wwPDB EM Validation Summary Report

Nov 20, 2022 – 04:47 PM EST

PDB ID	:	7MKO
EMDB ID	:	EMD-23901
Title	:	Escherichia coli RNA polymerase elongation complex
Authors	:	Qayyum, M.Z.; Murakami, K.S.
Deposited on	:	2021-04-26
Resolution	:	3.15 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:

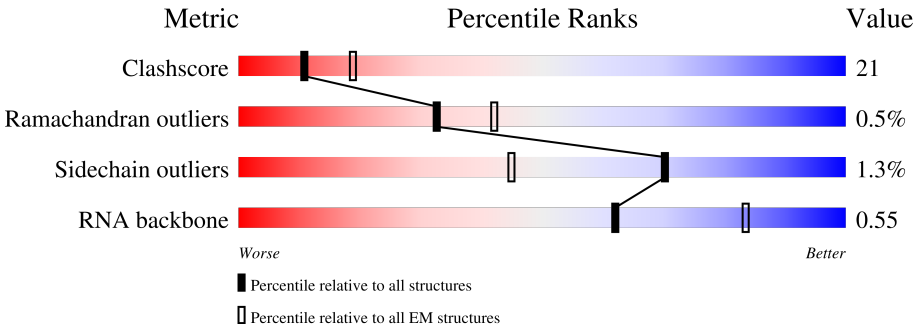
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	237	6% 63% 34%
1	B	237	8% 56% 39%
2	C	1340	9% 56% 42%
3	D	1363	13% 56% 41%
4	E	91	68% 42% 34% 24%
5	N	29	48% 28% 24%
6	R	11	64% 18% 18%

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Mol	Chain	Length	Quality of chain
7	T	29	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 26269 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	A	231	Total	C	N	O	S	0	0
			1794	1117	318	353	6		
1	B	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1320	Total	C	N	O	S	0	0
			10414	6532	1815	2024	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1344	Total	C	N	O	S	0	0
			10419	6546	1856	1967	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	69	Total	C	N	O	S	0	0
			546	335	105	105	1		

- Molecule 5 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	22	Total	C	N	O	P	0	0
			451	214	89	127	21		

- Molecule 6 is a RNA chain called RNA (20-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	11	Total	C	N	O	P	0	0
			244	108	50	75	11		

- Molecule 7 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	29	Total	C	N	O	P	0	0
			583	279	99	177	28		

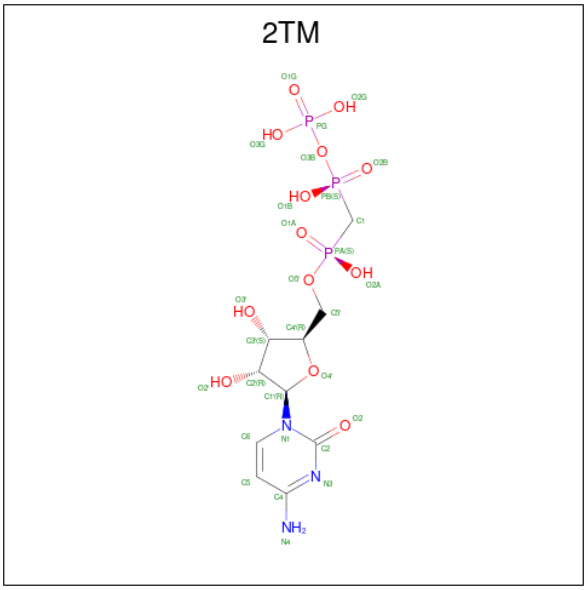
- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 10 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]methyl}phosphoryl]cytidine (three-letter code: 2TM) (formula: $C_{10}H_{18}N_3O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

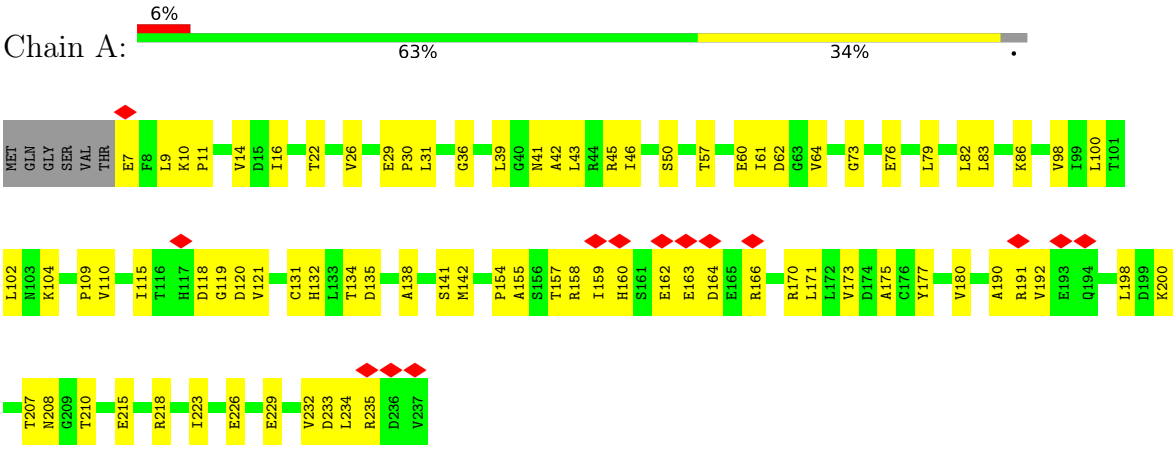


Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			29	10	3	13	3	

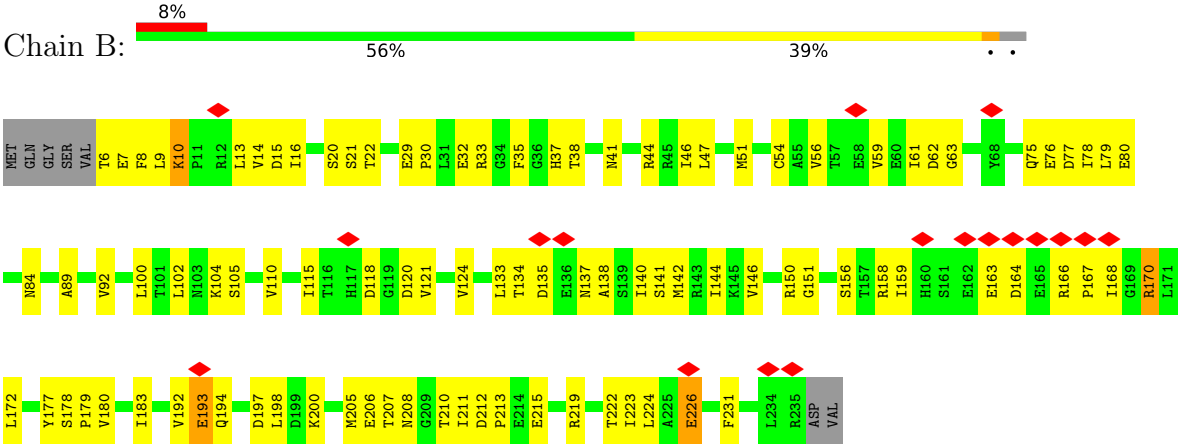
3 Residue-property plots (i)

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.

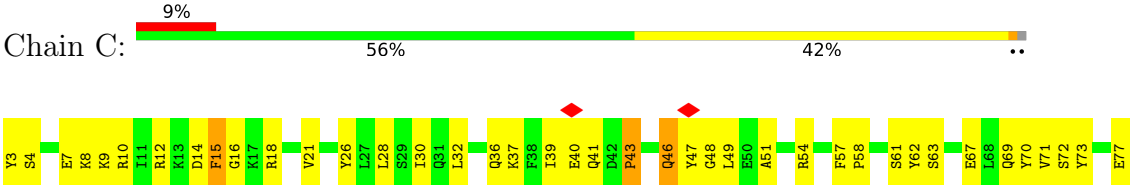
• Molecule 1: DNA-directed RNA polymerase subunit alpha

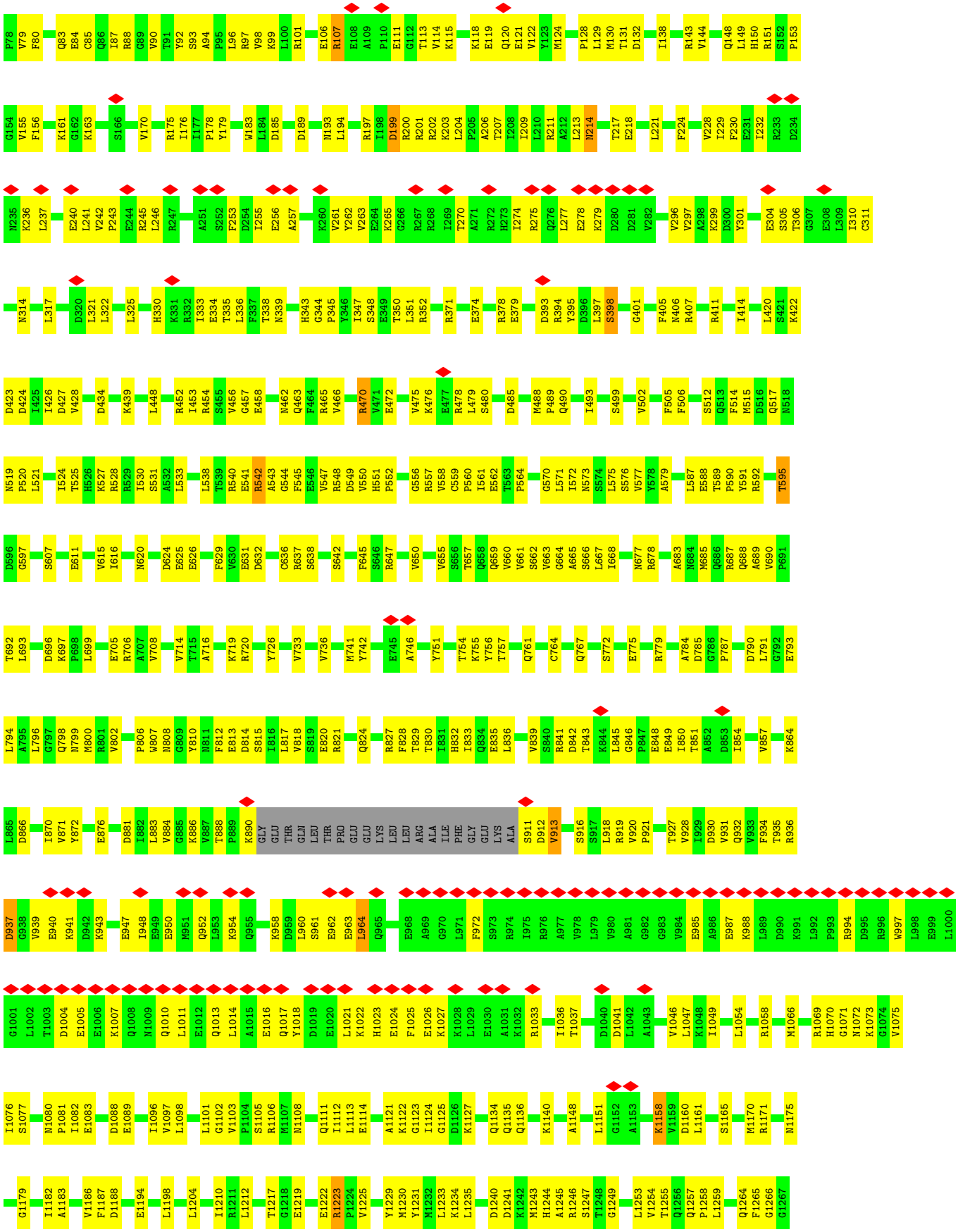


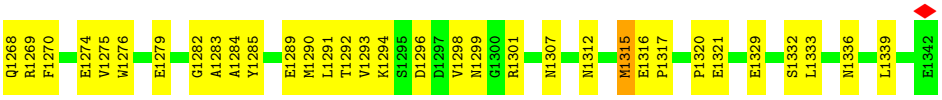
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

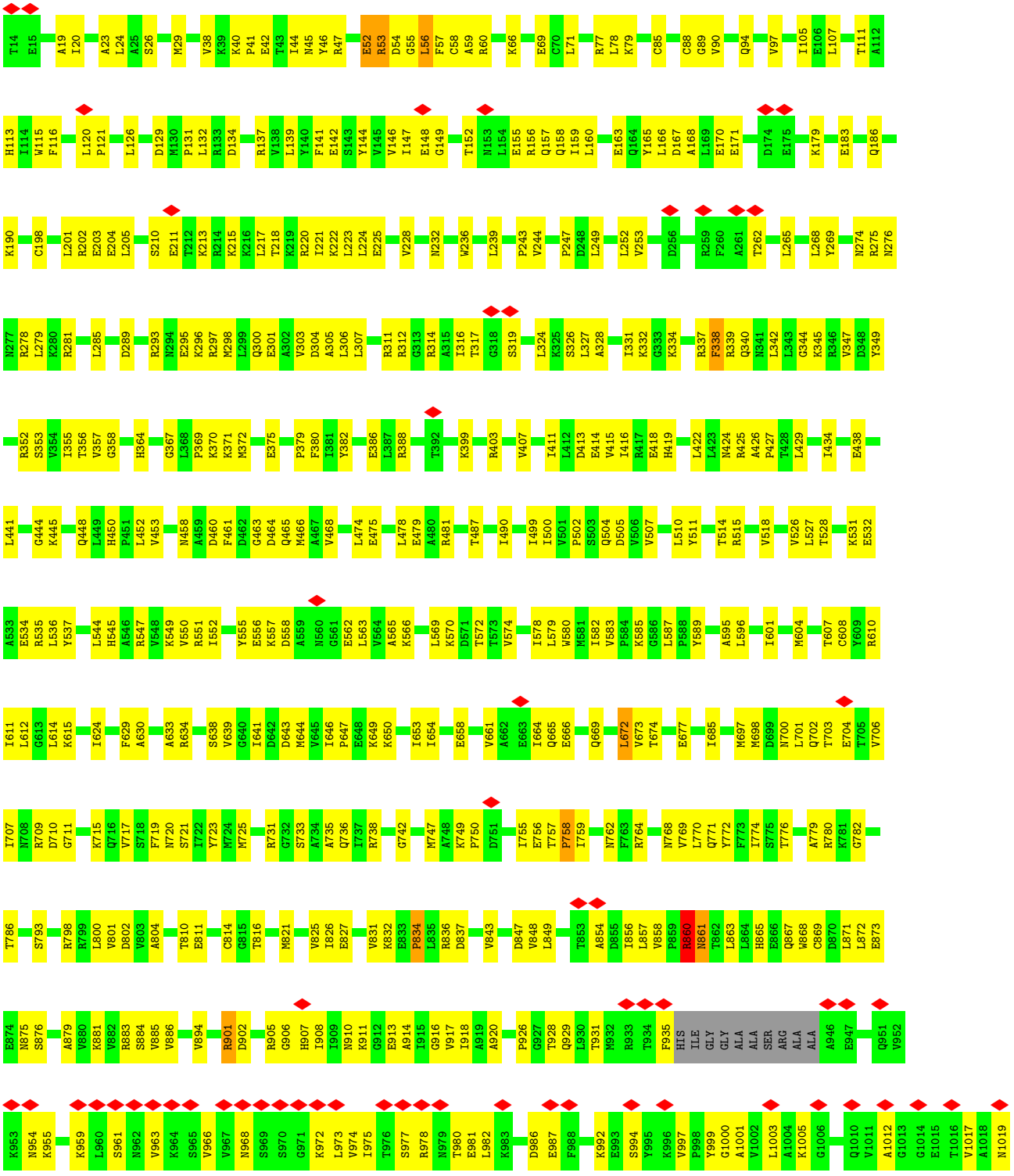


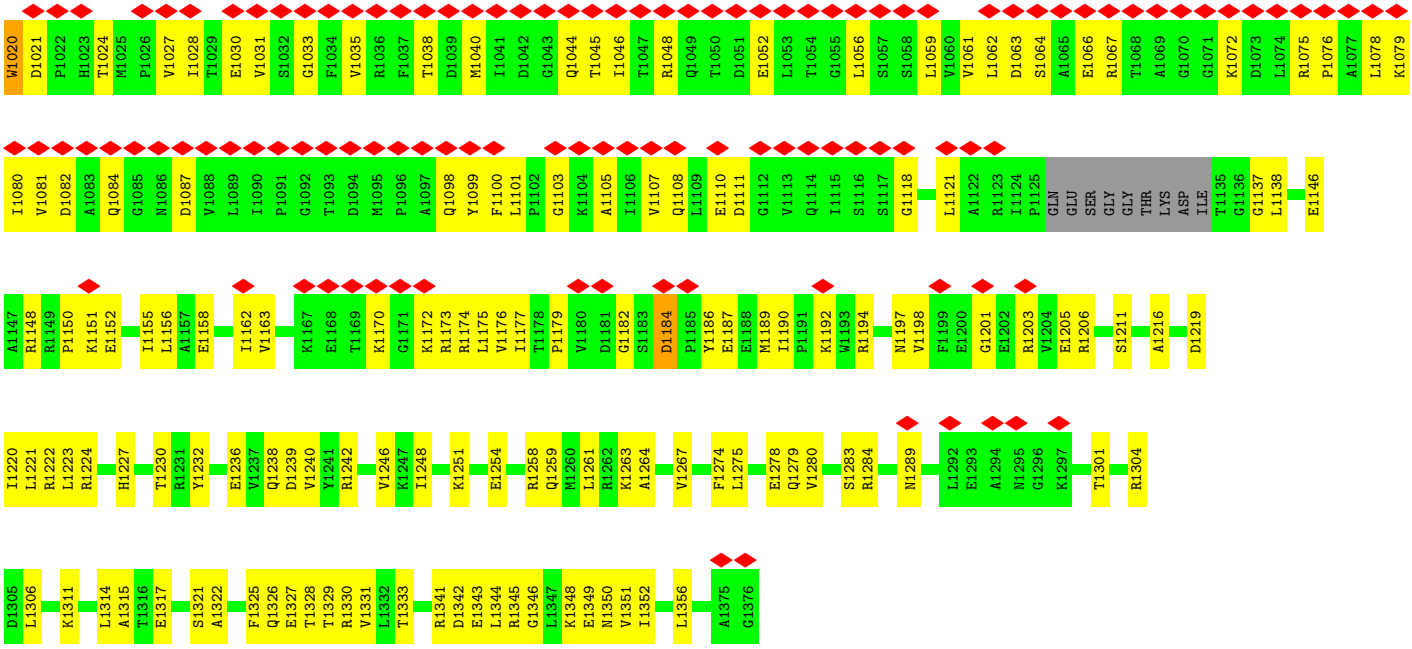

P78 V79 F80 Q83 E84 C85 Q86 I87 R88 G89 V90 T91 Y92 S93 A94 P95 L96 R97 V98 K99 L100 R101 E106 R107 E108 A109 P110 E111 G112 T113 V114 K115 K118 E119 Q120 E121 V122 Y123 M124 P128 L129 M130 T131 D132 I138 R143 V144 Q148 L149 H150 R151 S152 P153
G154 V155 F156 K161 G162 K163 S166 V170 R175 I176 I177 P178 Y179 W183 L184 D185 D189 N193 L194 R197 I198 D199 R200 R201 R202 K203 L204 P205 A206 T207 I208 I209 L210 R211 A212 L213 N214 T217 E218 L221 F224 V228 I229 F230 E231 I232 R233 D234
N235 K236 L237 E240 L241 V242 P243 E244 R245 L246 R247 A251 S252 F253 D254 I255 E256 A257 K260 V261 Y262 V263 E264 K265 G266 R267 R268 I269 T270 A271 R272 H273 I274 R275 Q276 L277 E278 K279 D280 D281 V282 V296 V297 A298 K299 D300 Y301 E304 S305 T306 G307 E308 L309 I310 C311
N314 L317 D320 L321 L322 L325 H330 K331 R332 I333 E334 T335 L336 F337 T338 N339 H343 G344 P345 Y346 I347 S348 E349 T350 L351 R352 R371 E374 R378 E379 D393 R394 Y395 D396 L397 S398 G401 F405 N406 R407 R411 I414 L420 S421 K422
D423 D424 I425 I426 D427 V428 D434 K439 L448 R452 I453 R454 S455 V456 G457 E458 N462 Q463 F464 R465 V466 R470 V471 E472 V475 K476 E477 R478 L479 S480 D485 M488 P489 Q490 I493 S499 V502 F505 F506 S512 Q513 F514 M515 D516 Q517 N518
N519 P520 L521 I524 T525 H526 K527 R528 R529 I530 S531 A532 L533 L538 T539 R540 E541 R542 A543 G544 F545 E546 V547 R548 D549 V550 H551 P552 G556 R557 V558 C559 P560 I561 E562 T563 P564 G570 L571 I572 N573 S574 L575 S576 V577 Y578 A579 L587 E588 T589 P590 Y591 R592 T595
D596 G597 S607 E611 V615 I616 N620 D624 E625 E626 F629 V630 E631 D632 C636 R637 S638 S642 F645 S646 R647 V650 V655 S656 T657 Q658 Q659 V660 V661 S662 V663 G664 A665 S666 I667 I668 N677 R678 A683 N684 M685 Q686 R687 Q688 A689 V690 P691
T692 L693 D696 K697 P698 L699 E705 R706 A707 V708 V714 T715 A716 K719 R720 Y726 V733 V736 M741 Y742 E745 A746 Y751 T754 K755 Y756 T757 Q761 C764 Q767 S772 E775 R779 A784 D785 G786 P787 D790 L791 G792 E793
L794 A795 L796 G797 Q798 N799 M800 R801 V802 P806 W807 N808 G809 Y810 N811 F812 E813 D814 S815 K816 L817 V818 S819 E820 R821 Q824 R827 F828 T829 T830 I831 H832 I833 Q834 E835 L836 V839 S840 R841 D842 T843 K844 L845 G846 P847 E848 E849 I850 T851 A852 D853 I854 V857 K864
L865 D866 I870 V871 Y872 E876 D881 I882 L883 V884 G885 K886 V887 T888 P889 K890 GLY GLU THR GLN LEU THR PRO GLU GLU LYS LEU LEU ARG ALA ILE PHE GLY GLU LYS ALA S911 D912 V913 S916 S917 L918 R919 V920 P921 T927 V928 I929 D930 V931 Q932 V933 F934 T935 R936
D937 G938 V939 E940 K941 D942 K943 E947 I948 E949 E950 M951 Q952 L953 K954 Q955 K958 D959 L960 S961 E962 E963 L964 Q965 E968 A969 G970 L971 F972 S973 R974 I975 R976 A977 Y978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988 L989 D990 K991 L992 P993 R994 D995 R996 W997 L998 E999 L1000
G1001 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012 Q1013 L1014 A1015 E1016 Q1017 Y1018 D1019 E1020 L1021 K1022 H1023 E1024 F1025 E1026 K1027 K1028 L1029 E1030 A1031 K1032 R1033 I1036 T1037 D1040 D1041 L1042 A1043 V1046 L1047 K1048 I1049 L1054 R1058 M1066 R1069 H1070 G1071 N1072 K1073 G1074 V1075
I1076 S1077 N1080 P1081 I1082 E1083 D1088 E1089 I1096 V1097 L1098 L1101 G1102 V1103 P1104 S1105 R1106 M1107 N1108 Q1111 I1112 L1113 E1114 A1121 K1122 G1123 I1124 G1125 D1126 K1127 Q1134 Q1135 Q1136 K1140 A1148 L1151 G1152 A1153 K1158 V1159 D1160 L1161 S1165 M1170 R1171 N1175
G1179 I1182 A1183 V1186 F1187 D1188 E1194 L1198 L1204 I1210 R1211 L1212 T1217 G1218 E1219 E1222 R1223 P1224 V1225 Y1229 M1230 Y1231 M1232 L1233 K1234 L1235 D1240 D1241 K1242 M1243 H1244 A1245 R1246 S1247 T1248 G1249 L1253 V1254 T1255 Q1256 Q1257 P1258 L1259 Q1264 F1265 G1266 G1267



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

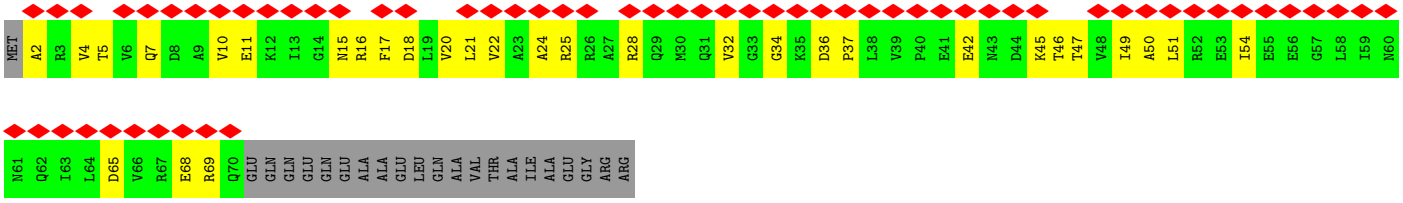
Chain D:





• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

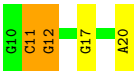


• Molecule 5: DNA (29-MER)

Chain N:

• Molecule 6: RNA (20-MER)

Chain R:



• Molecule 7: DNA (29-MER)

Chain T:


G1
G2
C11
G12
T13
G14
T15
A16
C17
C18
T19
C20
T21
C22
C23
T24
A25
G26
C27
C28
C29

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	256565	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 ($e^-/Å^2$)	40	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	0.204	Depositor
Minimum map value	-0.111	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	343.2, 343.2, 343.2	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2TM, 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	A	0.33	0/1816	0.63	0/2461
1	B	0.34	0/1808	0.69	2/2450 (0.1%)
2	C	0.38	0/10580	0.66	4/14274 (0.0%)
3	D	0.35	0/10577	0.67	7/14284 (0.0%)
4	E	0.27	0/548	0.63	0/738
5	N	0.59	0/506	0.96	0/777
6	R	0.66	0/274	1.18	2/427 (0.5%)
7	T	0.85	0/650	1.08	2/1000 (0.2%)
All	All	0.39	0/26759	0.70	17/36411 (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
2	C	0	2
3	D	0	3
All	All	0	5

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	758	PRO	CA-N-CD	-7.55	100.93	111.50
3	D	757	THR	C-N-CD	-6.51	106.27	120.60
3	D	802	ASP	CB-CG-OD1	6.05	123.75	118.30
3	D	1020	TRP	CA-CB-CG	6.02	125.14	113.70
3	D	802	ASP	CB-CG-OD2	-5.95	112.94	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	236	LYS	Peptide
2	C	595	THR	Peptide
3	D	1184	ASP	Peptide
3	D	860	ARG	Peptide
3	D	901	ARG	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	A	1794	0	1819	64	0
1	B	1786	0	1813	78	0
2	C	10414	0	10420	475	0
3	D	10419	0	10606	500	0
4	E	546	0	565	72	0
5	N	451	0	248	9	0
6	R	244	0	120	5	0
7	T	583	0	329	17	0
8	D	1	0	0	0	0
9	D	2	0	0	0	0
10	D	29	0	14	2	0
All	All	26269	0	25934	1077	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 21.

The worst 5 of 1077 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:D:474:LEU:HD23	4:E:28:ARG:CG	1.56	1.32
3:D:910:ASN:ND2	4:E:15:ASN:OD1	1.74	1.20
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.15	1.08
3:D:474:LEU:CD2	4:E:28:ARG:CG	2.35	1.05
3:D:474:LEU:CD2	4:E:28:ARG:HG2	1.85	1.04

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	229/237 (97%)	213 (93%)	16 (7%)	0	100	100
1	B	228/237 (96%)	209 (92%)	17 (8%)	2 (1%)	17	53
2	C	1316/1340 (98%)	1209 (92%)	99 (8%)	8 (1%)	25	62
3	D	1338/1363 (98%)	1219 (91%)	114 (8%)	5 (0%)	34	68
4	E	67/91 (74%)	61 (91%)	6 (9%)	0	100	100
All	All	3178/3268 (97%)	2911 (92%)	252 (8%)	15 (0%)	32	65

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	SER
2	C	199	ASP
2	C	913	VAL
2	C	1041	ASP
3	D	338	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/204 (98%)	199 (100%)	0	100	100
1	B	198/204 (97%)	195 (98%)	3 (2%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C	1139/1155 (99%)	1117 (98%)	22 (2%)	57 80
3	D	1117/1136 (98%)	1108 (99%)	9 (1%)	81 92
4	E	59/75 (79%)	59 (100%)	0	100 100
All	All	2712/2774 (98%)	2678 (99%)	34 (1%)	70 86

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	56	LEU
3	D	157	GLN
3	D	1289	ASN
2	C	936	ARG
2	C	935	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	932	GLN
3	D	1108	GLN
2	C	1023	HIS
3	D	1279	GLN
3	D	458	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	10/11 (90%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	11	C
6	R	12	G

There are no RNA pucker outliers to report.

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 4 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
10	2TM	D	2004	-	27,30,30	3.01	12 (44%)	39,47,47	1.12	4 (10%)

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	2TM	D	2004	-	-	6/19/38/38	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	2004	2TM	O2-C2	8.63	1.39	1.23
10	D	2004	2TM	PB-O3B	6.16	1.65	1.58
10	D	2004	2TM	PA-O5'	5.29	1.65	1.57
10	D	2004	2TM	C4-N4	4.96	1.45	1.33
10	D	2004	2TM	C2-N3	3.89	1.44	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	2004	2TM	C3'-C2'-C1'	2.89	106.93	101.43
10	D	2004	2TM	PB-O3B-PG	-2.88	122.49	132.62
10	D	2004	2TM	C4'-O4'-C1'	-2.20	104.62	109.47
10	D	2004	2TM	C2'-C3'-C4'	2.06	106.64	102.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	2004	2TM	C5'-O5'-PA-O1A
10	D	2004	2TM	O4'-C4'-C5'-O5'
10	D	2004	2TM	PA-C1-PB-O3B
10	D	2004	2TM	PA-C1-PB-O1B
10	D	2004	2TM	PA-C1-PB-O2B

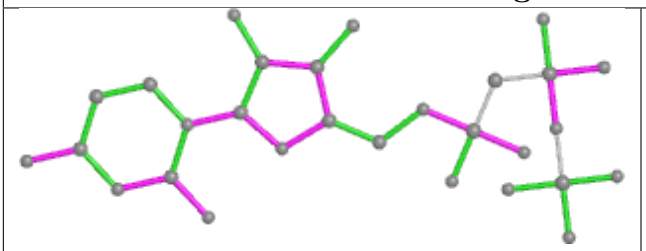
There are no ring outliers.

1 monomer is involved in 2 short contacts:

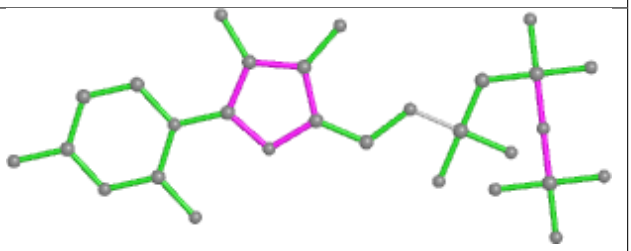
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	2004	2TM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

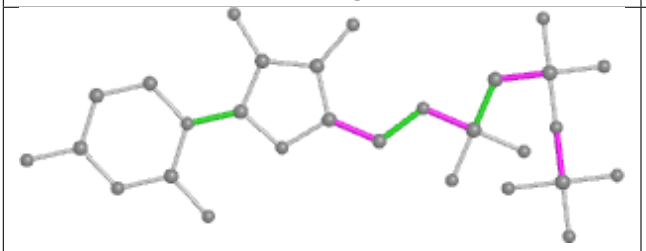
Ligand 2TM D 2004



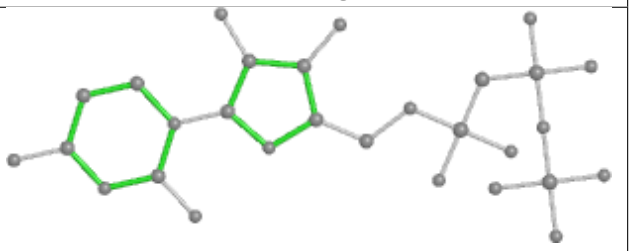
Bond lengths



Bond angles



Torsions



Rings

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.

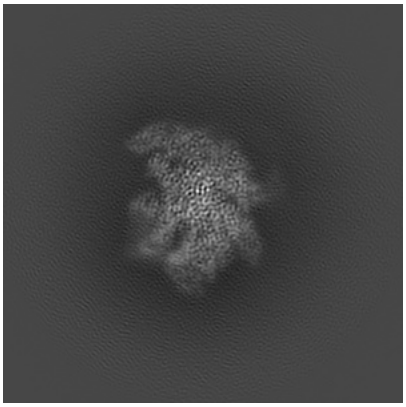
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23901. These allow visual inspection of the internal detail of the map and identification of artifacts.

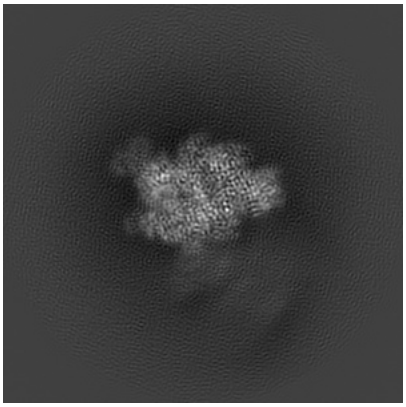
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

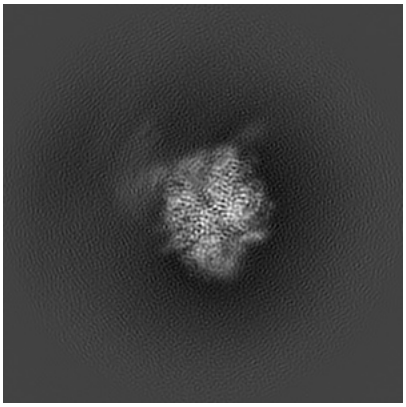
6.1.1 Primary map



X



Y

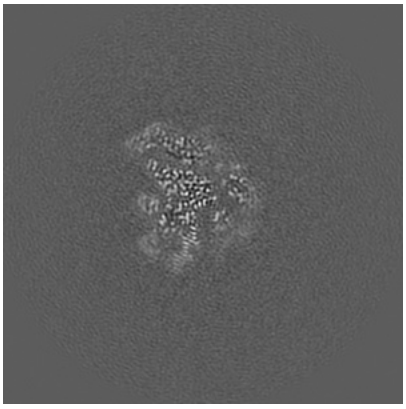


Z

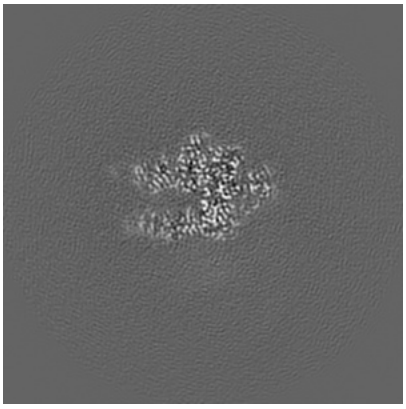
The images above show the map projected in three orthogonal directions.

6.2 Central slices

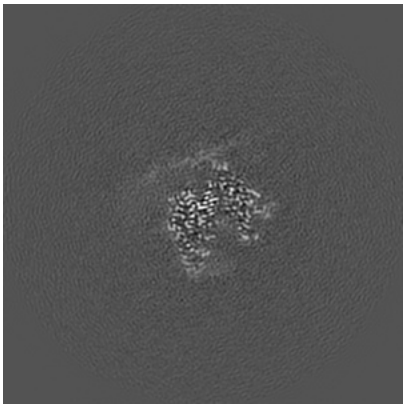
6.2.1 Primary map



X Index: 130



Y Index: 130

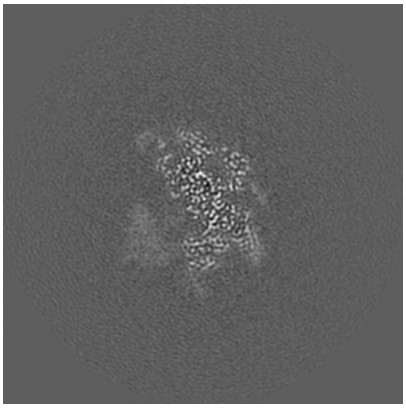


Z Index: 130

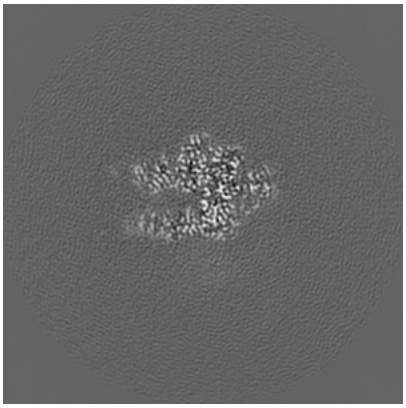
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

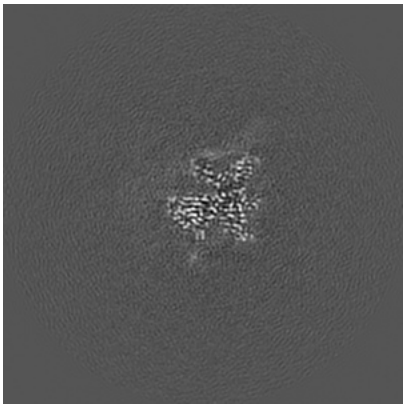
6.3.1 Primary map



X Index: 147



Y Index: 130



Z Index: 138

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

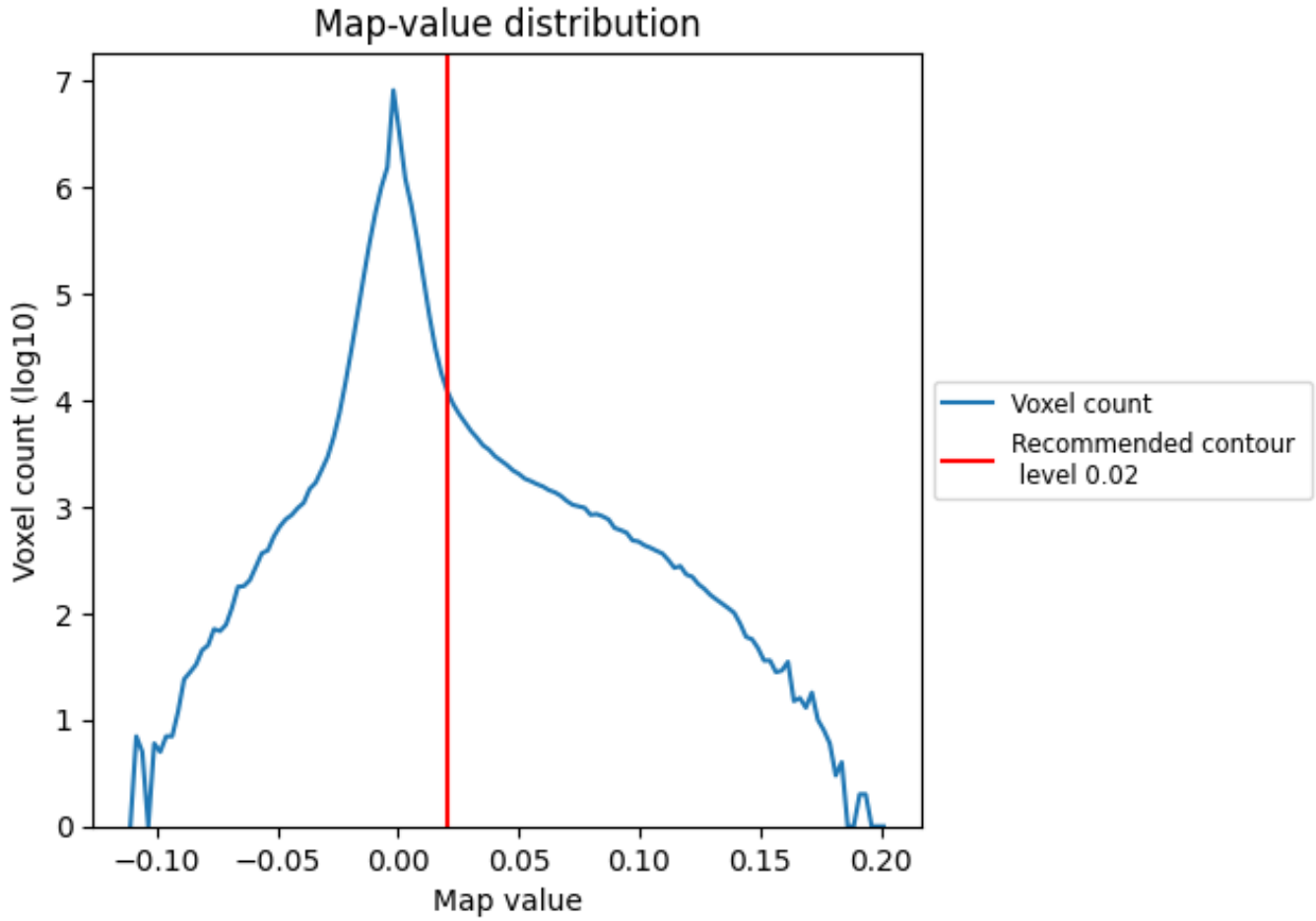
6.5 Mask visualisation (i)

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

7 Map analysis

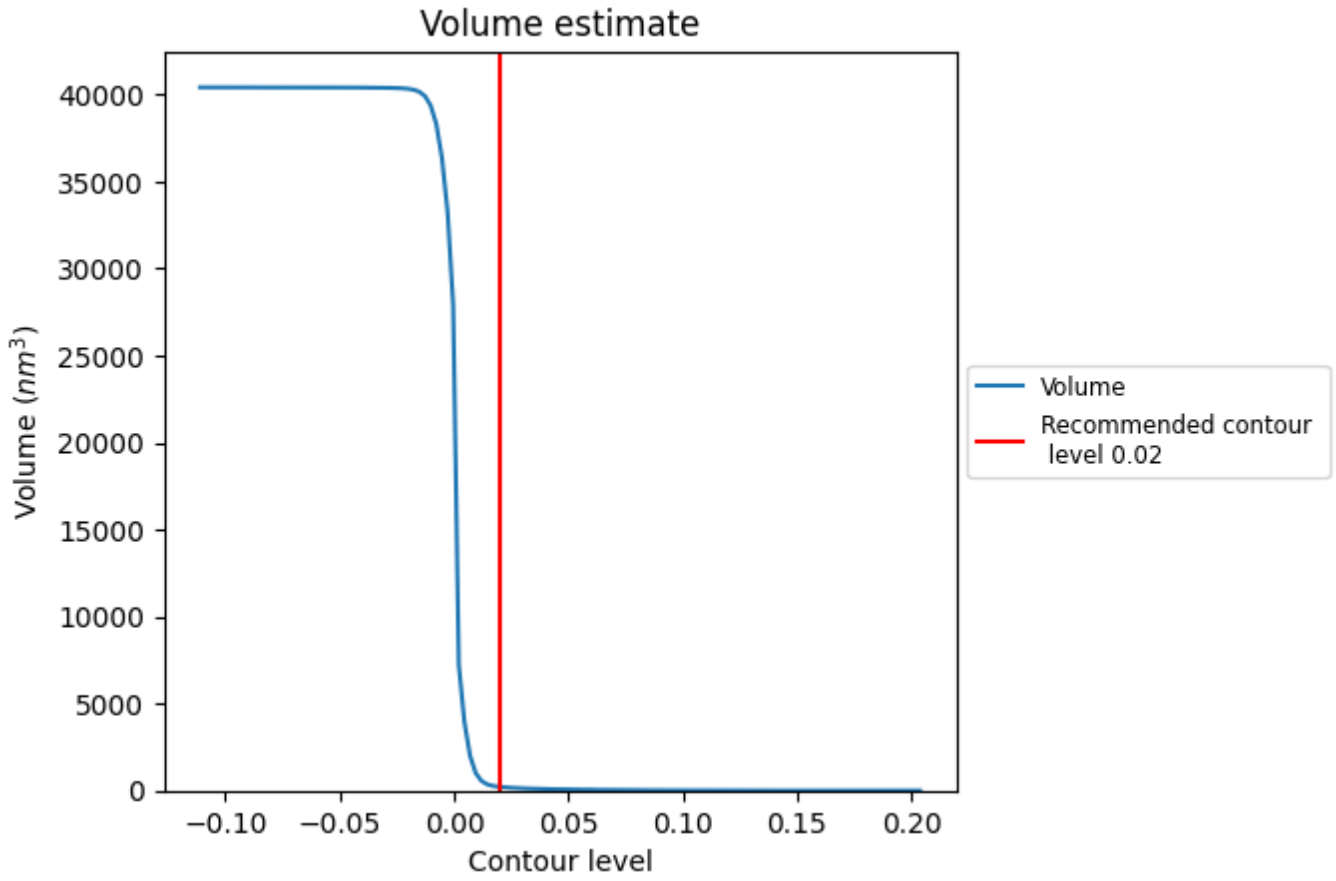
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

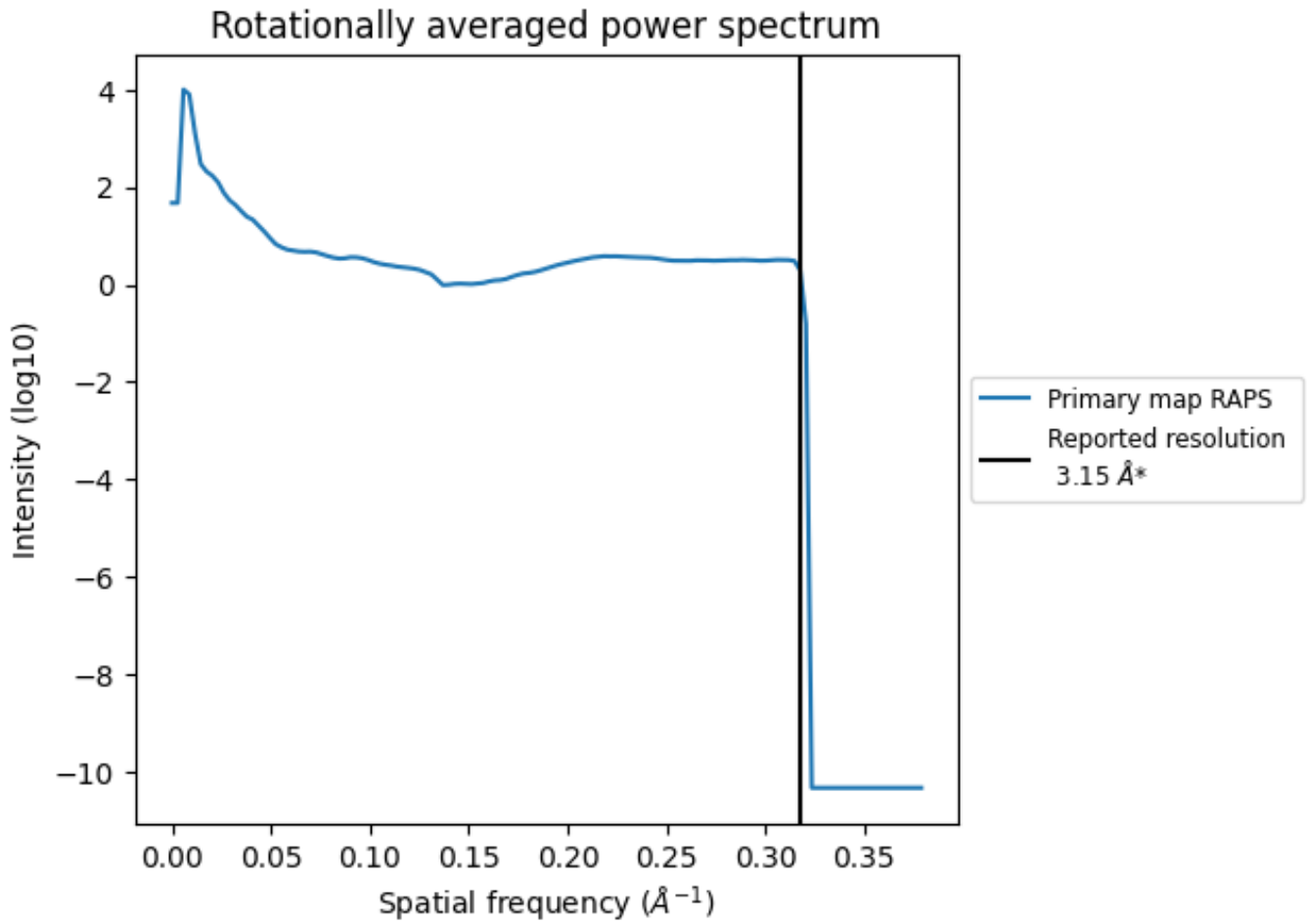
7.2 Volume estimate (i)



The volume at the recommended contour level is 211 nm^3; this corresponds to an approximate mass of 191 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 0.317 Å^{-1}

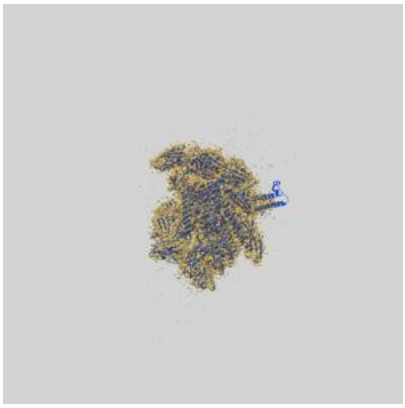
8 Fourier-Shell correlation

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

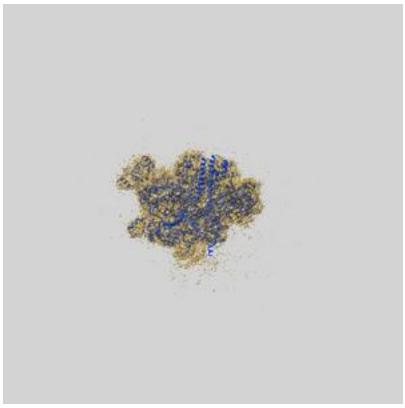
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23901 and PDB model 7MKO. Per-residue inclusion information can be found in section 3 on page 7.

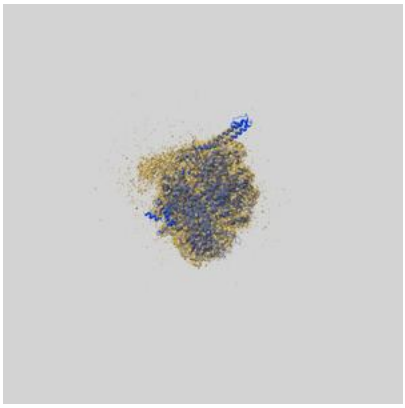
9.1 Map-model overlay



X



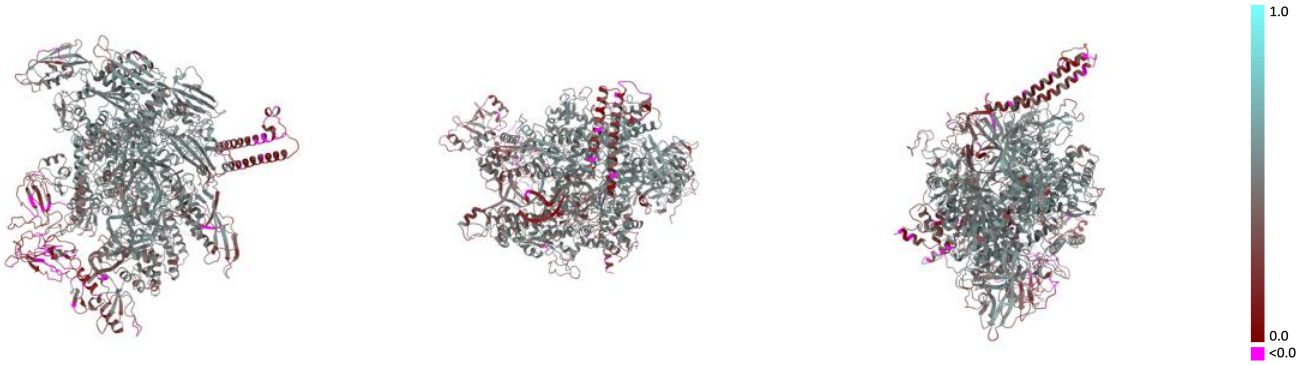
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

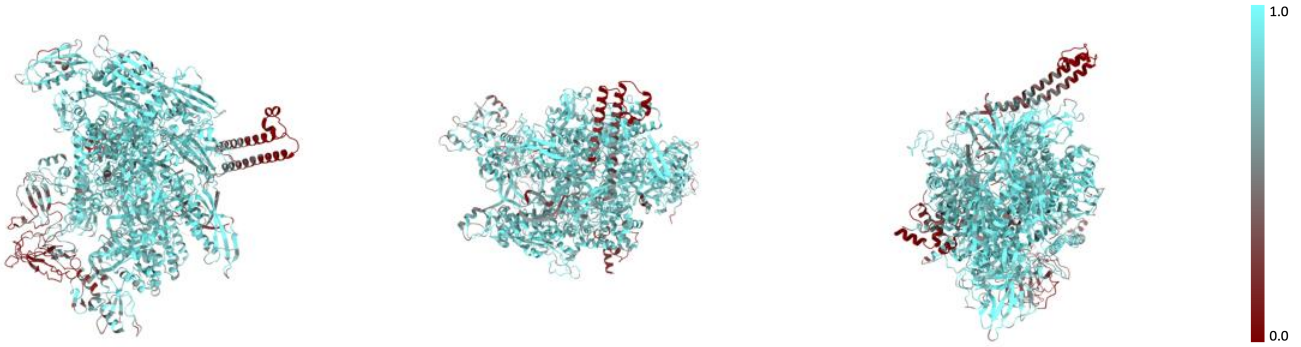
9.2 Q-score mapped to coordinate model (i)



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.

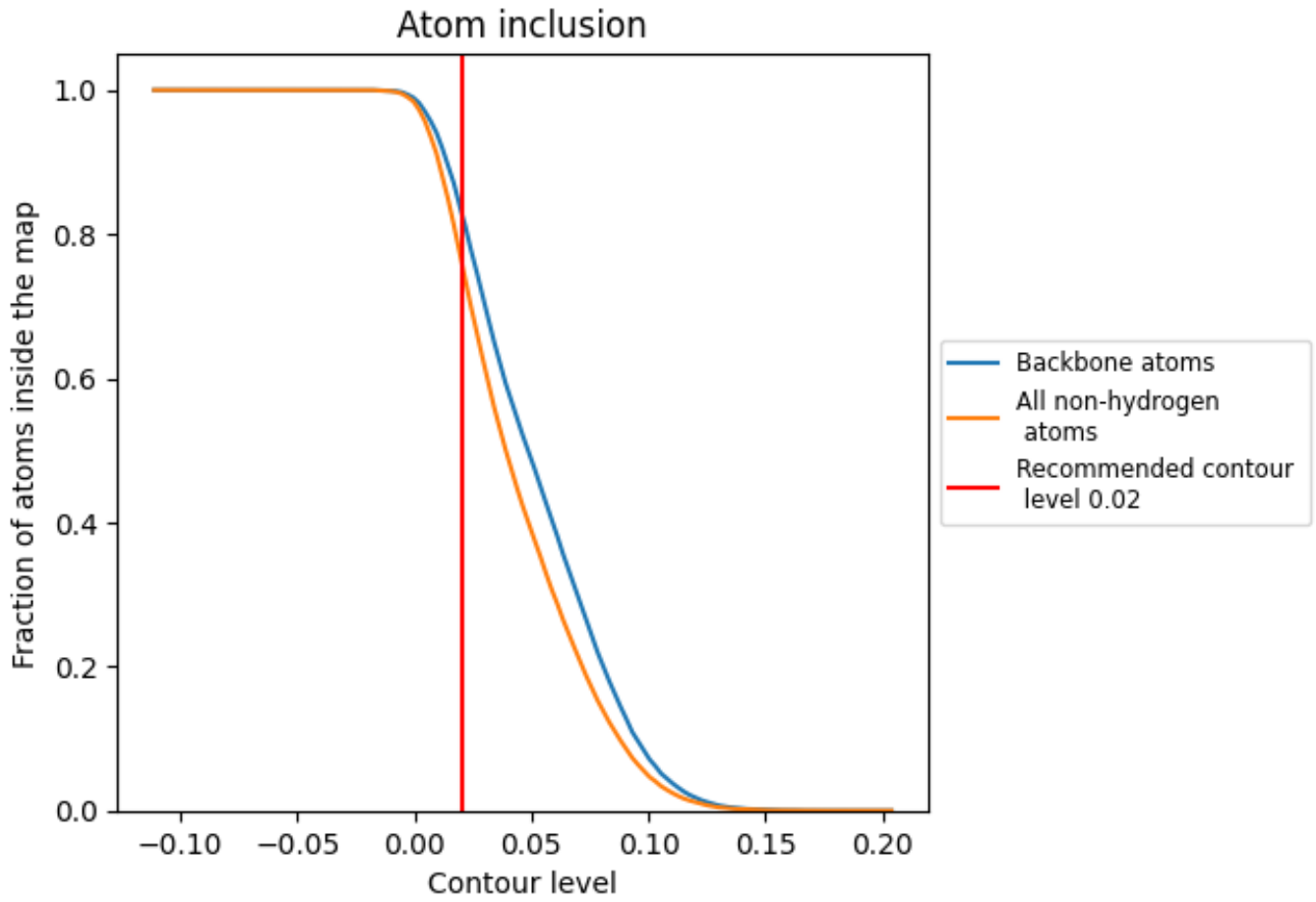
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7637	0.4330
A	0.8246	0.4790
B	0.7838	0.4440
C	0.7922	0.4520
D	0.7490	0.4170
E	0.1434	0.2290
N	0.7783	0.3800
R	0.8975	0.5160
T	0.7753	0.4030