wwPDB EM Validation Summary Report (i)

Apr 19, 2025 – 12:19 PM EDT

PDB ID	:	8T0L / pdb_00008t0l
EMDB ID	:	EMD-40943
Title	:	E. coli Sw2/Snf2 ATPase RapA bound to both ADP-AlF3 and reconstituted E. coli RNA polymerase post-termination complex on negatively-supercoiled DNA
Authors	:	Brewer, J.J.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2023-06-01
Resolution	:	3.62 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 (i) 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 (i)) were used in the production of this report:

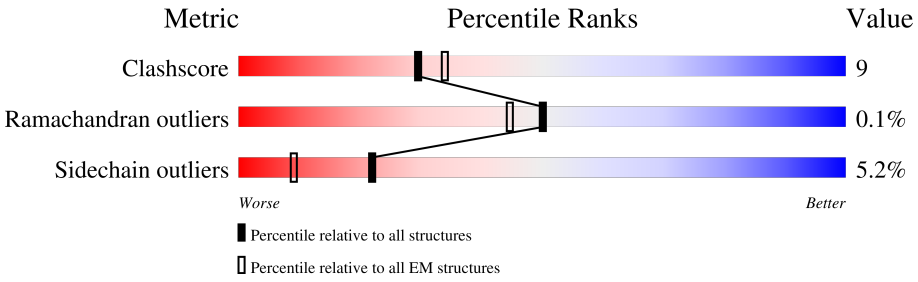
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.62 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

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	G	232	77% 19%
1	H	232	73% 19% 6%
2	I	1340	12% 75% 24%
3	J	1358	13% 72% 25%
4	K	72	11% 82% 17%
5	F	966	89% 79% 19%
6	A	23	74% 100%
7	B	23	100% 65% 35%

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
11	AF3	F	1001	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 33530 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 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	223	Total	C	N	O	S	0	0
			1706	1068	298	334	6		
1	H	218	Total	C	N	O	S	0	0
			1667	1043	291	327	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	235	ALA	-	expression tag	UNP C3SR67
H	235	ALA	-	expression tag	UNP C3SR67

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1333	Total	C	N	O	S	0	0
			10366	6514	1848	1954	50		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	262	ALA	THR	conflict	UNP A0A369F490

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	72	Total	C	N	O	S	0	0
			577	352	110	114	1		

- Molecule 5 is a protein called RNA polymerase-associated protein RapA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	966	Total	C	N	O	S	0	0
			7670	4800	1370	1471	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	144	ALA	TYR	conflict	UNP B7MAI2
F	413	ALA	THR	conflict	UNP B7MAI2
F	428	ALA	PHE	conflict	UNP B7MAI2
F	596	ALA	ARG	conflict	UNP B7MAI2
F	640	ALA	ARG	conflict	UNP B7MAI2
F	685	ALA	ARG	conflict	UNP B7MAI2
F	714	ALA	ASN	conflict	UNP B7MAI2
F	725	ALA	ILE	conflict	UNP B7MAI2

- Molecule 6 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	23	Total	C	N	O	P	0	0
			483	230	115	115	23		

- Molecule 7 is a DNA chain called DNA (5'-D(P*TP*CP*TP*GP*AP*AP*TP*TP*TP*AP *AP*AP*TP*TP*CP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	23	Total	C	N	O	P	0	0
			460	230	46	161	23		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

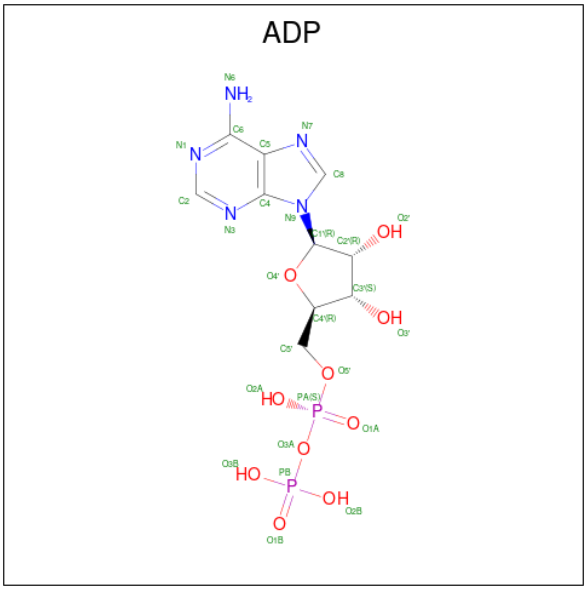
Mol	Chain	Residues	Atoms		AltConf
8	J	1	Total	Mg	0
			1	1	

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	J	2	Total	Zn	0
			2	2	

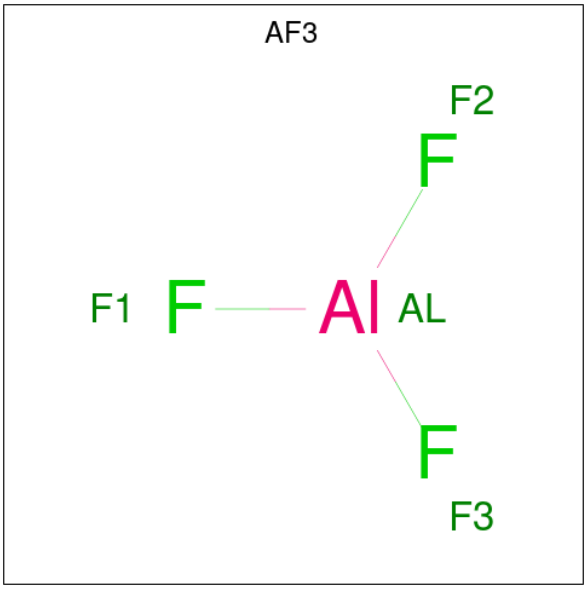
- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$)

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 11 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



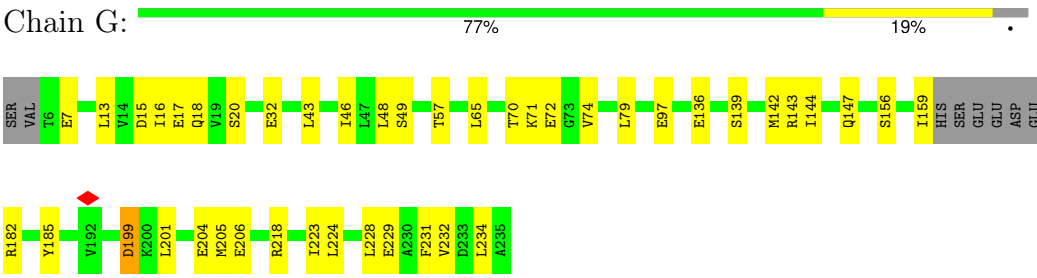
Mol	Chain	Residues	Atoms			AltConf
11	F	1	Total	Al	F	0
			4	1	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

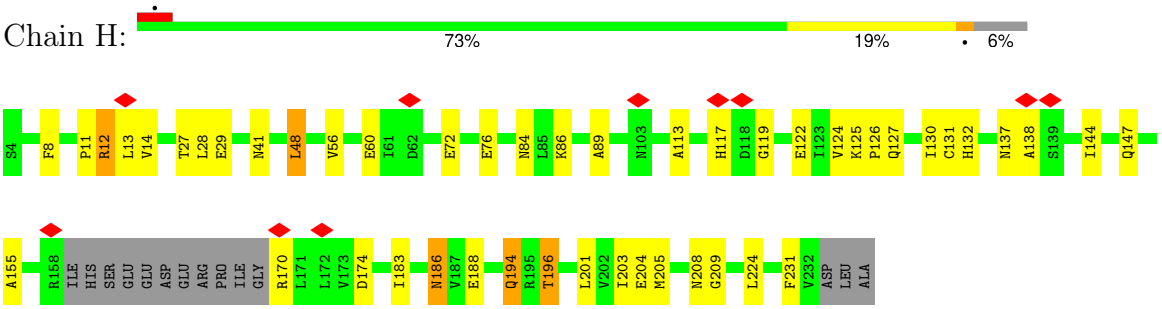
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



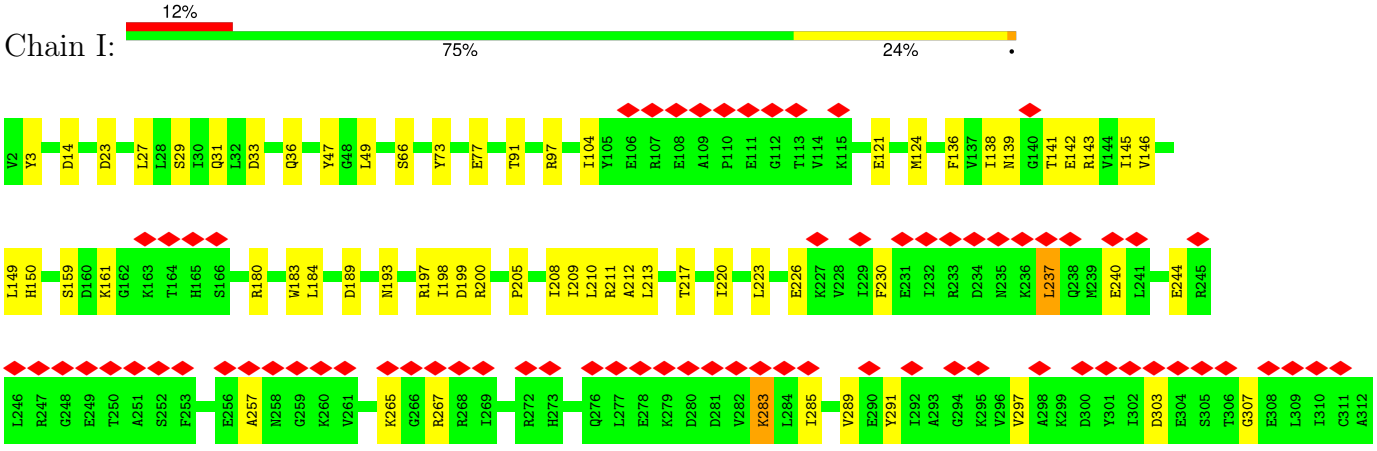
• Molecule 1: DNA-directed RNA polymerase subunit alpha

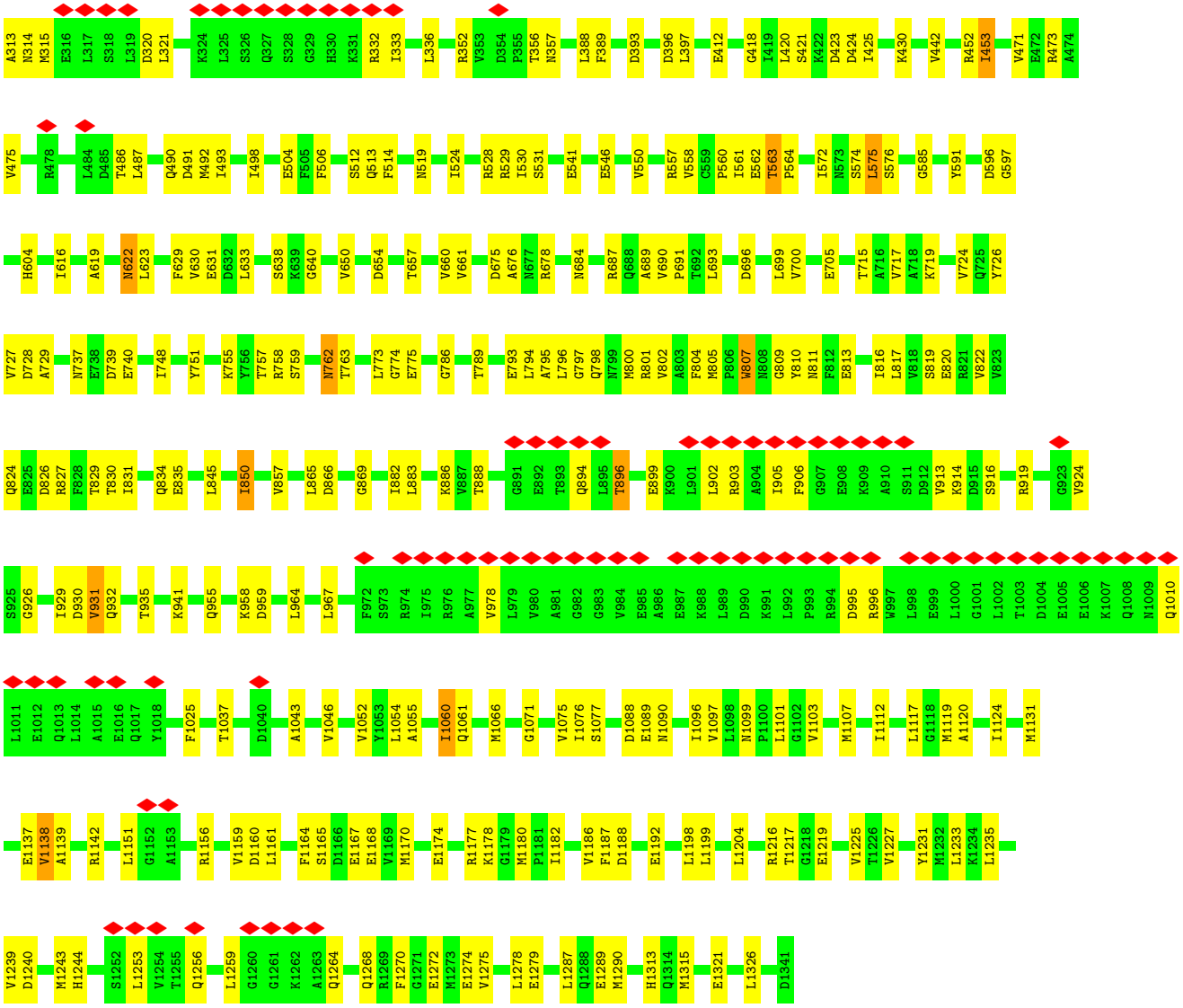
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

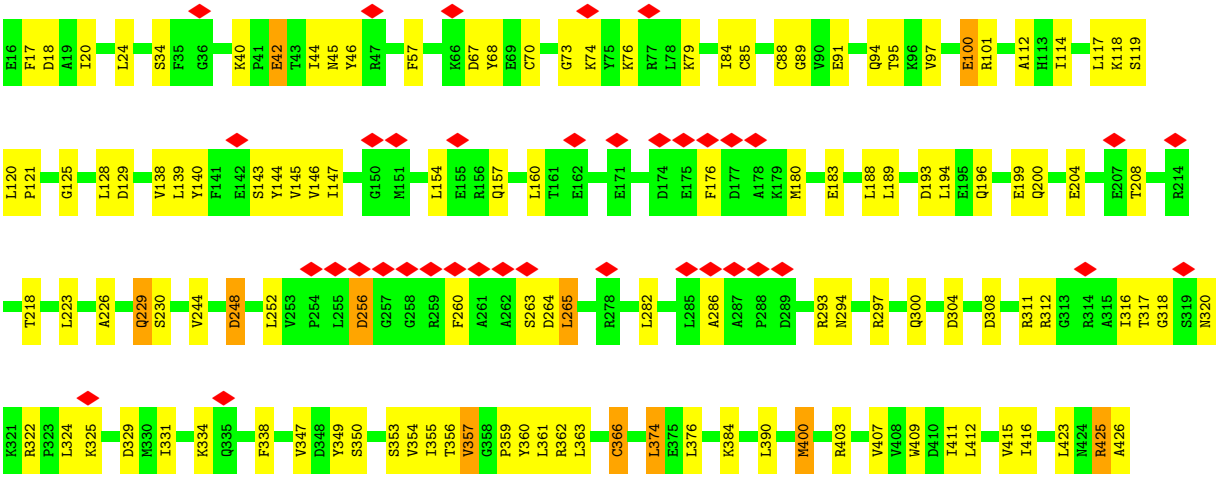
Chain I:

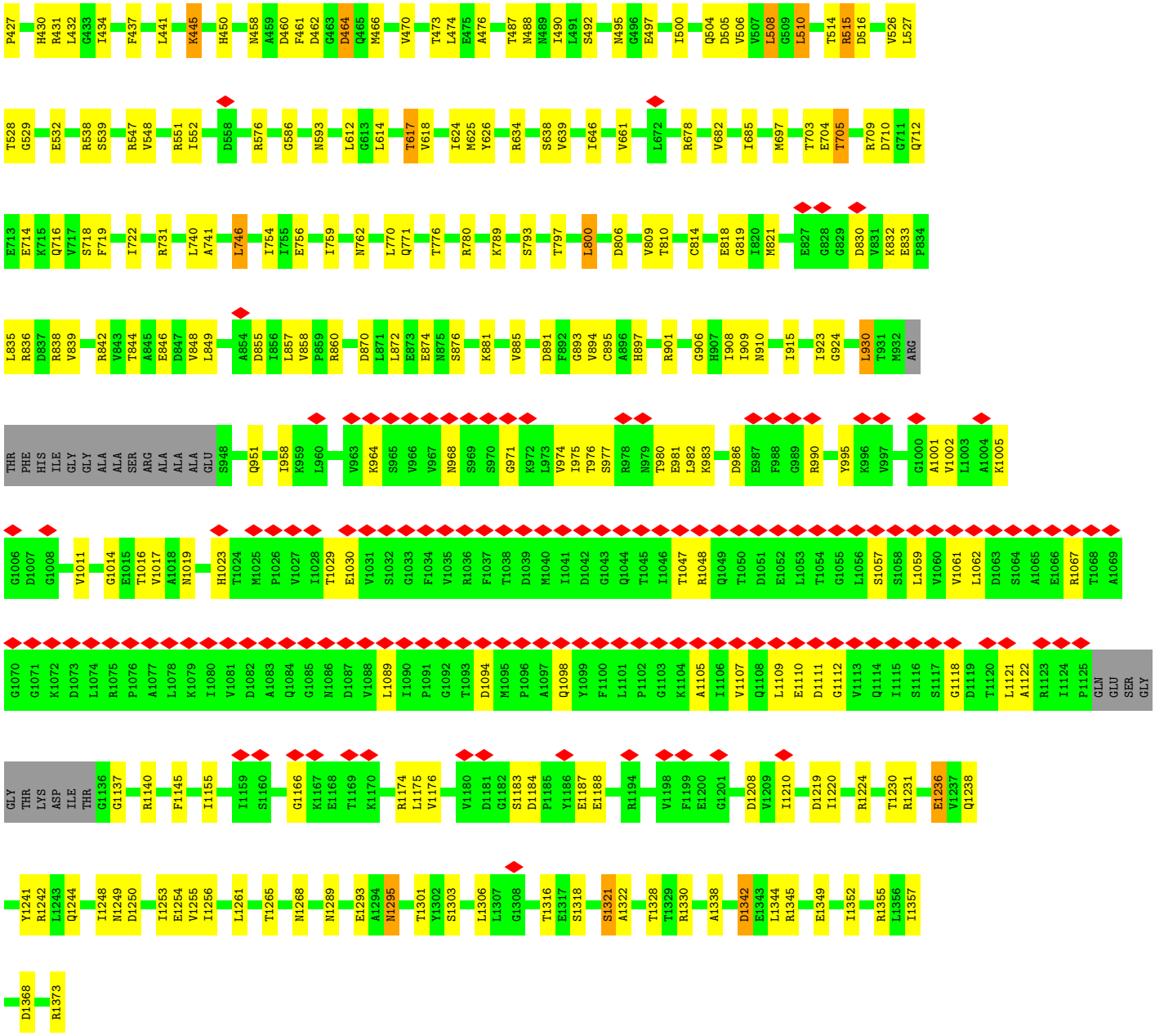




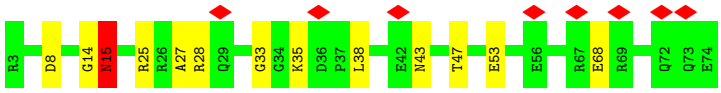
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:

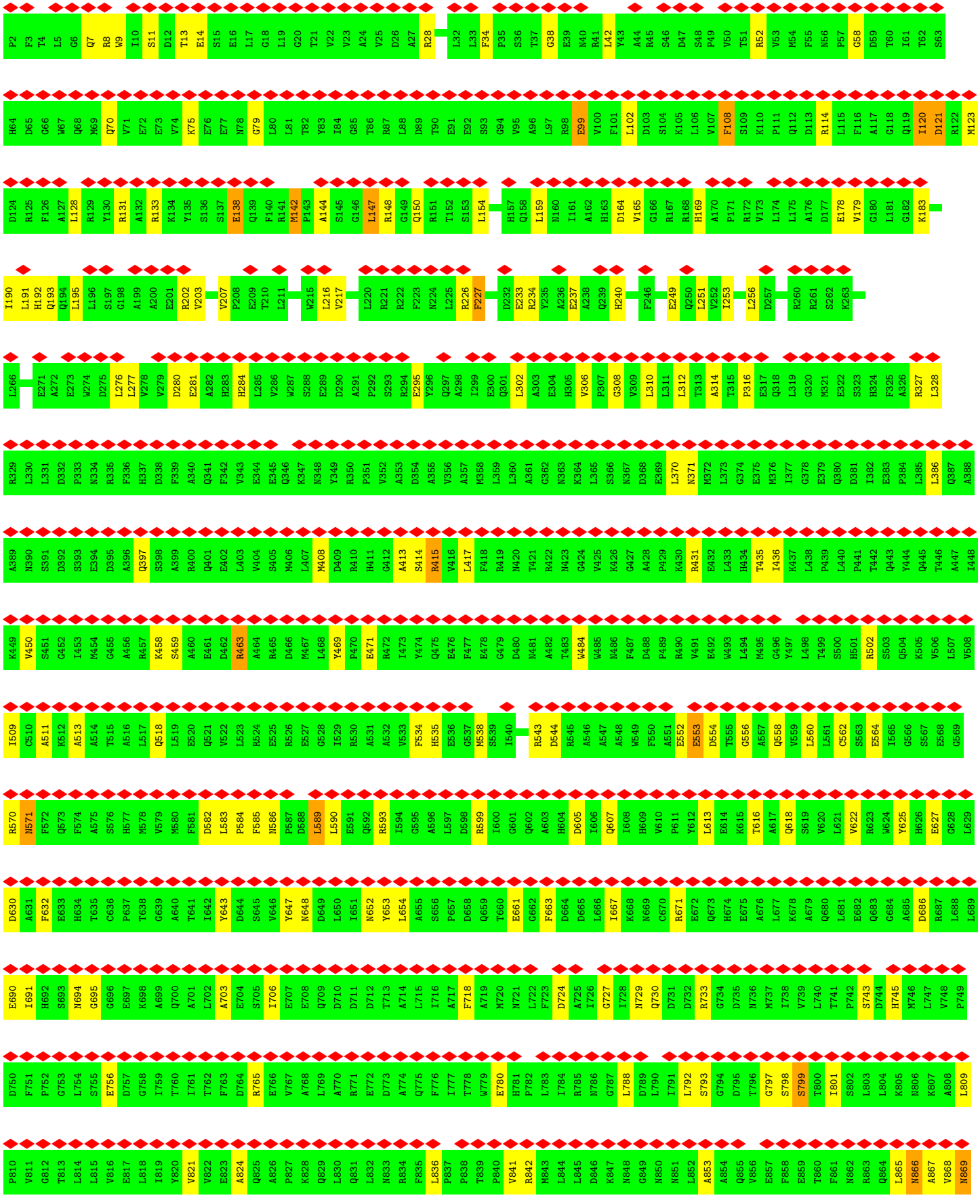


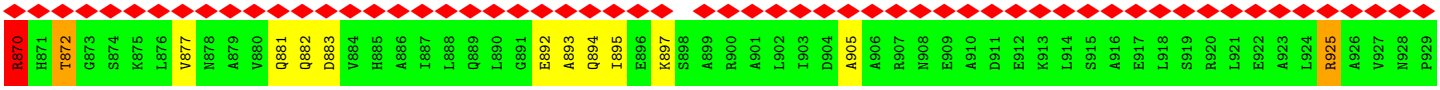


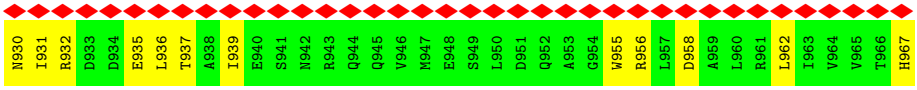
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase-associated protein RapA

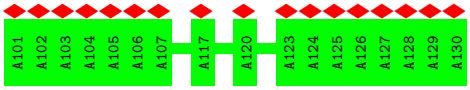

P2 F3 T4 L5 G6 Q7 R8 W9 I10 S11 D12 T13 E14 S15 E16 L17 G18 L19 G20 T21 V22 V23 A24 V25 D26 A27 R28 L32 L33 F34 P35 S36 T37 G38 E39 N40 R41 L42 Y43 A44 R45 S46 D47 S48 P49 V50 T51 R52 V53 M54 F55 N56 P57 G58 D59 T60 I61 T62 S63
H64 D65 G66 W67 Q68 M69 Q70 V71 E72 E73 V74 K75 E76 E77 N78 G79 L80 L81 T82 Y83 I84 G85 T86 R87 L88 D89 T90 E91 E92 S93 G94 V95 A96 L97 R98 E99 V100 F101 L102 D103 S104 K105 L106 V107 F108 S109 K110 P111 Q112 D113 R114 L115 F116 A117 G118 Q119 I120 D121 R122 M123
D124 R125 F126 A127 L128 R129 Y130 R131 A132 R133 K134 Y135 S136 S137 E138 Q139 F140 R141 M142 P143 A144 S145 G146 L147 R148 G149 Q150 R151 T152 S153 L154 H157 Q158 L159 N160 I161 A162 H163 D164 V165 G166 R167 R168 H169 A170 P171 R172 V173 L174 L175 A176 D177 E178 V179 G180 L181 G182 K183
I190 L191 H192 Q193 Q194 L195 L196 S197 G198 A199 A200 E201 R202 V203 V207 P208 E209 T210 L211 W215 L216 V217 L220 R221 R222 F223 N224 L225 R226 F227 D232 E233 R234 Y235 A236 E237 A238 Q239 H240 F246 E249 Q250 L251 V252 I253 L256 D257 R260 R261 S262 K263
L266 E271 A272 E273 W274 D275 L276 L277 V278 V279 D280 E281 A282 H283 H284 L285 V286 W287 S288 E289 D290 A291 P292 S293 R294 E295 Y296 Q297 A298 I299 E300 Q301 L302 A303 E304 H305 V306 P307 G308 V309 L310 L311 L312 T313 A314 T315 P316 E317 Q318 L319 G320 M321 E322 S323 H324 F325 A326 R327 L328
R329 L330 L331 D332 P333 N334 R335 F336 H337 D338 F339 A340 Q341 F342 Y343 E344 E345 Q346 K347 N348 Y349 R350 P351 Y352 A353 D354 A355 Y356 A357 M358 L359 L360 A361 G362 N363 K364 L365 S366 N367 D368 E369 L370 N371 M372 L373 G374 E375 M376 I377 G378 E379 Q380 D381 I382 E383 P384 L385 L386 Q387 A388
A389 N390 S391 D392 S393 E394 D395 A396 Q397 S398 A399 R400 Q401 E402 L403 V404 S405 M406 L407 M408 D409 R410 H411 G412 A413 S414 R415 V416 L417 F418 R419 N420 T421 R422 N423 G424 V425 K426 G427 A428 P429 K430 R431 E432 L433 H434 T435 I436 K437 L438 P439 L440 P441 T442 Q443 Y444 Q445 T446 A447 I448
K449 V450 S451 G452 I453 M454 G455 A456 R457 K458 S459 A460 E461 D462 R463 A464 R465 D466 M467 L468 Y469 P470 E471 R472 I473 Y474 Q475 E476 F477 E478 G479 D480 N481 A482 T483 W484 W485 N486 F487 D488 P489 R490 V491 E492 W493 L494 M495 G496 Y497 L498 T499 S500 H501 R502 S503 Q504 K505 V506 L507 V508
I509 C510 A511 K512 A513 A514 T515 A516 L517 Q518 L519 E520 Q521 V522 L523 R524 E525 R526 E527 G528 I529 R530 A531 A532 V533 F534 H535 E536 G537 M538 S539 I540 R543 D544 R545 A546 A547 A548 W549 F550 A551 E552 E553 D554 T555 G556 A557 Q558 V559 L560 L561 C562 S563 E564 I565 G566 S567 E568 G569
R570 N571 F572 Q573 F574 A575 S576 H577 M578 V579 M580 F581 D582 L583 P584 F585 N586 P587 D588 L589 L590 E591 Q592 R593 I594 G595 A596 L597 D598 R599 I600 G601 Q602 A603 H604 D605 I606 Q607 I608 H609 V610 P611 Y612 L613 E614 K615 T616 A617 Q618 S619 V620 L621 V622 R623 W624 Y625 H626 E627 G628 L629
D630 A631 F632 E633 H634 T635 C636 P637 T638 G639 A640 T641 I642 Y643 D644 S645 V646 Y647 N648 D649 L650 I651 N652 Y653 L654 A655 S656 P657 D658 Q659 T660 E661 G662 F663 D664 D665 L666 I667 K668 N669 C670 R671 E672 Q673 H674 E675 A676 L677 K678 A679 Q680 L681 E682 Q683 G684 A685 D686 R687 L688 L689
E690 I691 H692 S693 N694 G695 G696 E697 K698 A699 Q700 A701 L702 A703 E704 S705 I706 E707 E708 Q709 D710 D711 D712 T713 A714 L715 I716 A717 F718 A719 M720 N721 L722 F723 D724 A725 I726 G727 I728 N729 Q730 D731 D732 R733 G734 D735 N736 M737 I738 V739 L740 T741 P742 S743 D744 H745 M746 L747 V748 P749
D750 F751 P752 G753 L754 S755 E756 D757 G758 I759 T760 I761 T762 F763 D764 R765 E766 V767 A768 L769 A770 R771 E772 D773 A774 Q775 F776 I777 T778 W779 E780 H781 P782 L783 I784 R785 N786 G787 L788 D789 L790 I791 L792 S793 G794 D795 T796 G797 S798 S799 T800 I801 S802 L803 L804 K805 N806 K807 A808 L809
P810 V811 G812 T813 L814 L815 V816 E817 L818 I819 Y820 V821 V822 E823 A824 Q825 A826 P827 K828 Q829 L830 Q831 L832 N833 R834 F835 L836 P837 P838 T839 P840 V841 R842 M843 L844 L845 D846 K847 N848 G849 N850 N851 L852 A853 A854 Q855 V856 E857 F858 E859 T860 F861 N862 R863 Q864 L865 N866 A867 V868 N869





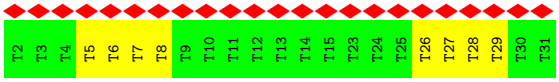
• Molecule 6: DNA (29-MER)

Chain A:



• Molecule 7: DNA (5’-D(P*TP*CP*TP*GP*AP*AP*TP*TP*TP*AP*AP*AP*TP*TP*CP*AP*GP*A)-3’)

Chain B:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100010	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 ($e^-/Å^2$)	55.9	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.838	Depositor
Minimum map value	-1.797	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.186	Depositor
Map size (Å)	275.456, 275.456, 275.456	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, MG, AF3

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	G	0.32	0/1726	0.56	0/2340
1	H	0.29	0/1686	0.54	0/2287
2	I	0.35	0/10736	0.55	0/14487
3	J	0.33	0/10523	0.57	0/14207
4	K	0.25	0/579	0.57	0/779
5	F	0.26	0/7812	0.53	0/10586
6	A	0.55	0/550	0.75	0/843
7	B	0.75	0/504	1.30	0/774
All	All	0.33	0/34116	0.58	0/46303

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
3	J	0	1
5	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	870	ARG	Peptide
3	J	76	LYS	Peptide

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	G	1706	0	1734	24	0
1	H	1667	0	1693	32	0
2	I	10567	0	10585	210	0
3	J	10366	0	10587	224	0
4	K	577	0	588	7	0
5	F	7670	0	7534	123	0
6	A	483	0	255	0	0
7	B	460	0	278	6	0
8	J	1	0	0	0	0
9	J	2	0	0	0	0
10	F	27	0	12	6	0
11	F	4	0	0	3	0
All	All	33530	0	33266	599	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 9.

The worst 5 of 599 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)
3:J:460:ASP:OD2	3:J:462:ASP:OD1	1.58	1.22
2:I:826:ASP:OD1	2:I:829:THR:OG1	1.99	0.81
2:I:684:ASN:OD1	2:I:687:ARG:NH2	2.14	0.80
3:J:806:ASP:OD1	3:J:1345:ARG:NH1	2.15	0.80
5:F:727:GLY:O	5:F:743:SER:OG	2.00	0.78

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	G	219/232 (94%)	197 (90%)	22 (10%)	0	100	100
1	H	214/232 (92%)	195 (91%)	19 (9%)	0	100	100
2	I	1338/1340 (100%)	1186 (89%)	151 (11%)	1 (0%)	48	79
3	J	1327/1358 (98%)	1180 (89%)	147 (11%)	0	100	100
4	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	9	39
5	F	964/966 (100%)	897 (93%)	66 (7%)	1 (0%)	48	79
All	All	4132/4200 (98%)	3719 (90%)	410 (10%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	1138	VAL
4	K	15	ASN
5	F	905	ALA

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	G	187/199 (94%)	174 (93%)	13 (7%)	12	39
1	H	184/199 (92%)	174 (95%)	10 (5%)	18	47
2	I	1155/1155 (100%)	1103 (96%)	52 (4%)	23	52
3	J	1117/1133 (99%)	1049 (94%)	68 (6%)	15	44
4	K	63/63 (100%)	60 (95%)	3 (5%)	21	50
5	F	819/819 (100%)	782 (96%)	37 (4%)	23	52
All	All	3525/3568 (99%)	3342 (95%)	183 (5%)	22	48

5 of 183 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	705	THR
4	K	15	ASN
3	J	746	LEU
3	J	1030	GLU
5	F	121	ASP

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

Mol	Chain	Res	Type
5	F	268	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
11	AF3	F	1001	-	0,3,3	-	-	-		
10	ADP	F	1000	-	24,29,29	0.87	0	29,45,45	1.21	2 (6%)

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
10	ADP	F	1000	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	1000	ADP	N3-C2-N1	-4.18	123.00	128.67
10	F	1000	ADP	C4-C5-N7	-2.28	106.92	109.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	1000	ADP	C5'-O5'-PA-O1A
10	F	1000	ADP	C5'-O5'-PA-O3A
10	F	1000	ADP	C5'-O5'-PA-O2A

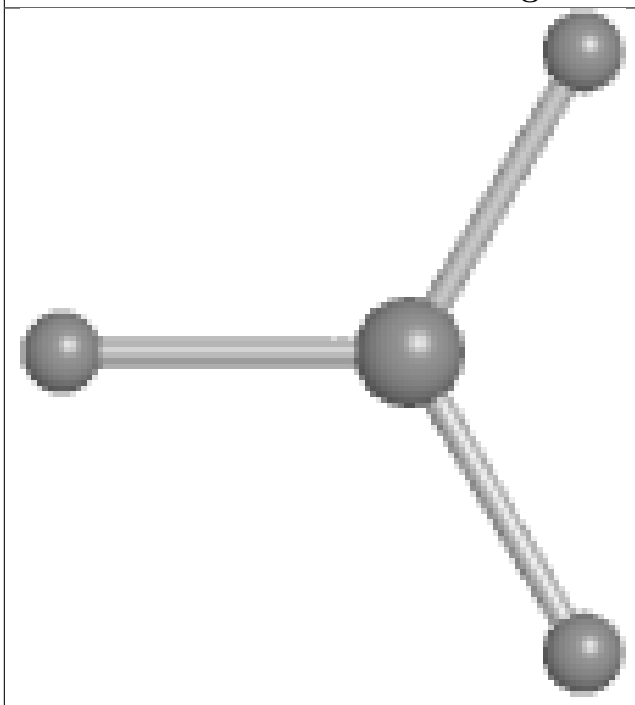
There are no ring outliers.

2 monomers are involved in 6 short contacts:

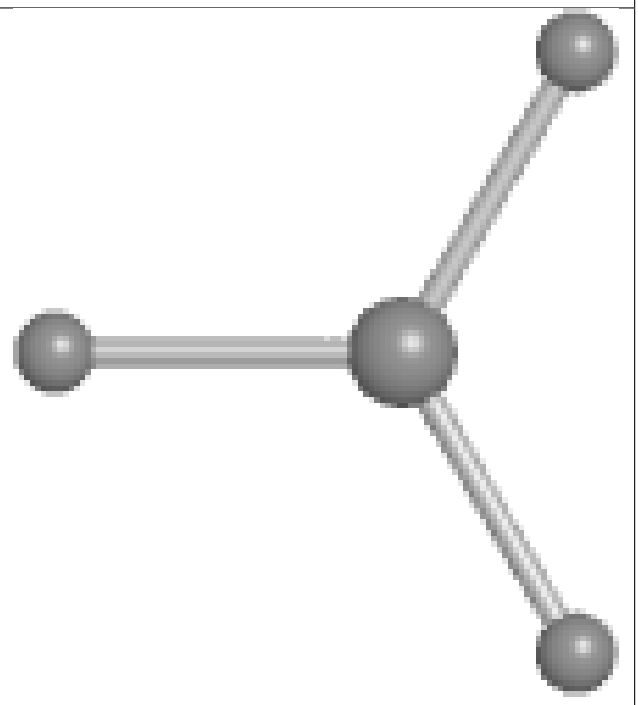
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	1001	AF3	3	0
10	F	1000	ADP	6	0

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 then 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.

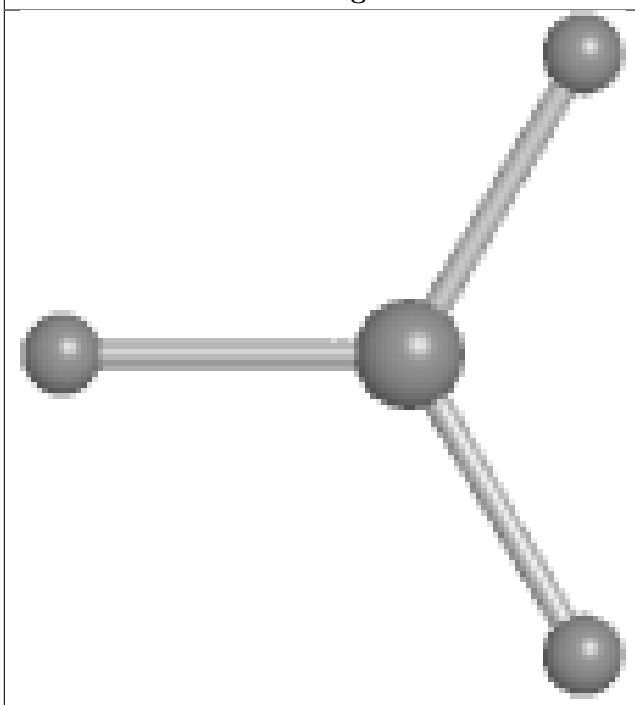
Ligand AF3 F 1001



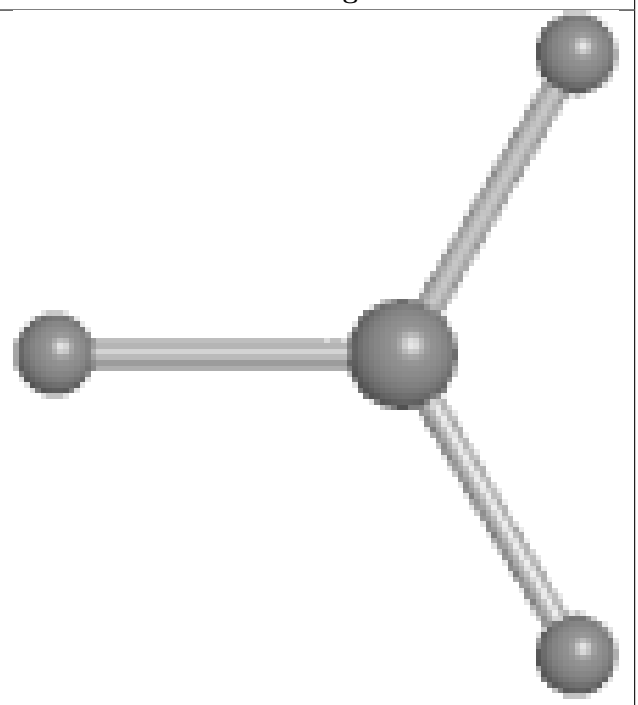
Bond lengths



Bond angles

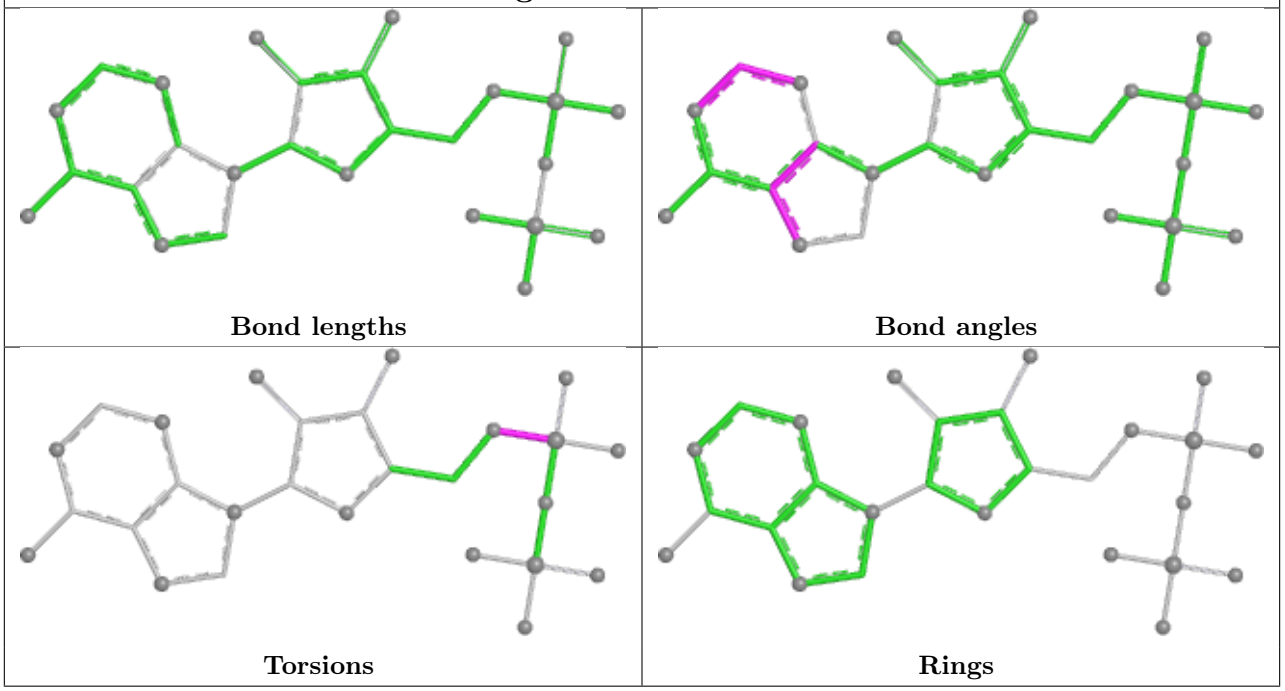


Torsions



Rings

Ligand ADP F 1000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	B	1
6	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	15:DT	O3'	23:DT	P	30.33
1	A	109:DA	O3'	117:DA	P	17.32

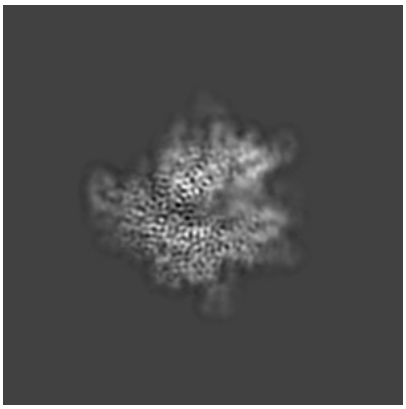
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-40943. These allow visual inspection of the internal detail of the map and identification of artifacts.

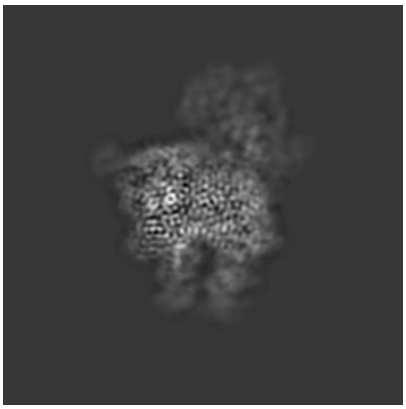
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

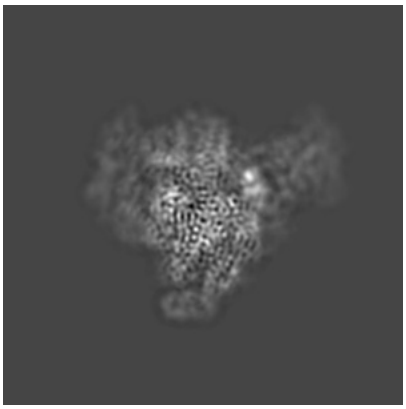
6.1.1 Primary map



X

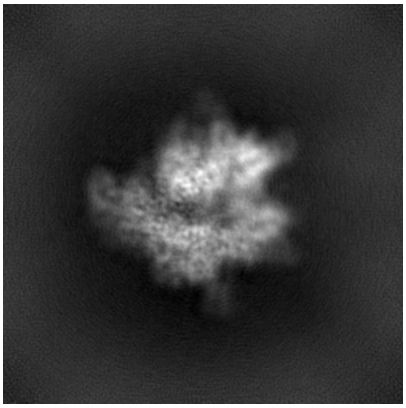


Y

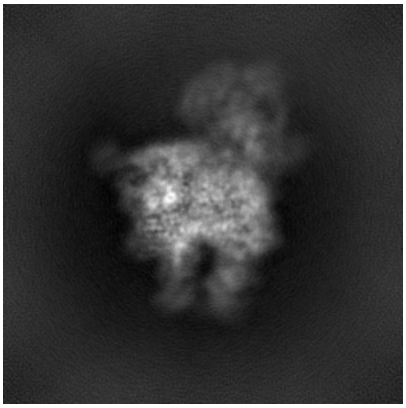


Z

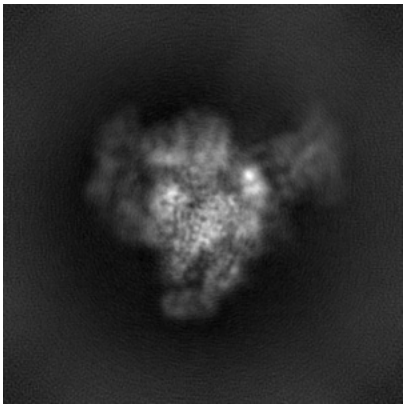
6.1.2 Raw map



X



Y

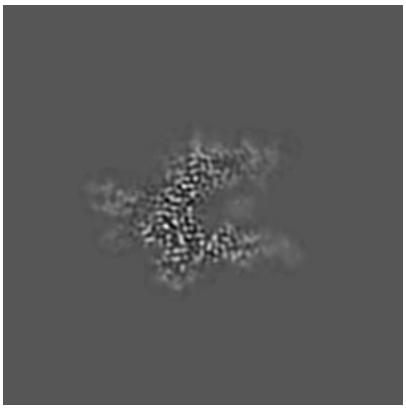


Z

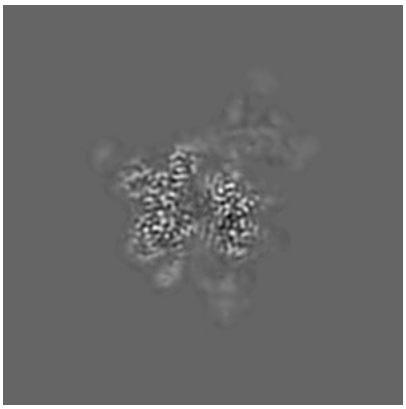
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

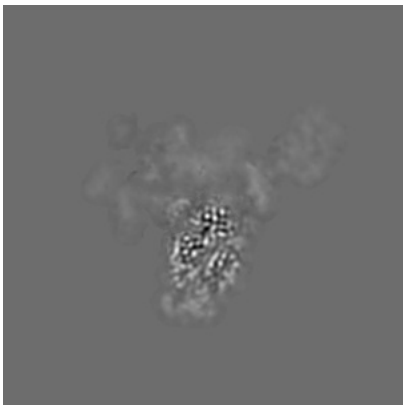
6.2.1 Primary map



X Index: 128

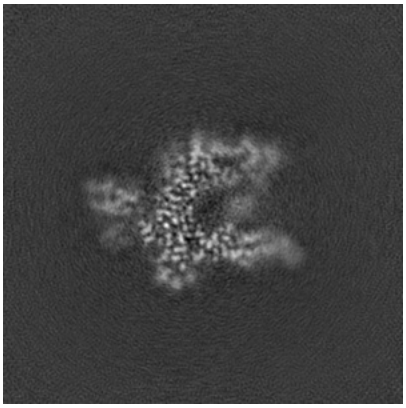


Y Index: 128

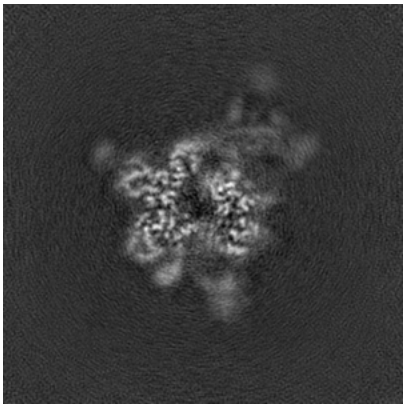


Z Index: 128

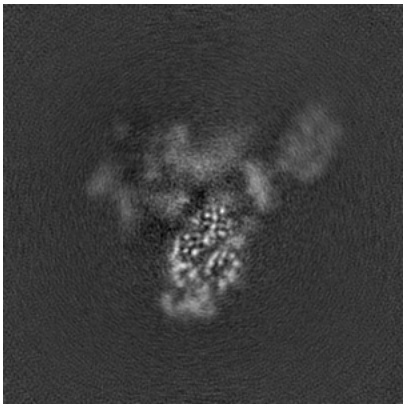
6.2.2 Raw map



X Index: 128



Y Index: 128

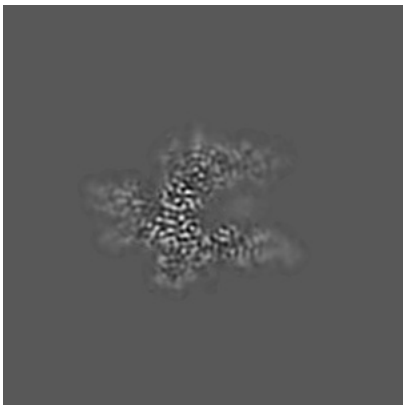


Z Index: 128

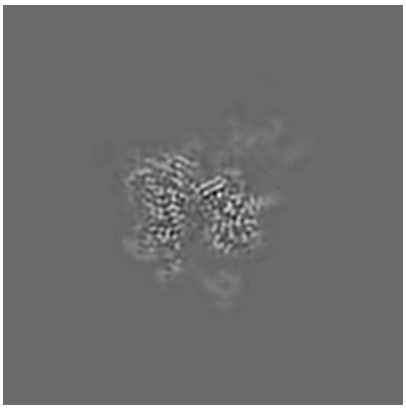
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

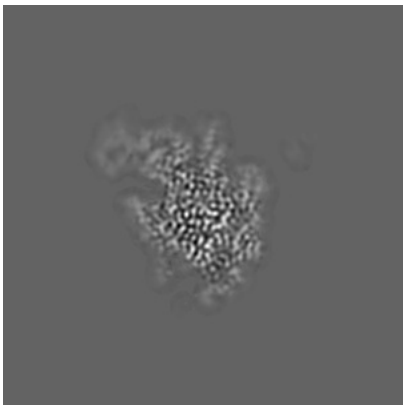
6.3.1 Primary map



X Index: 130

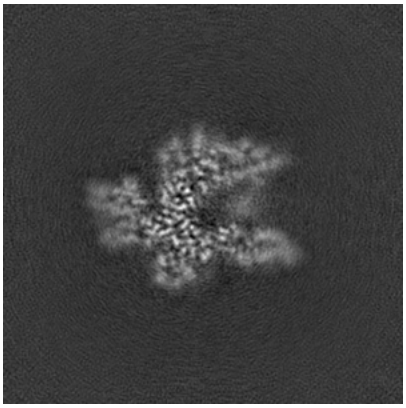


Y Index: 123

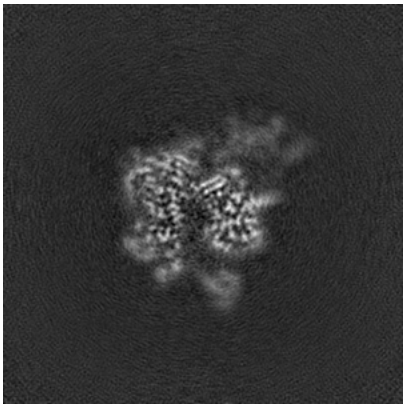


Z Index: 109

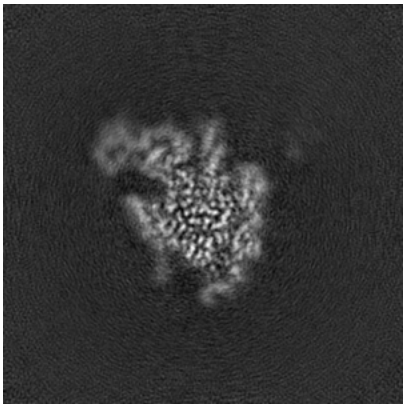
6.3.2 Raw map



X Index: 131



Y Index: 123

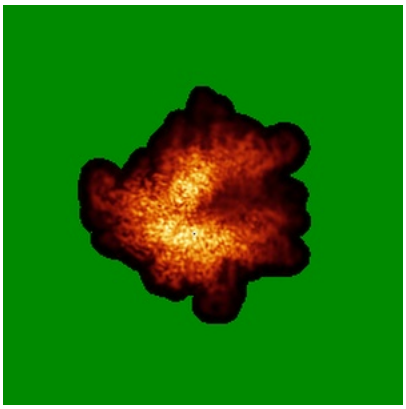


Z Index: 109

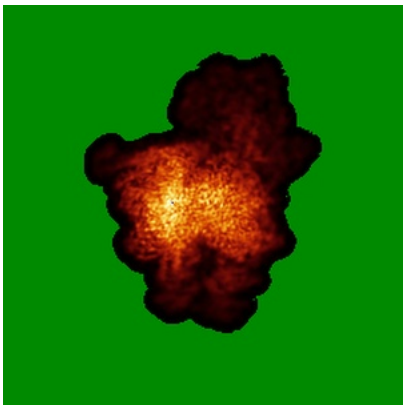
The images above show the largest variance slices of the map in three orthogonal directions.

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

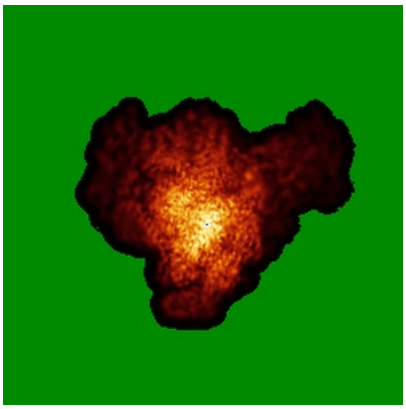
6.4.1 Primary map



X

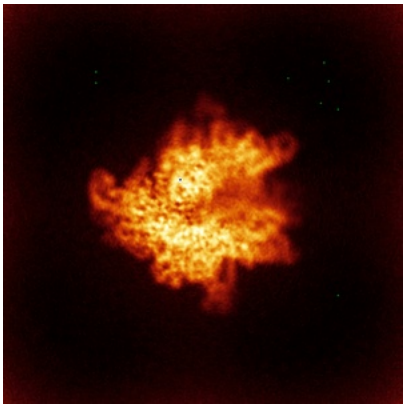


Y

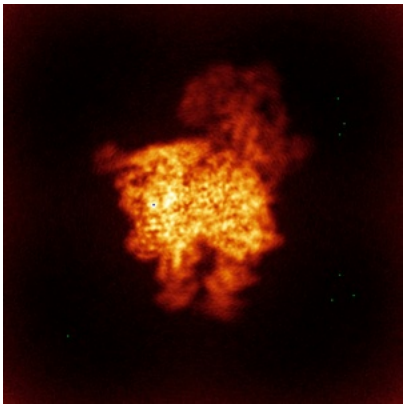


Z

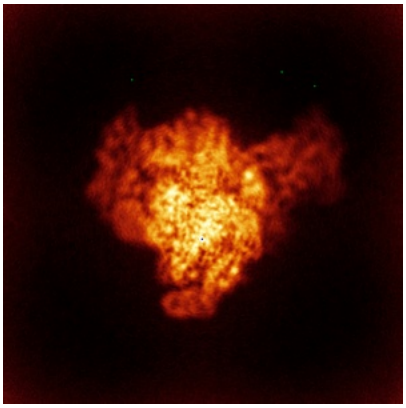
6.4.2 Raw map



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 0.186. 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.

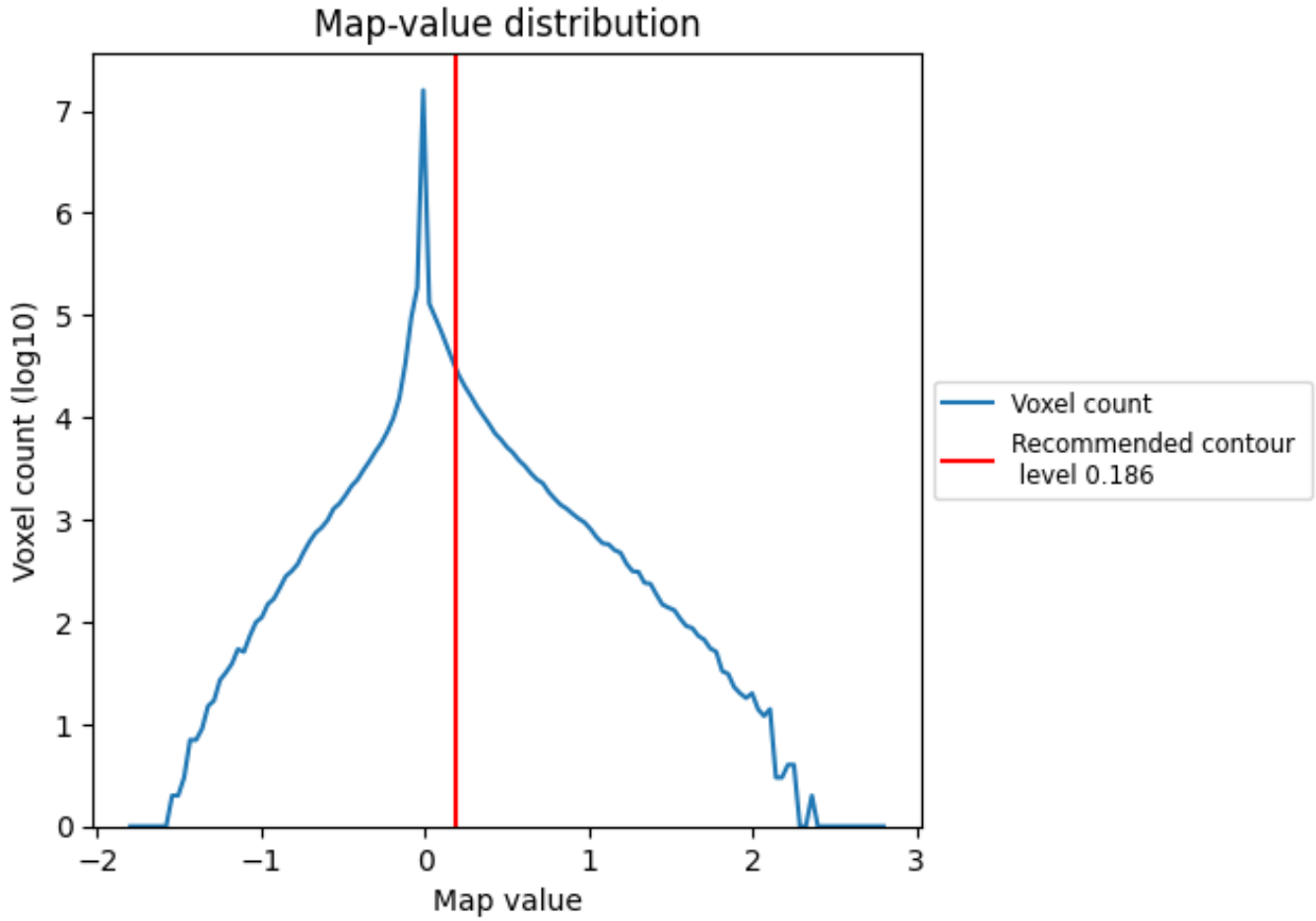
6.6 Mask visualisation (i)

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

7 Map analysis

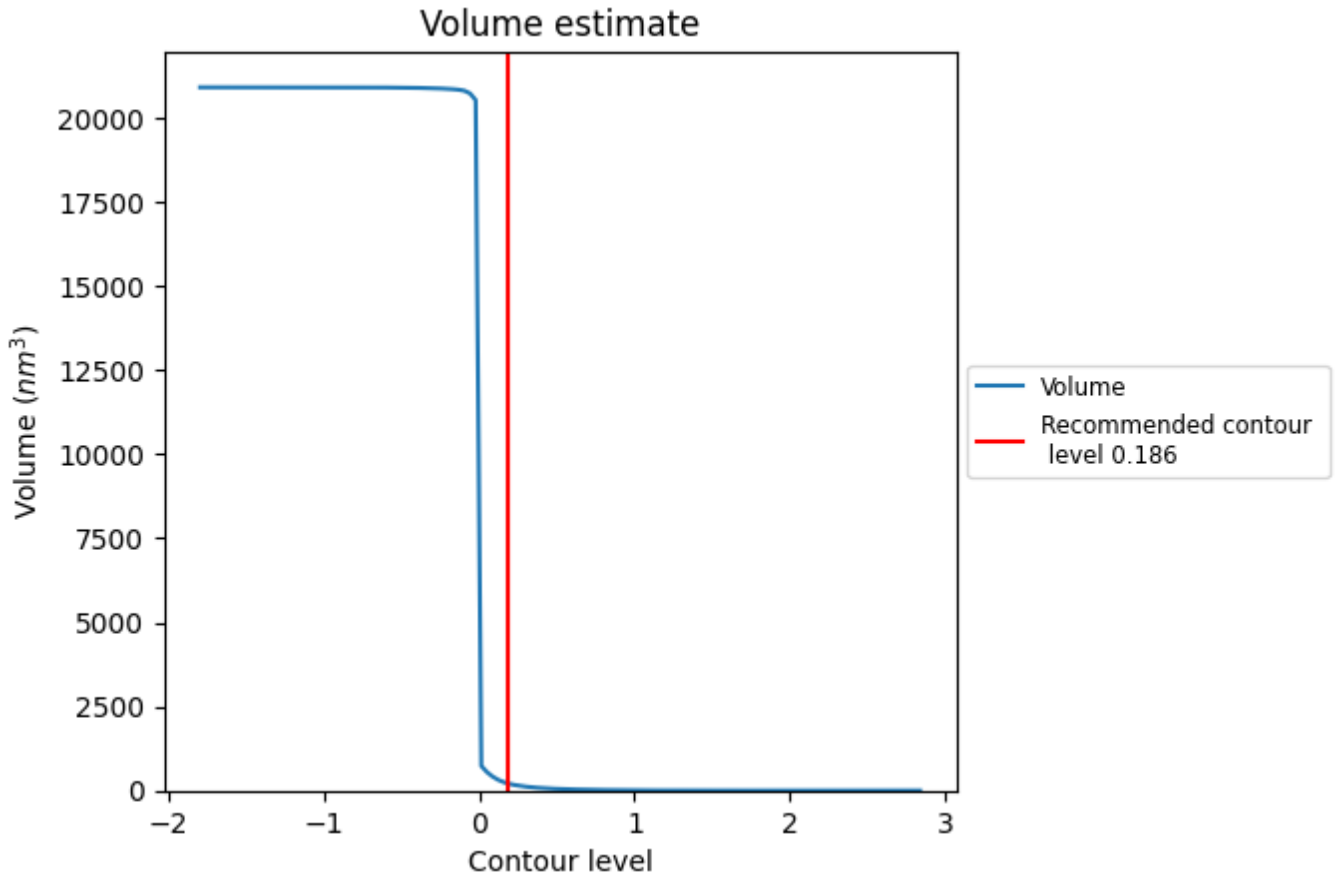
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

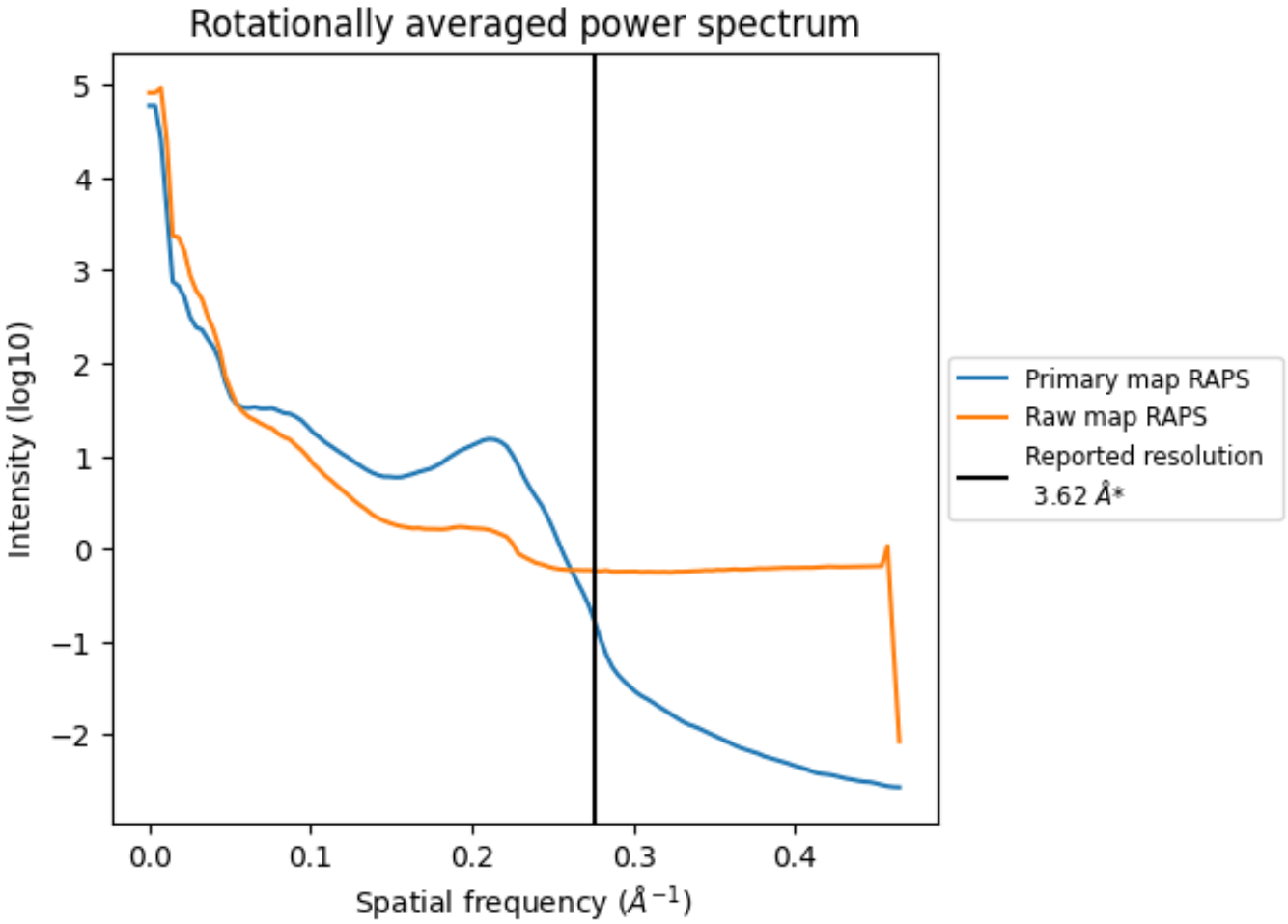
7.2 Volume estimate (i)



The volume at the recommended contour level is 211 nm^3; this corresponds to an approximate mass of 190 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)

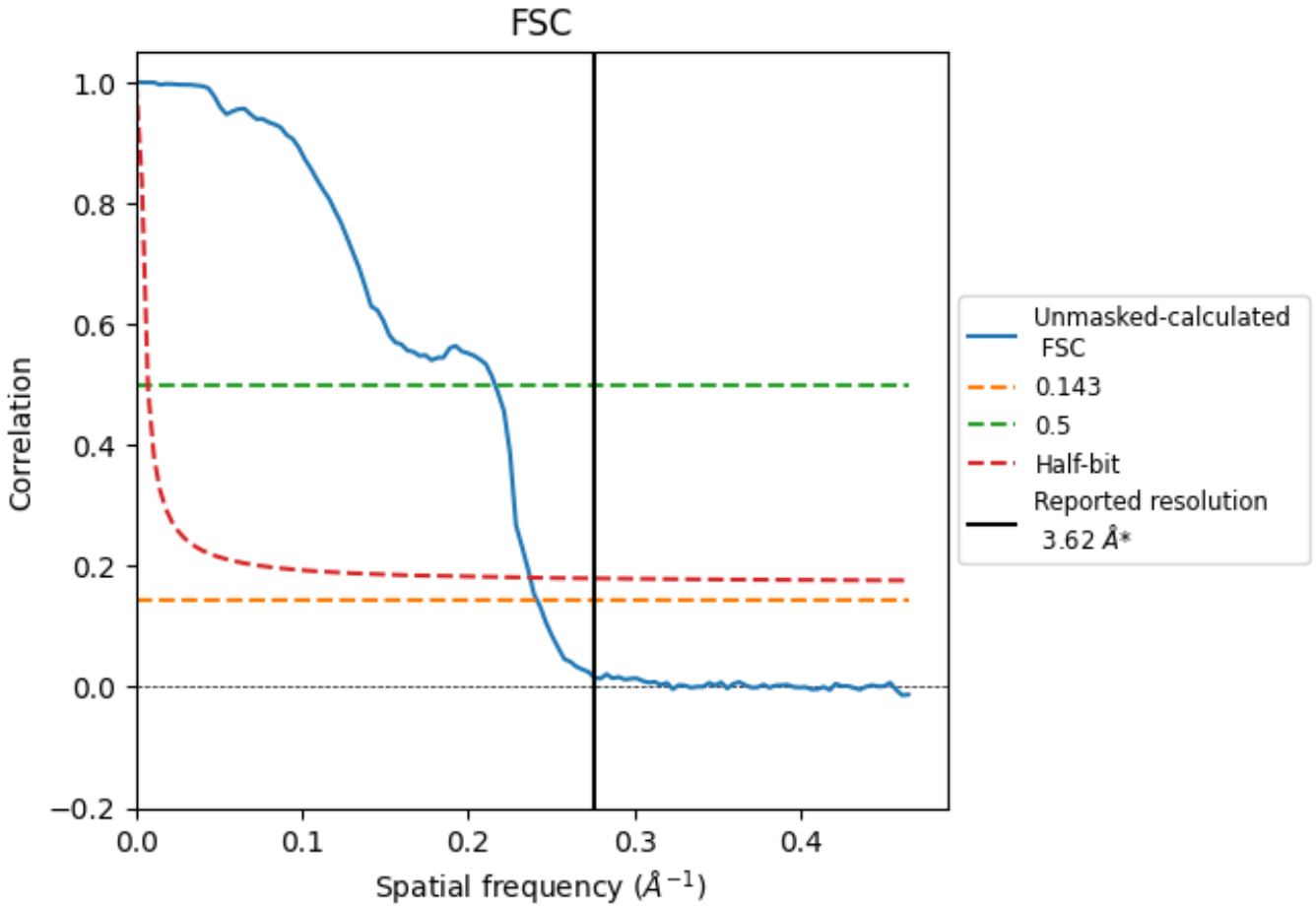


*Reported resolution corresponds to spatial frequency of 0.276 Å^{-1}

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 0.276 Å^{-1}

8.2 Resolution estimates (i)

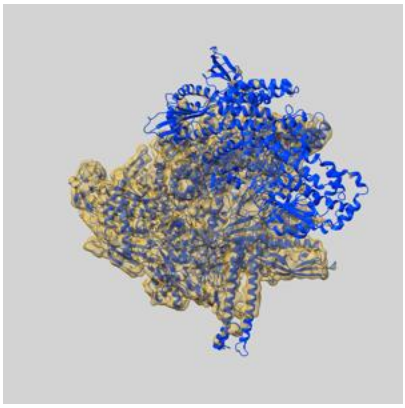
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	4.63	4.22

*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 4.14 differs from the reported value 3.62 by more than 10 %

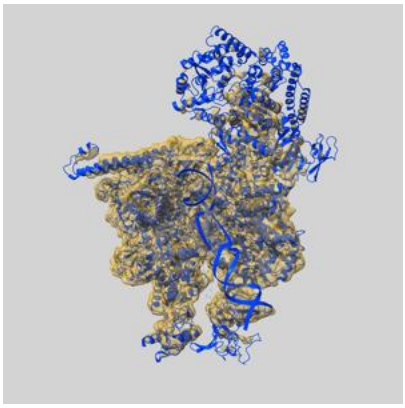
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-40943 and PDB model 8T0L. Per-residue inclusion information can be found in section 3 on page 7.

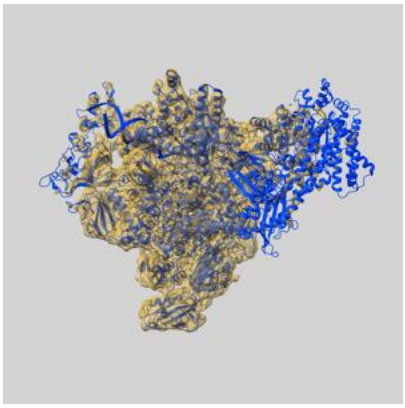
9.1 Map-model overlay



X



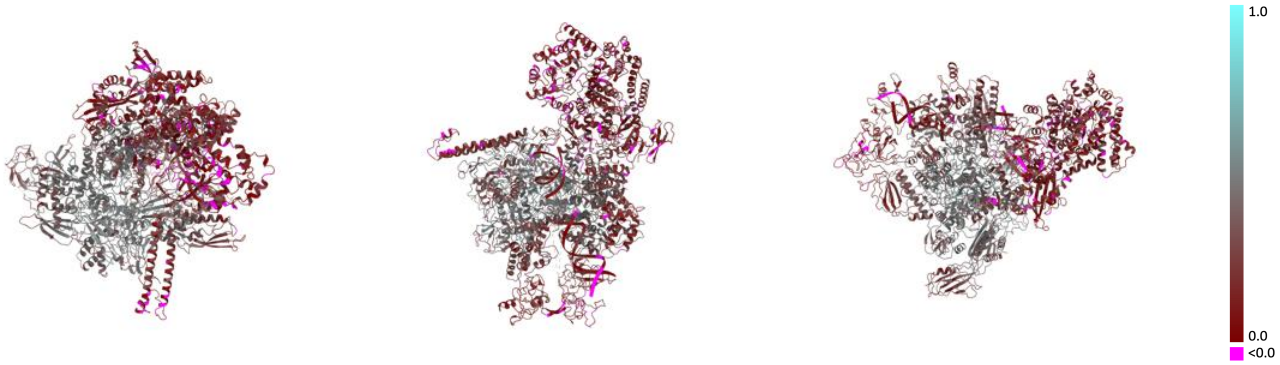
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.186 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.

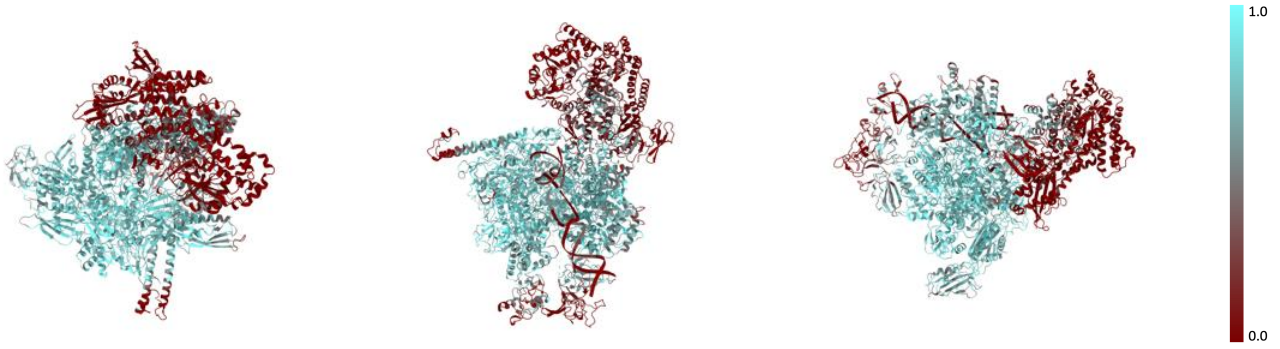
9.2 Q-score mapped to coordinate model (i)



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.

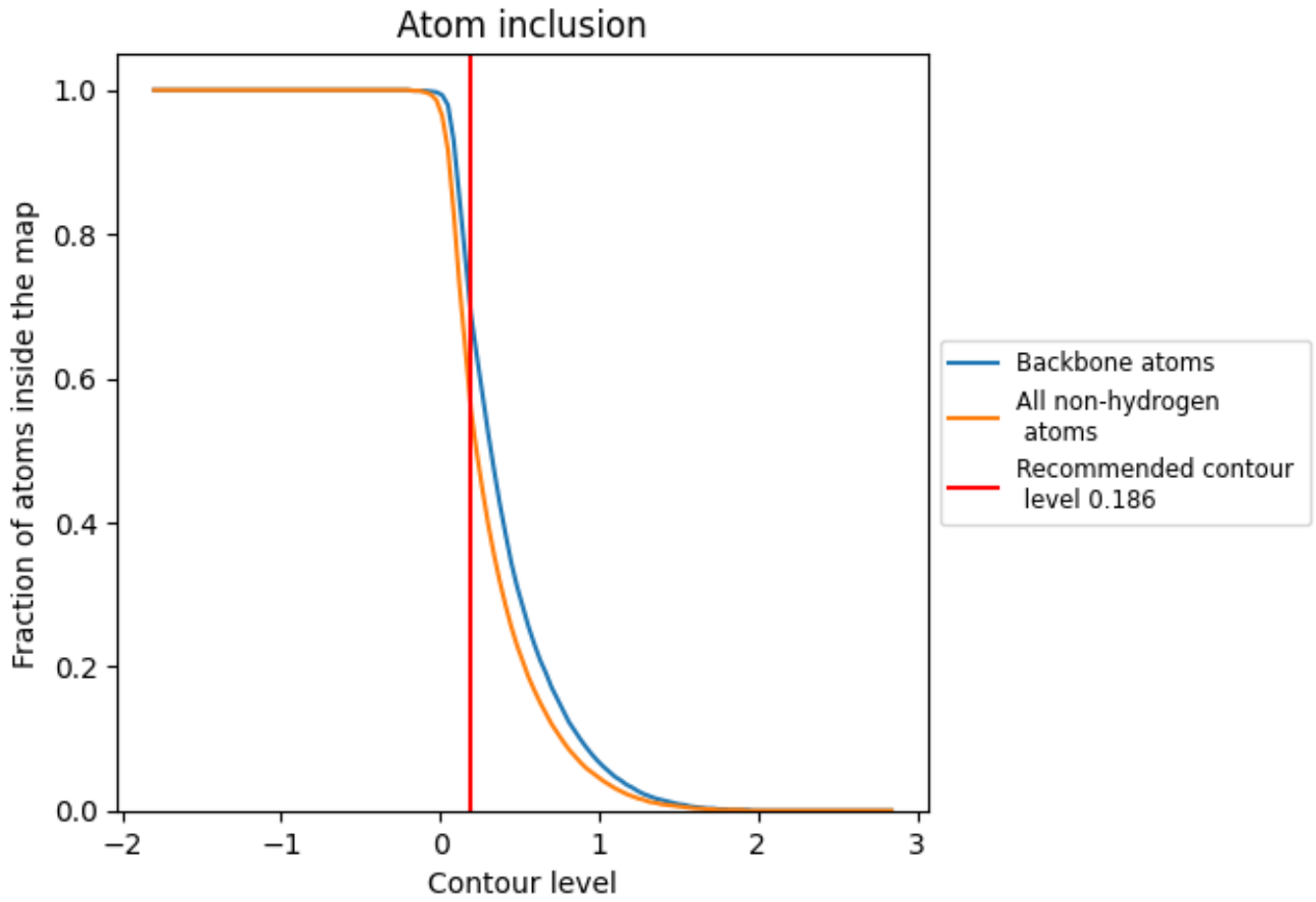
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.186).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 57% 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 (0.186) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5730	0.3070
A	0.1950	0.0980
B	0.1000	0.0870
F	0.1100	0.1590
G	0.8340	0.4300
H	0.7320	0.3630
I	0.7380	0.3700
J	0.7140	0.3420
K	0.6650	0.3140