Full wwPDB EM Validation Report ⓘ

Mar 3, 2024 – 02:08 PM EST

PDB ID	:	6C9Y
EMDB ID	:	EMD-7438
Title	:	Cryo-EM structure of E. coli RNAP sigma70 holoenzyme
Authors	:	Narayanan, A.; Vago, F.; Li, K.; Qayyum, M.Z.; Yenool, D.; Jiang, W.; Murakami, K.S.
Deposited on	:	2018-01-29
Resolution	:	4.25 Å(reported)

This is a Full wwPDB EM Validation 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:

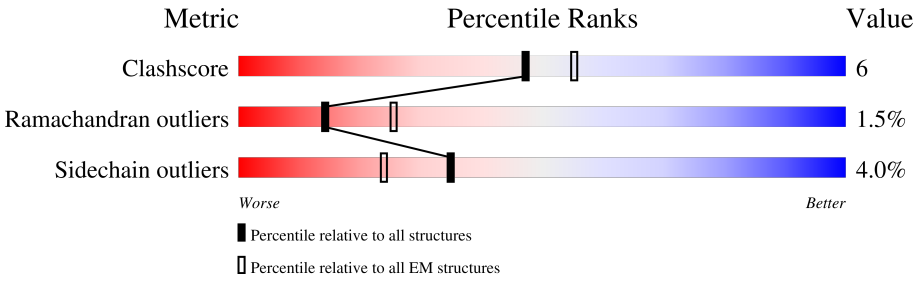
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 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 4.25 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

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	329	37% 55% 14% · 30%
1	B	329	34% 52% 14% · 33%
2	C	1342	65% 82% 16% ·
3	D	1407	63% 73% 21% · ·
4	E	91	75% 73% 10% · 16%
5	F	613	70% 62% 13% · 24%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28920 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	230	Total	C	N	O	S	0	0
			1787	1112	317	352	6		
1	B	221	Total	C	N	O	S	0	0
			1708	1067	302	333	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1350	Total	C	N	O	S	0	0
			10434	6553	1856	1976	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	76	Total	C	N	O	S	0	0
			605	368	115	121	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	468	Total	C	N	O	S	0	0
			3813	2389	678	723	23		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

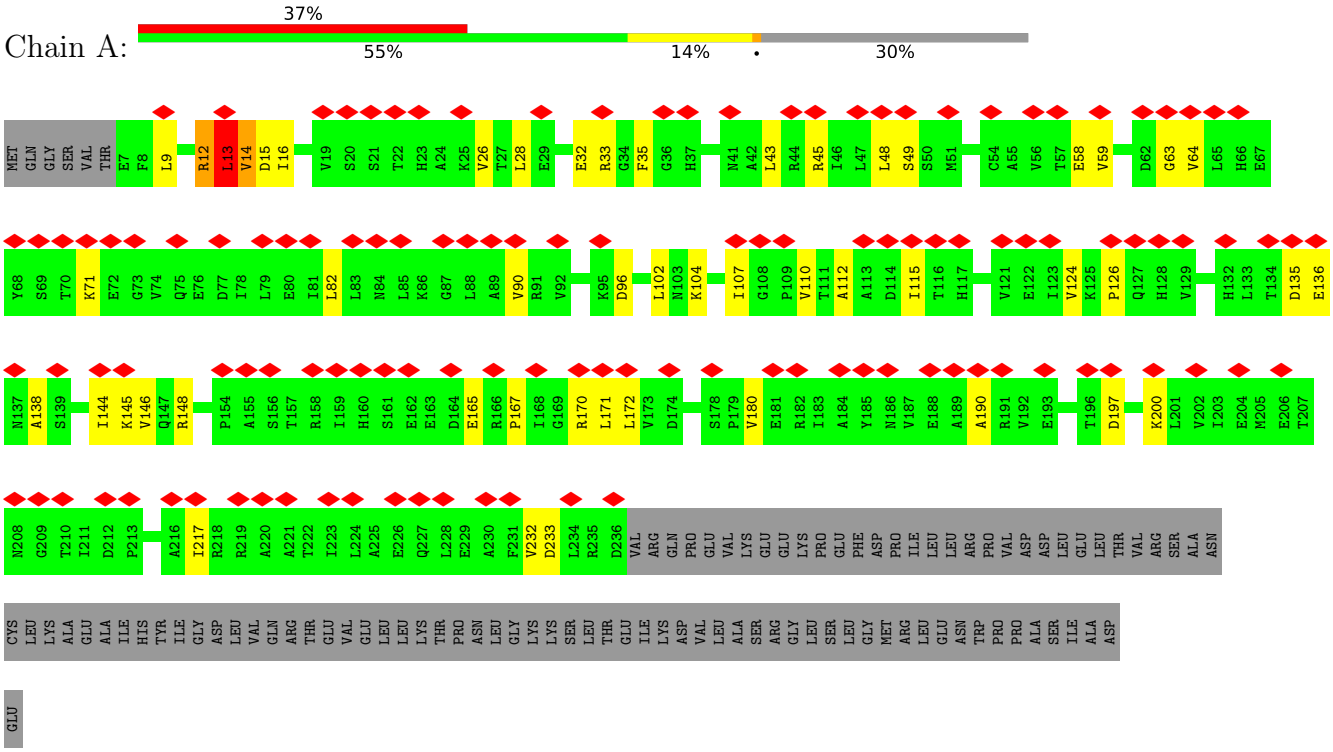
Mol	Chain	Residues	Atoms	AltConf
7	D	2	Total Zn 2 2	0

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.

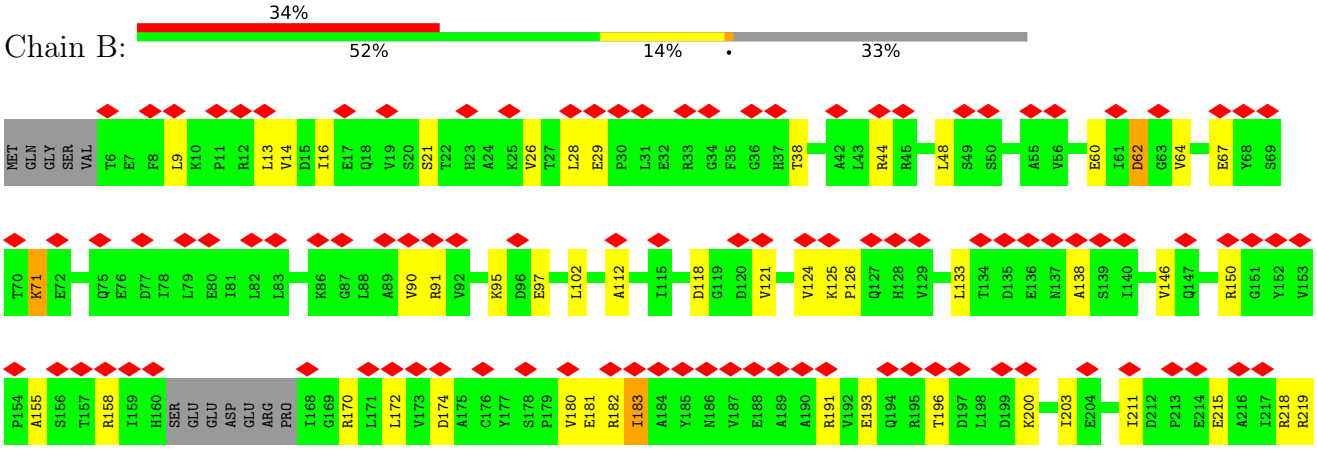
• Molecule 1: DNA-directed RNA polymerase subunit alpha

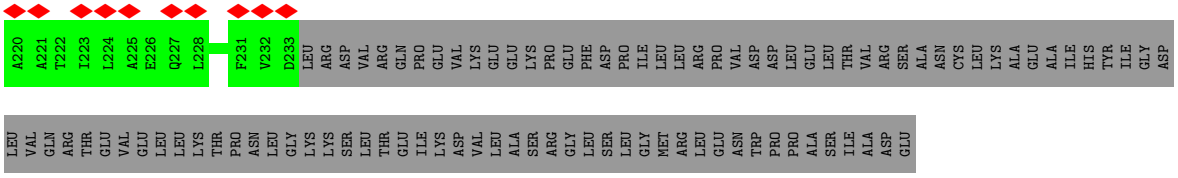
Chain A:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

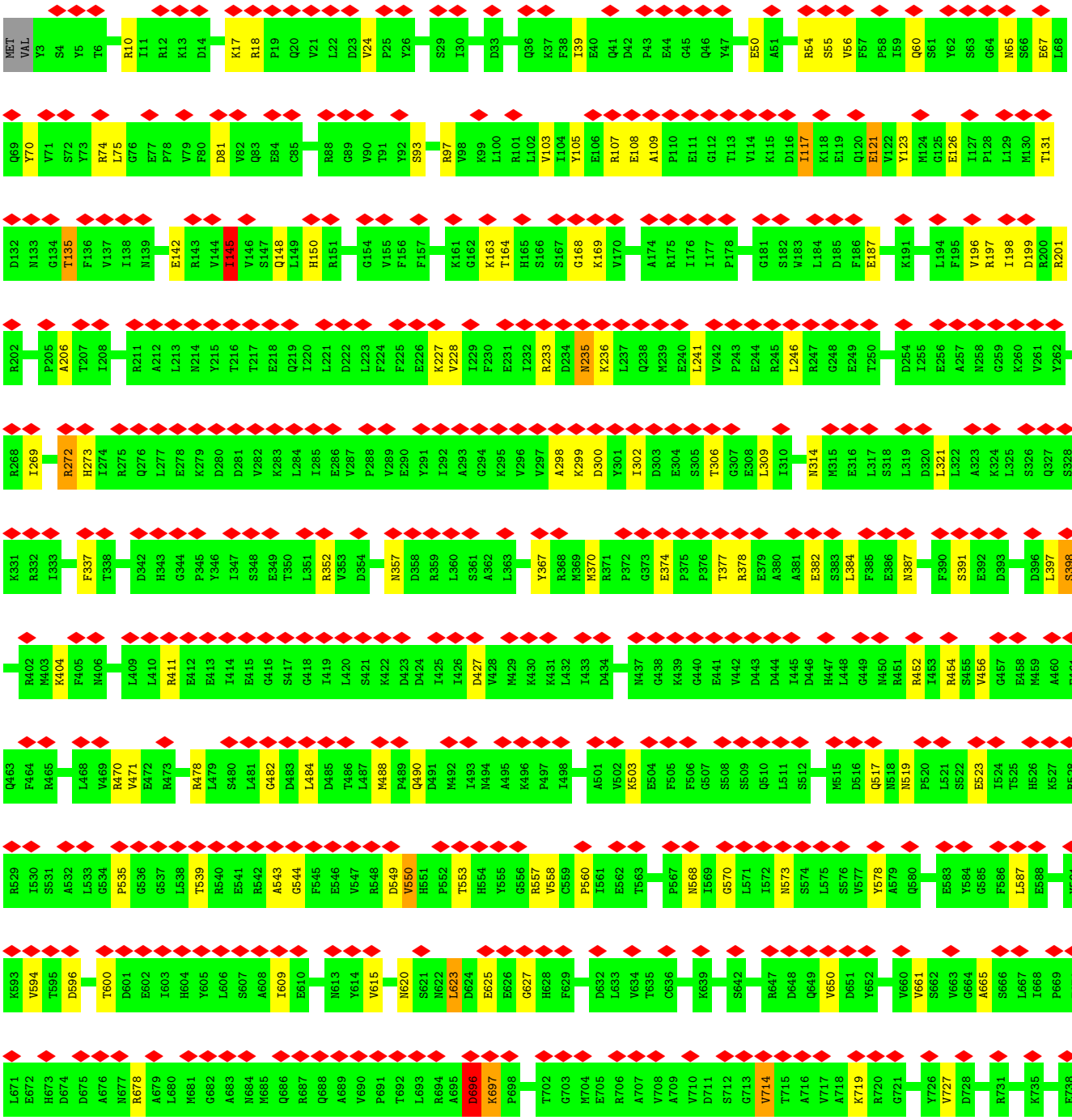
Chain B:

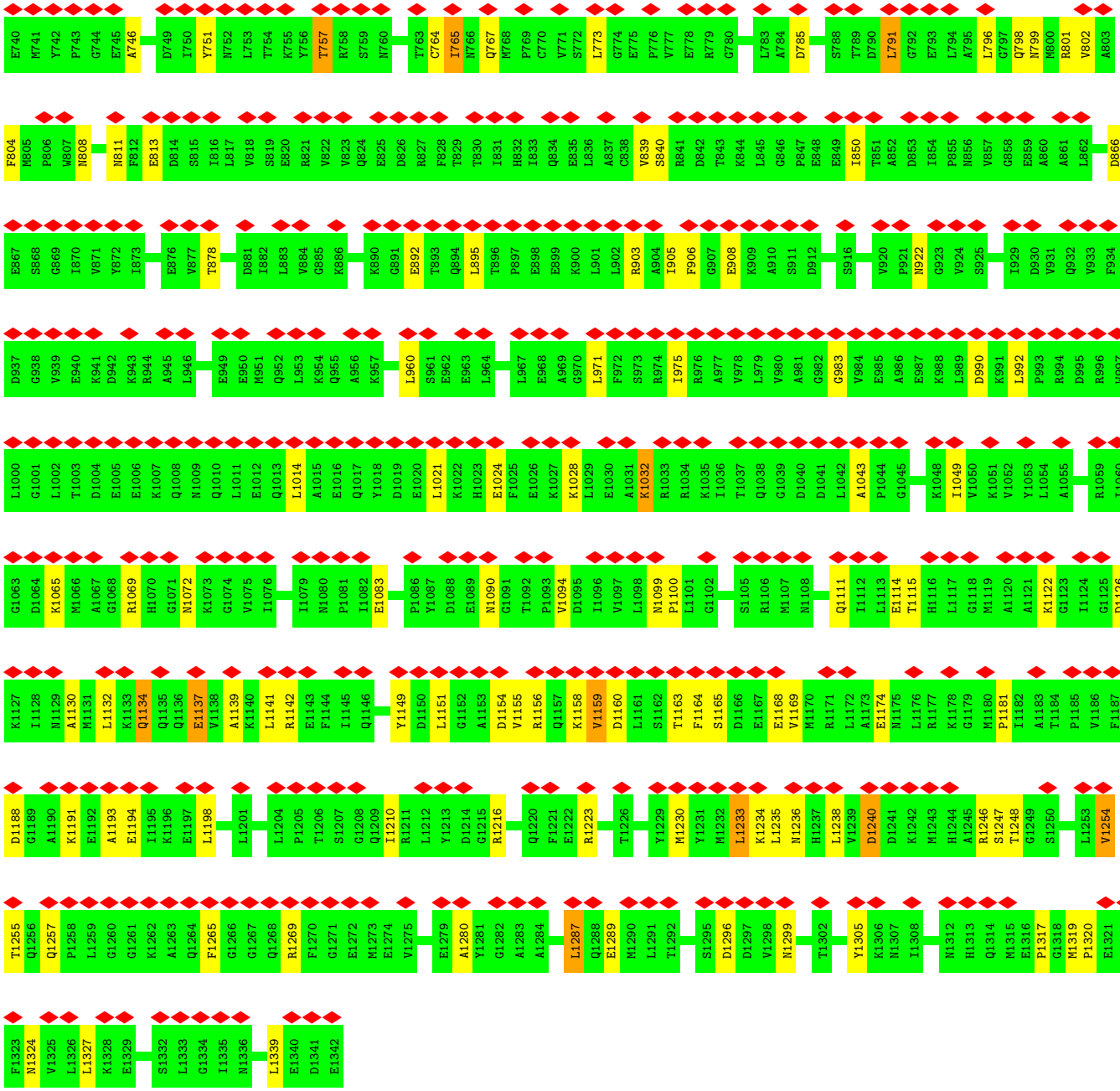




• Molecule 2: DNA-directed RNA polymerase subunit beta

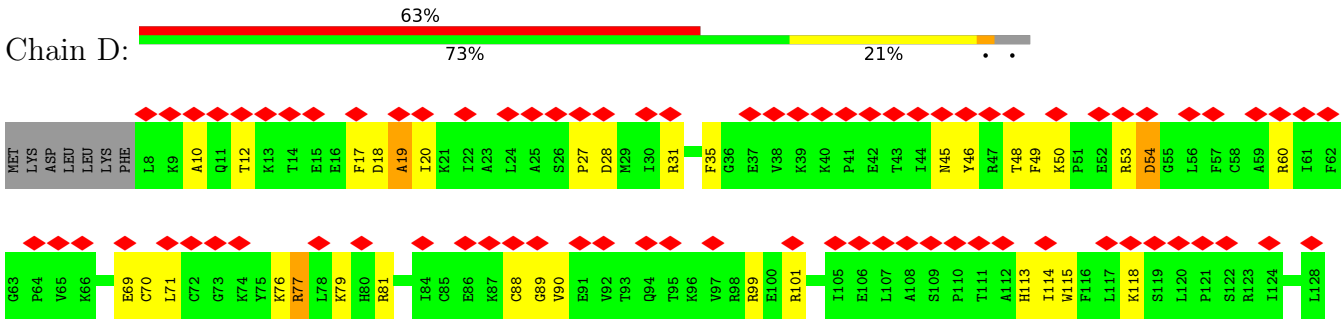
Chain C:

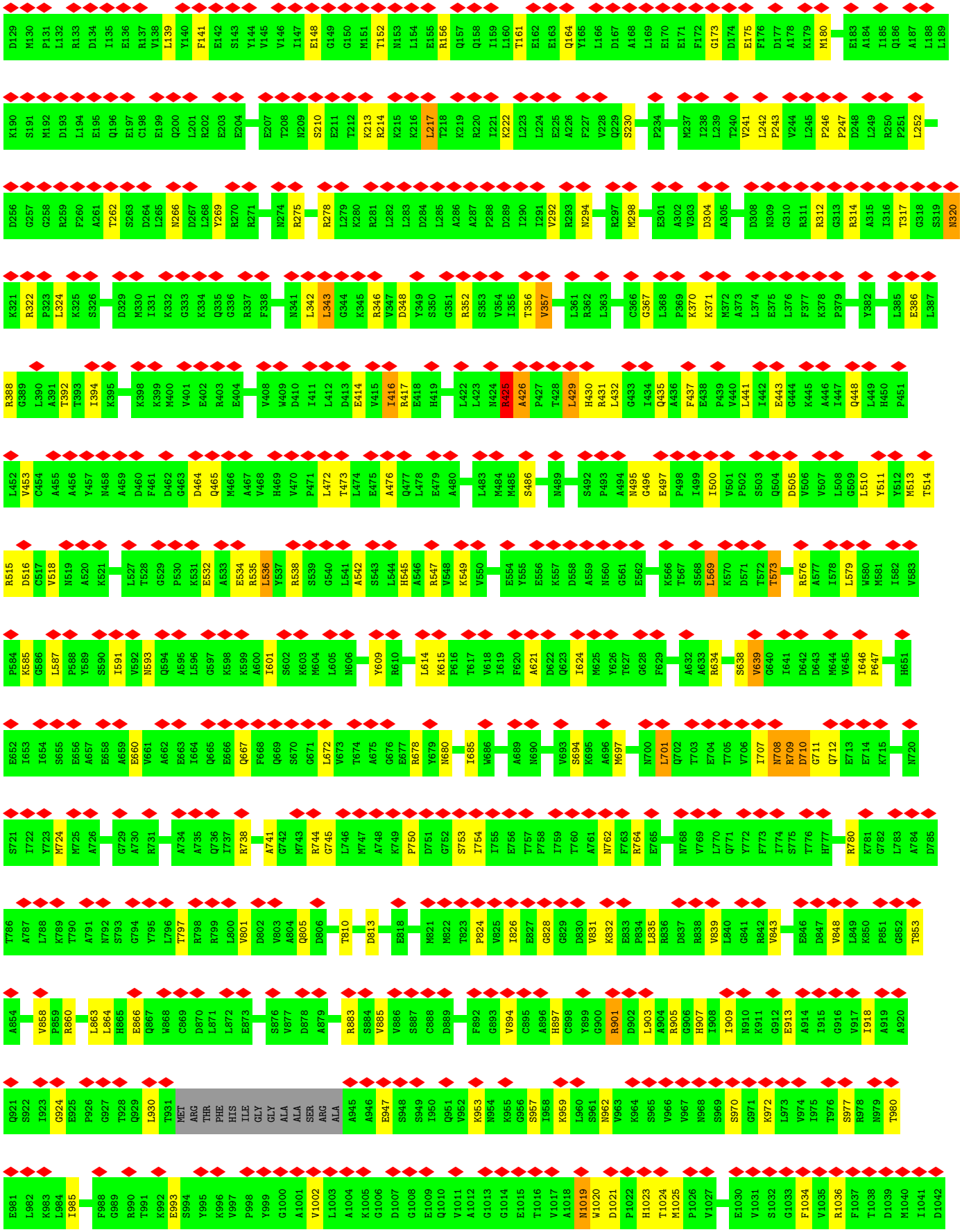


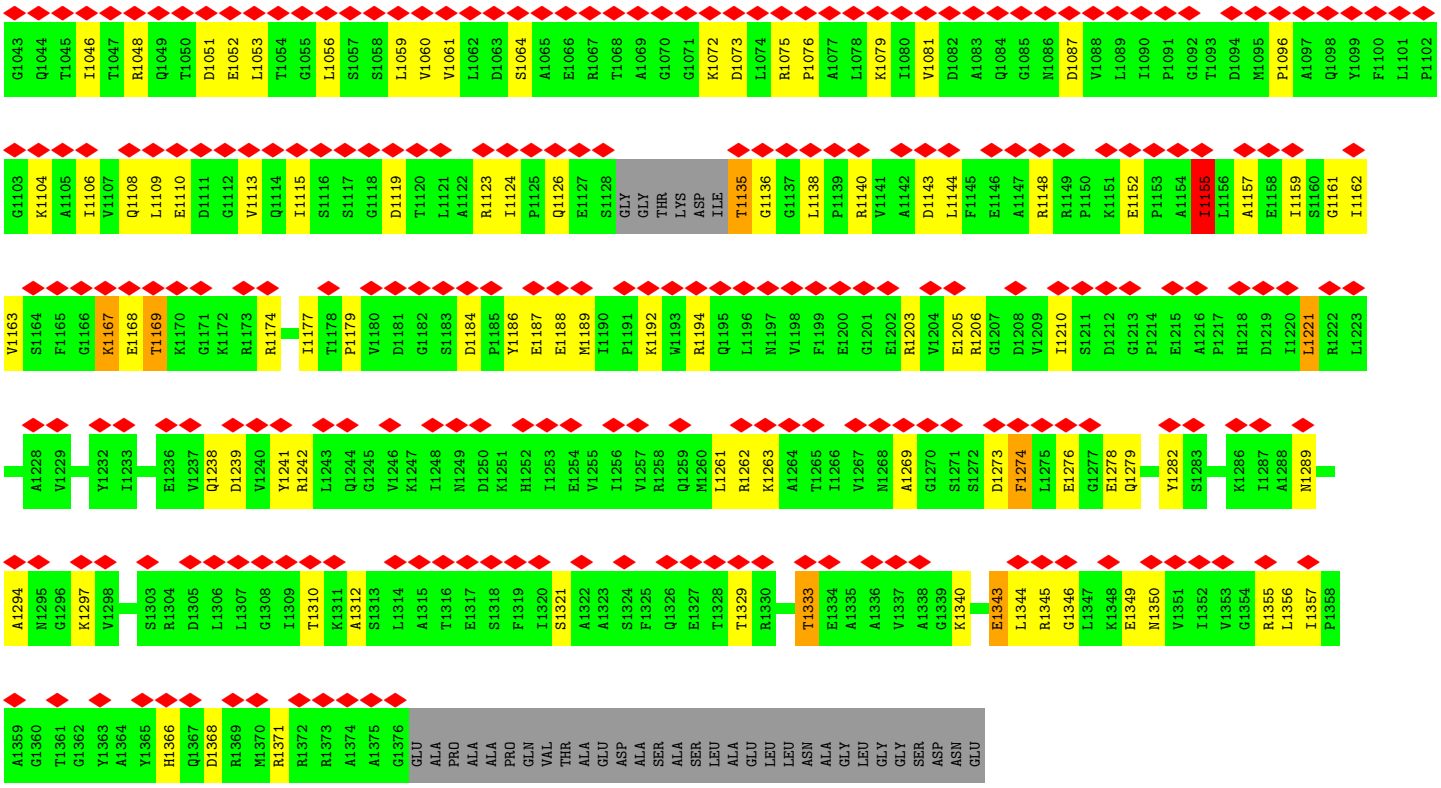


• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

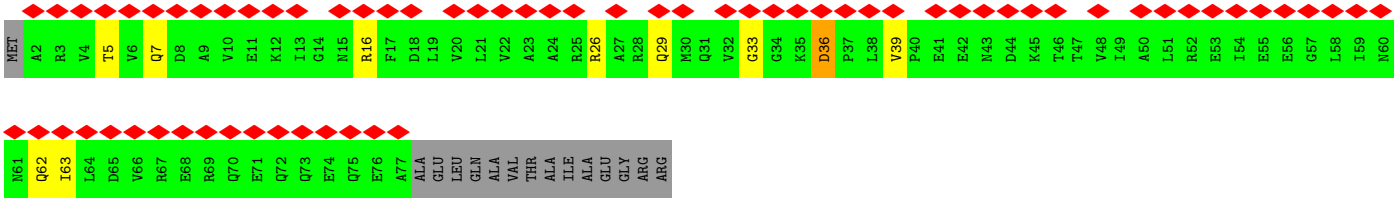



D129 M130 P131 L132 R133 D134 I135 E136 R137 V138 L139 Y140 F141 E142 S143 Y144 V145 V146 I147 E148 G149 G150 M151 T152 N153 L154 E155 R156 Q157 Q158 I159 L160 T161 E162 E163 Q164 Y165 L166 D167 A168 L169 E170 E171 F172 G173 D174 E175 F176 D177 A178 K179 M180 E183 A184 I185 Q186 A187 L188 L189
K190 S191 M192 D193 L194 E195 Q196 E197 C198 E199 Q200 L201 R202 E203 E204 E207 T208 N209 S210 E211 T212 K213 R214 K215 K216 L217 T218 K219 R220 I221 K222 L223 L224 E225 A226 F227 V228 Q229 S230 P234 M237 I238 L239 T240 V241 L242 P243 V244 L245 P246 P247 D248 L249 R250 P251 L252
D256 G257 G258 R259 F260 A261 T262 S263 D264 L265 N266 D267 L268 Y269 R270 R271 N274 R275 R278 L279 K280 R281 L282 L283 D284 L285 A286 A287 P288 D289 I290 I291 V292 R293 N294 R297 M298 E301 A302 V303 D304 A305 D308 N309 G310 R311 R312 G313 R314 A315 I316 T317 G318 S319 M320
K321 R322 P323 L324 K325 S326 D329 M330 I331 K332 G333 K334 Q335 G336 R337 F338 N341 L342 L343 G344 K345 R346 V347 D348 Y349 S350 G351 R352 S353 V354 I355 T356 V357 L361 R362 L363 C366 G367 L368 P369 K370 K371 M372 A373 L374 E375 L376 F377 K378 P379 Y382 L385 E386 L387
R388 G389 L390 A391 T392 T393 I394 K395 K398 K399 M400 V401 E402 R403 E404 V408 W409 D410 I411 L412 D413 E414 V415 I416 R417 E418 H419 L422 L423 N424 R425 A426 P427 T428 L429 H430 R431 L432 G433 I434 Q435 A436 F437 E438 P439 V440 L441 I442 E443 G444 K445 A446 I447 Q448 L449 H450 P451
L452 V453 C454 A455 A456 Y457 N458 A459 D460 F461 D462 G463 D464 Q465 M466 A467 V468 H469 V470 P471 L472 T473 L474 E475 A476 Q477 L478 E479 A480 L483 M484 M485 S486 N489 S492 P493 A494 N495 G496 E497 P498 I499 I500 V501 P502 S503 Q504 D505 V506 V507 L508 G509 L510 Y511 Y512 M513 T514
R515 D516 C517 V518 N519 A520 K521 L527 T528 G529 P530 K531 E532 A533 E534 R535 L536 Y537 R538 S539 G540 L541 A542 S543 L544 H545 A546 R547 V548 K549 V550 E554 Y555 E556 K557 D558 A559 N560 G561 E562 K566 T567 S568 L569 K570 D571 T572 T573 R576 A577 I578 L579 W580 M581 I582 V583
P584 K585 G586 L587 P588 Y589 S590 I591 V592 N593 Q594 A595 L596 G597 K598 K599 A600 I601 S602 K603 M604 L605 N606 Y609 R610 L614 K615 P616 T617 V618 I619 F620 A621 D622 Q623 I624 M625 Y626 T627 G628 F629 A632 A633 R634 S638 V639 G640 I641 D642 D643 M644 V645 I646 P647 H651
E652 I653 I654 S655 E656 A657 E658 A659 E660 V661 A662 E663 I664 Q665 E666 Q667 F668 Q669 S670 G671 L672 V673 T674 A675 G676 E677 R678 Y679 N680 I685 W686 A689 N690 V693 S694 K695 A696 M697 N700 L701 Q702 T703 E704 T705 V706 I707 N708 R709 D710 G711 Q712 E713 E714 K715 N720
S721 I722 Y723 M724 M725 A726 G729 A730 R731 A734 A735 Q736 I737 R738 A741 G742 M743 R744 G745 L746 M747 A748 K749 P750 D751 G752 S753 I754 I755 E756 T757 P758 I759 T760 A761 N762 F763 R764 E765 N768 V769 L770 Q771 Y772 F773 I774 S775 T776 H777 R780 K781 G782 L783 A784 D785
T786 A787 L788 K789 T790 A791 N792 S793 G794 Y795 L796 T797 R798 R799 L800 V801 D802 V803 A804 Q805 D806 T810 D813 E818 M821 M822 T823 P824 V825 I826 E827 G828 G829 D830 V831 K832 E833 P834 L835 R836 D837 R838 V839 L840 G841 R842 V843 E846 D847 V848 L849 K850 P851 G852 T853
A854 V858 P859 R860 L863 L864 H865 E866 Q867 W868 C869 D870 L871 L872 E873 S876 V877 D878 A879 R883 S884 V885 V886 S887 C888 D889 F892 G893 V894 C895 A896 H897 C898 Y899 G900 R901 D902 L903 A904 R905 G906 H907 I908 I909 N910 K911 G912 E913 A914 I915 G916 V917 I918 A919 A920
Q921 S922 I923 G924 E925 P926 G927 T928 Q929 L930 T931 MET ARG THR PHE HIS ILE GLY GLY ALA ALA SER ARG ALA A945 A946 E947 S948 S949 I950 Q951 V952 K953 N954 K955 G956 S957 I958 K959 L960 S961 N962 V963 K964 S965 V966 V967 N968 S969 S970 G971 K972 L973 Y974 I975 T976 S977 R978 N979 T980
E981 L982 K983 L984 I985 F988 G989 R990 T991 K992 E993 S994 Y995 K996 V997 P998 Y999 G1000 A1001 V1002 L1003 A1004 K1005 G1006 D1007 G1008 E1009 Q1010 V1011 A1012 G1013 G1014 E1015 T1016 V1017 A1018 N1019 W1020 D1021 P1022 H1023 T1024 M1025 P1026 V1027 E1030 V1031 S1032 G1033 F1034 V1035 R1036 F1037 T1038 D1039 M1040 I1041 D1042



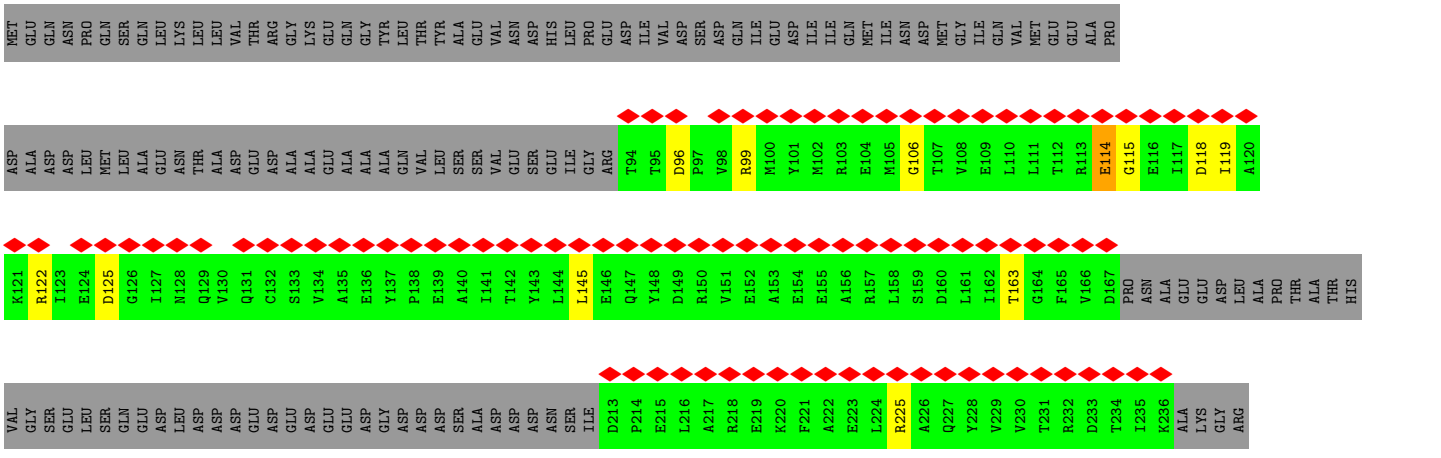
• Molecule 4: DNA-directed RNA polymerase subunit omega

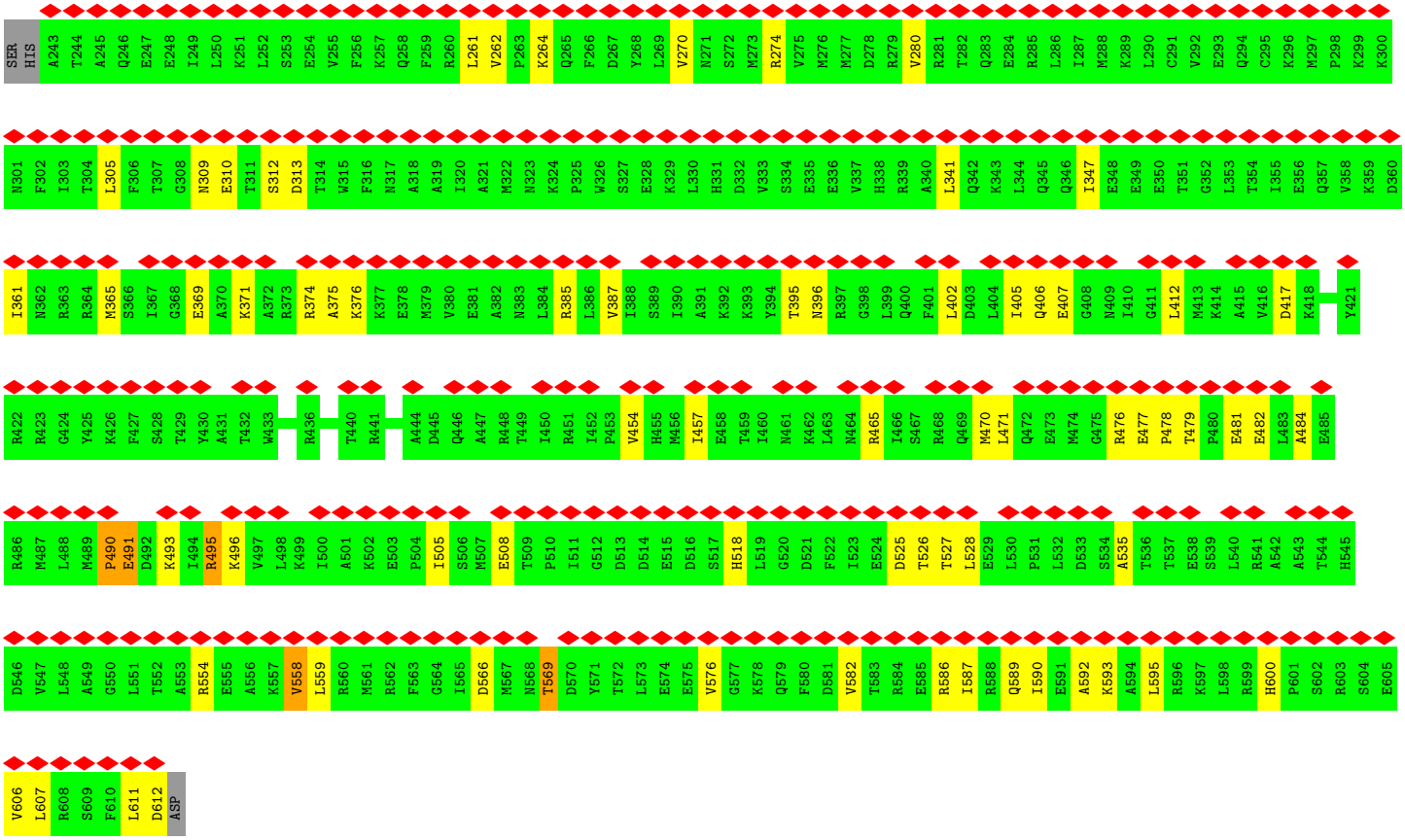
Chain E:



• Molecule 5: RNA polymerase sigma factor RpoD

Chain F:




SER HIS A243 T244 A245 Q246 E247 E248 I249 L250 K251 L252 S253 E254 V255 F256 K257 Q258 F259 R260 L261 V262 P263 K264 Q265 F266 D267 Y268 L269 V270 N271 S272 M273 R274 V275 M276 M277 D278 R279 V280 R281 T282 Q283 E284 R285 L286 I287 M288 K289 L290 C291 V292 E293 Q294 C295 K296 M297 P298 K299 K300
N301 F302 I303 T304 L305 F306 T307 G308 N309 E310 T311 S312 D313 T314 W315 F316 N317 A318 A319 I320 A321 M322 N323 K324 P325 W326 S327 E328 K329 L330 H331 D332 V333 S334 E335 E336 V337 H338 R339 A340 L341 Q342 K343 L344 Q345 Q346 I347 E348 E349 E350 T351 G352 L353 T354 I355 E356 Q357 V358 K359 D360
I361 N362 R363 R364 M365 S366 I367 G368 E369 A370 K371 A372 R373 R374 A375 K376 K377 E378 M379 V380 E381 A382 N383 L384 R385 L386 V387 I388 S389 I390 A391 K392 K393 Y394 T395 N396 R397 G398 L399 Q400 F401 L402 D403 L404 I405 Q406 E407 G408 N409 I410 G411 L412 M413 K414 A415 V416 D417 K418 Y421
R422 R423 G424 Y425 K426 F427 S428 T429 Y430 A431 T432 W433 R436 T440 R441 A444 D445 Q446 A447 R448 T449 I450 R451 I452 P453 V454 H455 M456 I457 E458 T459 I460 N461 K462 L463 N464 R465 I466 S467 R468 Q469 M470 L471 Q472 E473 M474 G475 R476 E477 P478 T479 P480 E481 E482 L483 A484 E485
R486 M487 L488 M489 P490 E491 D492 K493 I494 R495 K496 V497 L498 K499 I500 A501 K502 E503 P504 I505 S506 M507 E508 T509 P510 I511 G512 D513 D514 E515 D516 S517 H518 L519 G520 D521 F522 I523 E524 D525 T526 T527 L528 E529 L530 P531 L532 D533 S534 A535 T536 T537 E538 S539 L540 R541 A542 A543 T544 H545
D546 V547 L548 A549 G550 L551 T552 A553 R554 E555 A556 K557 V558 L559 R560 M561 R562 F563 G564 I565 D566 M567 N568 T569 D570 Y571 T572 L573 E574 E575 V576 G577 K578 Q579 F580 D581 V582 T583 R584 E585 R586 I587 R588 Q589 I590 E591 A592 K593 A594 L595 R596 K597 L598 R599 H600 P601 S602 R603 S604 E605
V606 L607 R608 S609 F610 L611 D612 ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96067	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 ($e^-/Å^2$)	45	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	0.159	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	315.84, 315.84, 315.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.316, 1.316, 1.316	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	0/1809	0.82	3/2451 (0.1%)
1	B	0.40	0/1728	0.80	4/2341 (0.2%)
2	C	0.41	1/10739 (0.0%)	0.75	14/14489 (0.1%)
3	D	0.39	0/10591	0.75	11/14307 (0.1%)
4	E	0.34	0/607	0.66	0/817
5	F	0.34	0/3864	0.76	3/5194 (0.1%)
All	All	0.39	1/29338 (0.0%)	0.76	35/39599 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	4
3	D	0	2
5	F	0	3
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	550	VAL	C-N	-5.44	1.21	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	70	TYR	CB-CG-CD1	-9.71	115.17	121.00
2	C	70	TYR	CB-CG-CD2	8.85	126.31	121.00
2	C	1021	LEU	CA-CB-CG	7.09	131.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	91	ARG	CG-CD-NE	-6.80	97.52	111.80
3	D	1221	LEU	CA-CB-CG	6.78	130.89	115.30
2	C	145	ILE	CG1-CB-CG2	-6.78	96.49	111.40
2	C	168	GLY	N-CA-C	-6.72	96.31	113.10
3	D	1343	GLU	C-N-CA	6.66	138.34	121.70
1	A	28	LEU	CA-CB-CG	6.64	130.57	115.30
3	D	709	ARG	NE-CZ-NH1	-6.20	117.20	120.30
3	D	426	ALA	CB-CA-C	5.92	118.98	110.10
2	C	1160	ASP	CB-CA-C	5.88	122.17	110.40
1	B	150	ARG	C-N-CA	-5.84	110.03	122.30
2	C	81	ASP	CB-CG-OD1	5.63	123.36	118.30
3	D	1155	ILE	CG1-CB-CG2	-5.52	99.25	111.40
3	D	77	ARG	CA-CB-CG	5.52	125.55	113.40
1	A	13	LEU	CA-CB-CG	5.48	127.90	115.30
2	C	866	ASP	CB-CG-OD1	5.42	123.18	118.30
3	D	500	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	B	102	LEU	CA-CB-CG	5.42	127.76	115.30
5	F	471	LEU	CA-CB-CG	5.39	127.71	115.30
3	D	46	TYR	CA-CB-CG	5.38	123.61	113.40
3	D	217	LEU	CA-CB-CG	5.37	127.65	115.30
5	F	586	ARG	NE-CZ-NH1	-5.30	117.65	120.30
3	D	701	LEU	CA-CB-CG	5.29	127.46	115.30
2	C	1158	LYS	CA-CB-CG	5.26	124.97	113.40
5	F	341	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	14	VAL	CA-CB-CG2	5.17	118.66	110.90
2	C	1160	ASP	C-N-CA	5.15	134.58	121.70
2	C	1233	LEU	CA-CB-CG	5.14	127.13	115.30
2	C	233	ARG	C-N-CA	5.12	134.49	121.70
2	C	696	ASP	C-N-CA	5.08	134.39	121.70
3	D	425	ARG	C-N-CA	5.07	134.38	121.70
1	B	48	LEU	CA-CB-CG	5.04	126.88	115.30
2	C	398	SER	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	198	ILE	Peptide
2	C	236	LYS	Peptide
2	C	397	LEU	Peptide
3	D	1184	ASP	Peptide

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Mol	Chain	Res	Type	Group
3	D	901	ARG	Peptide
5	F	569	THR	Peptide
5	F	582	VAL	Peptide
5	F	600	HIS	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	1787	0	1810	32	0
1	B	1708	0	1741	28	0
2	C	10570	0	10581	115	0
3	D	10434	0	10599	174	0
4	E	605	0	612	6	0
5	F	3813	0	3880	49	0
6	D	1	0	0	0	0
7	D	2	0	0	0	0
All	All	28920	0	29223	373	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 6.

All (373) 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:1140:ARG:HH12	3:D:1144:LEU:HG	1.32	0.94
1:A:233:ASP:HA	1:B:218:ARG:HH12	1.40	0.87
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.06	0.87
2:C:299:LYS:NZ	2:C:300:ASP:O	2.11	0.81
2:C:719:LYS:HZ3	2:C:751:TYR:HE1	1.28	0.80
1:A:33:ARG:NH2	1:A:197:ASP:OD2	2.13	0.79
3:D:518:VAL:HA	3:D:547:ARG:HH12	1.45	0.79
3:D:1263:LYS:NZ	3:D:1279:GLN:OE1	2.16	0.79
1:A:232:VAL:O	1:B:218:ARG:NH1	2.16	0.77
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.15	0.76
2:C:17:LYS:NZ	2:C:1194:GLU:OE2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:GLU:OE2	2:C:54:ARG:NE	2.20	0.74
3:D:1278:GLU:OE2	3:D:1279:GLN:NE2	2.21	0.73
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.22	0.72
3:D:77:ARG:HG3	3:D:79:LYS:HG2	1.72	0.71
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.25	0.70
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.74	0.69
5:F:493:LYS:NZ	5:F:496:LYS:NZ	2.41	0.69
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.26	0.68
1:B:211:ILE:HG12	1:B:219:ARG:HH22	1.59	0.68
1:A:49:SER:HB3	2:C:1083:GLU:OE2	1.95	0.67
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.77	0.66
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.76	0.66
2:C:378:ARG:NE	2:C:382:GLU:OE2	2.27	0.65
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.78	0.65
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.77	0.65
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.30	0.65
5:F:493:LYS:HZ3	5:F:496:LYS:HZ1	1.43	0.64
5:F:479:THR:HG22	5:F:482:GLU:HG3	1.80	0.64
5:F:587:ILE:HD12	5:F:590:ILE:HD12	1.79	0.64
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.80	0.64
1:A:63:GLY:O	1:A:71:LYS:NZ	2.29	0.63
3:D:615:LYS:HZ2	4:E:7:GLN:HB3	1.63	0.63
1:B:180:VAL:O	3:D:535:ARG:NH2	2.30	0.63
3:D:214:ARG:HA	3:D:217:LEU:HB3	1.80	0.63
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.31	0.62
3:D:31:ARG:HE	3:D:241:VAL:HG21	1.64	0.62
2:C:517:GLN:HG3	2:C:523:GLU:OE2	1.99	0.62
1:A:107:ILE:HD11	1:A:136:GLU:HG2	1.81	0.62
3:D:1073:ASP:HA	3:D:1168:GLU:HG2	1.80	0.62
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.81	0.62
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.82	0.61
2:C:272:ARG:HD3	2:C:273:HIS:HD2	1.65	0.61
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.34	0.61
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.33	0.61
5:F:493:LYS:NZ	5:F:496:LYS:HZ1	1.98	0.61
3:D:518:VAL:HA	3:D:547:ARG:NH1	2.15	0.61
3:D:741:ALA:O	3:D:762:ASN:ND2	2.32	0.61
2:C:374:GLU:OE1	5:F:99:ARG:NH1	2.34	0.60
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.81	0.60
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.83	0.60
4:E:36:ASP:N	4:E:36:ASP:OD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.34	0.60
3:D:1140:ARG:NH1	3:D:1144:LEU:HG	2.12	0.60
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.83	0.59
3:D:709:ARG:NH1	3:D:710:ASP:HB3	2.16	0.59
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.35	0.59
2:C:960:LEU:HD21	2:C:1032:LYS:NZ	2.18	0.59
3:D:708:ASN:OD1	3:D:708:ASN:N	2.35	0.59
3:D:532:GLU:HB2	3:D:535:ARG:NH1	2.18	0.59
3:D:1238:GLN:HG3	3:D:1242:ARG:HE	1.66	0.59
3:D:832:LYS:NZ	3:D:1242:ARG:NH1	2.51	0.59
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.84	0.59
3:D:1140:ARG:NH1	3:D:1140:ARG:O	2.36	0.59
2:C:93:SER:OG	2:C:126:GLU:OE1	2.13	0.58
5:F:479:THR:HG23	5:F:481:GLU:H	1.68	0.58
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.37	0.58
3:D:45:ASN:ND2	3:D:48:THR:OG1	2.36	0.58
1:A:64:VAL:HG13	1:A:71:LYS:HE2	1.85	0.58
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.36	0.58
3:D:435:GLN:HE21	3:D:486:SER:HA	1.69	0.58
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.68	0.58
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.37	0.57
5:F:115:GLY:HA2	5:F:118:ASP:HB2	1.86	0.57
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.85	0.57
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.18	0.57
3:D:832:LYS:HZ2	3:D:832:LYS:HB3	1.70	0.57
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.69	0.57
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.85	0.57
2:C:719:LYS:NZ	2:C:751:TYR:HE1	2.01	0.57
2:C:714:VAL:O	2:C:767:GLN:NE2	2.37	0.57
3:D:957:SER:HB3	3:D:985:ILE:HB	1.87	0.57
5:F:508:GLU:OE1	5:F:518:HIS:ND1	2.38	0.57
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.87	0.56
3:D:646:ILE:HD11	3:D:764:ARG:HD3	1.86	0.56
3:D:970:SER:HB2	3:D:972:LYS:HZ3	1.70	0.56
2:C:387:ASN:HA	2:C:391:SER:HB2	1.88	0.56
3:D:54:ASP:N	3:D:54:ASP:OD1	2.39	0.56
3:D:473:THR:HG23	3:D:476:ALA:H	1.70	0.56
3:D:538:ARG:NH1	3:D:634:ARG:NH1	2.54	0.56
3:D:437:PHE:HZ	3:D:453:VAL:HG11	1.71	0.56
1:A:233:ASP:HA	1:B:218:ARG:NH1	2.16	0.56
5:F:312:SER:OG	5:F:313:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.88	0.55
2:C:18:ARG:HE	2:C:620:ASN:HA	1.72	0.55
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.55
3:D:60:ARG:HA	3:D:90:VAL:HG22	1.90	0.55
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.71	0.55
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.21	0.54
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.89	0.54
3:D:1321:SER:HB2	3:D:1349:GLU:OE2	2.08	0.54
5:F:274:ARG:NH2	5:F:369:GLU:OE1	2.40	0.54
1:A:104:LYS:HD3	1:A:110:VAL:HG13	1.90	0.54
1:B:95:LYS:NZ	1:B:97:GLU:O	2.40	0.54
3:D:1061:VAL:O	3:D:1104:LYS:N	2.40	0.54
2:C:1142:ARG:HG2	2:C:1169:VAL:HG11	1.90	0.53
5:F:493:LYS:HZ2	5:F:496:LYS:NZ	2.05	0.53
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.11	0.53
3:D:1262:ARG:NH2	3:D:1312:ALA:O	2.42	0.53
3:D:388:ARG:NH2	3:D:414:GLU:OE1	2.42	0.53
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.91	0.53
2:C:1289:GLU:OE2	3:D:472:LEU:HB2	2.08	0.53
2:C:1269:ARG:HG3	3:D:346:ARG:NH1	2.24	0.53
3:D:1087:ASP:HB3	3:D:1096:PRO:HB3	1.91	0.53
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.91	0.53
3:D:1060:VAL:HG22	3:D:1106:ILE:HG12	1.90	0.53
3:D:615:LYS:NZ	4:E:7:GLN:HB3	2.23	0.53
3:D:1036:ARG:HD2	3:D:1079:LYS:HD3	1.90	0.53
5:F:612:ASP:OD1	5:F:612:ASP:N	2.39	0.53
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.24	0.52
3:D:1143:ASP:HA	3:D:1148:ARG:NH1	2.23	0.52
2:C:903:ARG:NH2	5:F:612:ASP:OD1	2.43	0.52
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.41	0.52
3:D:694:SER:OG	3:D:738:ARG:NE	2.43	0.52
3:D:1046:ILE:HD12	3:D:1059:LEU:HD22	1.92	0.52
5:F:262:VAL:HG11	5:F:264:LYS:HZ2	1.74	0.52
3:D:930:LEU:HD11	3:D:1241:TYR:HE1	1.75	0.52
5:F:376:LYS:NZ	5:F:417:ASP:HA	2.24	0.52
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.75	0.52
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.43	0.51
3:D:1340:LYS:HB2	3:D:1340:LYS:NZ	2.25	0.51
1:B:62:ASP:OD1	1:B:62:ASP:N	2.34	0.51
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.75	0.51
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:576:ARG:NH1	3:D:593:ASN:O	2.43	0.51
3:D:709:ARG:O	3:D:711:GLY:N	2.43	0.51
3:D:1109:LEU:HD22	3:D:1113:VAL:HG11	1.93	0.51
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.43	0.51
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.76	0.51
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.92	0.51
2:C:739:ASP:OD1	2:C:739:ASP:N	2.43	0.51
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.93	0.51
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.92	0.51
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.76	0.51
2:C:148:GLN:NE2	2:C:535:PRO:O	2.38	0.50
3:D:69:GLU:HG3	3:D:76:LYS:HG2	1.93	0.50
3:D:909:ILE:HD11	3:D:913:GLU:HG2	1.92	0.50
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.93	0.50
2:C:905:ILE:HG23	5:F:595:LEU:HD13	1.93	0.50
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.93	0.50
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.94	0.50
1:B:125:LYS:NZ	1:B:125:LYS:HB3	2.26	0.50
3:D:1002:VAL:N	3:D:1019:ASN:O	2.42	0.50
1:A:58:GLU:HG2	1:A:145:LYS:HE3	1.94	0.49
3:D:1051:ASP:HB2	3:D:1056:LEU:HB2	1.93	0.49
3:D:1034:PHE:N	3:D:1081:VAL:O	2.44	0.49
1:A:59:VAL:HG13	1:A:144:ILE:HG12	1.94	0.49
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.93	0.49
2:C:1240:ASP:N	2:C:1240:ASP:OD1	2.45	0.49
1:A:167:PRO:HB2	1:A:170:ARG:HG2	1.95	0.49
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.94	0.49
1:B:44:ARG:HG3	1:B:183:ILE:HD13	1.94	0.49
3:D:48:THR:O	3:D:50:LYS:N	2.43	0.49
2:C:1269:ARG:HB3	3:D:343:LEU:HD22	1.95	0.49
5:F:554:ARG:HH21	5:F:587:ILE:HD13	1.76	0.49
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.94	0.49
3:D:1329:THR:O	3:D:1333:THR:OG1	2.27	0.48
2:C:272:ARG:HD3	2:C:273:HIS:CD2	2.47	0.48
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.95	0.48
3:D:1059:LEU:HG	3:D:1110:GLU:OE2	2.14	0.48
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.96	0.48
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.95	0.48
3:D:1186:TYR:OH	3:D:1188:GLU:OE1	2.23	0.48
3:D:549:LYS:NZ	3:D:569:LEU:O	2.46	0.48
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:352:ARG:NH1	3:D:465:GLN:OE1	2.47	0.48
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.95	0.47
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.96	0.47
1:A:16:ILE:HG12	1:A:26:VAL:HG12	1.96	0.47
3:D:1064:SER:O	3:D:1072:LYS:NZ	2.47	0.47
5:F:122:ARG:HA	5:F:125:ASP:HB2	1.97	0.47
1:B:16:ILE:HB	1:B:26:VAL:HG13	1.96	0.47
2:C:201:ARG:HG3	2:C:201:ARG:HH11	1.79	0.47
2:C:201:ARG:HH12	2:C:370:MET:HA	1.78	0.47
1:B:133:LEU:HD23	1:B:138:ALA:HB1	1.97	0.47
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.96	0.47
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.29	0.47
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.97	0.47
5:F:145:LEU:O	5:F:225:ARG:NH2	2.47	0.47
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.96	0.47
2:C:314:ASN:O	2:C:352:ARG:NH1	2.43	0.47
3:D:35:PHE:CD2	3:D:101:ARG:HD3	2.50	0.46
2:C:107:ARG:HA	2:C:108:GLU:HA	1.56	0.46
3:D:495:ASN:O	3:D:497:GLU:N	2.48	0.46
2:C:785:ASP:OD2	2:C:791:LEU:N	2.48	0.46
2:C:906:PHE:HE2	5:F:607:LEU:HB3	1.81	0.46
3:D:356:THR:OG1	3:D:357:VAL:N	2.48	0.46
3:D:832:LYS:HZ2	3:D:1242:ARG:NH1	2.13	0.46
1:B:158:ARG:NH1	1:B:172:LEU:HD13	2.30	0.46
3:D:1036:ARG:HH21	3:D:1081:VAL:HG21	1.80	0.46
2:C:145:ILE:HG21	2:C:456:VAL:HG13	1.98	0.46
5:F:493:LYS:NZ	5:F:496:LYS:HZ2	2.12	0.46
2:C:488:MET:O	2:C:490:GLN:N	2.46	0.46
3:D:370:LYS:HD3	3:D:443:GLU:OE2	2.16	0.46
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.51	0.46
3:D:1203:ARG:NH1	3:D:1205:GLU:OE2	2.45	0.46
3:D:342:LEU:HA	3:D:343:LEU:HA	1.76	0.46
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.76	0.46
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.48	0.46
5:F:262:VAL:HG11	5:F:264:LYS:NZ	2.31	0.45
1:B:60:GLU:HB3	1:B:170:ARG:HG2	1.99	0.45
1:B:155:ALA:N	1:B:174:ASP:OD1	2.50	0.45
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	1.99	0.45
3:D:1161:GLY:HA3	3:D:1179:PRO:HA	1.98	0.45
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.77	0.45
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.87	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:962:ASN:O	3:D:980:THR:OG1	2.34	0.45
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.51	0.45
5:F:280:VAL:HG22	5:F:347:ILE:HG21	1.99	0.45
1:B:215:GLU:CD	1:B:219:ARG:HH12	2.19	0.45
3:D:53:ARG:HA	3:D:54:ASP:HA	1.58	0.45
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.19	0.45
3:D:609:TYR:HE1	3:D:614:LEU:HD12	1.82	0.45
3:D:947:GLU:O	3:D:1020:TRP:NE1	2.49	0.45
3:D:977:SER:OG	3:D:980:THR:OG1	2.34	0.45
2:C:990:ASP:OD1	2:C:990:ASP:N	2.49	0.45
2:C:1132:LEU:HD11	2:C:1174:GLU:OE2	2.17	0.45
1:A:43:LEU:HD13	1:A:217:ILE:HD11	1.99	0.45
1:A:45:ARG:HG2	1:B:38:THR:HB	1.98	0.45
2:C:568:ASN:OD1	2:C:568:ASN:N	2.50	0.45
3:D:953:LYS:HB2	3:D:993:GLU:OE2	2.16	0.45
1:B:215:GLU:OE2	1:B:219:ARG:NH1	2.50	0.45
2:C:549:ASP:OD1	2:C:550:VAL:N	2.49	0.45
3:D:638:SER:OG	3:D:639:VAL:N	2.47	0.45
5:F:558:VAL:HA	5:F:576:VAL:HG11	1.98	0.45
1:A:9:LEU:HB2	1:A:32:GLU:HG2	1.98	0.44
2:C:1024:GLU:HG2	2:C:1028:LYS:HD3	1.98	0.44
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.98	0.44
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.99	0.44
3:D:1023:HIS:ND1	3:D:1126:GLN:O	2.32	0.44
1:A:14:VAL:HG22	1:A:15:ASP:H	1.82	0.44
2:C:1247:SER:OG	2:C:1248:THR:N	2.50	0.44
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.48	0.44
5:F:525:ASP:OD2	5:F:528:LEU:HG	2.16	0.44
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.35	0.44
2:C:560:PRO:O	3:D:780:ARG:NH2	2.45	0.44
2:C:623:LEU:HD12	2:C:627:GLY:HA2	1.99	0.44
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.80	0.44
3:D:1075:ARG:HD2	3:D:1076:PRO:HD2	2.00	0.44
5:F:395:THR:OG1	5:F:396:ASN:N	2.51	0.44
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.99	0.44
5:F:470:MET:HB2	5:F:478:PRO:HG3	2.00	0.44
5:F:592:ALA:O	5:F:595:LEU:HB2	2.17	0.44
2:C:1130:ALA:O	2:C:1134:GLN:NE2	2.51	0.44
2:C:1319:MET:HA	2:C:1320:PRO:HD3	1.92	0.44
2:C:678:ARG:HA	2:C:678:ARG:HD3	1.79	0.44
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:975:ILE:HD11	2:C:1014:LEU:HB3	2.00	0.44
3:D:19:ALA:HA	3:D:1343:GLU:HA	2.00	0.44
3:D:88:CYS:O	3:D:90:VAL:N	2.51	0.44
3:D:275:ARG:NH1	3:D:298:MET:HB3	2.33	0.44
3:D:885:VAL:HG12	3:D:894:VAL:HG11	2.00	0.44
2:C:55:SER:OG	2:C:56:VAL:N	2.51	0.44
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	2.00	0.44
2:C:503:LYS:HD3	2:C:503:LYS:HA	1.84	0.43
2:C:1164:PHE:HB2	2:C:1168:GLU:HG3	2.01	0.43
3:D:70:CYS:SG	3:D:71:LEU:N	2.90	0.43
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.98	0.43
3:D:1269:ALA:HB2	3:D:1274:PHE:HD1	1.84	0.43
3:D:18:ASP:N	3:D:18:ASP:OD1	2.47	0.43
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.84	0.43
3:D:832:LYS:HD3	3:D:1242:ARG:HH12	1.84	0.43
3:D:848:VAL:HG12	3:D:858:VAL:HG22	2.00	0.43
3:D:1108:GLN:OE1	3:D:1123:ARG:NH1	2.51	0.43
5:F:270:VAL:HG13	5:F:365:MET:HE3	1.99	0.43
1:B:181:GLU:HA	3:D:535:ARG:HH22	1.83	0.43
2:C:357:ASN:OD1	2:C:357:ASN:N	2.49	0.43
3:D:959:LYS:NZ	3:D:985:ILE:HG13	2.34	0.43
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.86	0.43
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.55	0.43
2:C:1339:LEU:HA	3:D:20:ILE:HG12	2.00	0.43
3:D:516:ASP:HB3	3:D:573:THR:HG21	2.00	0.43
3:D:667:GLN:HG2	3:D:672:LEU:HD22	2.00	0.43
5:F:114:GLU:H	5:F:114:GLU:HG3	1.57	0.43
1:B:67:GLU:OE1	1:B:67:GLU:N	2.49	0.43
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.81	0.43
2:C:908:GLU:OE2	5:F:611:LEU:HB3	2.18	0.43
3:D:1163:VAL:HG23	3:D:1177:ILE:HG22	2.01	0.43
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.01	0.43
1:A:12:ARG:NH1	1:A:13:LEU:O	2.51	0.43
3:D:27:PRO:O	3:D:31:ARG:HG3	2.19	0.43
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.16	0.43
3:D:1344:LEU:O	3:D:1346:GLY:N	2.44	0.43
3:D:118:LYS:HB3	3:D:118:LYS:HE2	1.92	0.43
1:A:71:LYS:HD3	1:A:71:LYS:HA	1.90	0.42
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	2.01	0.42
2:C:696:ASP:HB3	2:C:697:LYS:H	1.54	0.42
1:B:196:THR:HG23	3:D:443:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:802:VAL:HG11	2:C:1230:MET:HB3	2.00	0.42
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.00	0.42
3:D:1273:ASP:HB2	3:D:1276:GLU:HB2	2.01	0.42
2:C:24:VAL:HG22	2:C:578:TYR:HE1	1.83	0.42
3:D:222:LYS:HA	3:D:222:LYS:HD2	1.85	0.42
3:D:511:TYR:HE2	3:D:724:MET:HG2	1.85	0.42
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.88	0.42
3:D:429:LEU:HD13	3:D:429:LEU:HA	1.92	0.42
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.44	0.42
3:D:1021:ASP:HB3	3:D:1024:THR:HB	2.00	0.42
3:D:1157:ALA:HB3	3:D:1206:ARG:HA	2.02	0.42
5:F:106:GLY:O	5:F:385:ARG:NH2	2.53	0.42
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.70	0.42
2:C:39:ILE:HD11	2:C:75:LEU:HG	2.01	0.42
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.00	0.42
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.40	0.42
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.80	0.42
2:C:570:GLY:O	2:C:573:ASN:ND2	2.45	0.42
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.35	0.42
5:F:387:VAL:HG21	5:F:412:LEU:HD22	2.01	0.42
5:F:476:ARG:HB3	5:F:477:GLU:H	1.62	0.42
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.89	0.41
1:B:112:ALA:HB3	1:B:126:PRO:HA	2.02	0.41
2:C:1137:GLU:HG3	2:C:1139:ALA:H	1.84	0.41
1:A:165:GLU:OE2	1:A:172:LEU:HD11	2.20	0.41
3:D:863:LEU:HD11	3:D:901:ARG:HB3	2.02	0.41
3:D:1152:GLU:OE2	3:D:1194:ARG:HG2	2.21	0.41
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.41
1:A:90:VAL:HG21	1:A:146:VAL:HG21	2.02	0.41
2:C:1305:TYR:HE2	5:F:535:ALA:HB2	1.85	0.41
5:F:495:ARG:HD3	5:F:495:ARG:H	1.86	0.41
1:B:71:LYS:HA	1:B:71:LYS:HD3	1.84	0.41
2:C:117:ILE:H	2:C:117:ILE:HG12	1.64	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.03	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.88	0.41
2:C:549:ASP:OD2	3:D:750:PRO:HB3	2.20	0.41
2:C:594:VAL:HG11	2:C:650:VAL:HG23	2.03	0.41
3:D:538:ARG:HA	3:D:538:ARG:HD2	1.93	0.41
2:C:135:THR:HG21	2:C:142:GLU:OE2	2.20	0.41
3:D:1115:ILE:HB	3:D:1119:ASP:HB2	2.02	0.41
5:F:309:ASN:HB3	5:F:310:GLU:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1025:MET:HB3	3:D:1124:ILE:HB	2.03	0.41
3:D:1174:ARG:NH2	3:D:1187:GLU:OE2	2.54	0.41
3:D:148:GLU:H	3:D:156:ARG:HG3	1.84	0.41
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.85	0.41
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.36	0.41
2:C:799:ASN:OD1	2:C:799:ASN:N	2.54	0.41
3:D:139:LEU:HD23	3:D:139:LEU:HA	1.84	0.41
1:B:26:VAL:O	1:B:203:ILE:N	2.47	0.41
1:B:118:ASP:HB2	1:B:121:VAL:HB	2.03	0.41
3:D:813:ASP:HB2	3:D:897:HIS:CE1	2.56	0.41
1:A:96:ASP:OD1	1:A:148:ARG:NH1	2.54	0.40
2:C:17:LYS:N	2:C:1188:ASP:OD2	2.54	0.40
3:D:161:THR:HG22	3:D:164:GLN:HB2	2.03	0.40
3:D:242:LEU:HA	3:D:243:PRO:HD3	1.90	0.40
3:D:278:ARG:HD3	5:F:407:GLU:OE2	2.20	0.40
3:D:587:LEU:HD23	3:D:591:ILE:HG21	2.02	0.40
3:D:1052:GLU:HG2	3:D:1053:LEU:H	1.86	0.40
4:E:63:ILE:HD13	4:E:63:ILE:HA	1.92	0.40
2:C:804:PHE:HE2	2:C:1115:THR:HG21	1.85	0.40
3:D:832:LYS:HZ2	3:D:1242:ARG:HH11	1.69	0.40
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	2.02	0.40
5:F:589:GLN:O	5:F:593:LYS:N	2.49	0.40
1:A:171:LEU:HD13	1:A:171:LEU:HA	1.91	0.40
2:C:123:TYR:OH	2:C:126:GLU:HG3	2.21	0.40
2:C:227:LYS:HZ3	2:C:298:ALA:HB1	1.84	0.40
3:D:371:LYS:HA	3:D:371:LYS:HD2	1.95	0.40
3:D:1036:ARG:HB3	3:D:1079:LYS:HB3	2.03	0.40
2:C:228:VAL:HG23	2:C:337:PHE:HB2	2.03	0.40
2:C:1255:THR:O	2:C:1257:GLN:N	2.55	0.40
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.03	0.40
5:F:505:ILE:HD12	5:F:505:ILE:HA	1.95	0.40
2:C:727:VAL:HG23	2:C:773:LEU:HD23	2.03	0.40
2:C:1236:ASN:HA	2:C:1238:LEU:HD12	2.04	0.40
3:D:1282:TYR:HD1	3:D:1282:TYR:HA	1.77	0.40

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	228/329 (69%)	204 (90%)	24 (10%)	0	100	100
1	B	217/329 (66%)	196 (90%)	18 (8%)	3 (1%)	11	47
2	C	1338/1342 (100%)	1209 (90%)	109 (8%)	20 (2%)	10	46
3	D	1344/1407 (96%)	1212 (90%)	105 (8%)	27 (2%)	7	40
4	E	74/91 (81%)	70 (95%)	3 (4%)	1 (1%)	11	47
5	F	462/613 (75%)	430 (93%)	27 (6%)	5 (1%)	14	52
All	All	3663/4111 (89%)	3321 (91%)	286 (8%)	56 (2%)	14	46

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	SER
1	B	193	GLU
2	C	398	SER
2	C	484	LEU
2	C	697	LYS
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	805	GLN
3	D	826	ILE
3	D	831	VAL
3	D	860	ARG
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO

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Mol	Chain	Res	Type
5	F	566	ASP
2	C	121	GLU
2	C	596	ASP
2	C	746	ALA
2	C	1137	GLU
2	C	1154	ASP
2	C	1165	SER
3	D	89	GLY
3	D	1167	LYS
5	F	569	THR
1	B	13	LEU
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	19	ALA
2	C	163	LYS
2	C	199	ASP
2	C	235	ASN
2	C	813	GLU
3	D	173	GLY
3	D	314	ARG
3	D	417	ARG
3	D	585	LYS
2	C	625	GLU
3	D	230	SER
3	D	1274	PHE
3	D	1345	ARG
2	C	169	LYS
2	C	983	GLY
2	C	1223	ARG
3	D	152	THR
3	D	1297	LYS
3	D	357	VAL
5	F	96	ASP
5	F	361	ILE
3	D	828	GLY

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	198/286 (69%)	195 (98%)	3 (2%)	65 80
1	B	189/286 (66%)	182 (96%)	7 (4%)	34 59
2	C	1155/1157 (100%)	1104 (96%)	51 (4%)	28 54
3	D	1115/1168 (96%)	1067 (96%)	48 (4%)	29 55
4	E	65/75 (87%)	61 (94%)	4 (6%)	18 46
5	F	417/540 (77%)	406 (97%)	11 (3%)	46 67
All	All	3139/3512 (89%)	3015 (96%)	124 (4%)	35 57

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	13	LEU
1	A	124	VAL
1	B	9	LEU
1	B	62	ASP
1	B	64	VAL
1	B	71	LYS
1	B	124	VAL
1	B	183	ILE
1	B	191	ARG
2	C	103	VAL
2	C	117	ILE
2	C	131	THR
2	C	135	THR
2	C	145	ILE
2	C	164	THR
2	C	235	ASN
2	C	272	ARG
2	C	306	THR
2	C	321	LEU
2	C	377	THR
2	C	452	ARG
2	C	470	ARG
2	C	471	VAL
2	C	539	THR
2	C	553	THR
2	C	558	VAL

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Mol	Chain	Res	Type
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	714	VAL
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	791	LEU
2	C	878	THR
2	C	895	LEU
2	C	922	ASN
2	C	992	LEU
2	C	1032	LYS
2	C	1090	ASN
2	C	1134	GLN
2	C	1141	LEU
2	C	1151	LEU
2	C	1155	VAL
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1198	LEU
2	C	1210	ILE
2	C	1233	LEU
2	C	1234	LYS
2	C	1240	ASP
2	C	1254	VAL
2	C	1265	PHE
2	C	1287	LEU
2	C	1296	ASP
2	C	1299	ASN
2	C	1324	ASN
2	C	1327	LEU
3	D	12	THR
3	D	54	ASP
3	D	81	ARG
3	D	175	GLU
3	D	252	LEU
3	D	269	TYR
3	D	292	VAL
3	D	320	ASN

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Mol	Chain	Res	Type
3	D	324	LEU
3	D	343	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	431	ARG
3	D	505	ASP
3	D	514	THR
3	D	515	ARG
3	D	536	LEU
3	D	545	HIS
3	D	569	LEU
3	D	573	THR
3	D	639	VAL
3	D	678	ARG
3	D	680	ASN
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	744	ARG
3	D	753	SER
3	D	754	ILE
3	D	801	VAL
3	D	810	THR
3	D	853	THR
3	D	903	LEU
3	D	1019	ASN
3	D	1048	ARG
3	D	1135	THR
3	D	1155	ILE
3	D	1162	ILE
3	D	1221	LEU
3	D	1261	LEU
3	D	1289	ASN
3	D	1310	THR
3	D	1333	THR
3	D	1366	HIS
4	E	5	THR
4	E	36	ASP

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Mol	Chain	Res	Type
4	E	39	VAL
4	E	62	GLN
5	F	114	GLU
5	F	163	THR
5	F	261	LEU
5	F	305	LEU
5	F	465	ARG
5	F	491	GLU
5	F	495	ARG
5	F	526	THR
5	F	527	THR
5	F	558	VAL
5	F	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	147	GLN
1	B	117	HIS
1	B	132	HIS
2	C	235	ASN
2	C	276	GLN
2	C	330	HIS
2	C	554	HIS
2	C	922	ASN
2	C	1090	ASN
2	C	1116	HIS
2	C	1134	GLN
2	C	1299	ASN
2	C	1324	ASN
3	D	45	ASN
3	D	294	ASN
3	D	320	ASN
3	D	430	HIS
3	D	435	GLN
3	D	680	ASN
3	D	1010	GLN
3	D	1019	ASN
3	D	1289	ASN
5	F	227	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

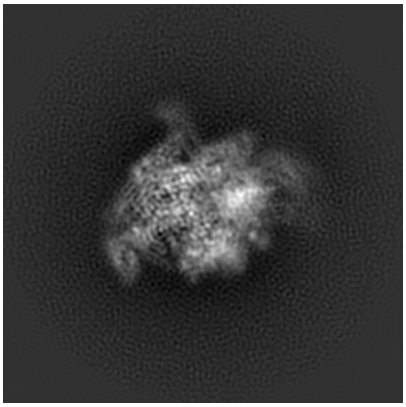
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7438. These allow visual inspection of the internal detail of the map and identification of artifacts.

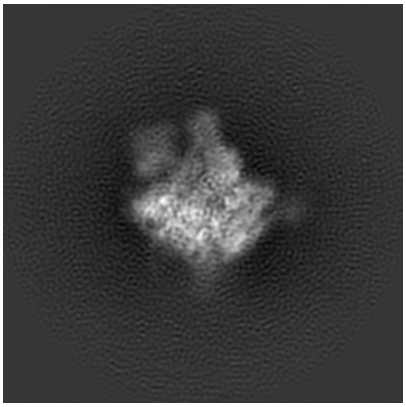
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

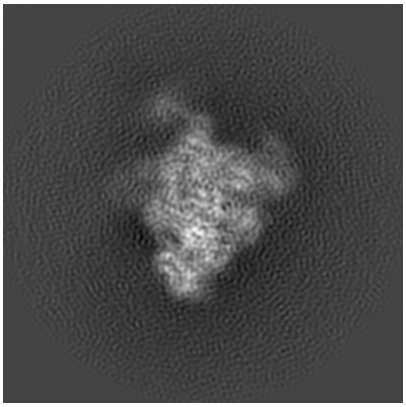
6.1.1 Primary map



X



Y

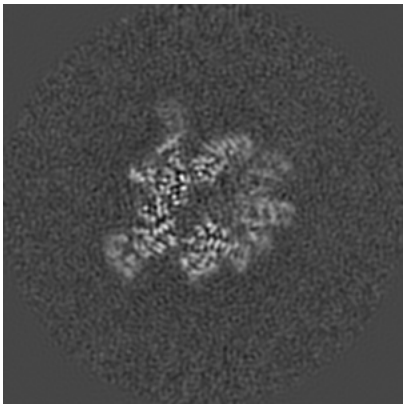


Z

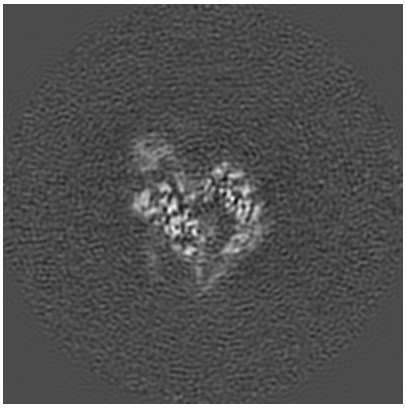
The images above show the map projected in three orthogonal directions.

6.2 Central slices

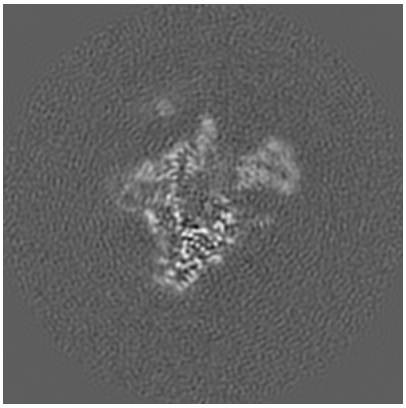
6.2.1 Primary map



X Index: 120



Y Index: 120

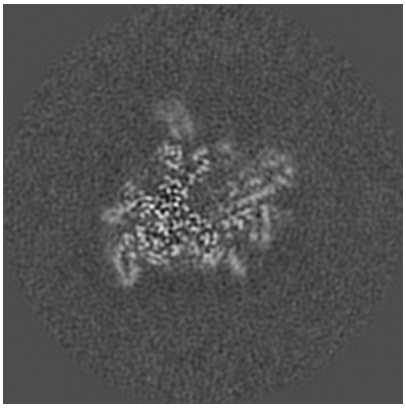


Z Index: 120

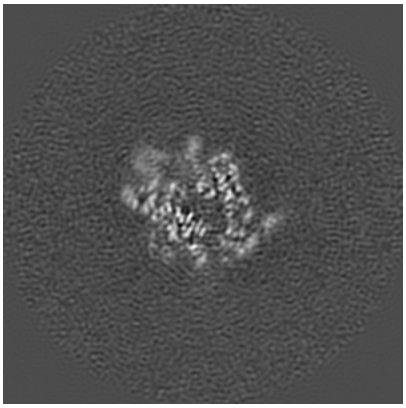
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

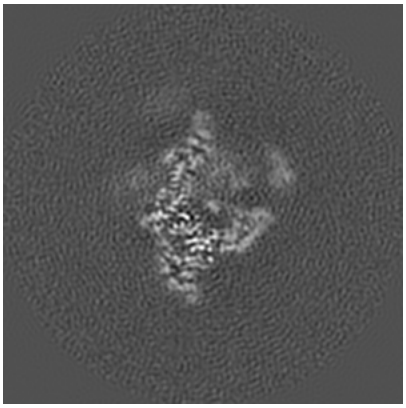
6.3.1 Primary map



X Index: 114



Y Index: 114

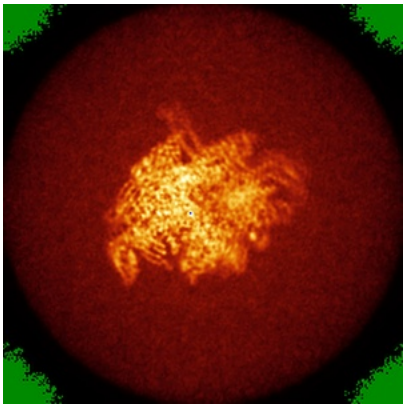


Z Index: 114

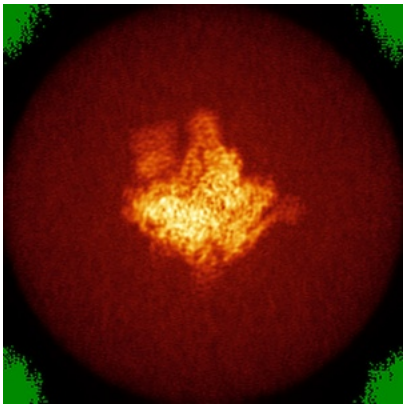
The images above show the largest variance slices of the map in three orthogonal directions.

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

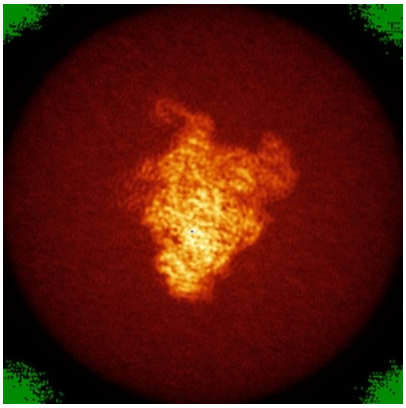
6.4.1 Primary map



X



Y

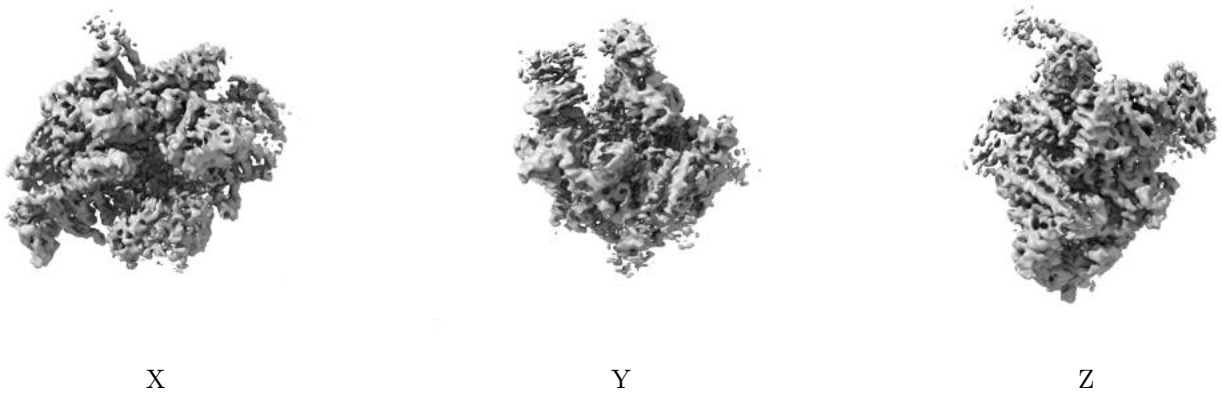


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

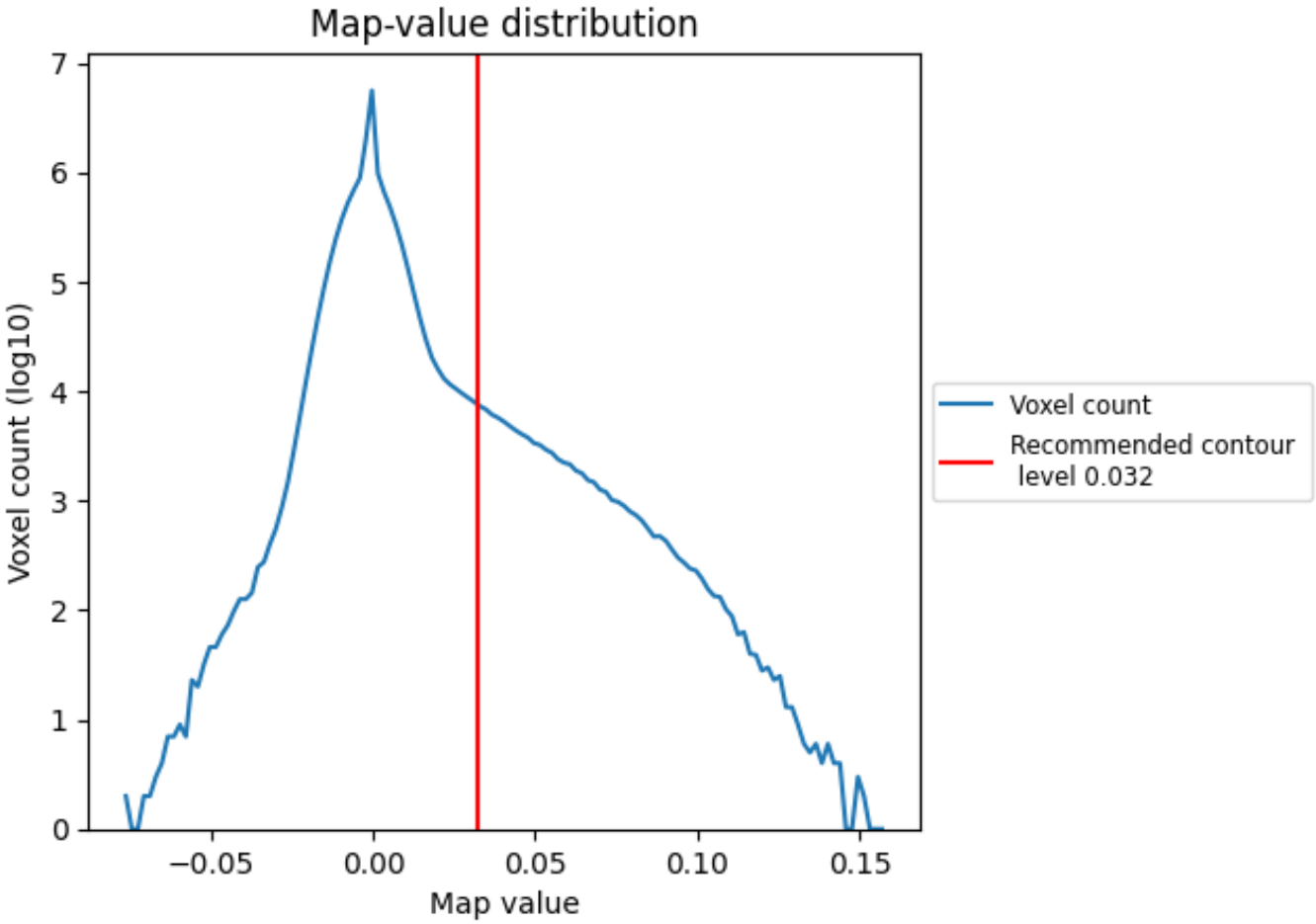
6.6 Mask visualisation (i)

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

7 Map analysis

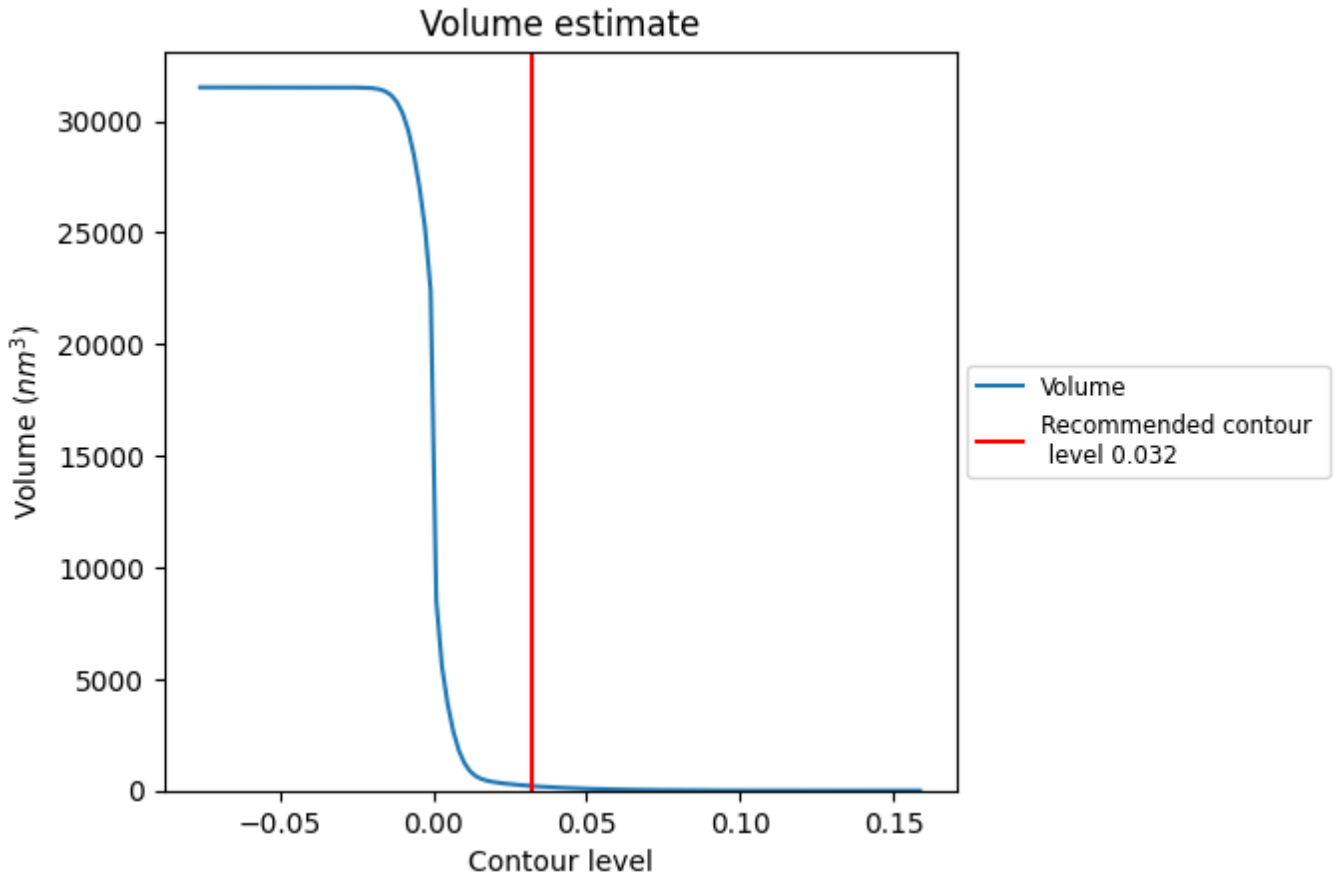
This section contains the results of statistical analysis of the map.

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.

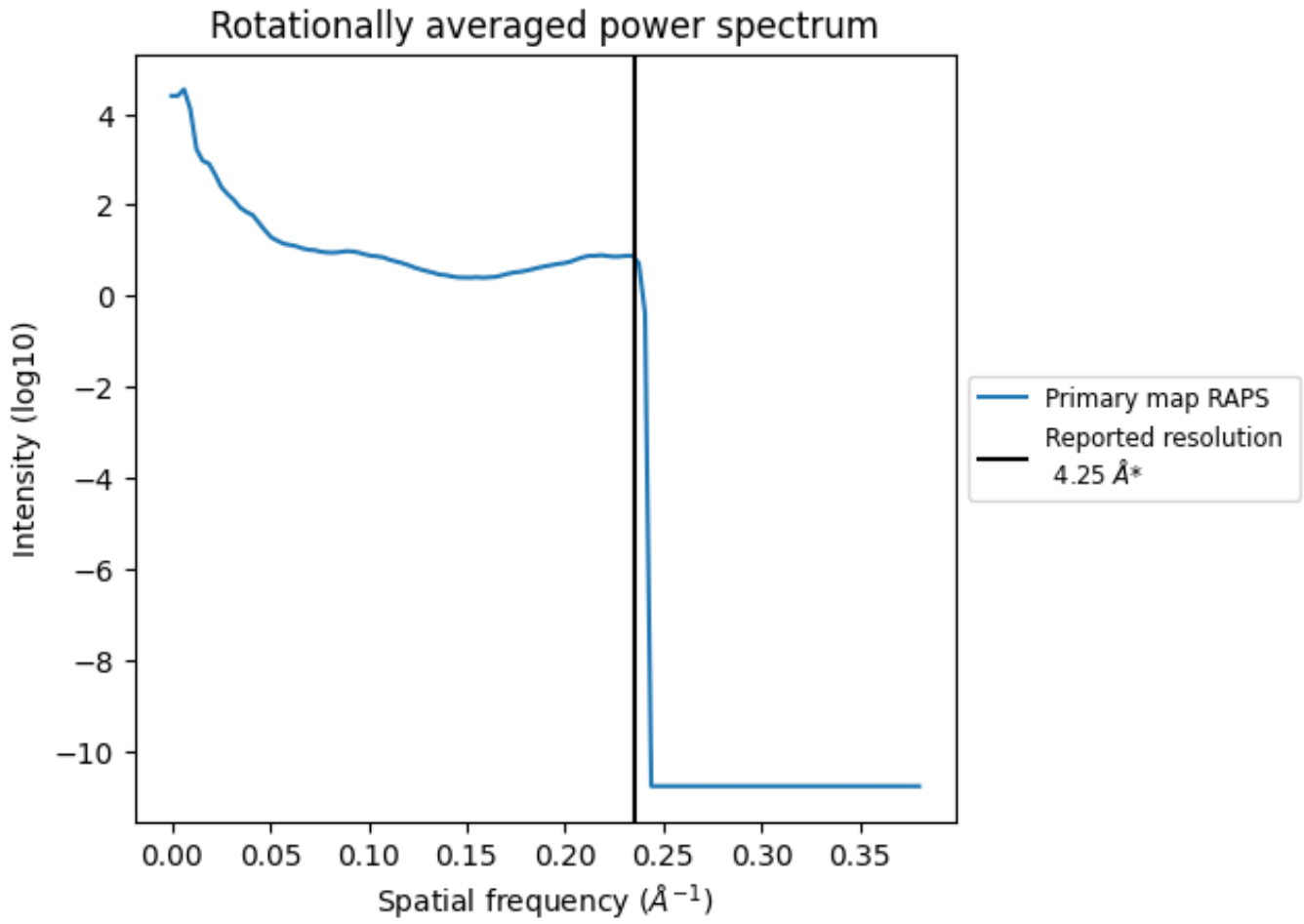
7.2 Volume estimate



The volume at the recommended contour level is 206 nm^3; this corresponds to an approximate mass of 186 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 0.235 Å^{-1}

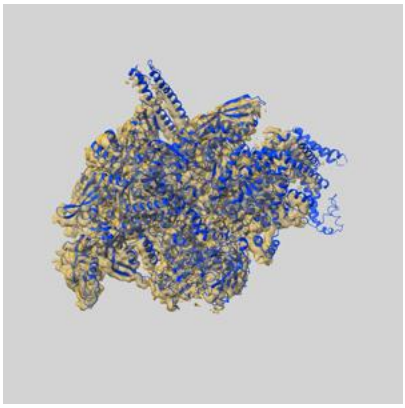
8 Fourier-Shell correlation (i)

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

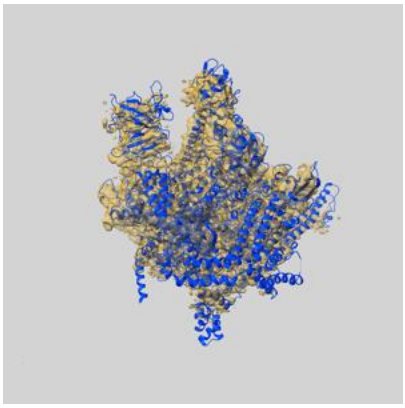
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7438 and PDB model 6C9Y. Per-residue inclusion information can be found in section 3 on page 5.

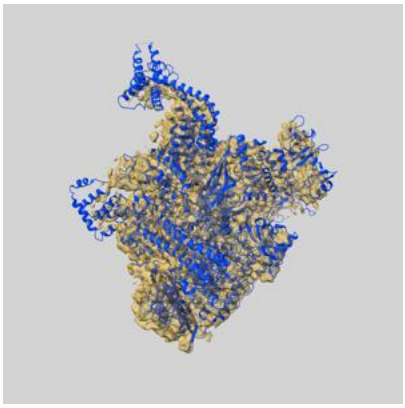
9.1 Map-model overlay



X



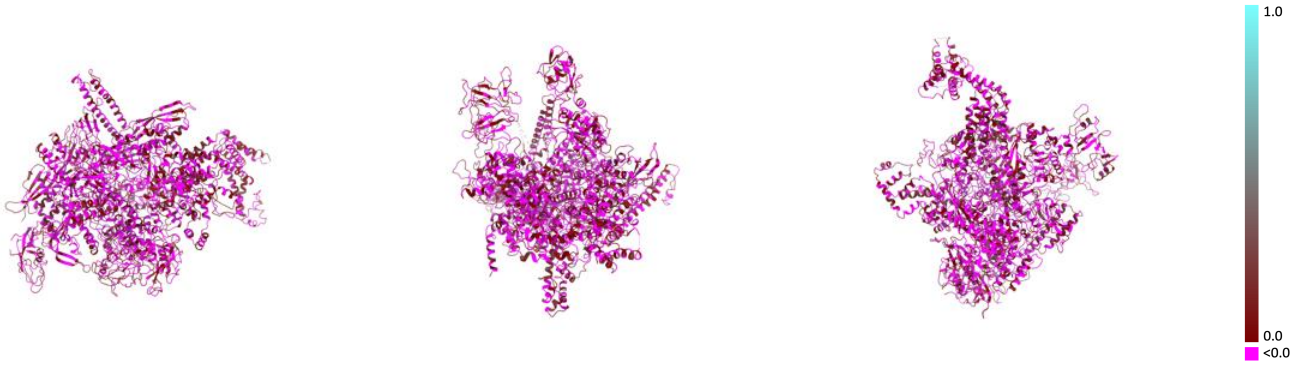
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.032 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.

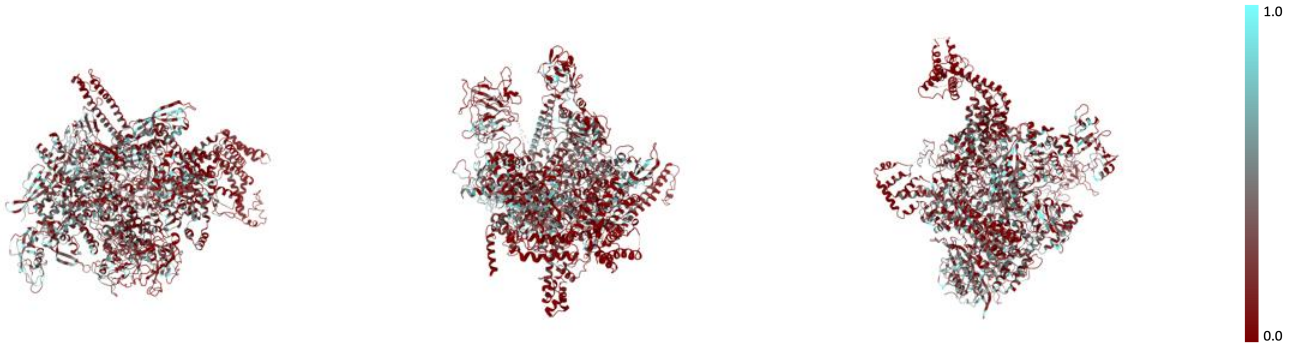
9.2 Q-score mapped to coordinate model (i)



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.

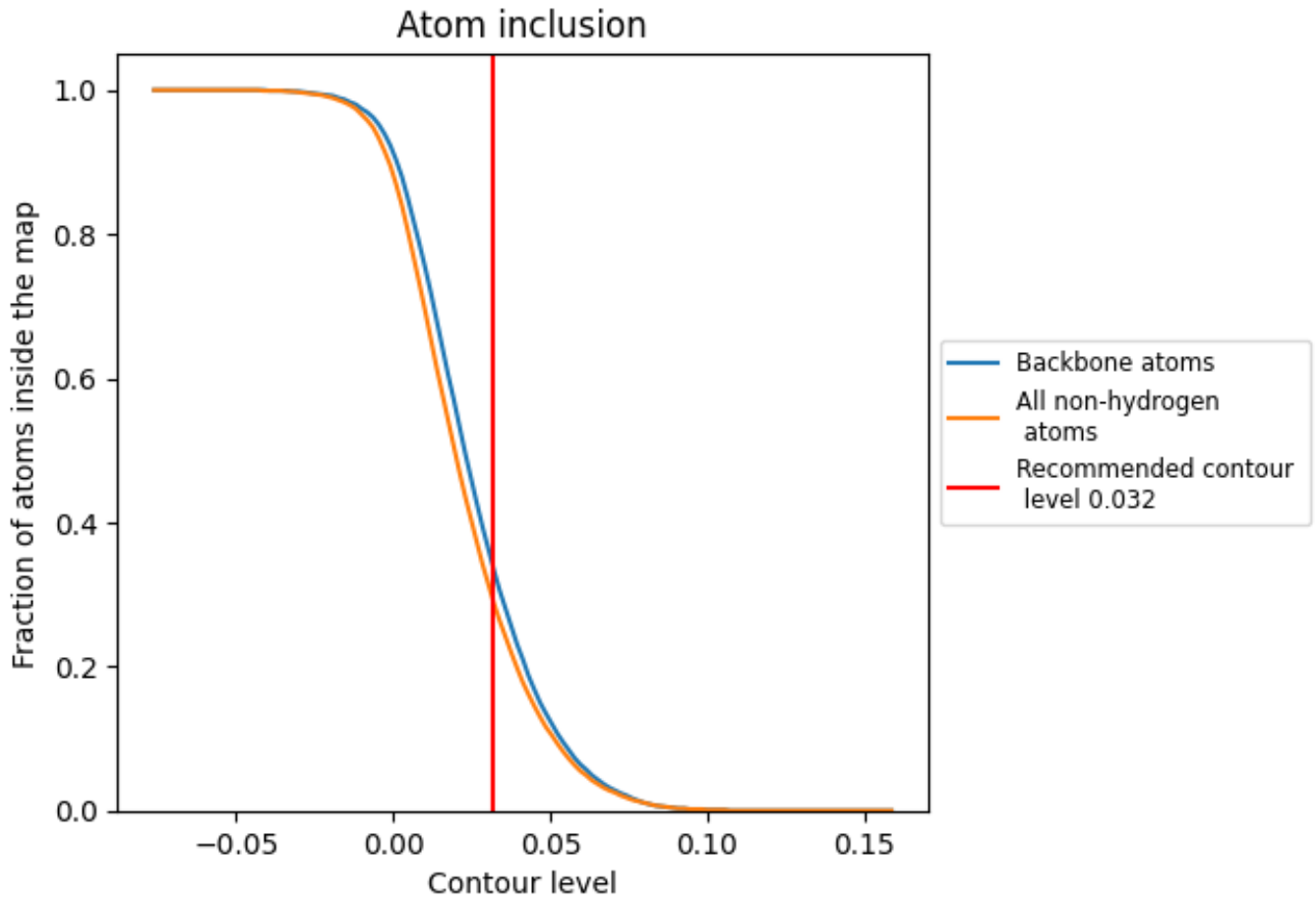
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.032).

9.4 Atom inclusion (i)



At the recommended contour level, 34% of all backbone atoms, 29% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2900	-0.0170
A	0.4000	-0.0020
B	0.4190	-0.0130
C	0.3110	-0.0300
D	0.3100	-0.0120
E	0.1140	-0.0490
F	0.0920	0.0030