wwPDB EM Validation Summary Report

Apr 6, 2024 – 12:55 PM EDT

PDB ID	:	8UHG
EMDB ID	:	EMD-42280
Title	:	Structure of paused transcription complex Pol II-DSIF-NELF - poised post-translocated
Authors	:	Vos, S.M.; Su, B.G.
Deposited on	:	2023-10-09
Resolution	:	2.70 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:

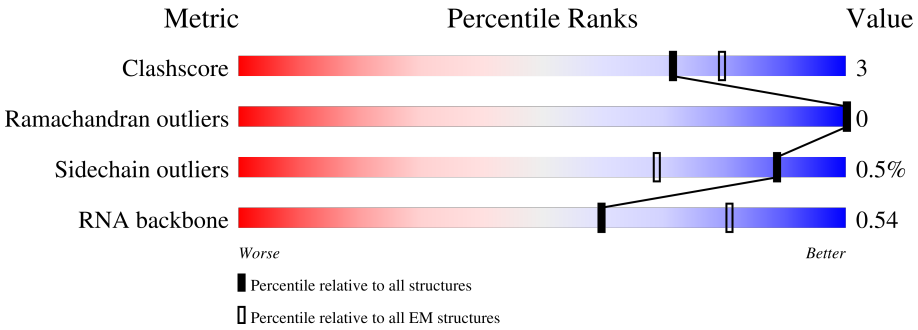
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.70 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	X	380	96%
2	V	554	56%, 85%, 14%
3	W	590	26%, 79%, 10%, 11%
4	A	1970	65%, 6%, 29%
5	B	1174	89%, 7%
6	C	271	87%, 6%, 6%
7	D	142	78%, 9%, 13%

Continued on next page...

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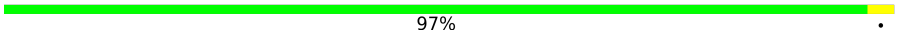
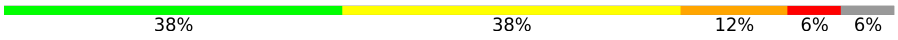
Mol	Chain	Length	Quality of chain
8	E	210	
9	F	127	
10	G	171	
11	H	150	
12	I	125	
13	J	67	
14	K	115	
15	L	58	
16	N	50	
17	P	16	
18	T	38	
19	U	528	
20	Z	1087	

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 89307 atoms, of which 44423 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 Negative elongation factor E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
1	X	15	283	85	159	23	16	0	0

- Molecule 2 is a protein called Negative elongation factor B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	V	550	8912	2825	4501	751	811	24	0	0

- Molecule 3 is a protein called Negative elongation factor C/D.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	W	526	8362	2673	4183	698	784	24	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	A	1399	22303	6976	11208	1985	2064	70	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	B	1136	18193	5739	9117	1597	1676	64	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	C	254	4031	1282	1993	348	402	6	0	0

- Molecule 7 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	124	Total	C	H	N	O	S	0	0
			2016	632	1004	173	203	4		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	E	207	Total	C	H	N	O	S	0	0
			3438	1083	1729	298	320	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	77	Total	C	H	N	O	S	0	0
			1271	397	653	105	111	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	G	171	Total	C	H	N	O	S	0	0
			2710	875	1358	219	250	8		

- 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	H	N	O	S	0	0
			2333	750	1147	194	237	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	114	Total	C	H	N	O	S	0	0
			1789	571	861	166	180	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	J	66	Total	C	H	N	O	S	0	0
			1064	339	540	88	91	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	K	115	Total	C	H	N	O	S	0	0
			1863	593	942	152	174	2		

- Molecule 15 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	L	44	Total	C	H	N	O	S	0	0
			752	231	379	72	64	6		

- Molecule 16 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	N	27	Total	C	H	N	O	P	0	0
			856	263	305	97	164	27		

- Molecule 17 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	P	15	Total	C	H	N	O	P	0	0
			474	141	158	50	110	15		

- Molecule 18 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	T	38	Total	C	H	N	O	P	0	0
			1207	371	425	148	225	38		

- Molecule 19 is a protein called Negative elongation factor A.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	U	196	Total	C	H	N	O	S	0	0
			3054	953	1556	253	284	8		

- Molecule 20 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Z	274	Total	C	H	N	O	S	0	0
			4387	1373	2205	393	405	11		

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

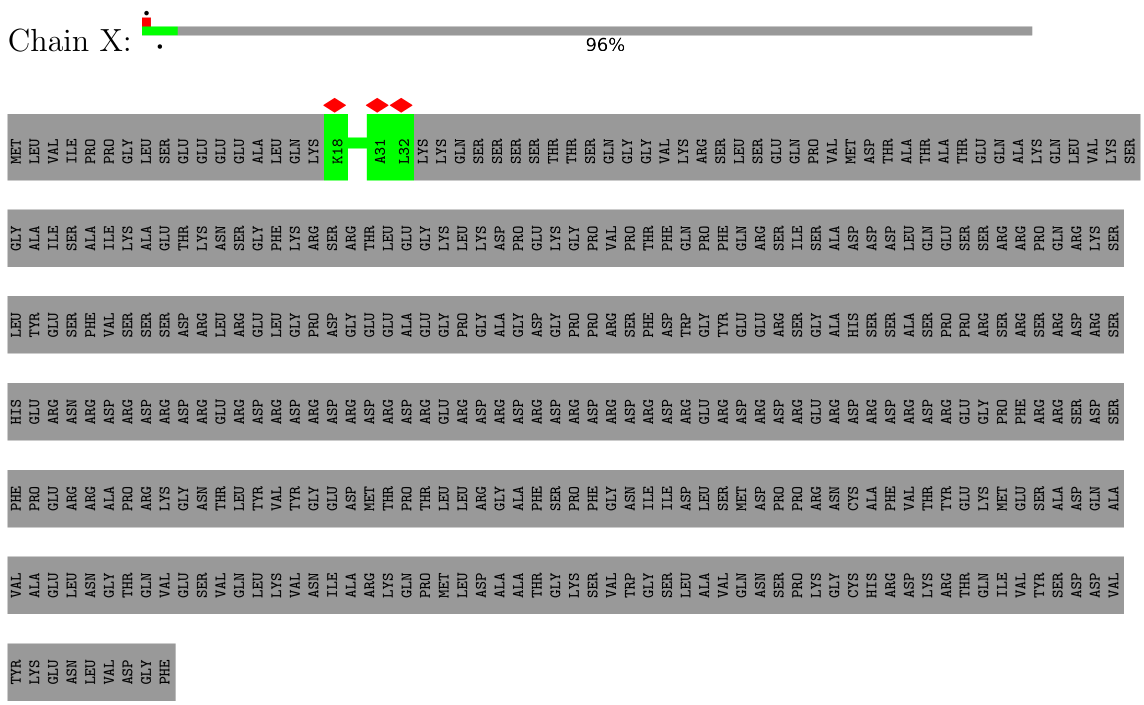
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total Mg 1 1	0

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.

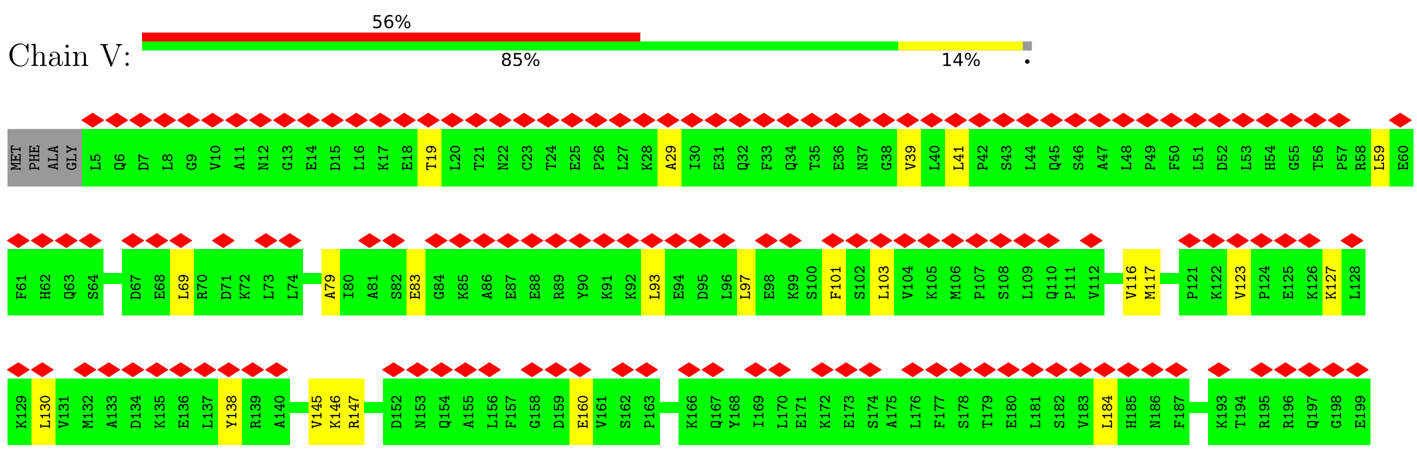
- Molecule 1: Negative elongation factor E

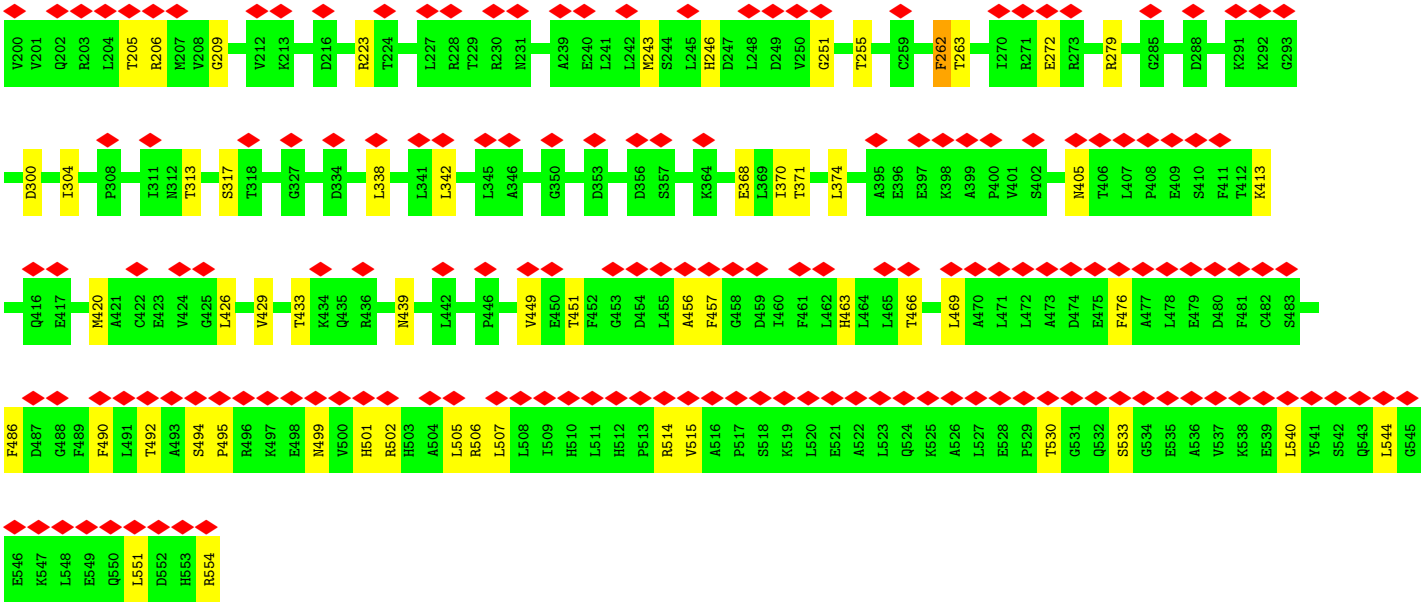
Chain X:



- Molecule 2: Negative elongation factor B

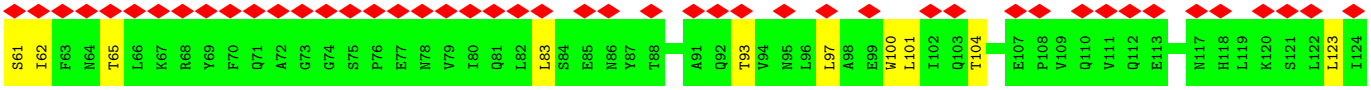
Chain V:

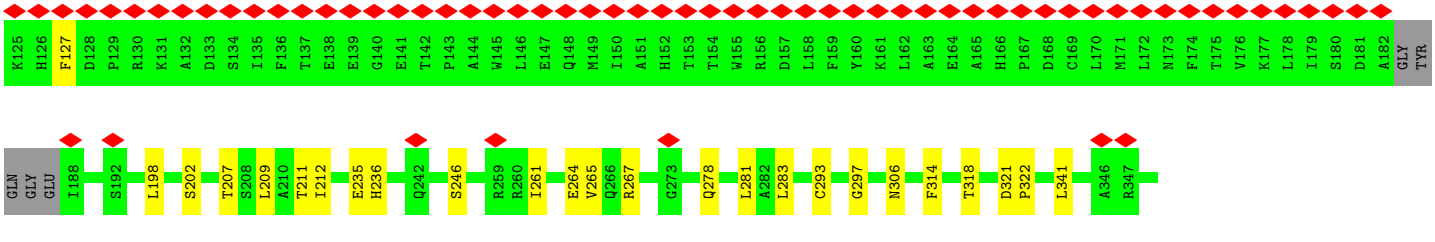




• Molecule 3: Negative elongation factor C/D

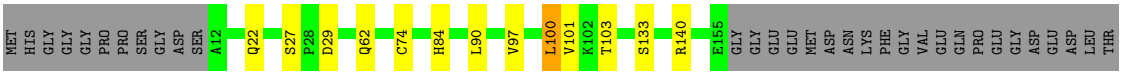
Chain W:

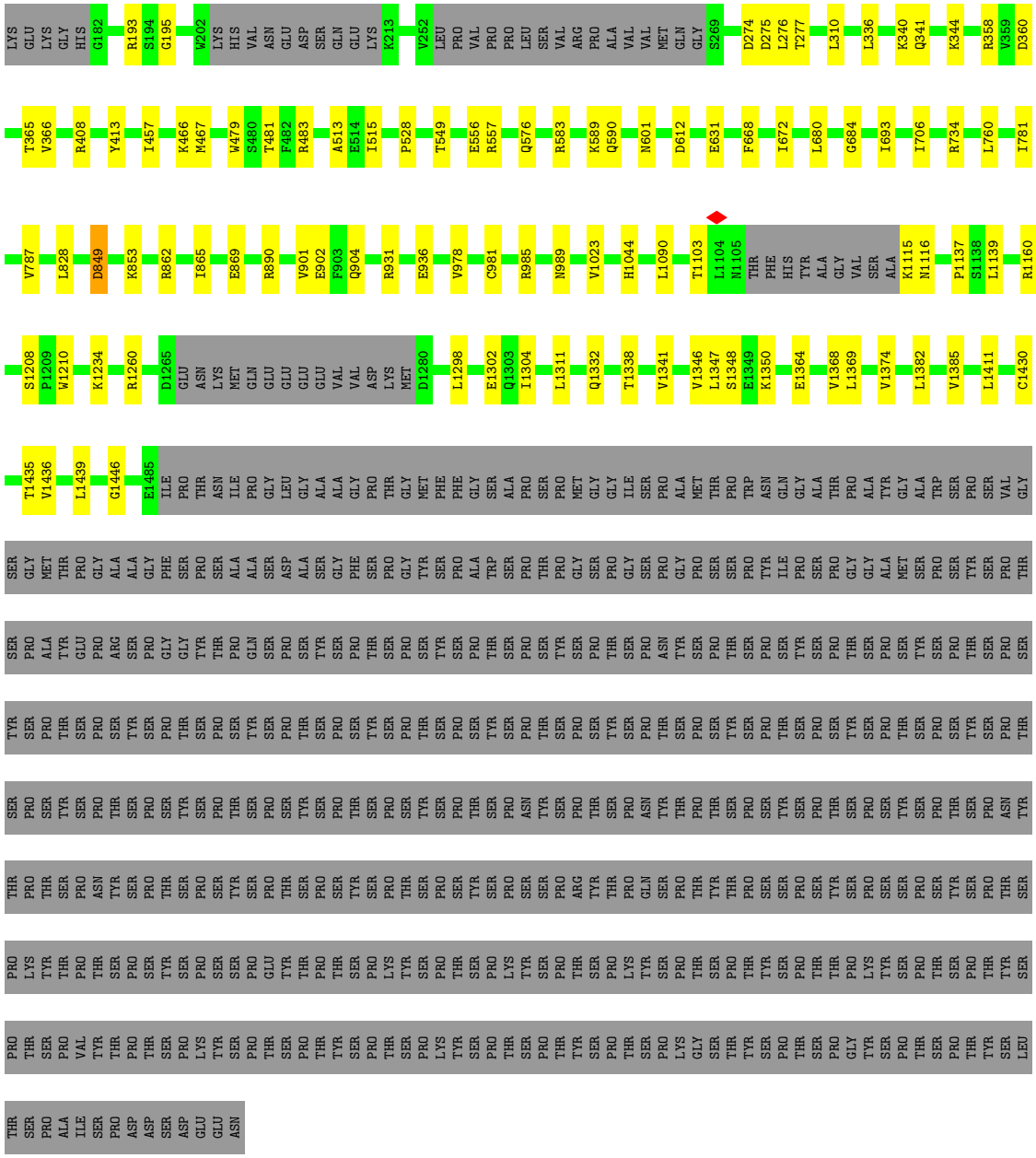




• Molecule 4: DNA-directed RNA polymerase subunit

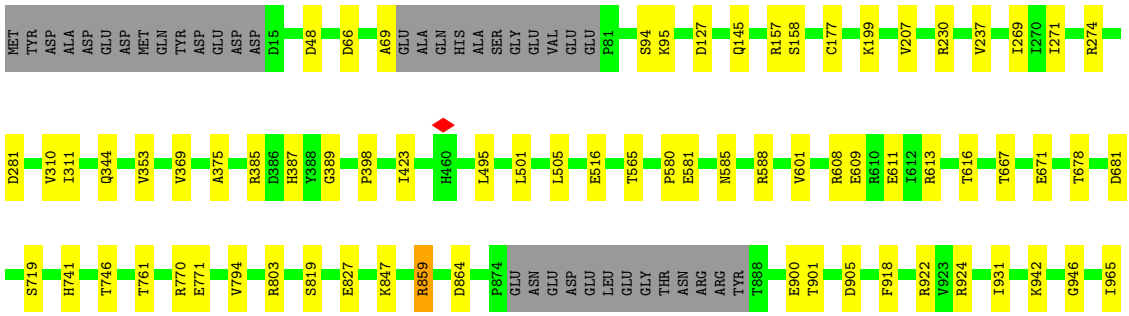
Chain A:





• Molecule 5: DNA-directed RNA polymerase subunit beta

Chain B:



• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

Chain C:

• Molecule 7: RNA polymerase Rpb4/RPC9 core domain-containing protein

Chain D:

• Molecule 8: DNA-directed RNA polymerase II subunit E

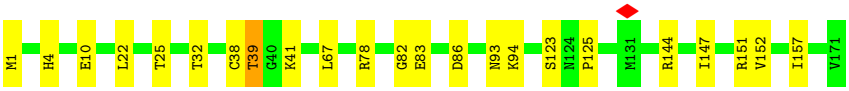
Chain E:

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

Chain F:

• Molecule 10: DNA-directed RNA polymerase subunit

Chain G:

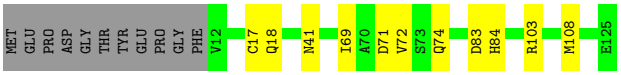


• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:

• Molecule 12: DNA-directed RNA polymerase II subunit RPB9

Chain I:

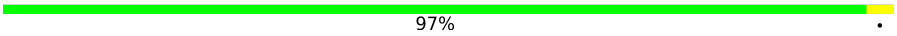


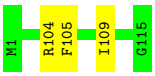
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

• Molecule 14: DNA-directed RNA polymerase II subunit RPB11-a

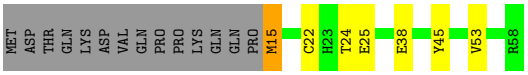
Chain K:





• Molecule 15: RNA polymerase II subunit K

Chain L:

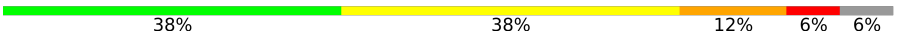


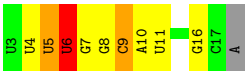
• Molecule 16: Non-template DNA

Chain N:

• Molecule 17: RNA

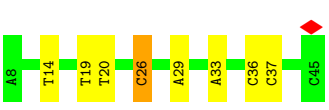
Chain P:





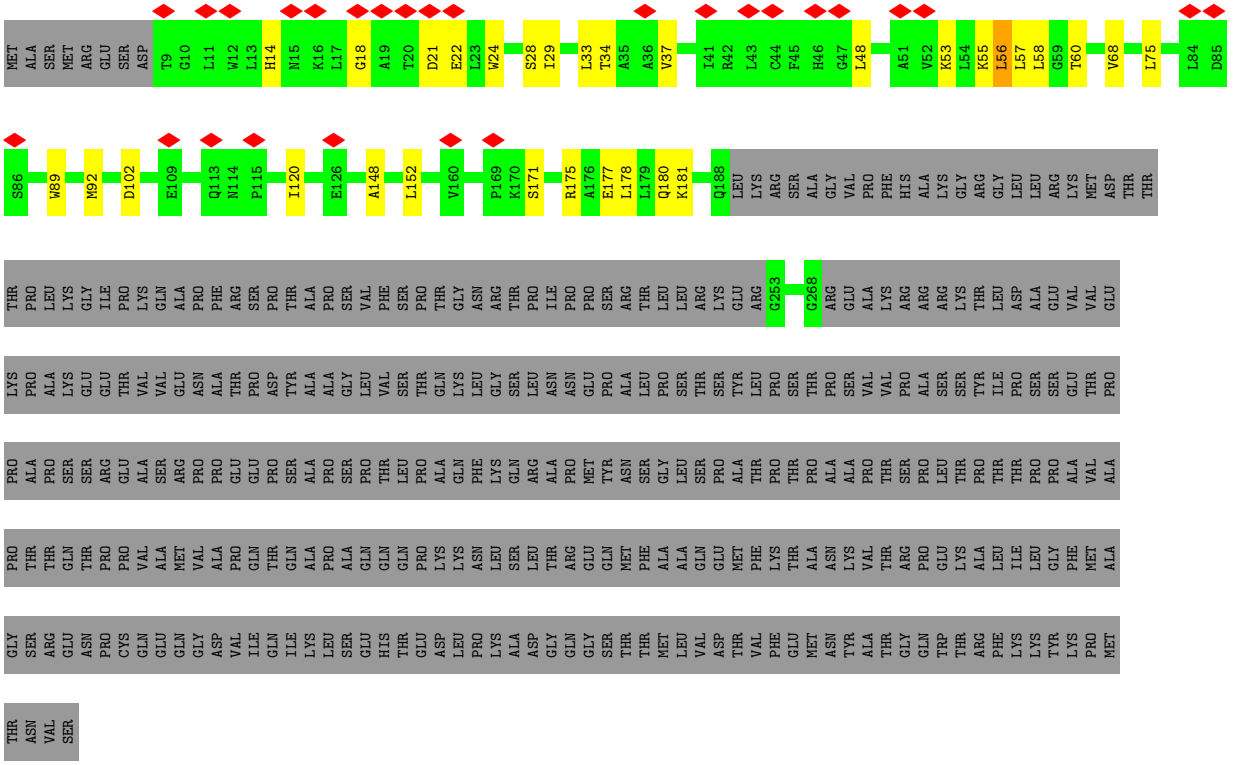
• Molecule 18: Template DNA

Chain T:



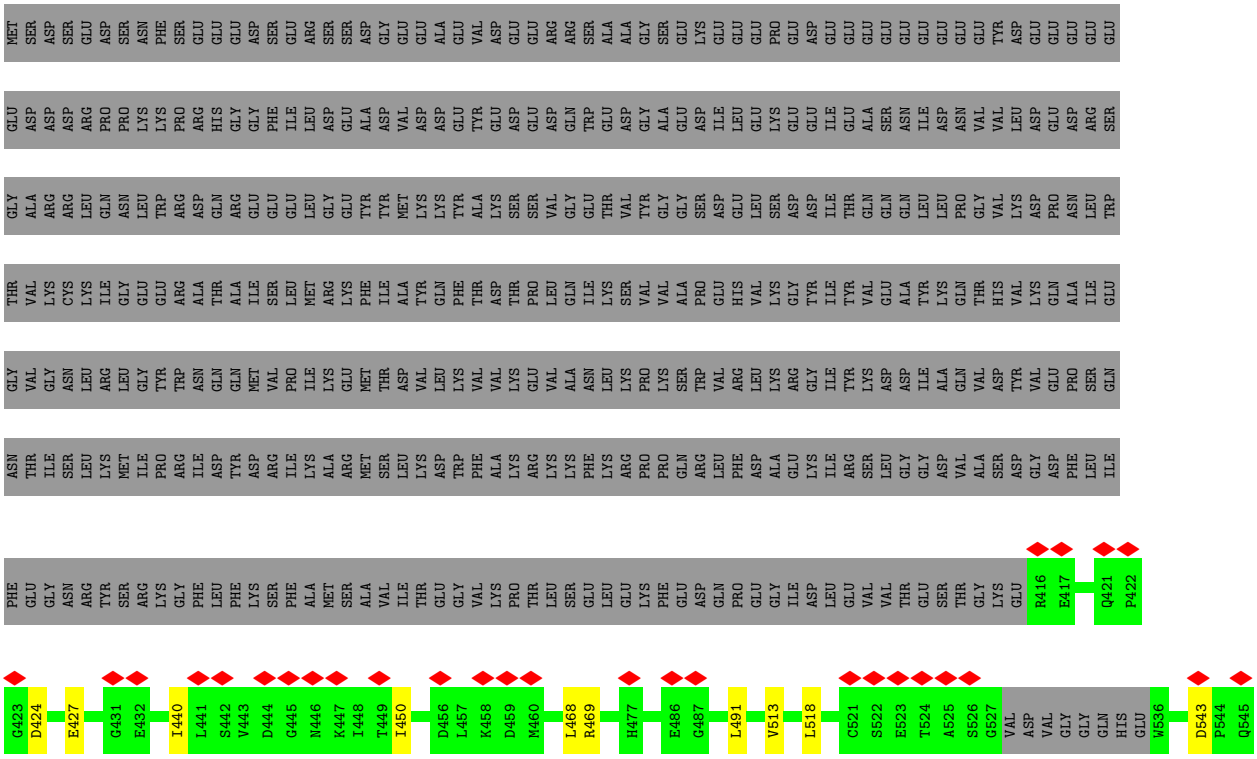
• Molecule 19: Negative elongation factor A

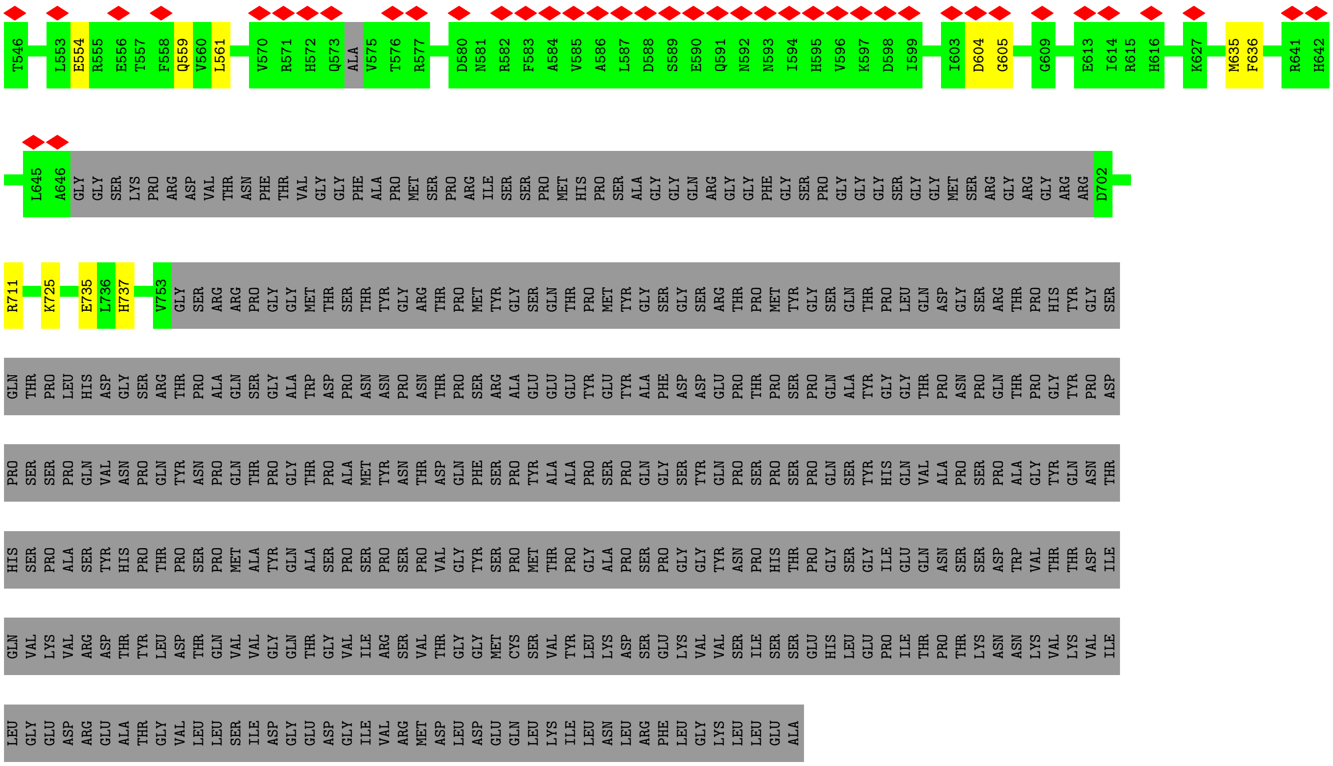
Chain U:



• Molecule 20: Transcription elongation factor SPT5

Chain Z:




T546 L553 E554 R555 E556 T557 F558 Q559 V560 L561 V570 R571 H572 Q573 ALA V575 T576 R577 D580 N581 R582 F583 A584 V585 A586 L587 D588 S589 E590 Q591 N592 N593 I594 H595 V596 K597 D598 I599 I603 D604 G605 G609 E613 I614 R615 H616 K627 M635 F636 R641 H642
L645 A646 GLY GLY SER LYS PRO ARG ASP VAL THR ASN PHE THR VAL GLY GLY PHE ALA PRO MET SER PRO ARG ILE SER SER PRO MET HIS PRO SER ALA GLY GLY GLN ARG GLY GLY PHE GLY SER PRO GLY GLY GLY SER GLY GLY MET SER ARG GLY ARG GLY ARG ARG D702
R711 K725 E735 L736 H737 V753 GLY SER ARG ARG PRO GLY GLY MET THR SER THR TYR GLY ARG THR PRO MET TYR GLY SER GLN THR PRO MET TYR GLY SER GLY SER ARG THR PRO MET TYR GLY SER GLN THR PRO LEU GLN ASP GLY SER ARG THR PRO HIS TYR GLY SER
GLN THR PRO LEU HIS ASP GLY SER ARG THR PRO ALA GLN SER GLY ALA TRP ASP PRO ASN ASN PRO ASN THR PRO SER ARG ALA GLU GLU TYR GLU TYR ALA PHE ASP ASP GLU PRO THR PRO SER PRO GLN ALA TYR GLY THR PRO ASN PRO GLN THR PRO GLY TYR PRO ASP
PRO SER SER PRO GLN VAL ASN PRO GLN TYR ASN PRO GLN THR PRO GLY THR PRO ALA MET TYR ASN THR ASP GLN PHE SER PRO TYR ALA ALA PRO SER PRO GLN GLY SER TYR GLN PRO SER PRO SER PRO GLN SER TYR HIS GLN VAL ALA PRO SER PRO ALA GLY TYR GLN ASN THR
HIS SER PRO ALA SER TYR HIS PRO THR PRO SER PRO MET ALA TYR GLN ALA SER PRO SER PRO SER PRO VAL GLY TYR SER PRO MET THR PRO GLY ALA PRO SER PRO GLY GLY TYR ASN PRO HIS THR PRO GLY SER GLY ILE GLU GLN ASN SER SER ASP TRP VAL THR THR ASP ILE
GLN VAL LYS VAL ARG ASP THR TYR LEU ASP THR GLN VAL VAL GLY GLN THR GLY VAL ILE ARG SER VAL THR GLY GLY MET CYS SER VAL TYR LEU LYS ASP SER GLU LYS VAL VAL SER ILE SER SER GLU HIS LEU GLU PRO ILE THR PRO THR LYS ASN ASN LYS VAL LYS VAL ILE
LEU GLY GLU ASP ARG GLU ALA THR GLY VAL LEU LEU SER ILE ASP GLY GLU ASP GLY ILE VAL ARG MET ASP LEU ASP GLU GLN LEU LYS ILE LEU ASN LEU ARG PHE LEU GLY LYS LEU LEU GLU ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90283	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.739	Depositor
Minimum map value	-0.921	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.085	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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: ZN, MG

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	X	0.28	0/124	0.47	0/159
2	V	0.33	0/4496	0.66	1/6074 (0.0%)
3	W	0.31	0/4261	0.57	0/5777
4	A	0.29	0/11294	0.62	1/15241 (0.0%)
5	B	0.29	0/9257	0.61	0/12493
6	C	0.28	0/2081	0.60	0/2828
7	D	0.29	0/1025	0.58	0/1376
8	E	0.30	0/1739	0.62	0/2347
9	F	0.30	0/628	0.61	0/848
10	G	0.31	0/1383	0.60	0/1874
11	H	0.28	0/1207	0.63	0/1628
12	I	0.30	0/949	0.62	0/1284
13	J	0.30	0/533	0.66	0/719
14	K	0.31	0/940	0.55	0/1271
15	L	0.29	0/378	0.72	0/500
16	N	0.94	0/615	1.12	1/944 (0.1%)
17	P	0.41	0/351	1.40	9/544 (1.7%)
18	T	0.93	2/878 (0.2%)	1.14	5/1353 (0.4%)
19	U	0.32	0/1521	0.62	1/2063 (0.0%)
20	Z	0.27	0/2214	0.61	0/2979
All	All	0.34	2/45874 (0.0%)	0.65	18/62302 (0.0%)

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
12	I	0	1
20	Z	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	36	DC	C1'-N1	6.62	1.57	1.49
18	T	26	DC	C1'-N1	5.03	1.55	1.49

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	P	9	C	C2-N1-C1'	12.22	132.25	118.80
17	P	9	C	C6-N1-C1'	-9.11	109.86	120.80
17	P	9	C	N1-C2-O2	8.12	123.78	118.90
2	V	262	PHE	CB-CG-CD1	7.37	125.95	120.80
17	P	9	C	O4'-C1'-N1	7.10	113.88	108.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	I	103	ARG	Peptide
20	Z	711	ARG	Sidechain

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	X	124	159	159	0	0
2	V	4411	4501	4501	58	0
3	W	4179	4183	4181	45	0
4	A	11095	11208	11207	73	0
5	B	9076	9117	9116	57	0
6	C	2038	1993	1989	13	0
7	D	1012	1004	1004	10	0
8	E	1709	1729	1729	14	0
9	F	618	653	653	3	0
10	G	1352	1358	1358	15	0
11	H	1186	1147	1147	5	0
12	I	928	861	859	7	0
13	J	524	540	540	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K	921	942	942	3	0
15	L	373	379	378	6	0
16	N	551	305	307	1	0
17	P	316	158	158	2	0
18	T	782	425	427	4	0
19	U	1498	1556	1556	19	0
20	Z	2182	2205	2205	14	0
21	A	2	0	0	0	0
21	B	1	0	0	0	0
21	C	1	0	0	0	0
21	I	2	0	0	0	0
21	J	1	0	0	0	0
21	L	1	0	0	0	0
22	A	1	0	0	0	0
All	All	44884	44423	44416	308	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 3.

The worst 5 of 308 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)
5:B:237:VAL:HG21	5:B:369:VAL:HG12	1.67	0.76
7:D:73:ARG:NE	7:D:102:ASN:O	2.19	0.75
2:V:79:ALA:O	2:V:83:GLU:N	2.22	0.72
2:V:138:TYR:OH	2:V:160:GLU:OE1	2.10	0.70
3:W:481:HIS:O	3:W:489:GLN:NE2	2.25	0.70

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	X	13/380 (3%)	13 (100%)	0	0	100	100
2	V	548/554 (99%)	531 (97%)	17 (3%)	0	100	100
3	W	512/590 (87%)	492 (96%)	20 (4%)	0	100	100
4	A	1387/1970 (70%)	1339 (96%)	48 (4%)	0	100	100
5	B	1130/1174 (96%)	1077 (95%)	53 (5%)	0	100	100
6	C	250/271 (92%)	241 (96%)	9 (4%)	0	100	100
7	D	122/142 (86%)	115 (94%)	7 (6%)	0	100	100
8	E	203/210 (97%)	196 (97%)	7 (3%)	0	100	100
9	F	75/127 (59%)	73 (97%)	2 (3%)	0	100	100
10	G	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
11	H	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
12	I	112/125 (90%)	105 (94%)	7 (6%)	0	100	100
13	J	64/67 (96%)	63 (98%)	1 (2%)	0	100	100
14	K	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
15	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
19	U	192/528 (36%)	189 (98%)	3 (2%)	0	100	100
20	Z	266/1087 (24%)	260 (98%)	6 (2%)	0	100	100
All	All	5344/7719 (69%)	5153 (96%)	191 (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	X	13/331 (4%)	13 (100%)	0	100	100
2	V	493/495 (100%)	490 (99%)	3 (1%)	86	95
3	W	466/513 (91%)	464 (100%)	2 (0%)	91	97
4	A	1232/1749 (70%)	1228 (100%)	4 (0%)	92	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	B	994/1027 (97%)	989 (100%)	5 (0%)	88 96
6	C	231/248 (93%)	231 (100%)	0	100 100
7	D	114/126 (90%)	114 (100%)	0	100 100
8	E	190/192 (99%)	188 (99%)	2 (1%)	73 90
9	F	67/111 (60%)	67 (100%)	0	100 100
10	G	152/152 (100%)	151 (99%)	1 (1%)	84 94
11	H	129/131 (98%)	128 (99%)	1 (1%)	81 93
12	I	103/112 (92%)	102 (99%)	1 (1%)	76 91
13	J	55/56 (98%)	54 (98%)	1 (2%)	59 83
14	K	104/104 (100%)	104 (100%)	0	100 100
15	L	41/55 (74%)	40 (98%)	1 (2%)	49 77
19	U	167/451 (37%)	164 (98%)	3 (2%)	59 83
20	Z	244/940 (26%)	244 (100%)	0	100 100
All	All	4795/6793 (71%)	4771 (100%)	24 (0%)	89 96

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	E	52	ARG
11	H	124	ARG
10	G	39	THR
12	I	41	ASN
4	A	612	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
11	H	131	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	P	14/16 (87%)	7 (50%)	1 (7%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	P	5	U
17	P	6	U
17	P	7	G
17	P	8	G
17	P	9	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
17	P	6	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 9 ligands modelled in this entry, 9 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.

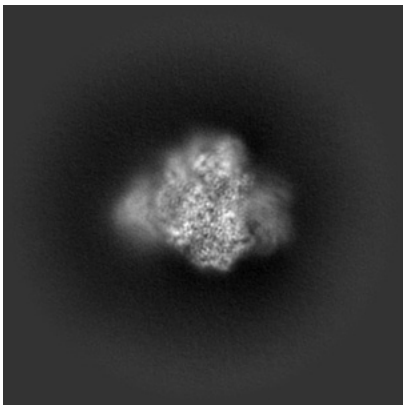
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42280. These allow visual inspection of the internal detail of the map and identification of artifacts.

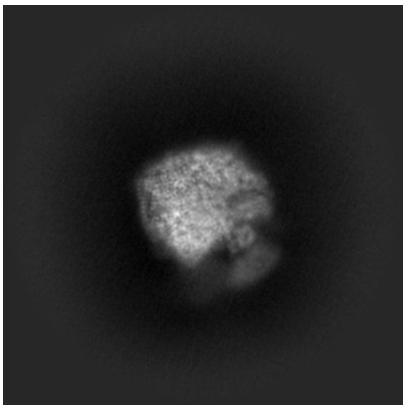
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

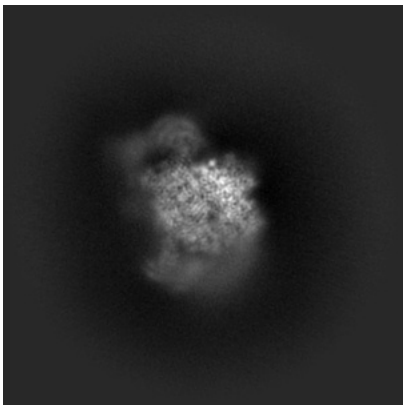
6.1.1 Primary map



X

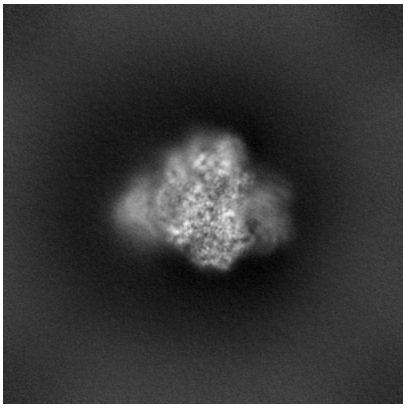


Y

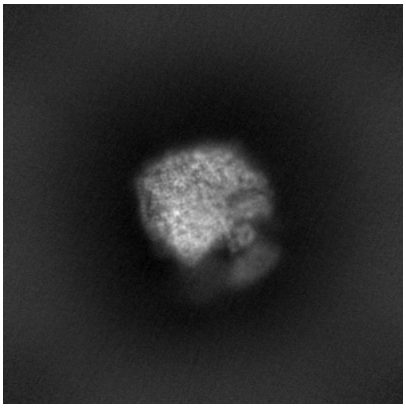


Z

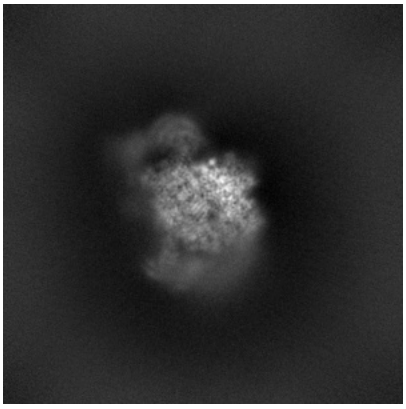
6.1.2 Raw map



X



Y

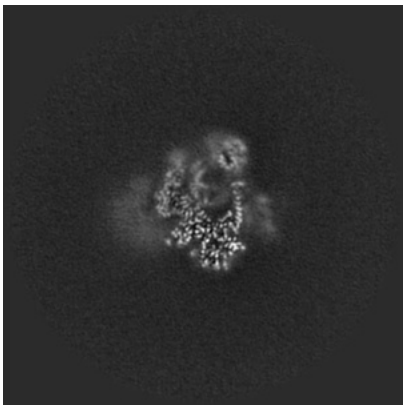


Z

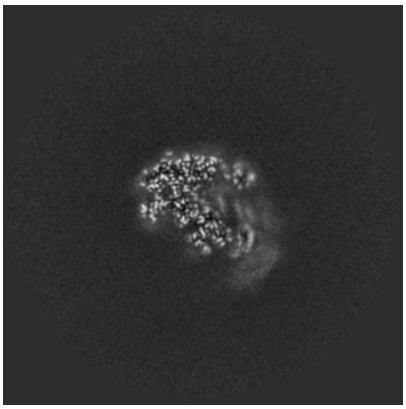
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

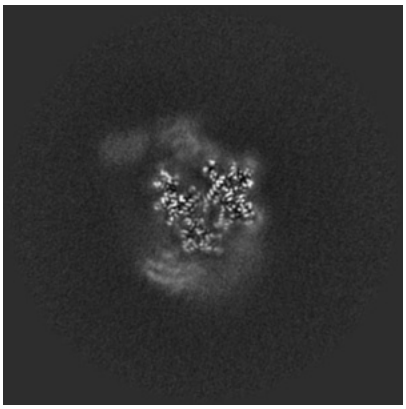
6.2.1 Primary map



X Index: 256

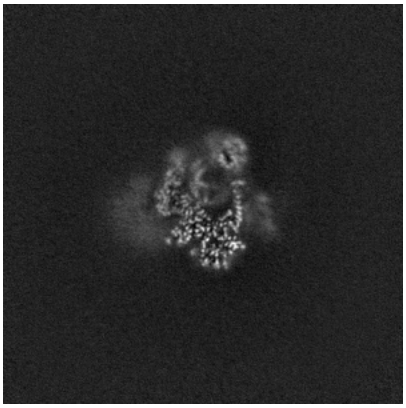


Y Index: 256

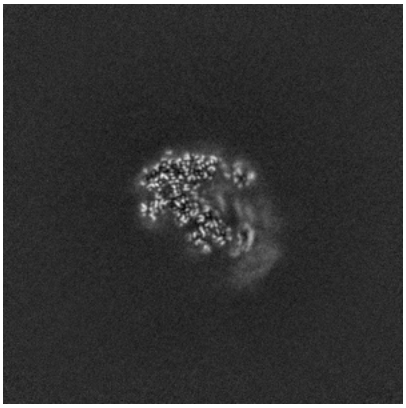


Z Index: 256

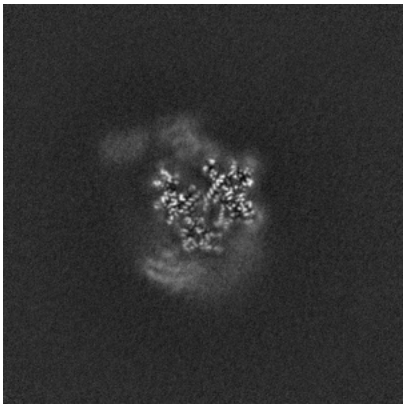
6.2.2 Raw map



X Index: 256



Y Index: 256

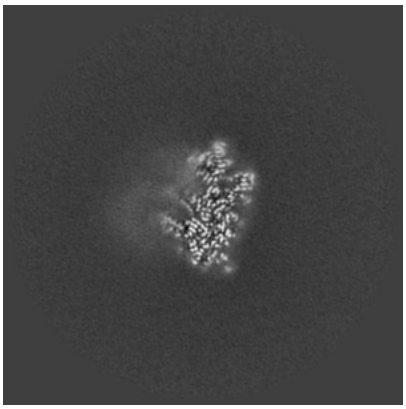


Z Index: 256

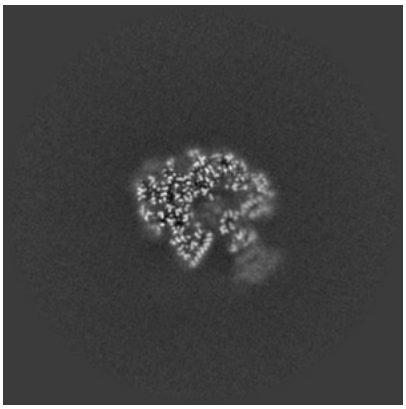
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

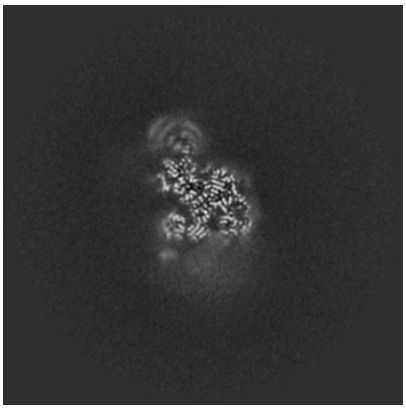
6.3.1 Primary map



X Index: 289

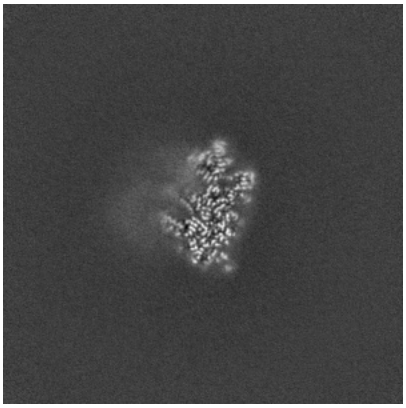


Y Index: 281

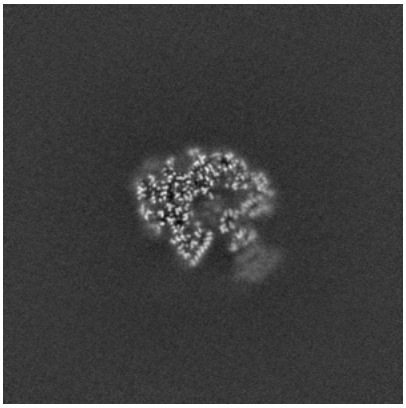


Z Index: 220

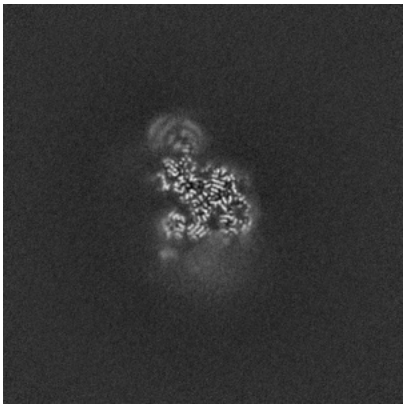
6.3.2 Raw map



X Index: 289



Y Index: 281

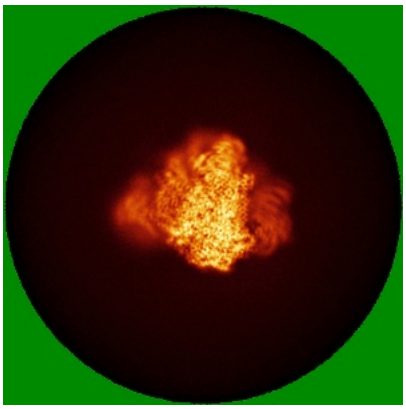


Z Index: 220

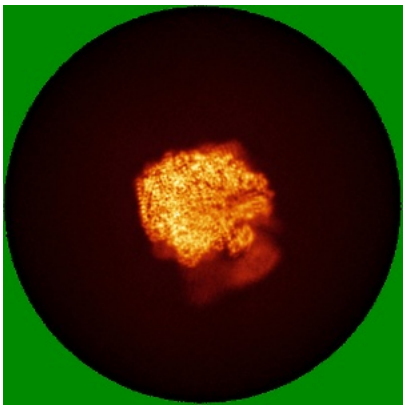
The images above show the largest variance slices of the map in three orthogonal directions.

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

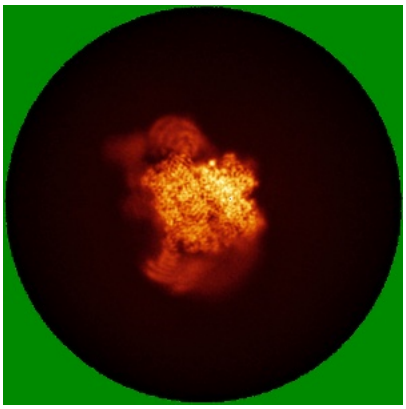
6.4.1 Primary map



X

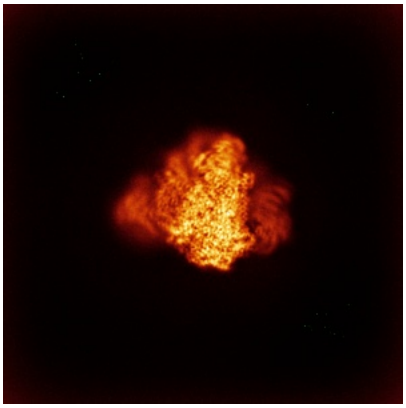


Y

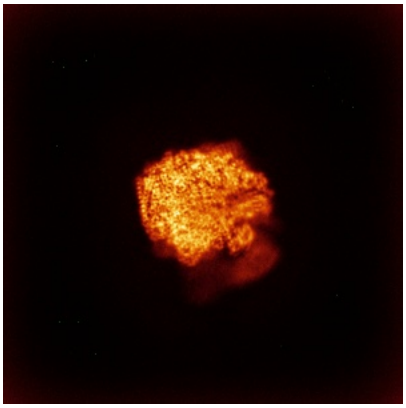


Z

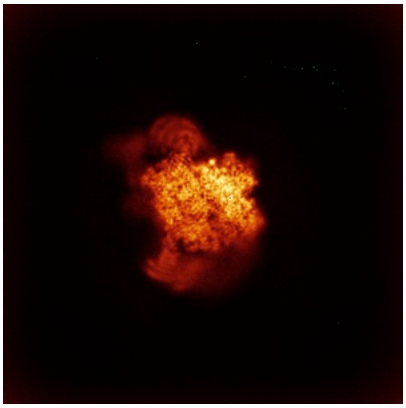
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. 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

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.

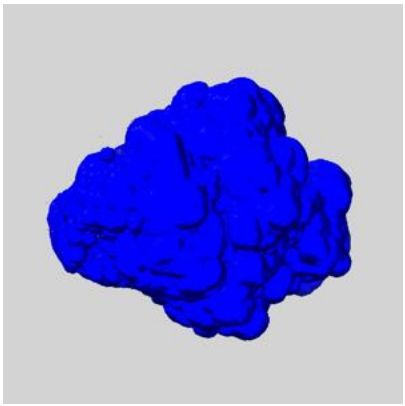
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

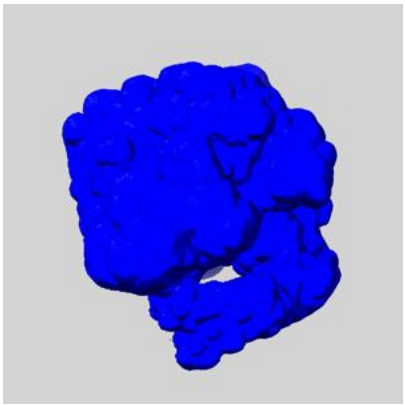
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

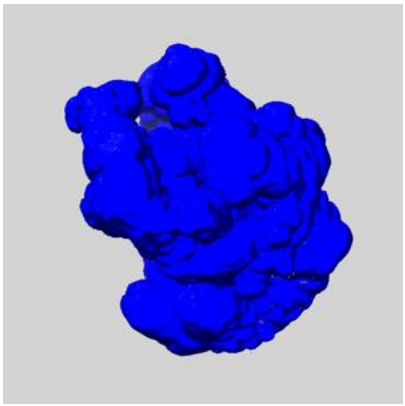
6.6.1 emd_42280_msk_1.map (i)



X



Y

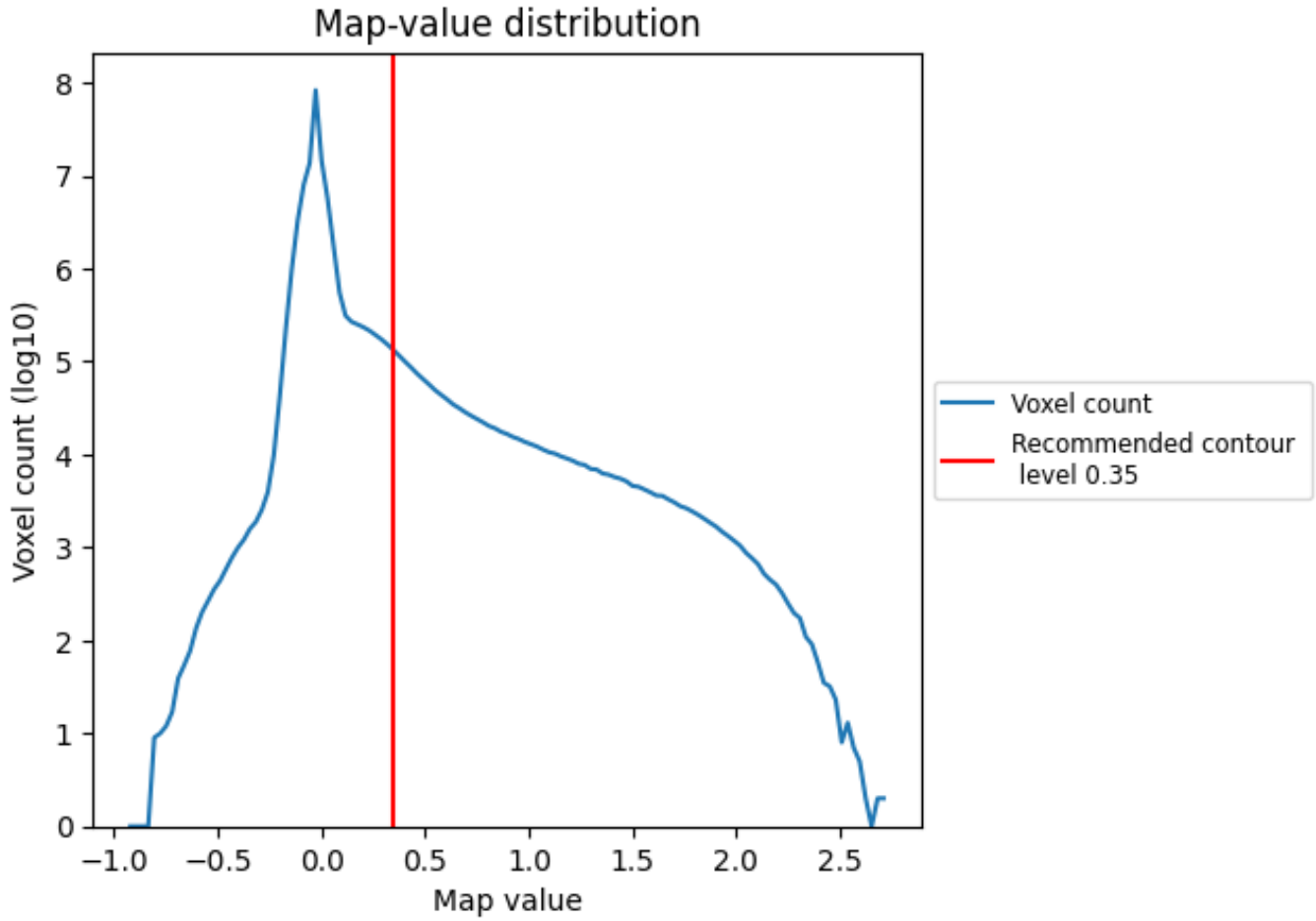


Z

7 Map analysis

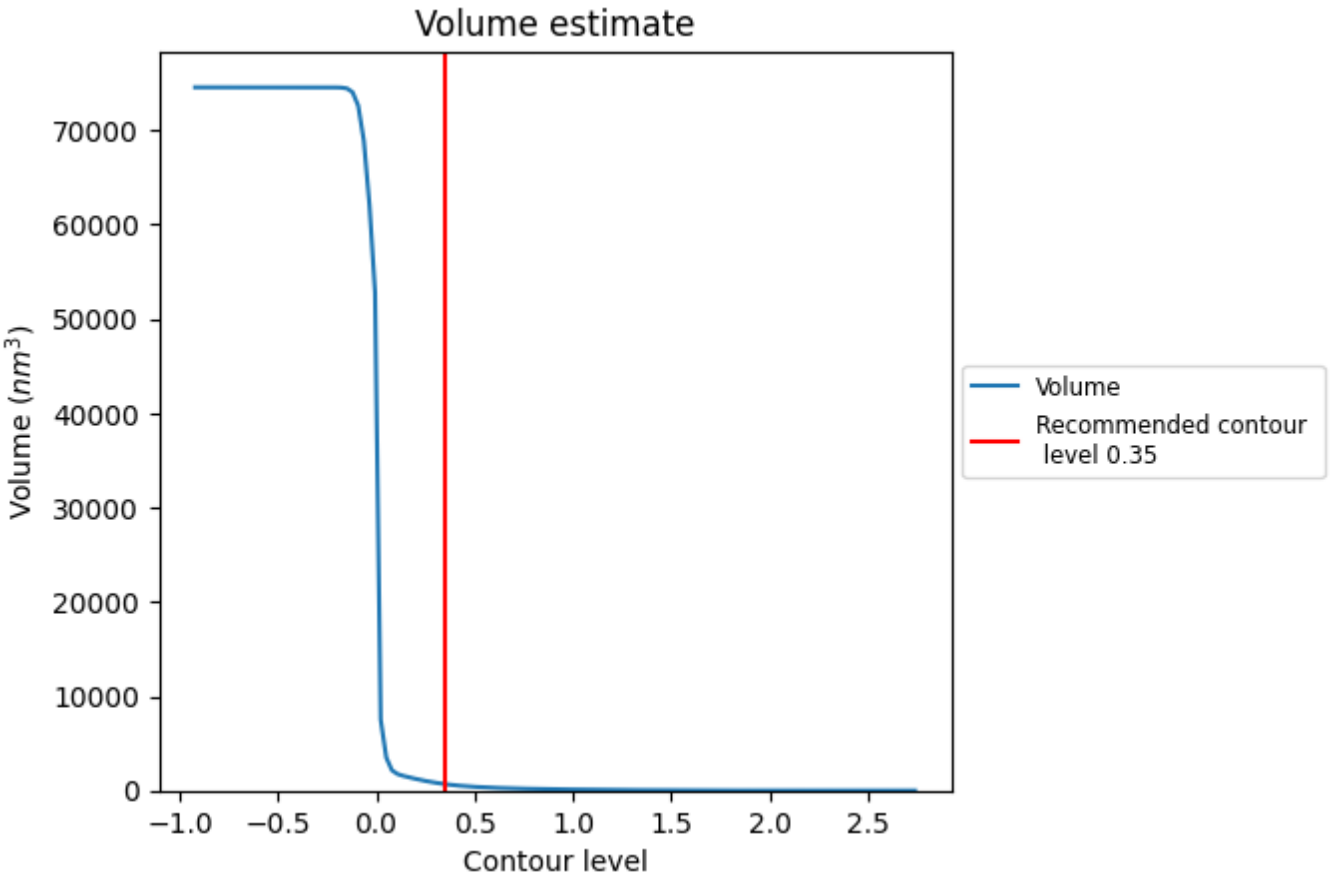
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

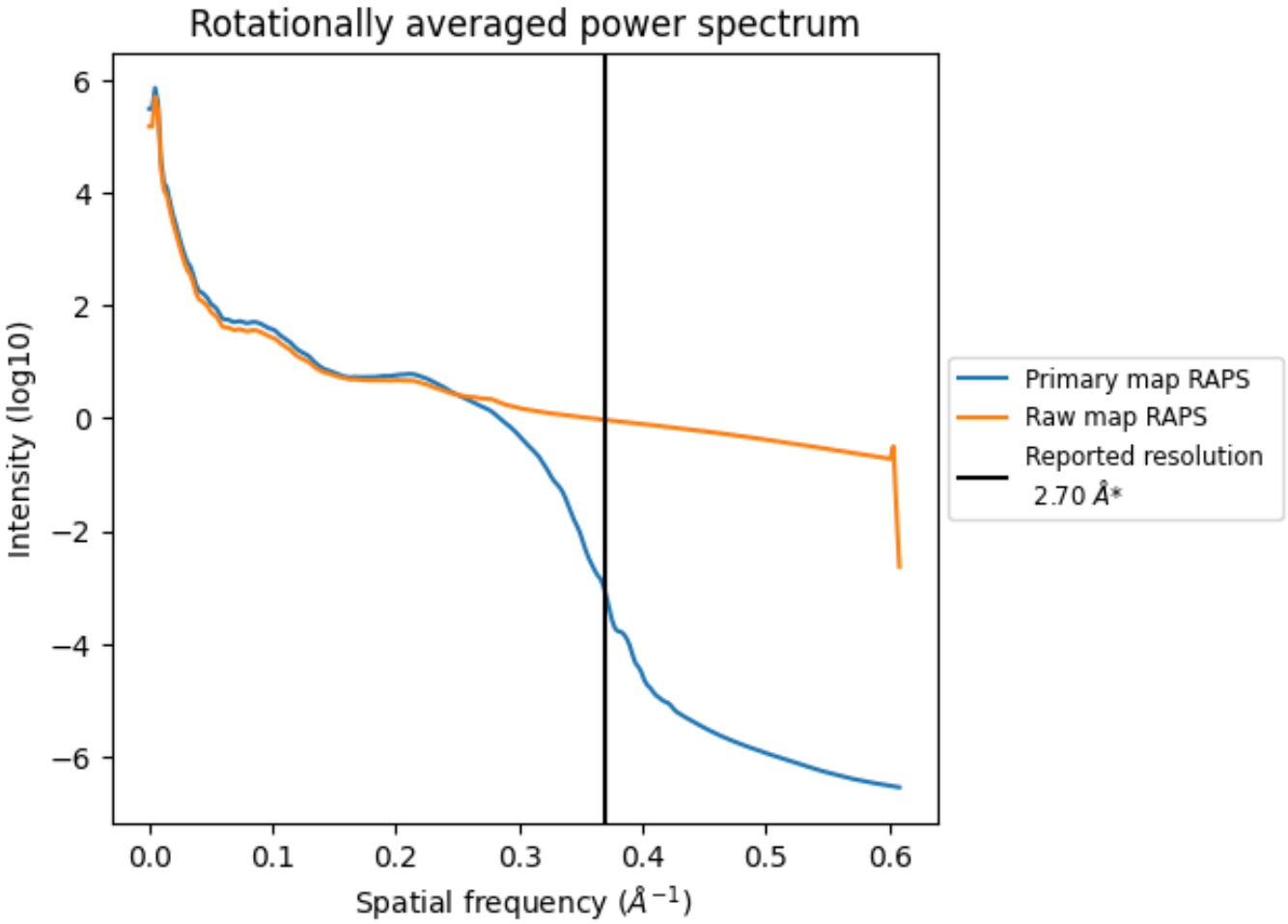
7.2 Volume estimate (i)



The volume at the recommended contour level is 683 nm^3; this corresponds to an approximate mass of 617 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)

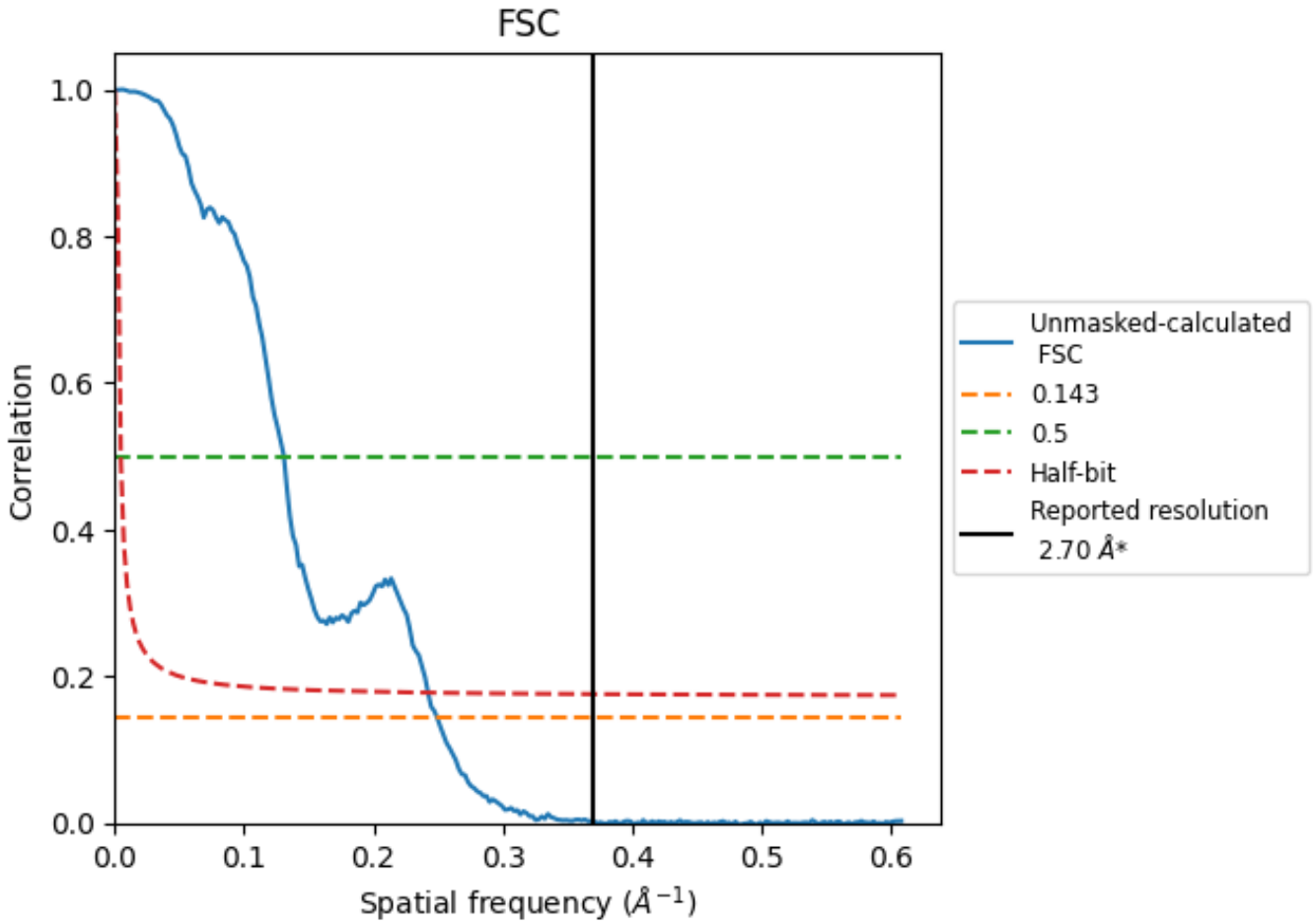


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

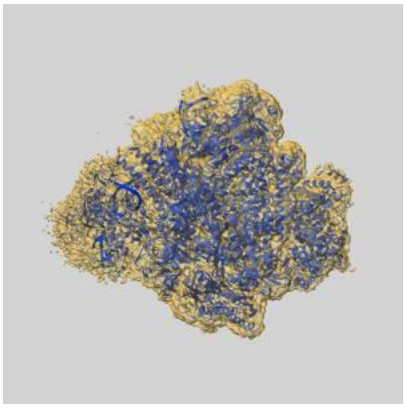
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.65	4.13

*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 4.01 differs from the reported value 2.7 by more than 10 %

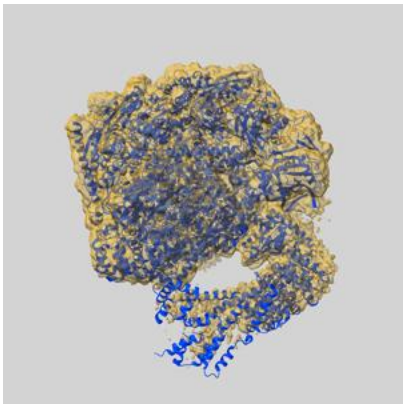
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42280 and PDB model 8UHG. Per-residue inclusion information can be found in section 3 on page 8.

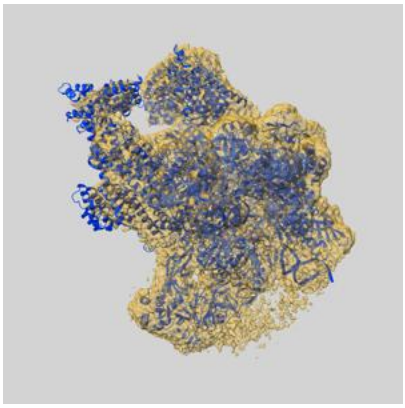
9.1 Map-model overlay



X



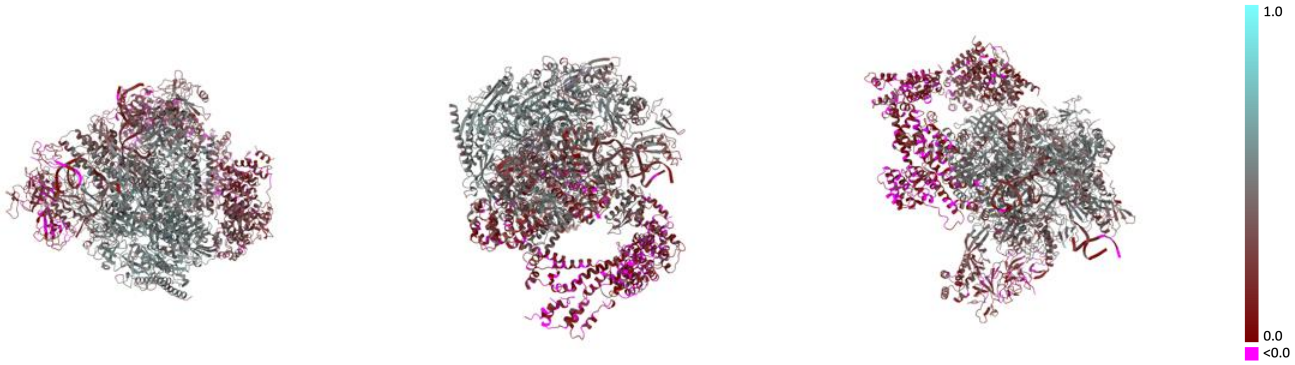
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.35 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.

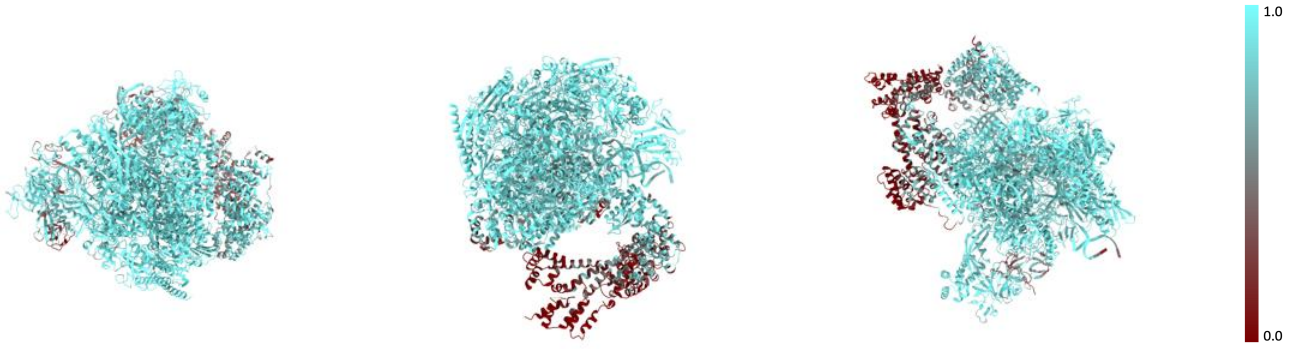
9.2 Q-score mapped to coordinate model (i)



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.

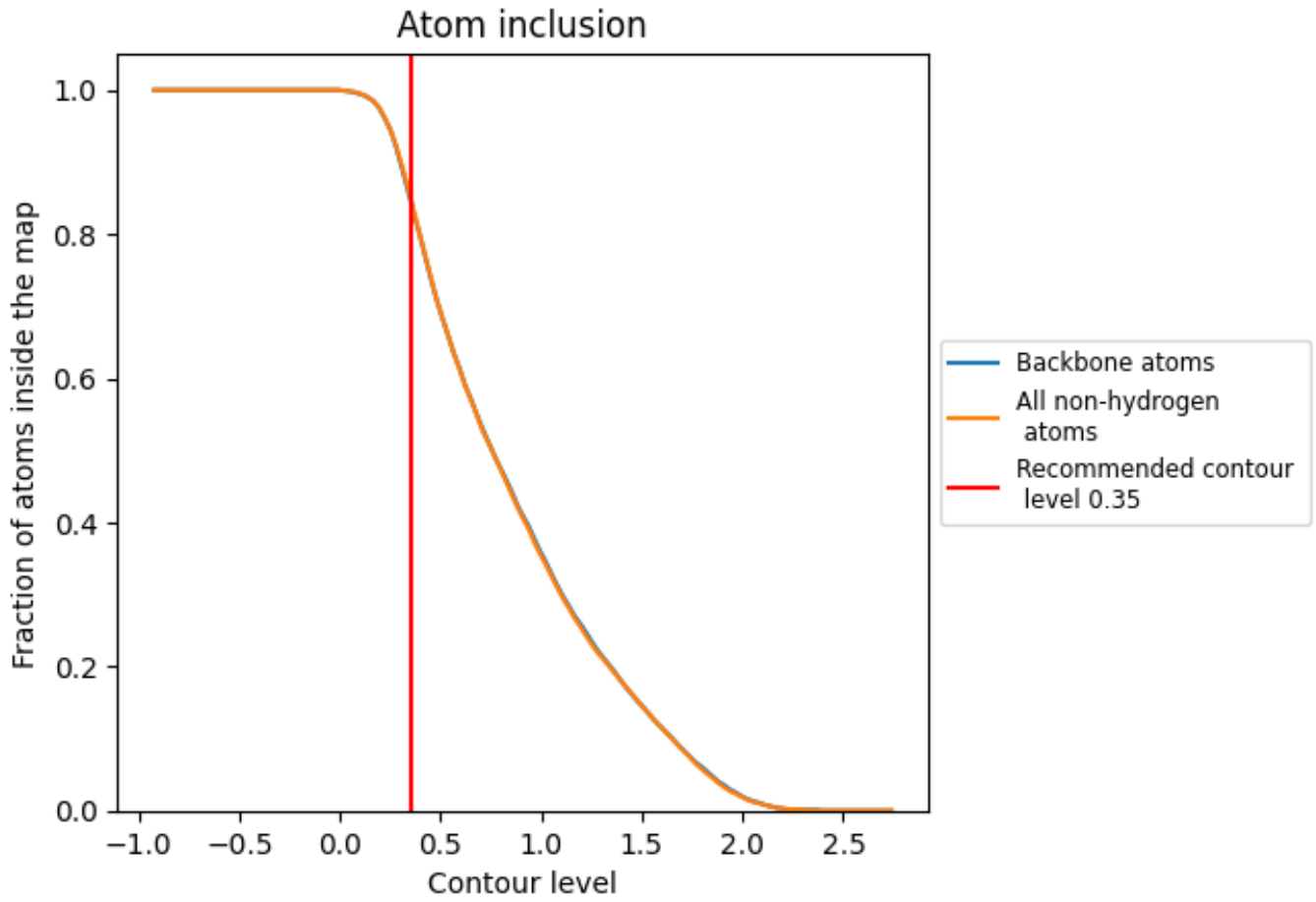
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8530	0.3530
A	0.9580	0.4470
B	0.9660	0.4720
C	0.9850	0.5020
D	0.9690	0.2100
E	0.9640	0.4140
F	0.9870	0.4910
G	0.9670	0.2600
H	0.9730	0.4830
I	0.9800	0.4170
J	0.9790	0.5150
K	0.9780	0.5030
L	0.9890	0.4710
N	0.8730	0.1520
P	0.9620	0.3350
T	0.9140	0.2540
U	0.7430	0.1840
V	0.3890	0.0780
W	0.6280	0.1790
X	0.7900	0.1130
Z	0.6690	0.1580