



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 05:33 AM JST

PDB ID : 7FJJ
EMDB ID : EMD-31622
Title : human Pol III pre-termination complex
Authors : Hou, H.; Xu, Y.
Deposited on : 2021-08-04
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

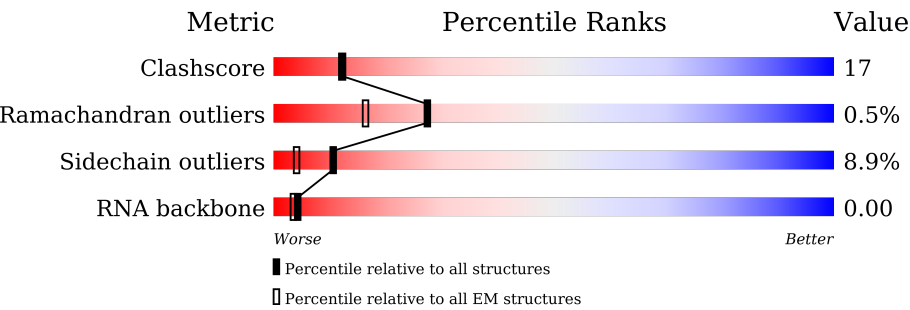
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 3.60 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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1390	<div><div></div><div>62%30%6%.</div></div>
2	B	1133	<div><div></div><div>70%22%5%.</div></div>
3	C	346	<div><div></div><div>75%22%..</div></div>
4	D	148	<div><div></div><div>34%34%14%18%</div></div>
5	E	210	<div><div></div><div>80%19%. .</div></div>
6	F	127	<div><div></div><div>48%10%.40%</div></div>
7	G	204	<div><div></div><div>52%28%.19%</div></div>

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Mol	Chain	Length	Quality of chain
8	H	150	
9	I	108	
10	J	67	
11	K	133	
12	L	58	
13	M	708	
14	N	398	
15	O	534	
16	P	316	
17	Q	223	
18	R	10	
19	X	54	
20	Y	54	

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
22	ZN	J	2000	-	-	X	-
23	SF4	P	401	-	-	X	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 39474 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1360	Total	C	N	O	S	0	0
			10675	6763	1865	1974	73		

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1095	Total	C	N	O	S	0	0
			8644	5473	1512	1591	68		

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	107	Total	C	N	O	S	0	0
			848	525	157	153	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	24	ALA	SER	variant	UNP Q9Y2Y1

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

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

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	202	Total	C	N	O	S	0	0
			1612	1012	274	316	10		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

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

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	443	Total	C	N	O	S	0	0
			3546	2233	620	673	20		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	130	Total	C	N	O	S	0	0
			1008	636	166	196	10		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	86	Total	C	N	O	S	0	0
			724	463	124	131	6		

- Molecule 18 is a RNA chain called RNA (5'-R(*CP*CP*GP*GP*GP*UP*GP*CP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	4	Total	C	N	O	P	0	0
			86	38	15	29	4		

- Molecule 19 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	X	22	Total	C	N	O	P	0	0
			449	215	76	136	22		

- Molecule 20 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	22	Total	C	N	O	P	0	0
			447	212	79	134	22		

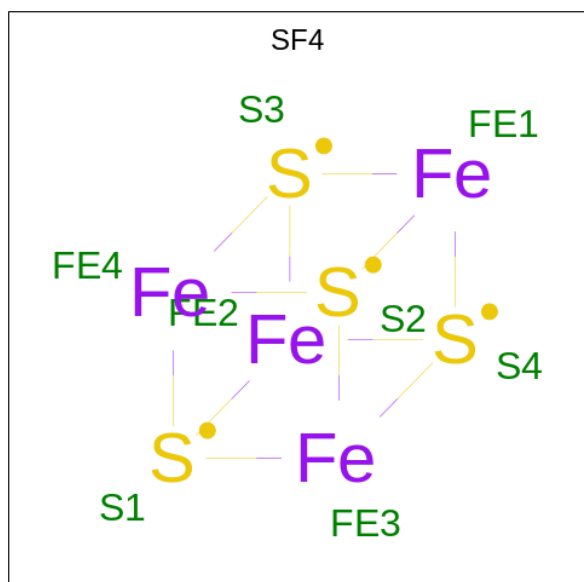
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).

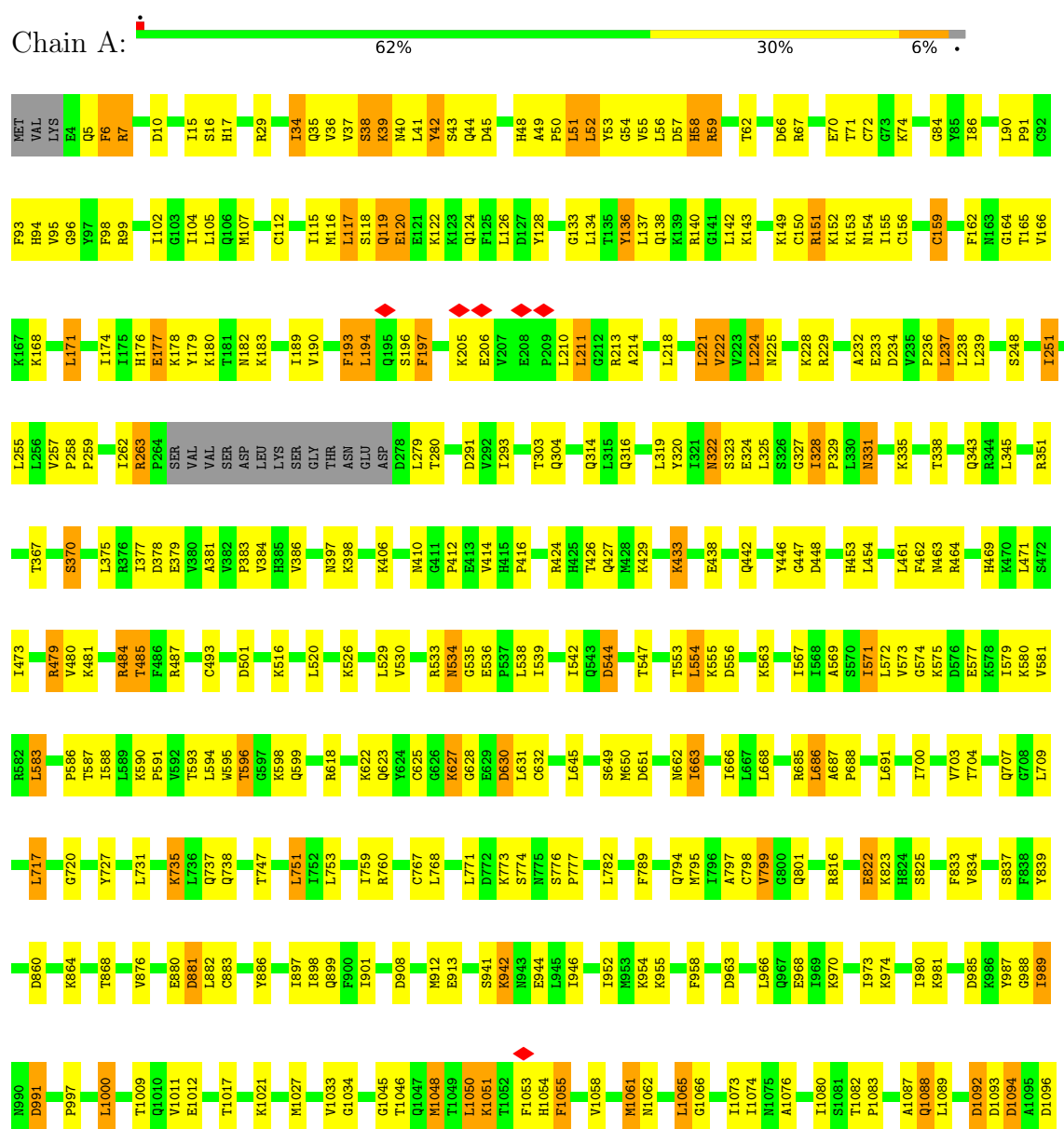


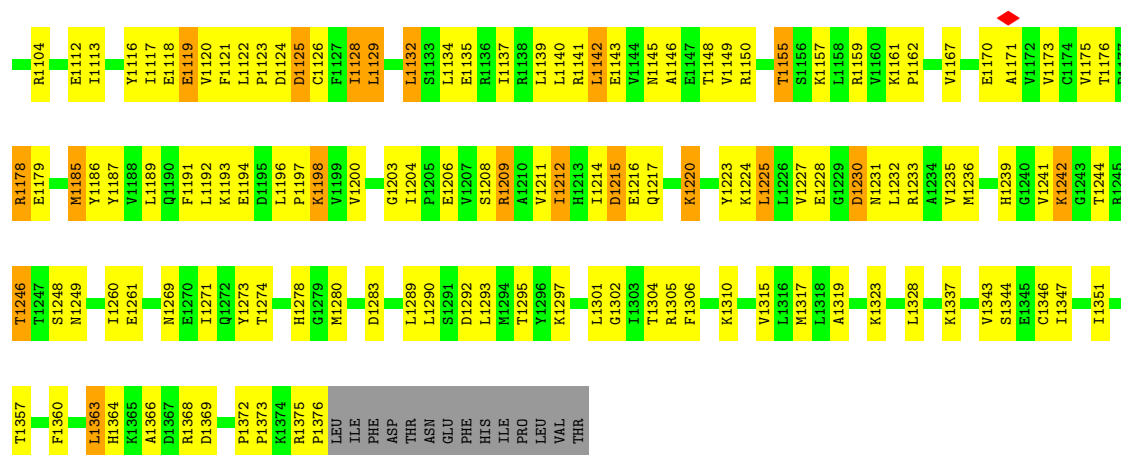
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
23	P	1	8	4	4	0

3 Residue-property plots

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.

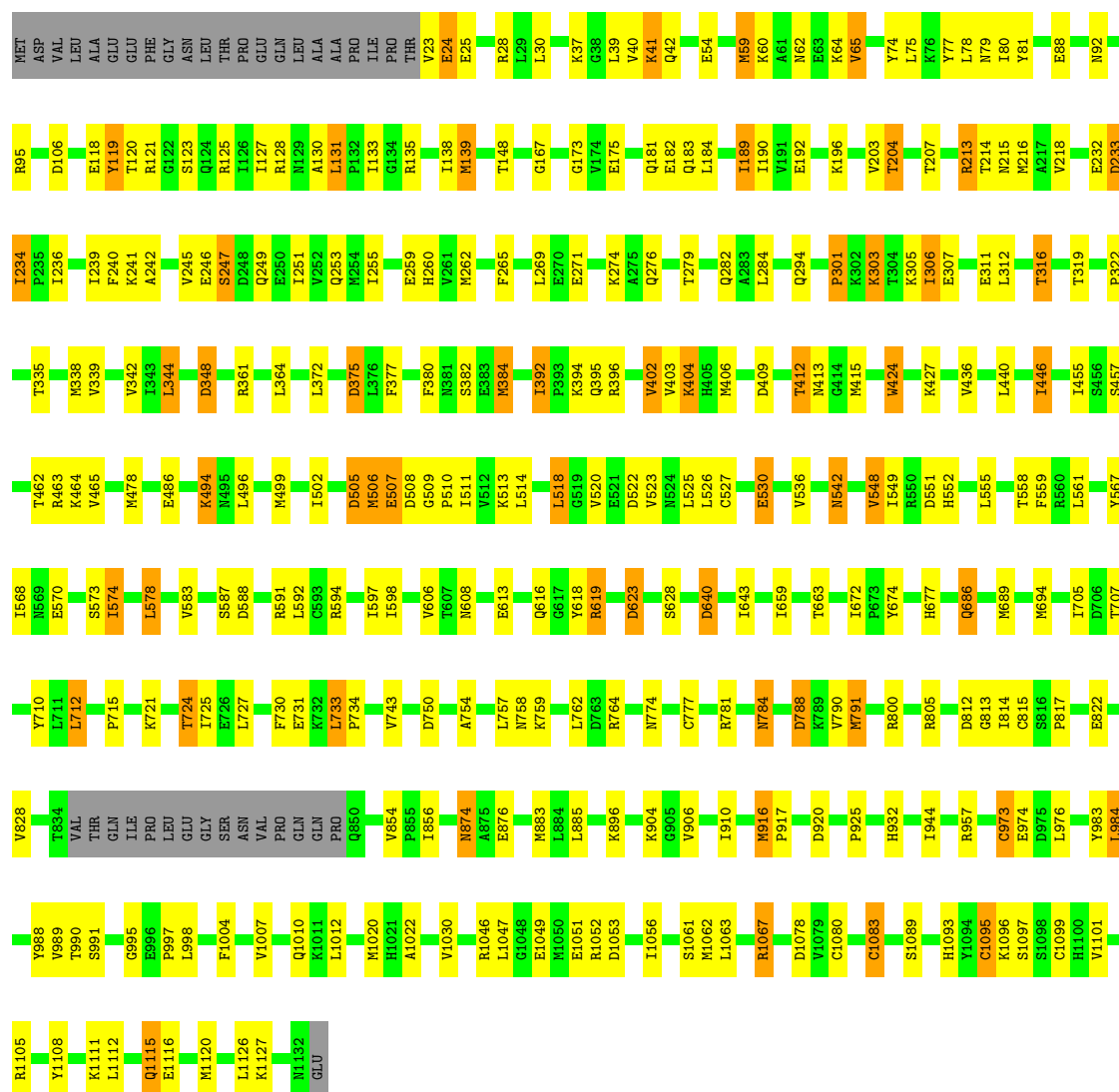
• Molecule 1: DNA-directed RNA polymerase III subunit RPC1



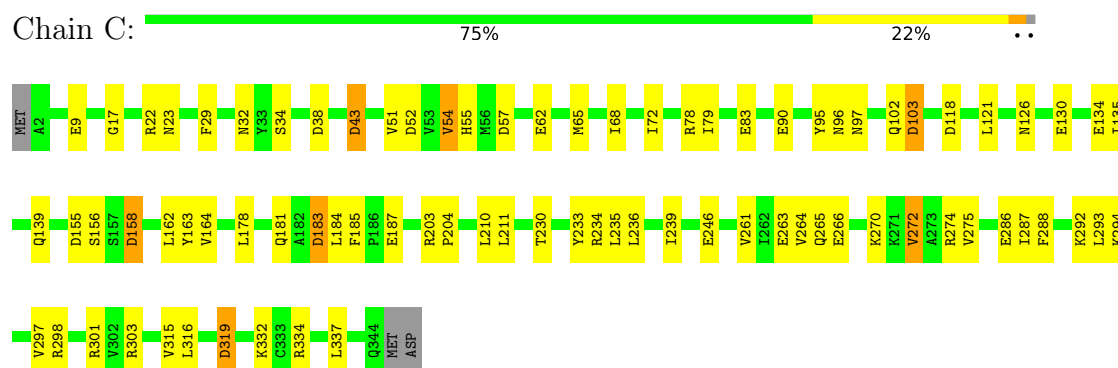


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

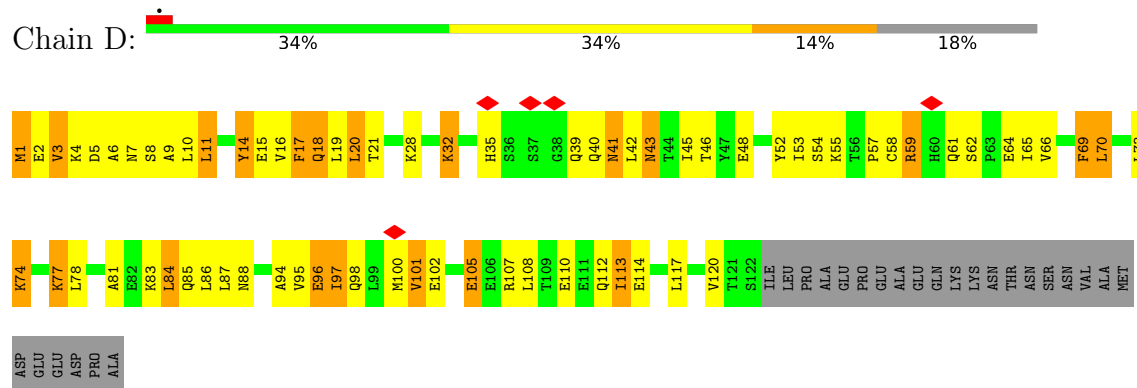
Chain B: 70% 22% 5% •



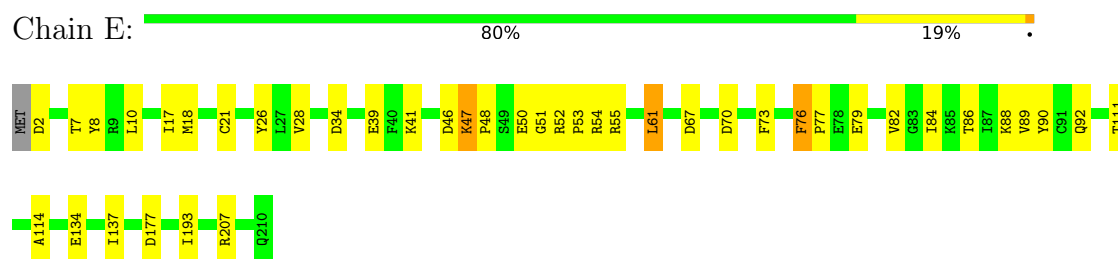
- Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1



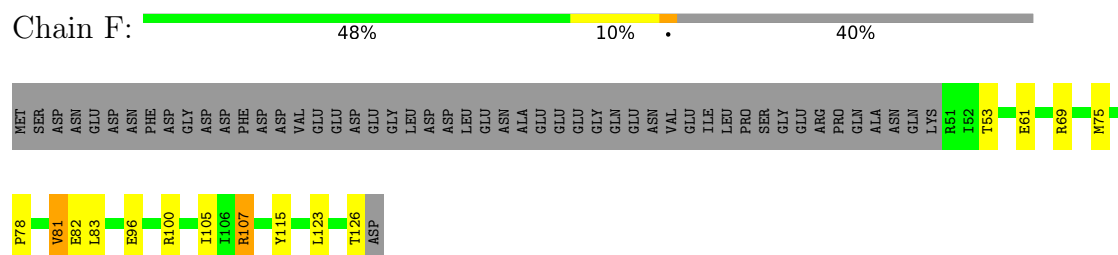
- Molecule 4: DNA-directed RNA polymerase III subunit RPC9



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

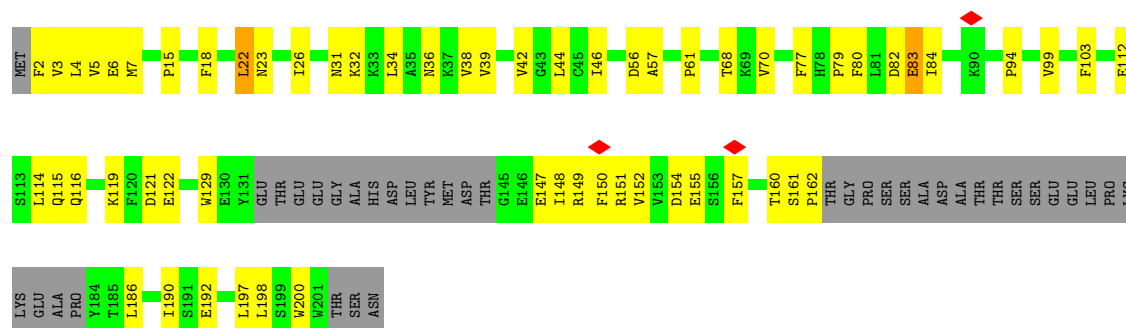


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



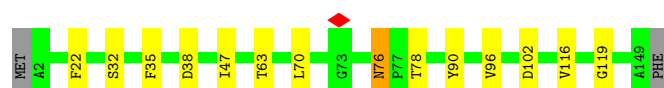
- Molecule 7: DNA-directed RNA polymerase III subunit RPC8





- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 89% 9% ..



- Molecule 9: DNA-directed RNA polymerase III subunit RPC10

Chain I: 12% 79% 19% ..



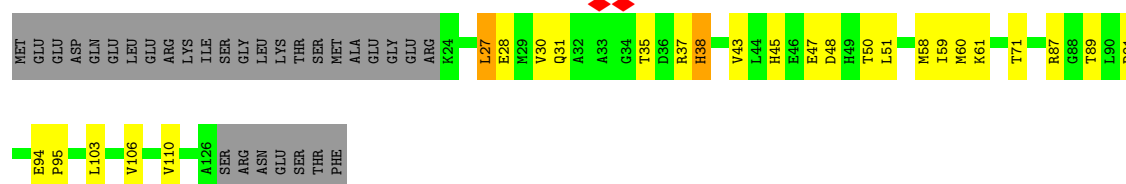
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 70% 21% 6% .



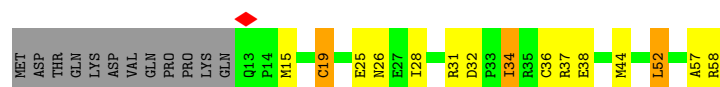
- Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 58% 18% . 23%

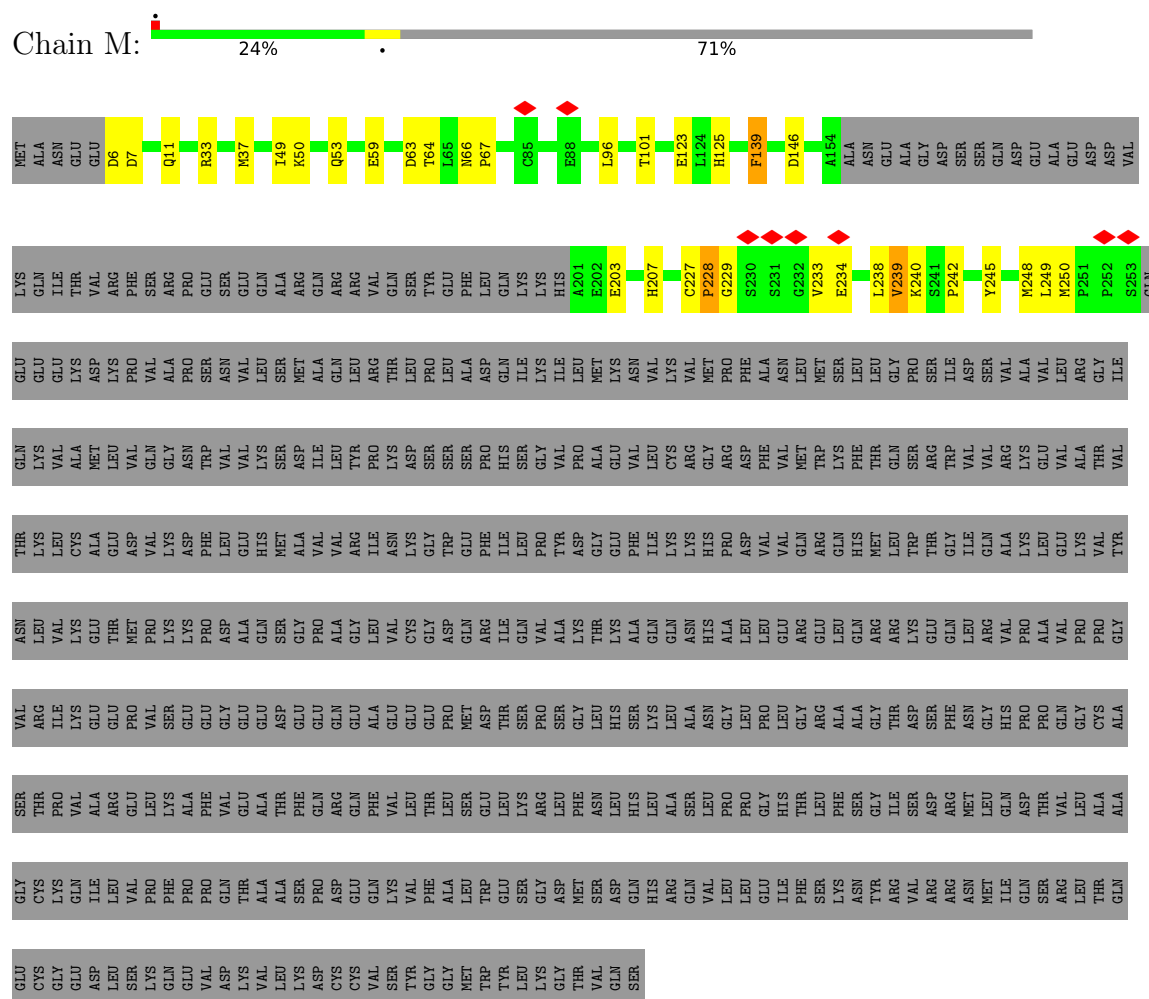


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

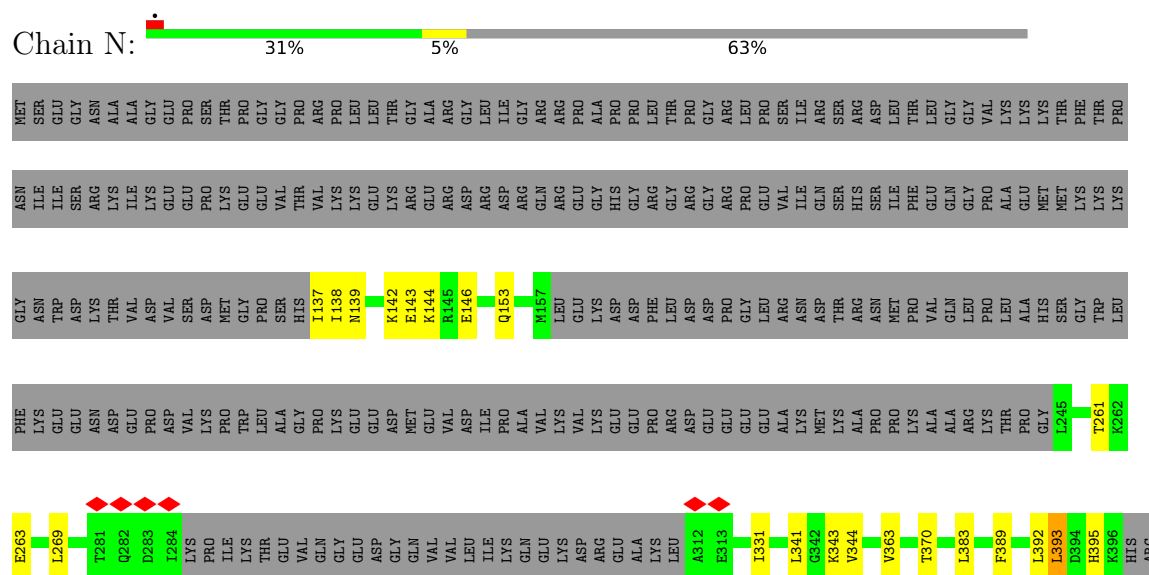
Chain L: 53% 21% 5% 21%



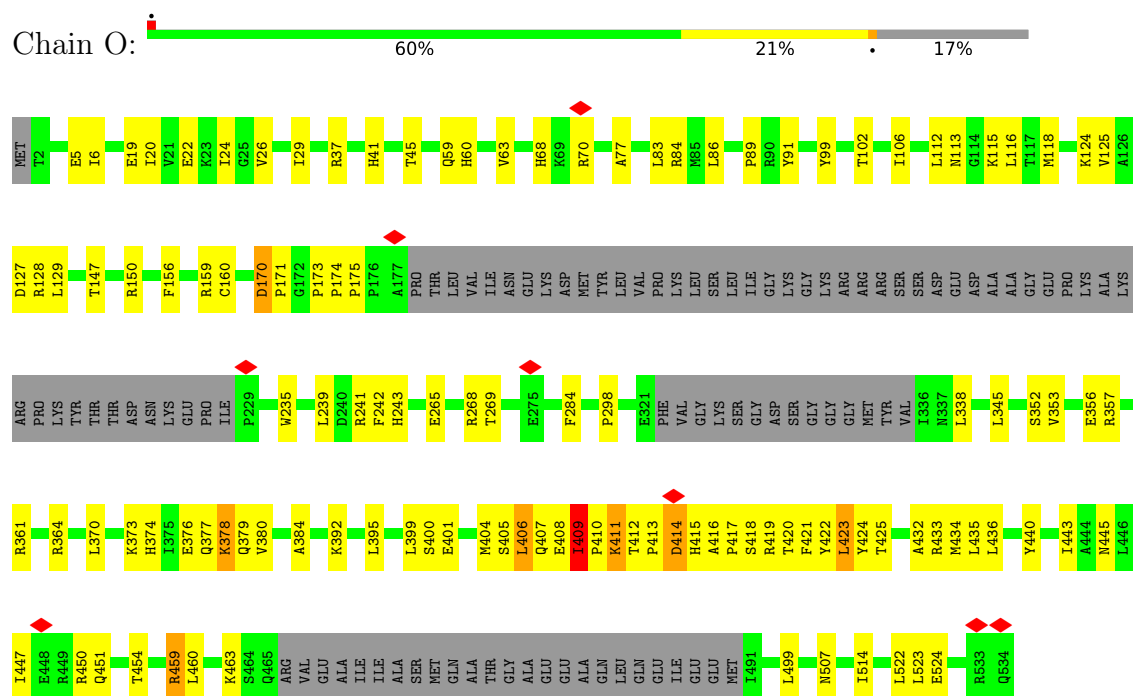
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5



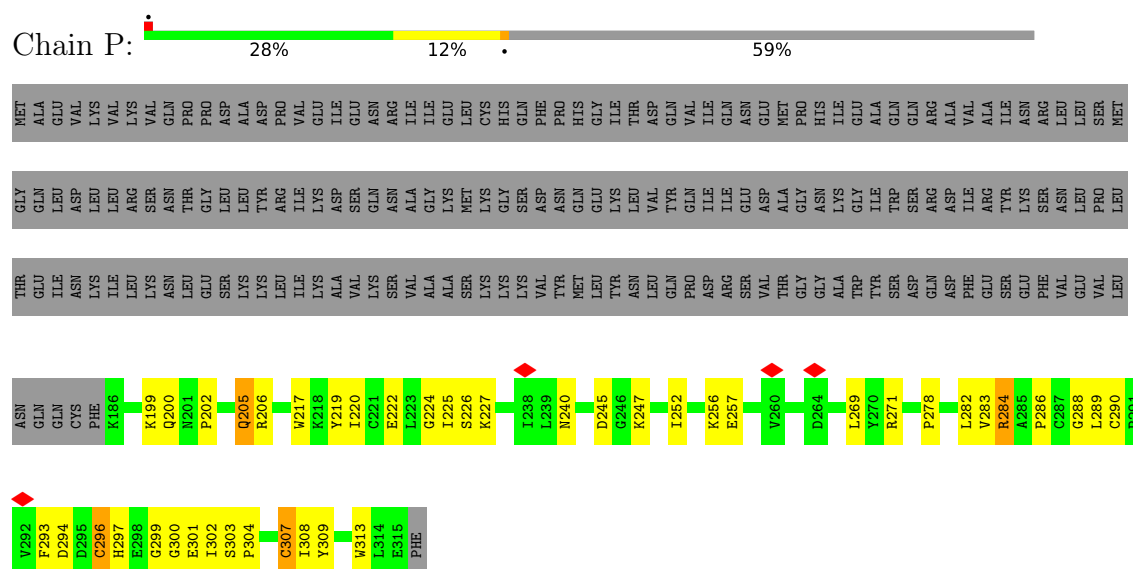
- Molecule 14: DNA-directed RNA polymerase III subunit RPC4



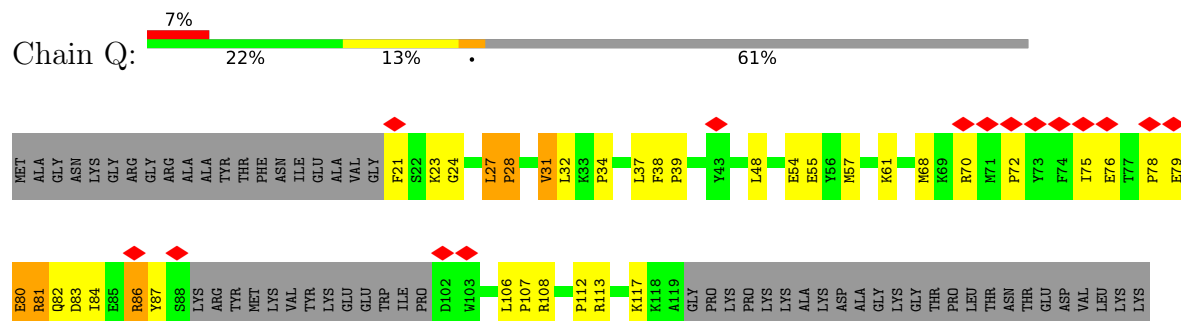
- Molecule 15: DNA-directed RNA polymerase III subunit RPC3



• Molecule 16: DNA-directed RNA polymerase III subunit RPC6



• Molecule 17: DNA-directed RNA polymerase III subunit RPC7



GLU
ASP
GLY
ASP
ASP
PHE
GLY
ALA
ASP
SER
ASP
ASP
ASN
MET
ASP
GLU
ALA
THR
TYR

- Chain R: 

A diagram of a 12-bit bus. It consists of a horizontal bar divided into 12 segments. The first 10 segments are grey and labeled 'C' (Control) from left to right. The 11th segment is yellow and labeled 'G8'. The 12th segment is orange and labeled 'G9'. To the right of the orange segment is a red diamond shape. Below the bar, the labels 'U10' and 'G11' are present, corresponding to the 10th and 11th segments respectively.

- Chain X: 17% 24% 59%

[illegible]

- Chain Y: 13% 24% . 59%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48593	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 ($e^-/\text{\AA}^2$)	1.38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (\AA)	379.44, 379.44, 379.44	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.054, 1.054, 1.054	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.62	0/10866	0.81	1/14648 (0.0%)
2	B	0.62	0/8807	0.80	5/11875 (0.0%)
3	C	0.58	0/2790	0.69	0/3782
4	D	0.58	0/997	0.79	0/1343
5	E	0.45	0/1745	0.64	0/2358
6	F	0.58	0/620	0.66	0/839
7	G	0.51	0/1374	0.69	0/1868
8	H	0.42	0/1207	0.67	0/1628
9	I	0.34	0/869	0.61	0/1174
10	J	0.56	0/521	0.81	2/703 (0.3%)
11	K	0.56	0/837	0.69	0/1129
12	L	0.57	0/394	0.66	0/524
13	M	0.53	0/1648	0.66	0/2232
14	N	0.58	0/1137	0.70	0/1530
15	O	0.40	0/3604	0.60	0/4872
16	P	0.45	0/1028	0.73	0/1391
17	Q	0.46	0/742	0.69	0/996
18	R	0.92	0/95	1.30	0/146
19	X	0.64	0/501	0.90	0/771
20	Y	0.71	1/499 (0.2%)	1.16	1/767 (0.1%)
All	All	0.57	1/40281 (0.0%)	0.75	9/54576 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	-1	DC	O3'-P	5.44	1.67	1.61

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1083	CYS	CB-CA-C	13.76	137.92	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1083	CYS	N-CA-CB	-9.75	93.05	110.60
2	B	1095	CYS	N-CA-C	-9.64	84.97	111.00
2	B	1095	CYS	N-CA-CB	-9.12	94.19	110.60
10	J	10	CYS	CA-CB-SG	-6.12	102.99	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10675	0	10918	453	0
2	B	8644	0	8748	236	0
3	C	2736	0	2712	80	0
4	D	985	0	1006	117	0
5	E	1715	0	1733	44	0
6	F	610	0	642	18	0
7	G	1337	0	1306	109	0
8	H	1186	0	1147	31	0
9	I	848	0	812	55	0
10	J	512	0	526	16	0
11	K	822	0	810	43	0
12	L	388	0	395	14	0
13	M	1612	0	1572	32	0
14	N	1128	0	1181	33	0
15	O	3546	0	3585	155	0
16	P	1008	0	998	59	0
17	Q	724	0	734	53	0
18	R	86	0	44	11	0
19	X	449	0	251	26	0
20	Y	447	0	248	31	0
21	A	1	0	0	0	0
22	A	2	0	0	1	0
22	B	1	0	0	1	0
22	I	2	0	0	0	0
22	J	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	L	1	0	0	0	0
23	P	8	0	0	4	0
All	All	39474	0	39368	1329	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 17.

The worst 5 of 1329 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:1116:TYR:CE1	9:I:43:TYR:HE1	1.36	1.43
8:H:76:ASN:HD21	11:K:87:ARG:CZ	1.29	1.42
8:H:78:THR:CB	11:K:87:ARG:HH22	1.34	1.39
1:A:1116:TYR:CE1	9:I:43:TYR:CE1	2.14	1.35
1:A:1116:TYR:CD1	9:I:43:TYR:CE1	2.12	1.35

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	1356/1390 (98%)	1274 (94%)	69 (5%)	13 (1%)	13	46
2	B	1091/1133 (96%)	1026 (94%)	57 (5%)	8 (1%)	19	53
3	C	341/346 (99%)	338 (99%)	3 (1%)	0	100	100
4	D	120/148 (81%)	109 (91%)	10 (8%)	1 (1%)	16	51
5	E	207/210 (99%)	200 (97%)	7 (3%)	0	100	100
6	F	74/127 (58%)	72 (97%)	2 (3%)	0	100	100
7	G	160/204 (78%)	137 (86%)	23 (14%)	0	100	100
8	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	105/108 (97%)	98 (93%)	7 (7%)	0	100	100
10	J	63/67 (94%)	63 (100%)	0	0	100	100
11	K	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	M	198/708 (28%)	189 (96%)	8 (4%)	1 (0%)	25	59
14	N	140/398 (35%)	140 (100%)	0	0	100	100
15	O	435/534 (82%)	416 (96%)	18 (4%)	1 (0%)	44	73
16	P	128/316 (40%)	102 (80%)	25 (20%)	1 (1%)	16	51
17	Q	82/223 (37%)	72 (88%)	9 (11%)	1 (1%)	11	43
All	All	4791/6253 (77%)	4519 (94%)	246 (5%)	26 (0%)	27	59

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	177	GLU
1	A	1185	MET
1	A	1209	ARG
2	B	1096	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1182/1212 (98%)	1023 (86%)	159 (14%)	3	18
2	B	950/988 (96%)	837 (88%)	113 (12%)	4	22
3	C	299/302 (99%)	282 (94%)	17 (6%)	17	46
4	D	114/136 (84%)	88 (77%)	26 (23%)	0	4
5	E	191/192 (100%)	180 (94%)	11 (6%)	17	46
6	F	66/111 (60%)	64 (97%)	2 (3%)	36	63
7	G	149/181 (82%)	146 (98%)	3 (2%)	50	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	129/131 (98%)	128 (99%)	1 (1%)	79	88
9	I	92/93 (99%)	91 (99%)	1 (1%)	70	83
10	J	53/56 (95%)	44 (83%)	9 (17%)	1	11
11	K	92/119 (77%)	88 (96%)	4 (4%)	25	54
12	L	43/55 (78%)	38 (88%)	5 (12%)	4	23
13	M	180/622 (29%)	176 (98%)	4 (2%)	47	69
14	N	131/347 (38%)	129 (98%)	2 (2%)	60	78
15	O	400/476 (84%)	390 (98%)	10 (2%)	42	66
16	P	114/280 (41%)	110 (96%)	4 (4%)	31	60
17	Q	81/195 (42%)	72 (89%)	9 (11%)	5	25
All	All	4266/5496 (78%)	3886 (91%)	380 (9%)	10	32

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	583	VAL
3	C	261	VAL
2	B	686	GLN
2	B	976	LEU
4	D	41	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	7	ASN
15	O	113	ASN
4	D	43	ASN
9	I	21	HIS
15	O	415	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	R	4/10 (40%)	3 (75%)	1 (25%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	R	9	C
18	R	10	U
18	R	11	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	R	8	G

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 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	SF4	P	401	16	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
23	SF4	P	401	16	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

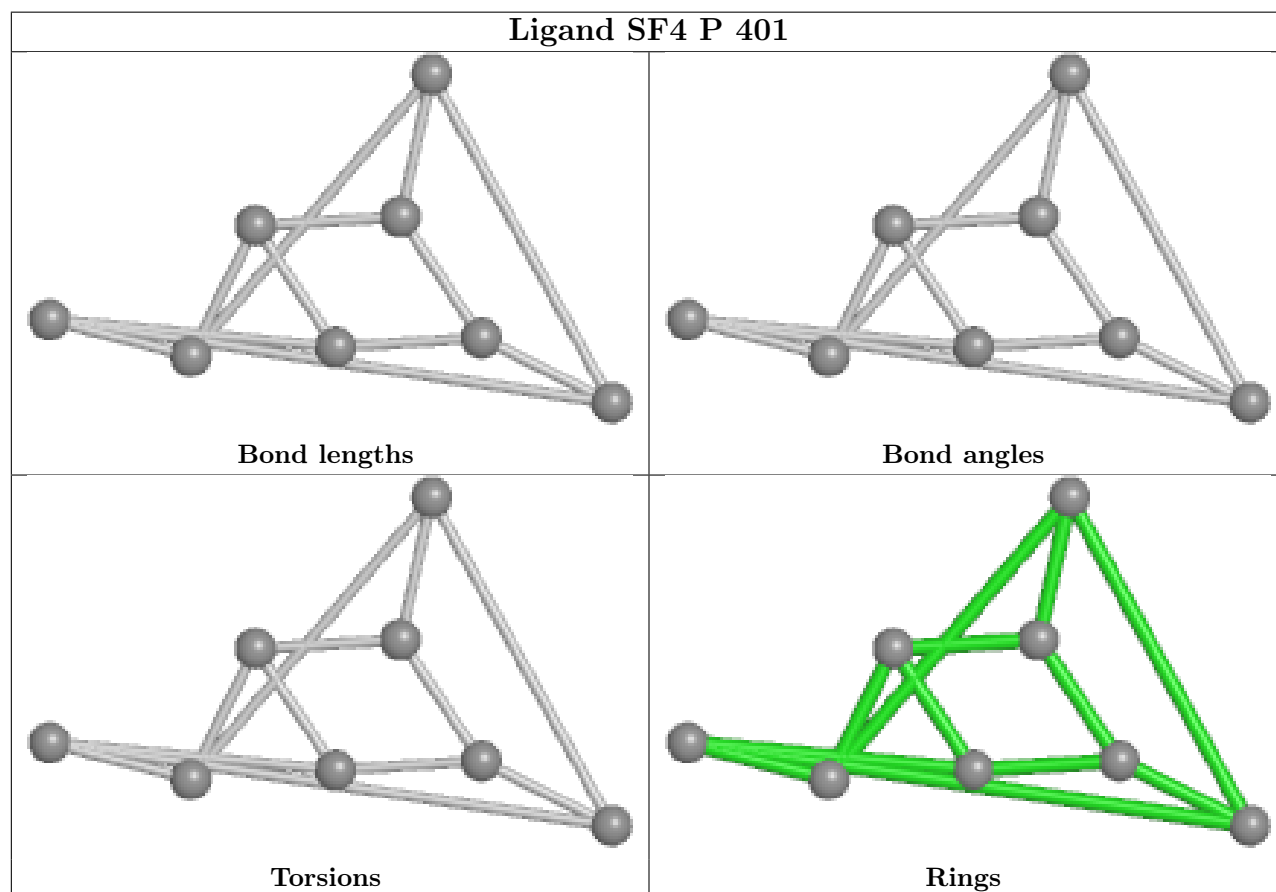
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	P	401	SF4	4	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.

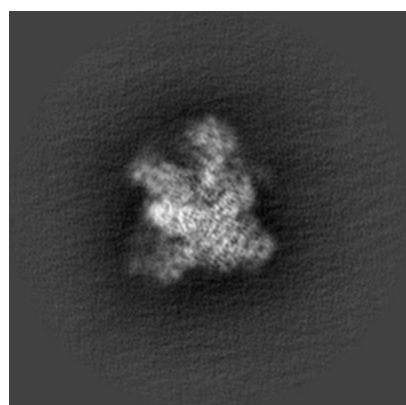
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31622. These allow visual inspection of the internal detail of the map and identification of artifacts.

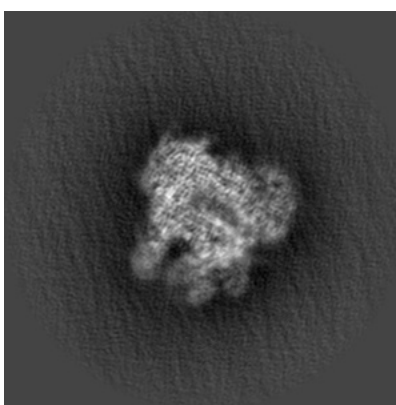
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

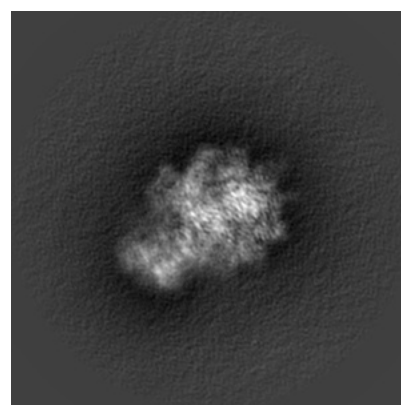
6.1.1 Primary map



X



Y

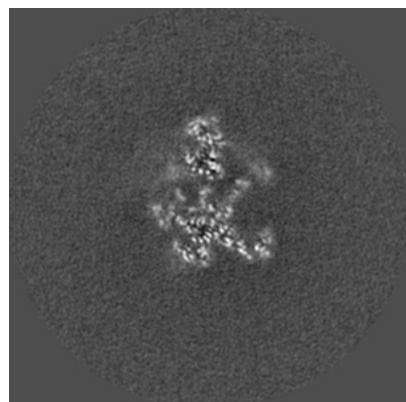


Z

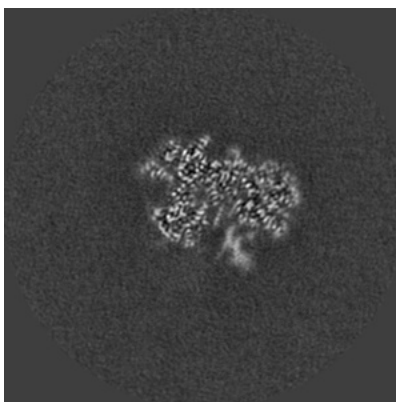
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

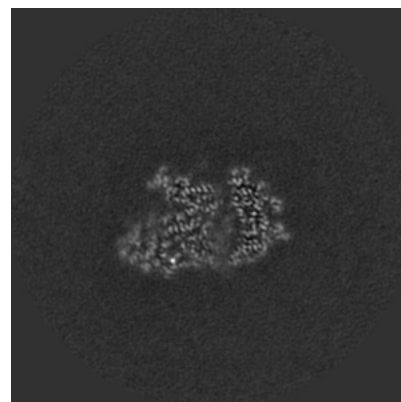
6.2.1 Primary map



X Index: 180



Y Index: 180

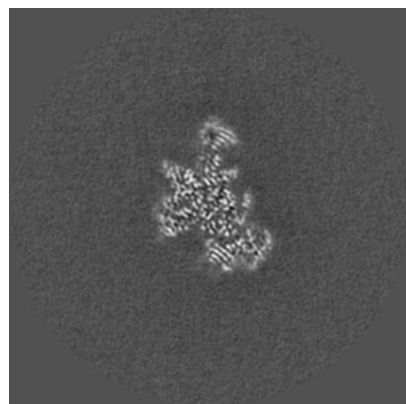


Z Index: 180

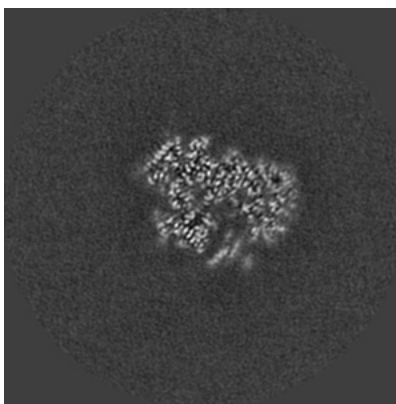
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

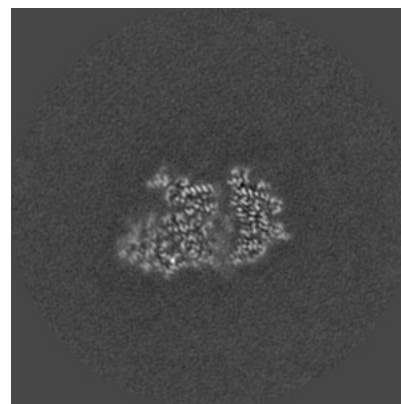
6.3.1 Primary map



X Index: 208



Y Index: 185

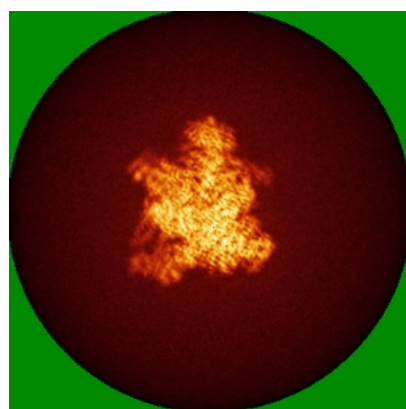


Z Index: 179

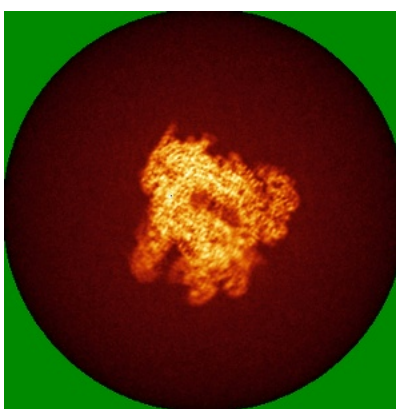
The images above show the largest variance slices of the map in three orthogonal directions.

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

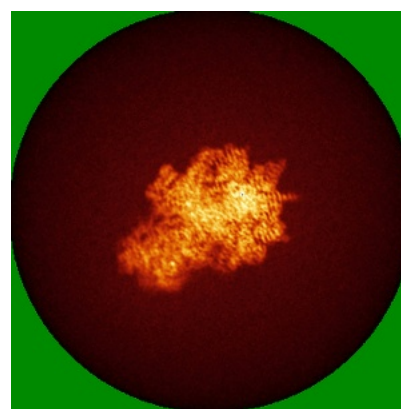
6.4.1 Primary map



X



Y

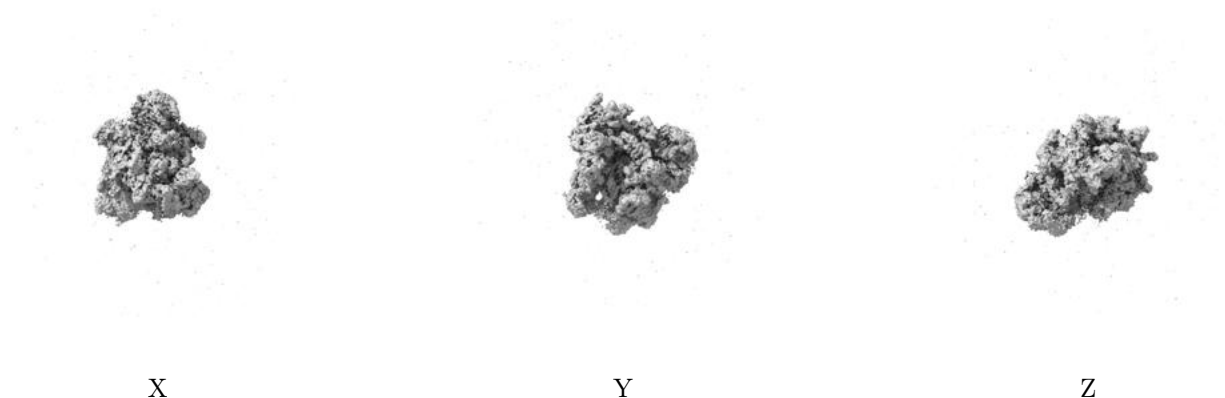


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

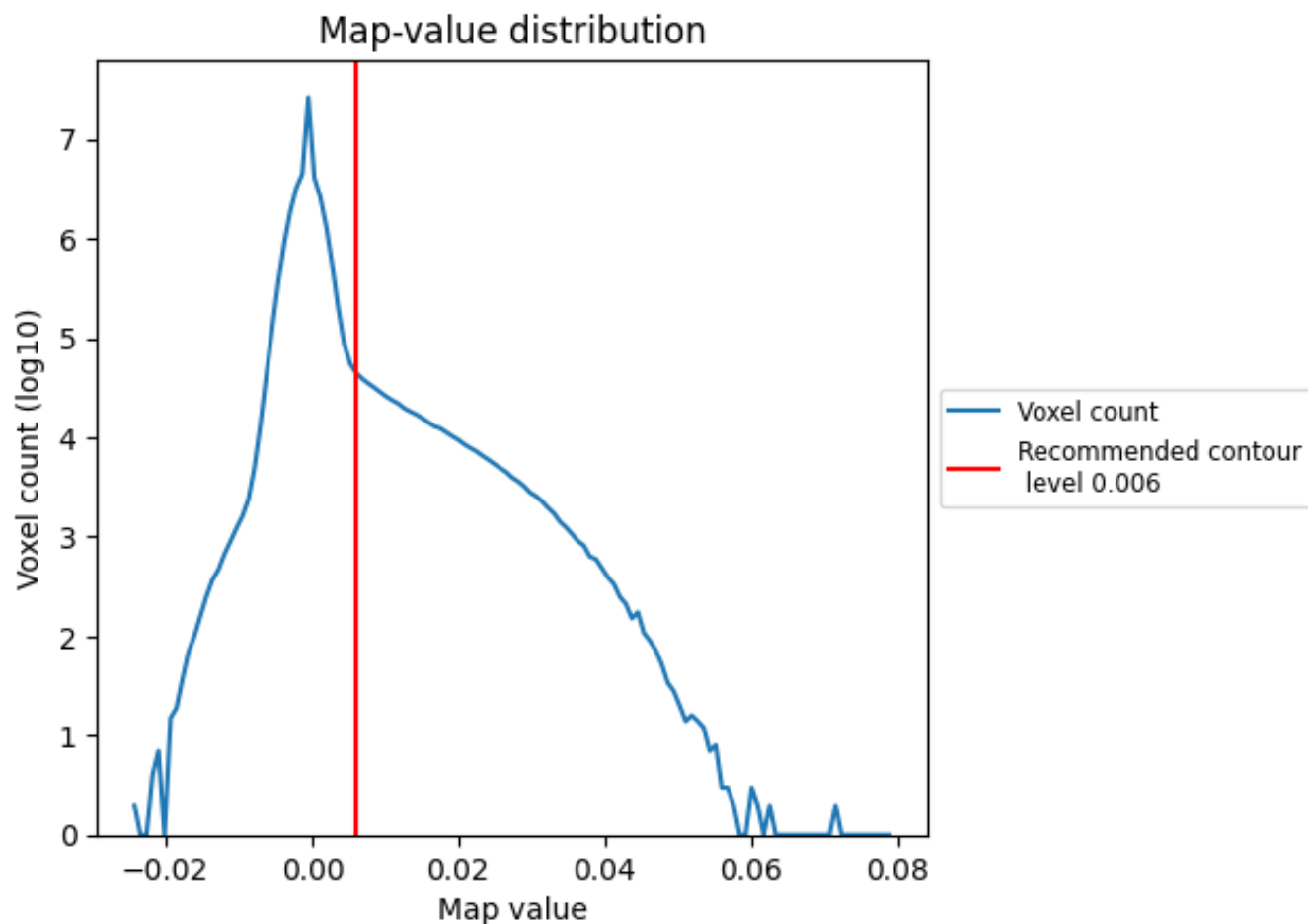
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

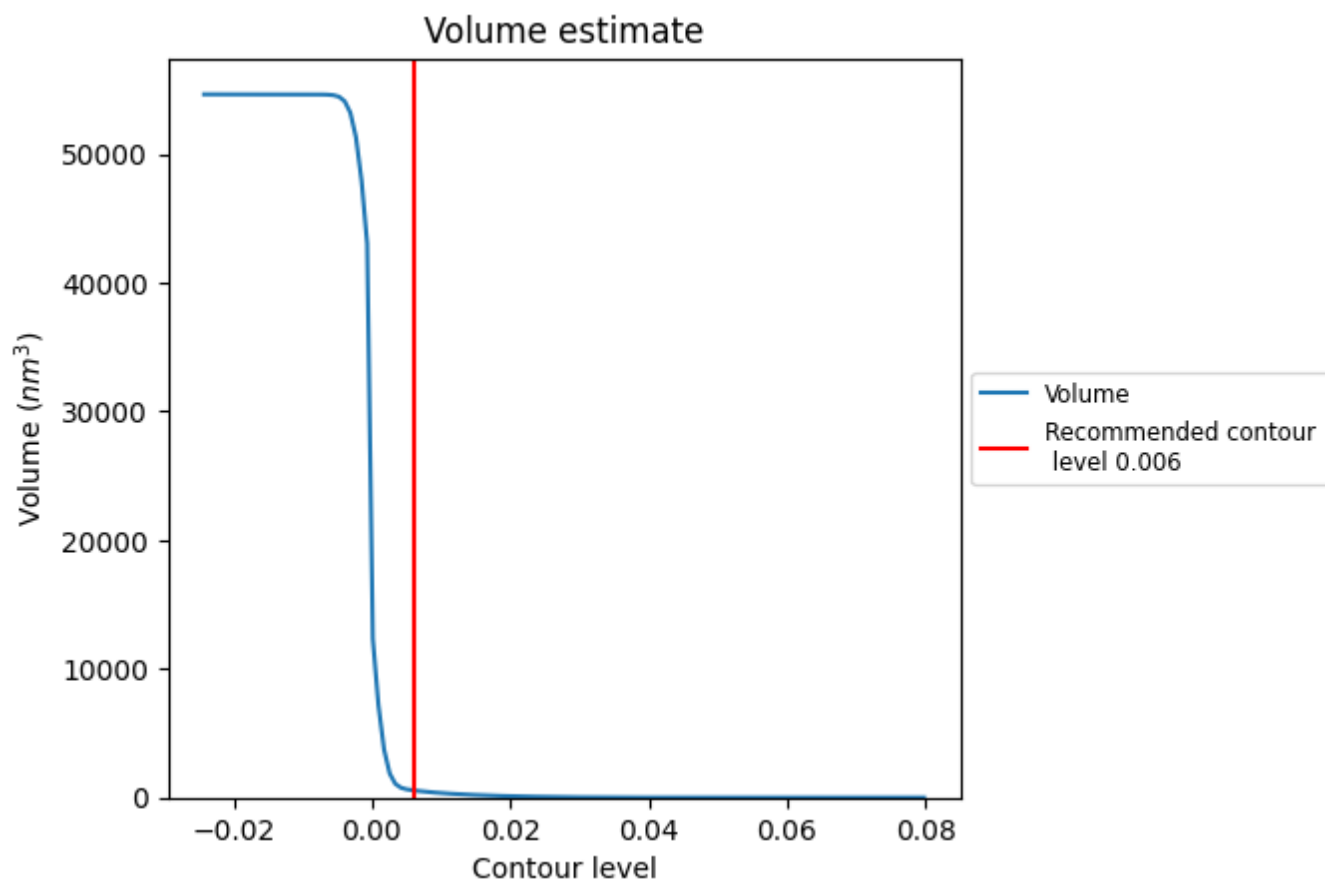
This section contains the results of statistical analysis of the map.

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.

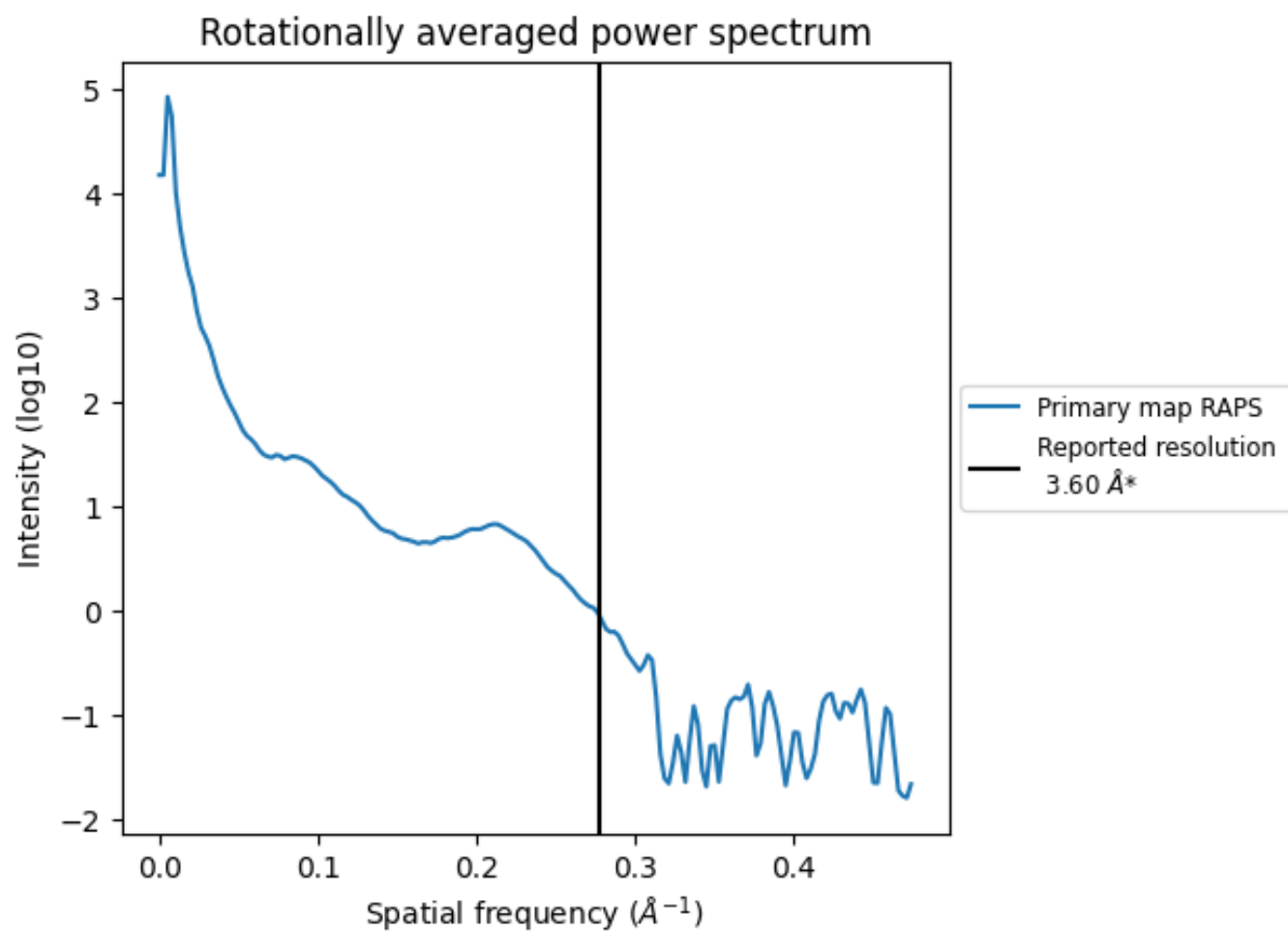
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 558 nm^3 ; this corresponds to an approximate mass of 504 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 0.278 Å⁻¹

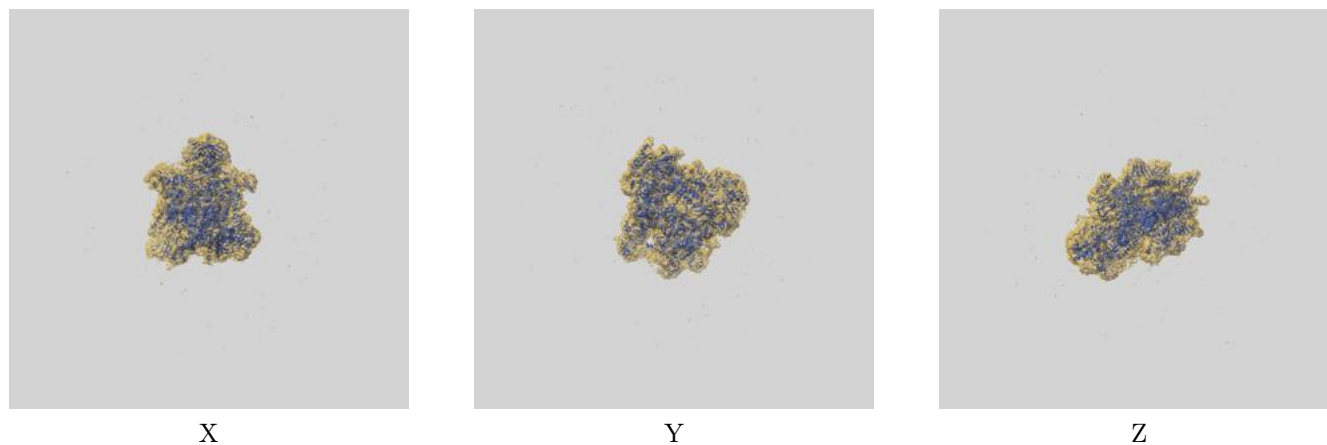
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

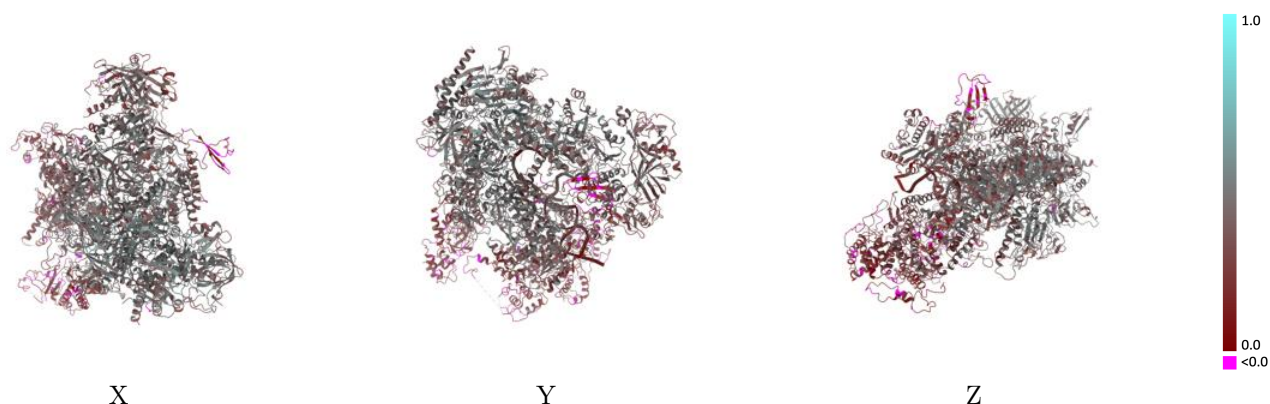
This section contains information regarding the fit between EMDB map EMD-31622 and PDB model 7FJJ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



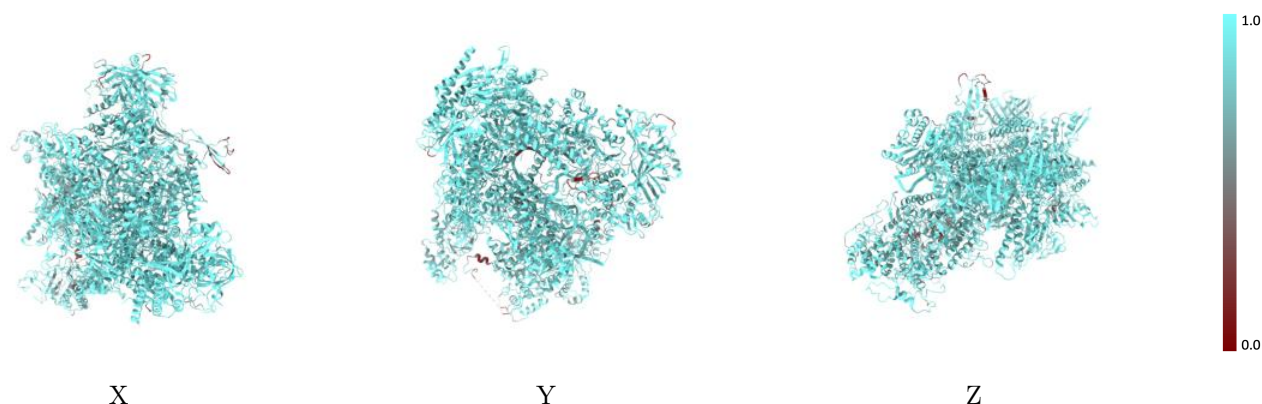
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



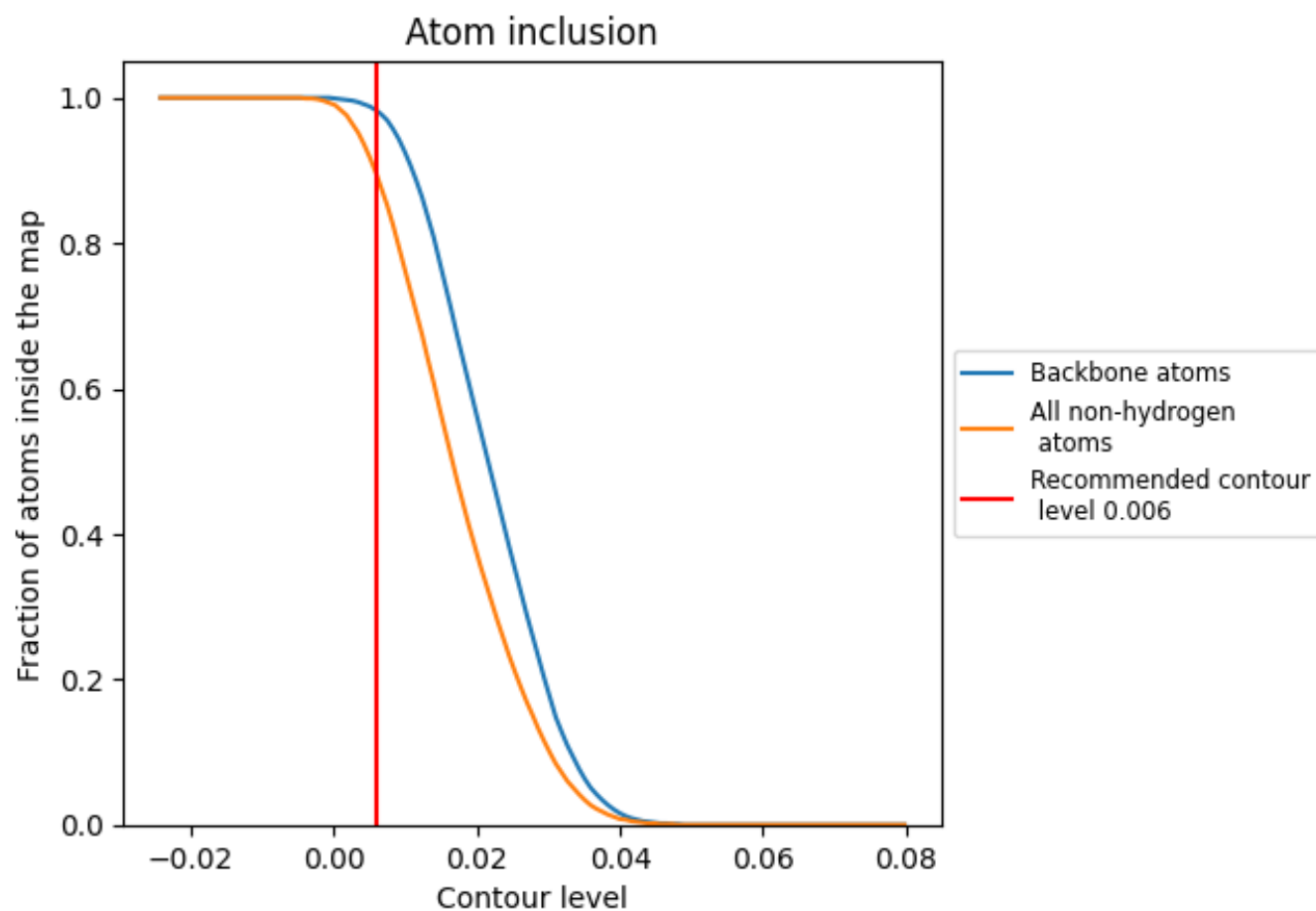
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 89% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8930	 0.3640
A	 0.9020	 0.4020
B	 0.9170	 0.4430
C	 0.9430	 0.4410
D	 0.8260	 0.1330
E	 0.9150	 0.3810
F	 0.9320	 0.4450
G	 0.8720	 0.2100
H	 0.9210	 0.4220
I	 0.7580	 0.2130
J	 0.9440	 0.4590
K	 0.9320	 0.4180
L	 0.9250	 0.3950
M	 0.8760	 0.3480
N	 0.8350	 0.3380
O	 0.8560	 0.2120
P	 0.8440	 0.1840
Q	 0.6810	 0.1280
R	 0.4880	 0.1650
X	 0.9380	 0.3380
Y	 0.9530	 0.2890

