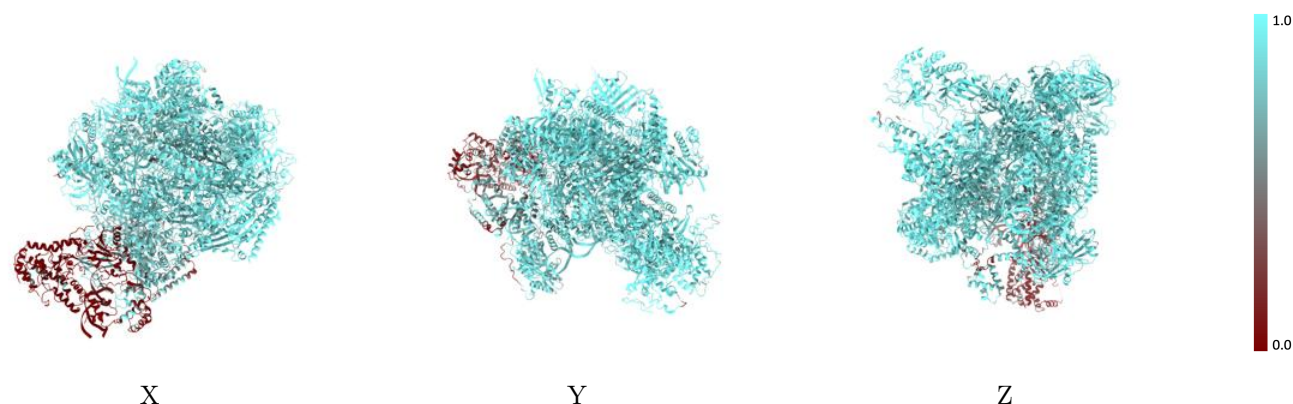
The images above show the 3D surface view of the map at the recommended contour level 0.172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



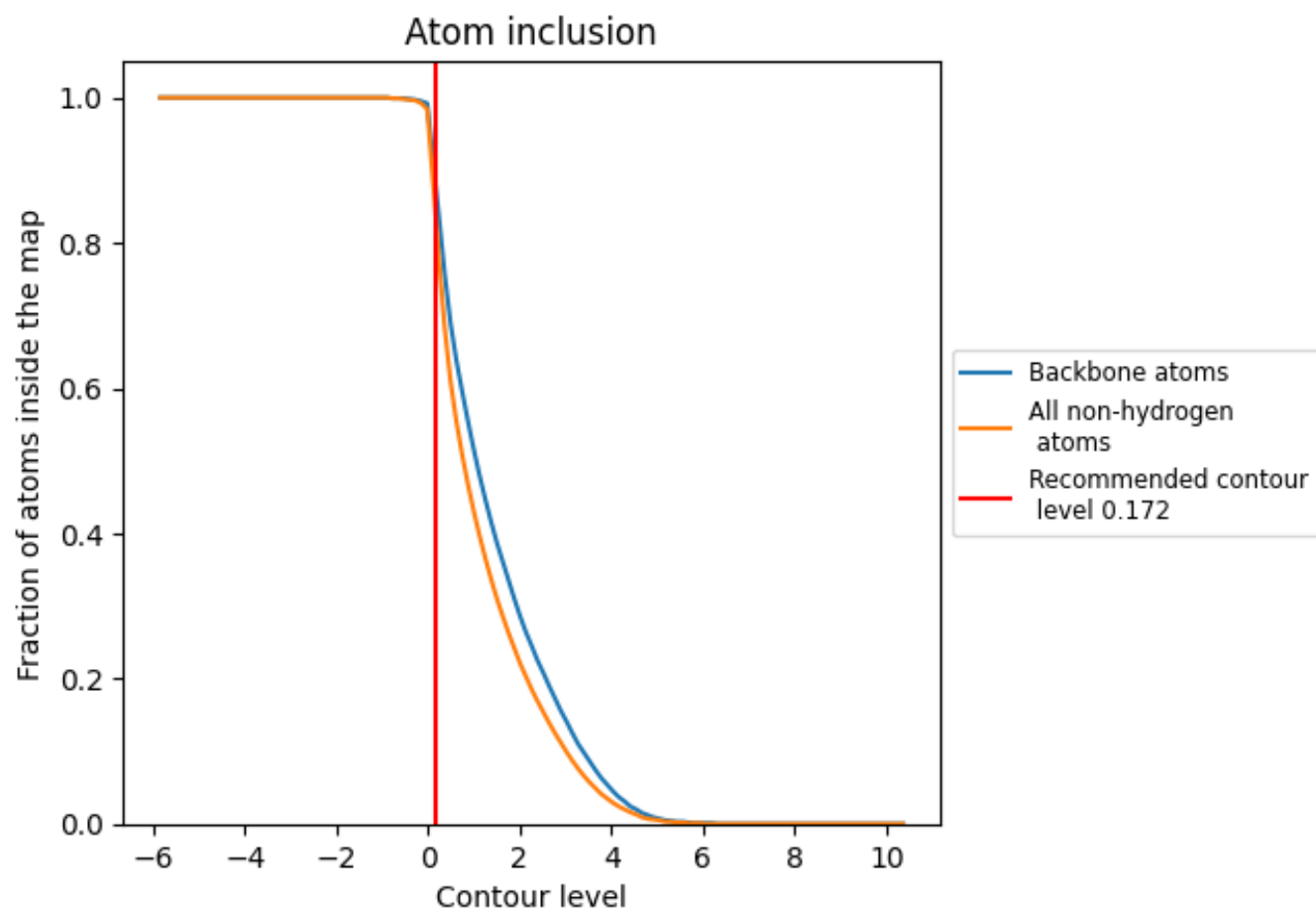
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.172).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (0.172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.3510
1	 0.0730	 0.0290
3	 0.1280	 0.0030
4	 0.3660	 0.0610
A	 0.9390	 0.4700
B	 0.9450	 0.4830
C	 0.9540	 0.4980
D	 0.9560	 0.2740
E	 0.9370	 0.4000
F	 0.9510	 0.4930
G	 0.9480	 0.3600
H	 0.9530	 0.4770
I	 0.9620	 0.4360
J	 0.9480	 0.4840
K	 0.9380	 0.4720
L	 0.9460	 0.4070
M	 0.8180	 0.3470
N	 0.9220	 0.3070
O	 0.9490	 0.3940
P	 0.9090	 0.2670
Q	 0.9400	 0.3450
U	 0.9030	 0.1670
V	 0.8360	 0.2700
W	 0.8280	 0.1260
X	 0.7550	 0.1720
Y	 0.7830	 0.2070
Z	 0.9220	 0.5250

