wwPDB EM Validation Summary Report ⓘ

Mar 10, 2024 – 06:38 am GMT

PDB ID	:	8QMA
EMDB ID	:	EMD-18496
Title	:	Structure of the plastid-encoded RNA polymerase complex (PEP) from Sinapis alba
Authors	:	do Prado, P.F.V.; Ahrens, F.M.; Pfannschmidt, T.; Hillen, H.S.
Deposited on	:	2023-09-21
Resolution	:	3.50 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:

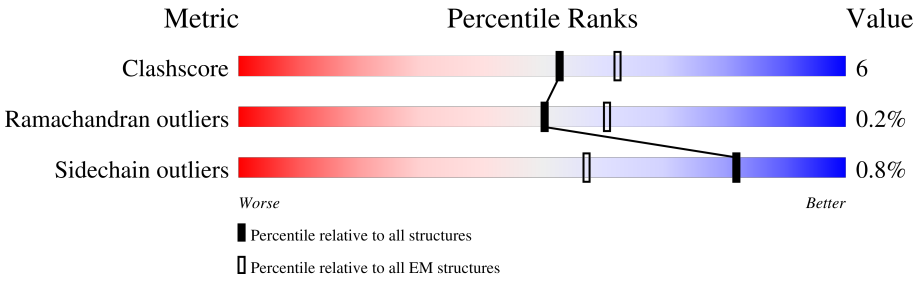
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	G	264	71% 10% 19%
2	H	529	35% 7% 58%
3	K	334	5% 50% 9% 40%
4	L	297	64% 9% 25%
5	M	184	47% 14% 38%
5	N	184	48% 10% 41%
6	O	768	16% 20% 5% 75%
7	P	162	13% 31% 9% 60%

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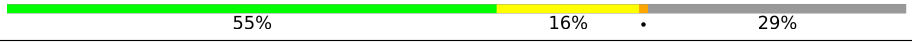
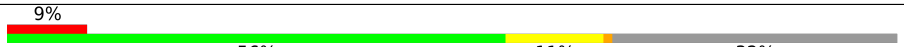
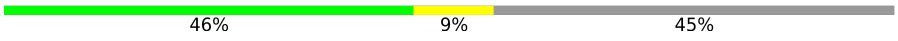
Mol	Chain	Length	Quality of chain
8	R	140	
9	S	460	
10	A	1072	
11	B	1373	
12	C	327	
12	D	327	
13	E	911	
14	F	675	
15	I	611	
16	J	483	
17	T	680	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 52064 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 PAP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	214	Total	C	N	O	S	0	0
			1766	1137	300	323	6		

- Molecule 2 is a protein called PAP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	224	Total	C	N	O	S	0	0
			1892	1193	341	348	10		

- Molecule 3 is a protein called PAP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	200	Total	C	N	O	S	0	0
			1681	1062	295	317	7		

- Molecule 4 is a protein called PAP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	222	Total	C	N	O	S	0	0
			1801	1158	306	333	4		

- Molecule 5 is a protein called PAP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	114	Total	C	N	O	S	0	0
			925	590	147	179	9		
5	N	108	Total	C	N	O	S	0	0
			867	552	138	168	9		

- Molecule 6 is a protein called PAP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	194	Total	C	N	O	S	0	0
			1538	950	272	306	10		

- Molecule 7 is a protein called PAP12 (DNA-directed RNA polymerase subunit omega).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	65	Total	C	N	O	S	0	0
			530	332	91	105	2		

- Molecule 8 is a protein called PTAC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	100	Total	C	N	O	S	0	0
			852	555	144	150	3		

- Molecule 9 is a protein called PAP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	384	Total	C	N	O	S	0	0
			3104	1985	520	584	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	789	Total	C	N	O	S	0	0
			6310	4042	1093	1154	21		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta".

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	931	Total	C	N	O	S	0	0
			7445	4765	1316	1339	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	210	Total	C	N	O	S	0	0
			1666	1054	294	310	8		
12	D	278	Total	C	N	O	S	0	0
			2249	1440	393	407	9		

- Molecule 13 is a protein called PAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	632	Total	C	N	O	S	0	0
			5075	3214	882	946	33		

- Molecule 14 is a protein called PAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	483	Total	C	N	O	S	0	0
			4060	2593	706	746	15		

- Molecule 15 is a protein called FLN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	338	Total	C	N	O	S	0	0
			2645	1684	439	502	20		

- Molecule 16 is a protein called PAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	426	Total	C	N	O	S	0	0
			3477	2227	591	639	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	509	Total	C	N	O	S	0	0
			4151	2674	726	732	19		

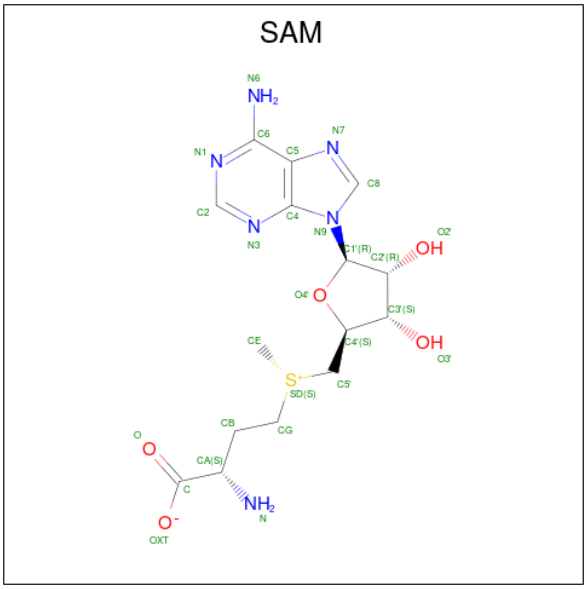
- Molecule 18 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	G	1	Total	Fe	0
			1	1	
18	L	1	Total	Fe	0
			1	1	

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Zn	0
			1	1	

- Molecule 20 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



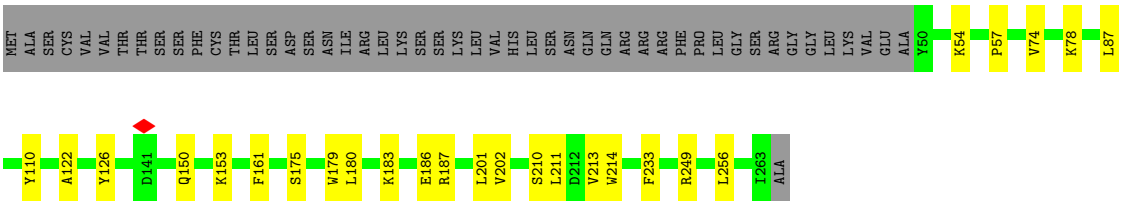
Mol	Chain	Residues	Atoms					AltConf
20	J	1	Total	C	N	O	S	0
			27	15	6	5	1	

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.

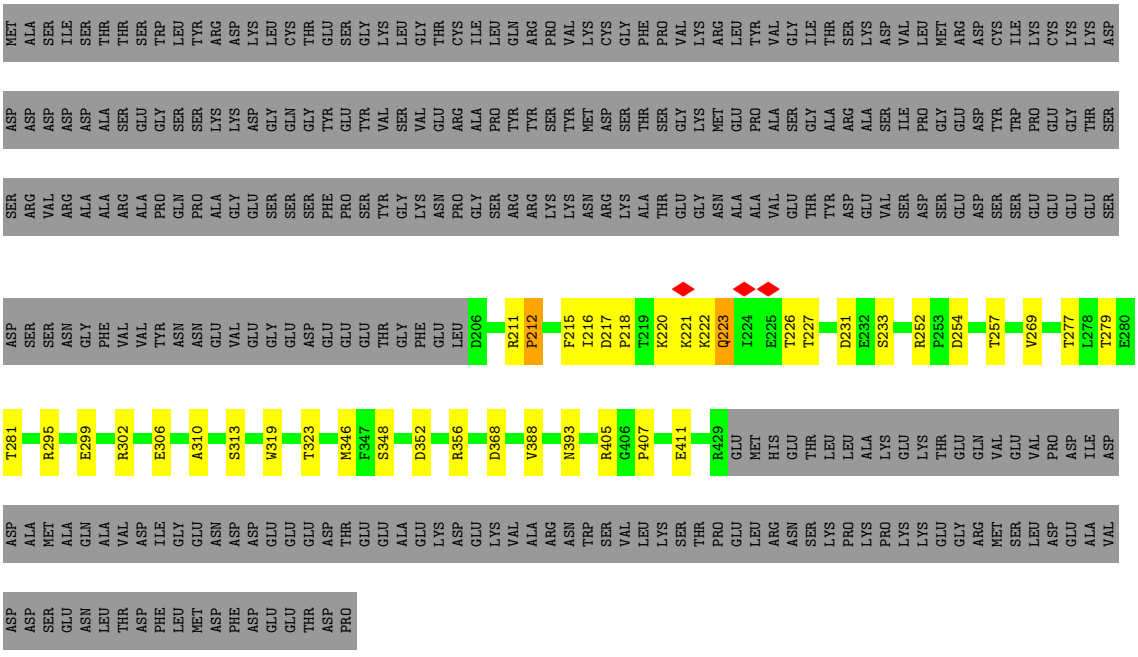
- Molecule 1: PAP4

Chain G:



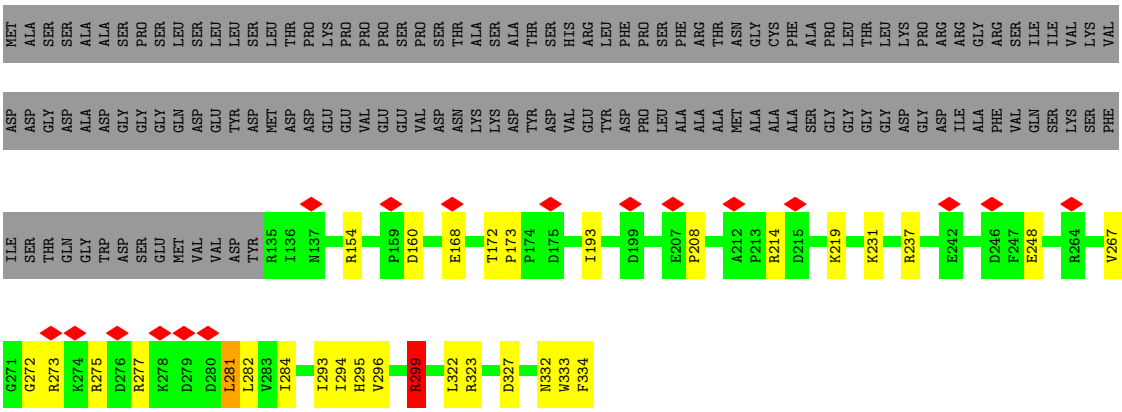
- Molecule 2: PAP5

Chain H:



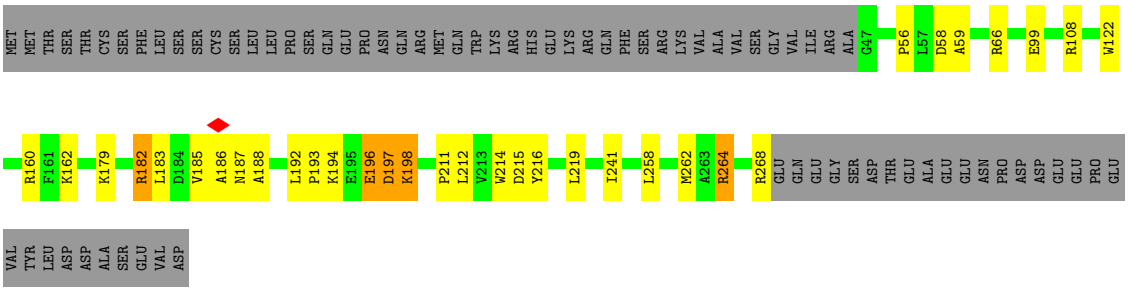
- Molecule 3: PAP8

Chain K:



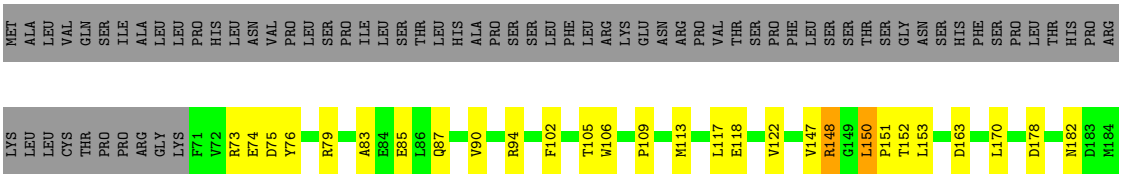
• Molecule 4: PAP9

Chain L:



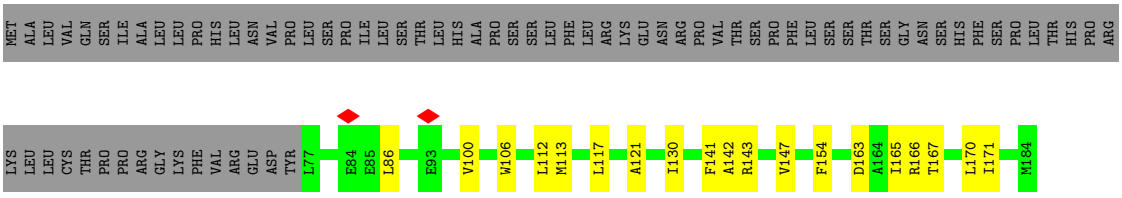
• Molecule 5: PAP10

Chain M:



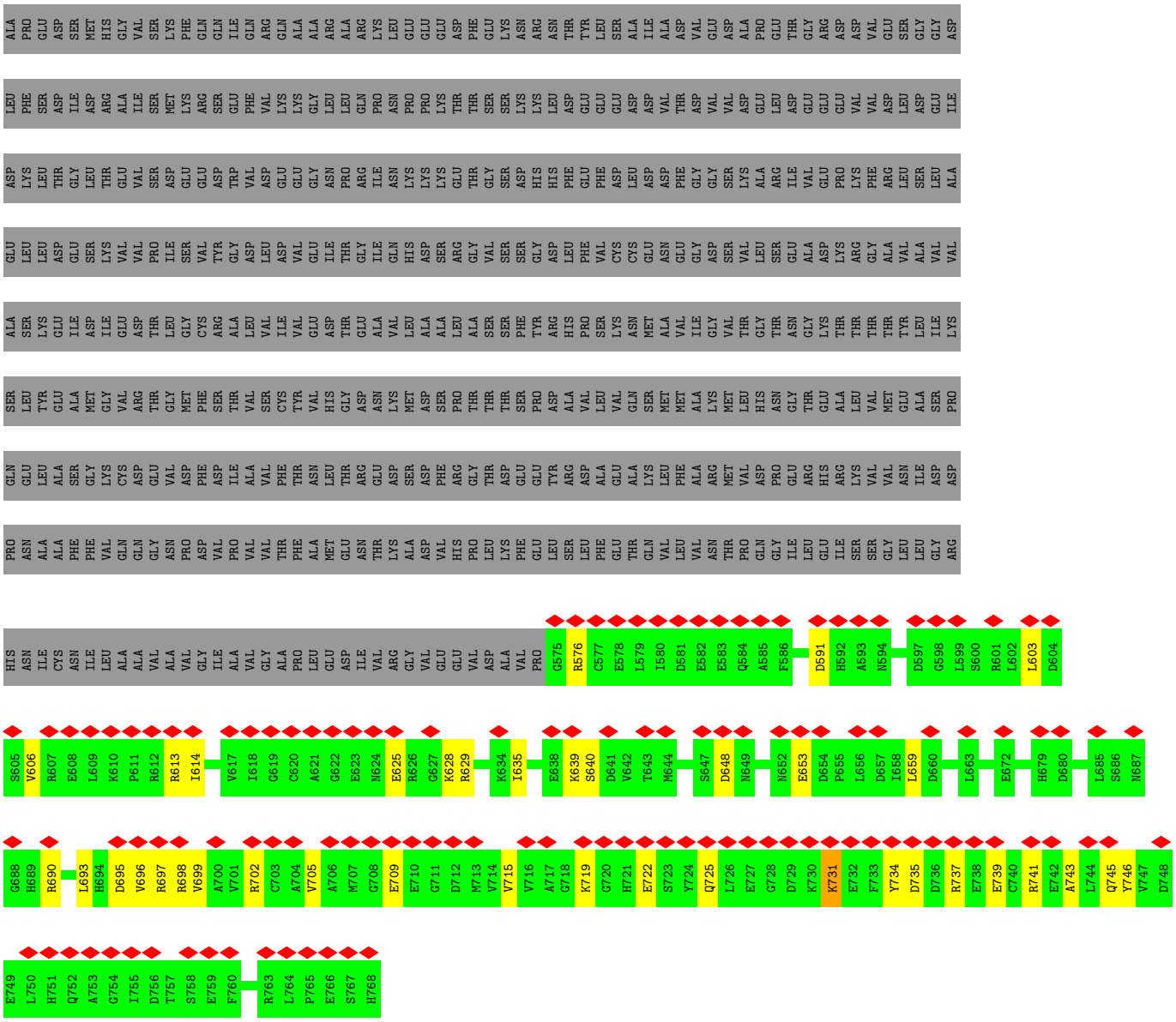
• Molecule 5: PAP10

Chain N:

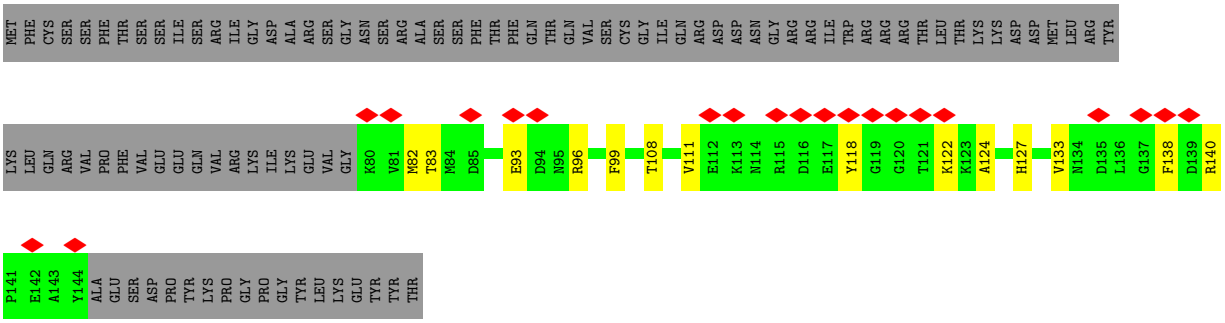


• Molecule 6: PAP11

Chain O:

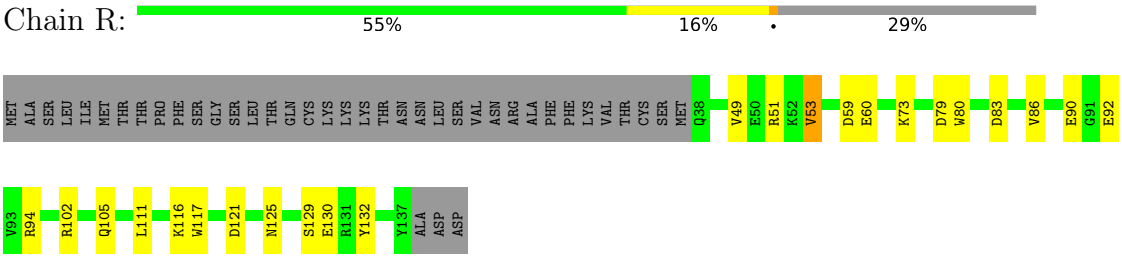


• Molecule 7: PAP12 (DNA-directed RNA polymerase subunit omega)



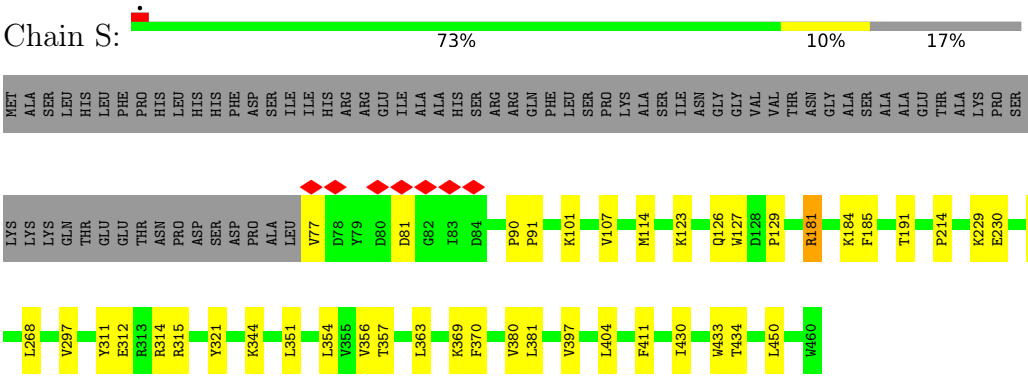
• Molecule 8: PTAC18

Chain R:



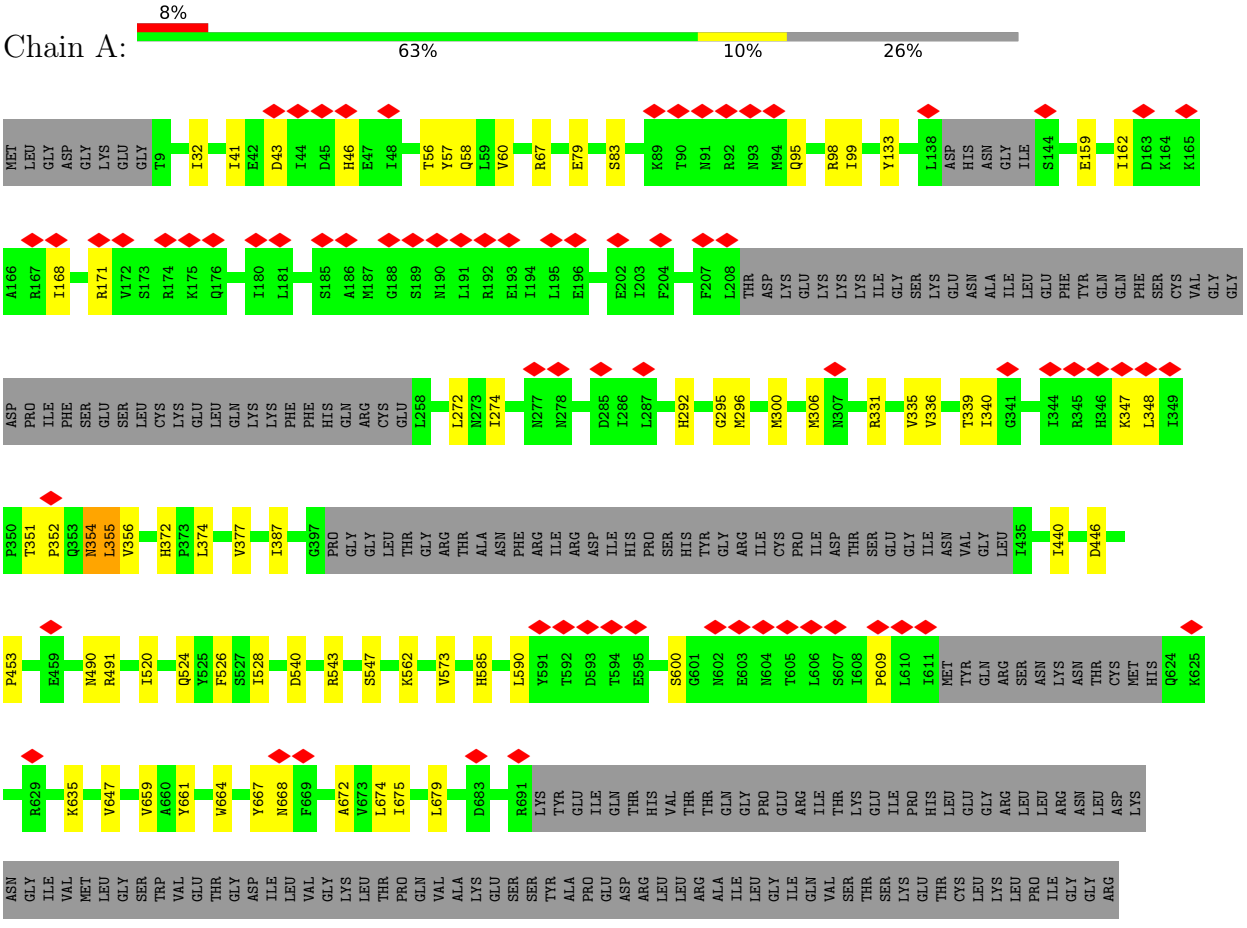
• Molecule 9: PAP6

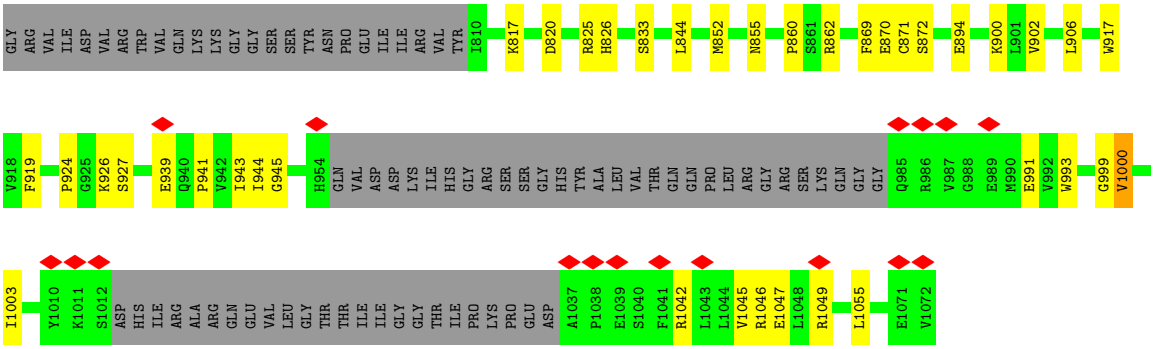
Chain S:



• Molecule 10: DNA-directed RNA polymerase subunit beta

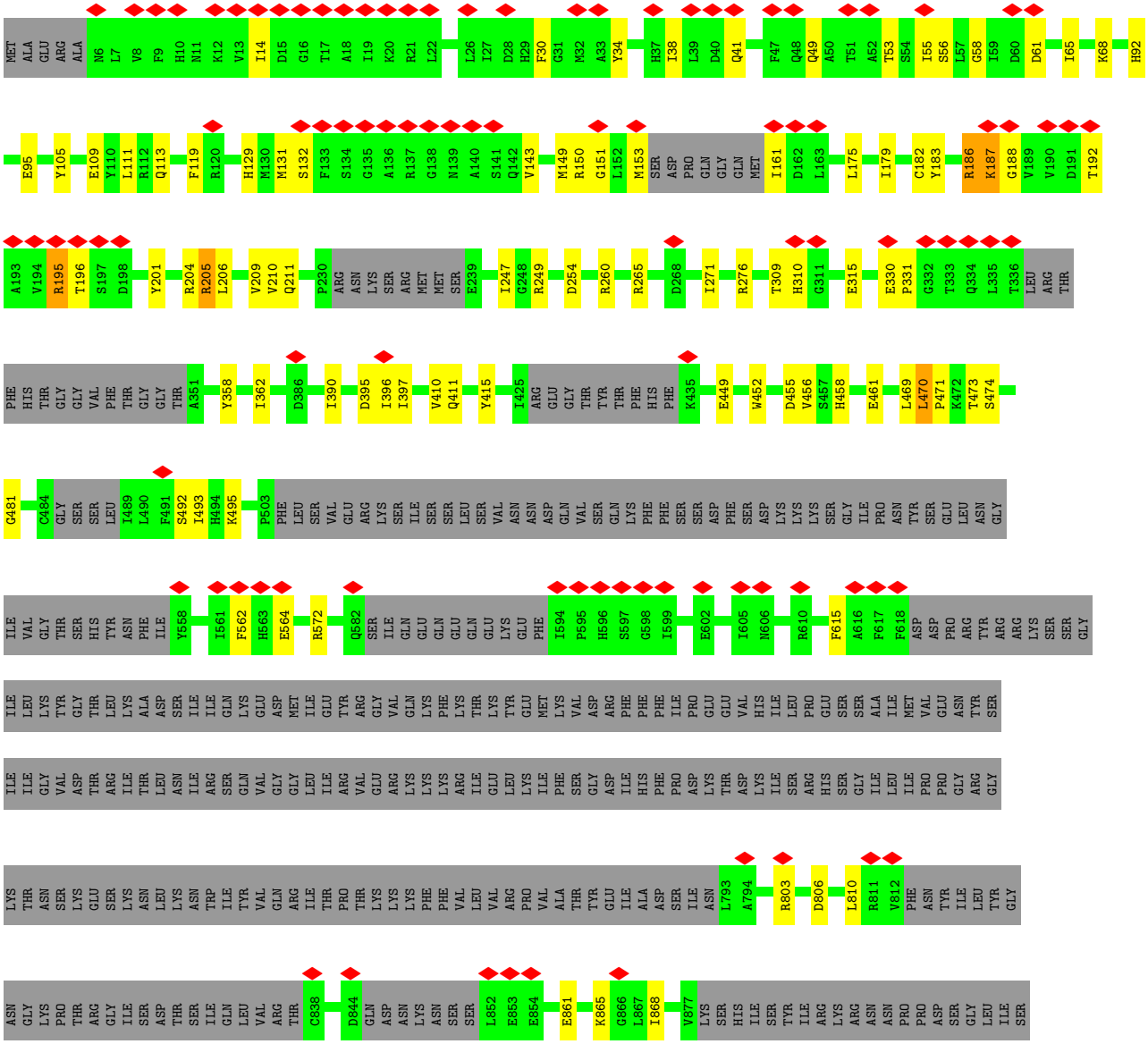
Chain A:

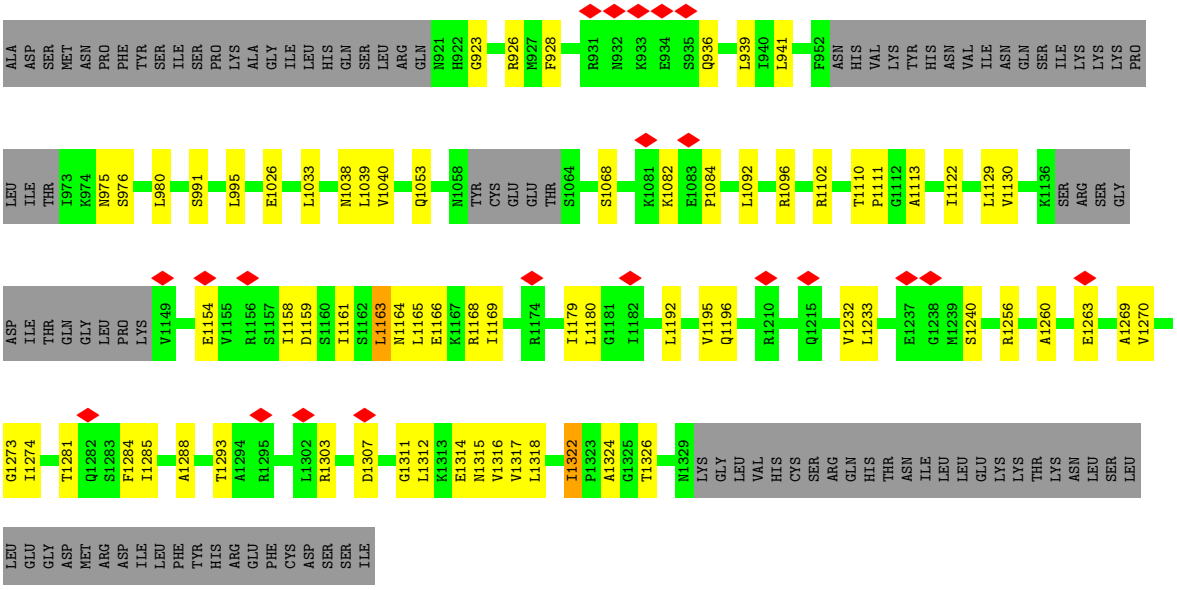




• Molecule 11: DNA-directed RNA polymerase subunit beta"

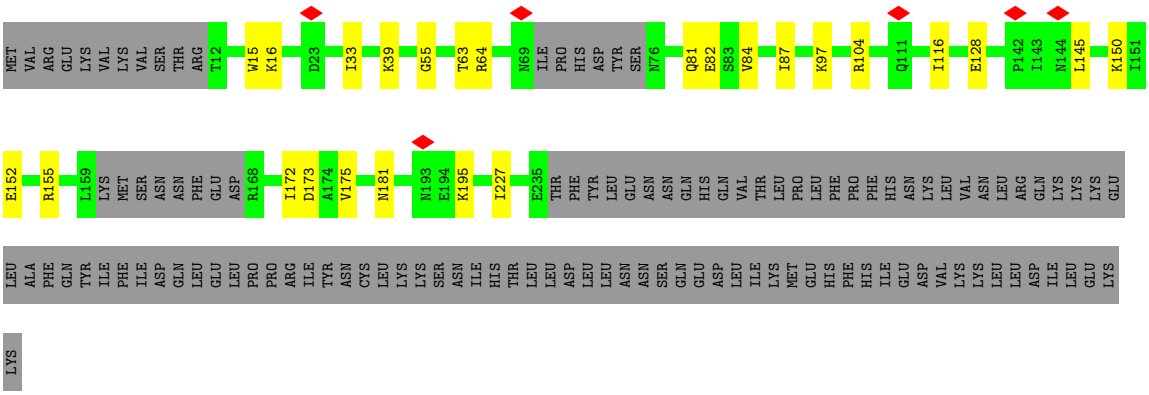
Chain B:





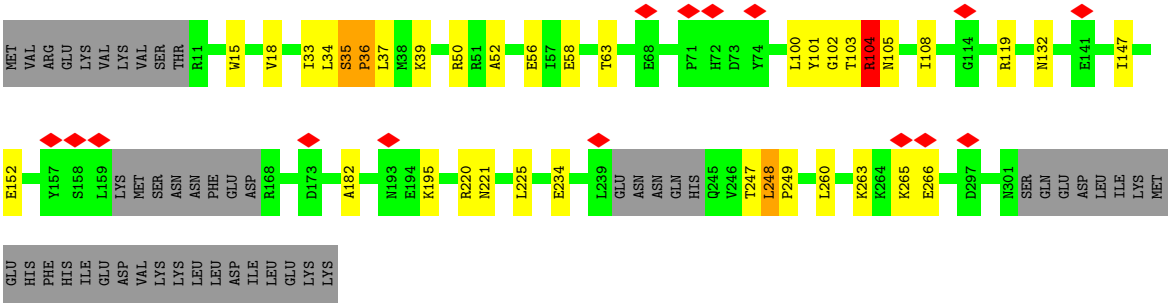
• Molecule 12: DNA-directed RNA polymerase subunit alpha

Chain C:



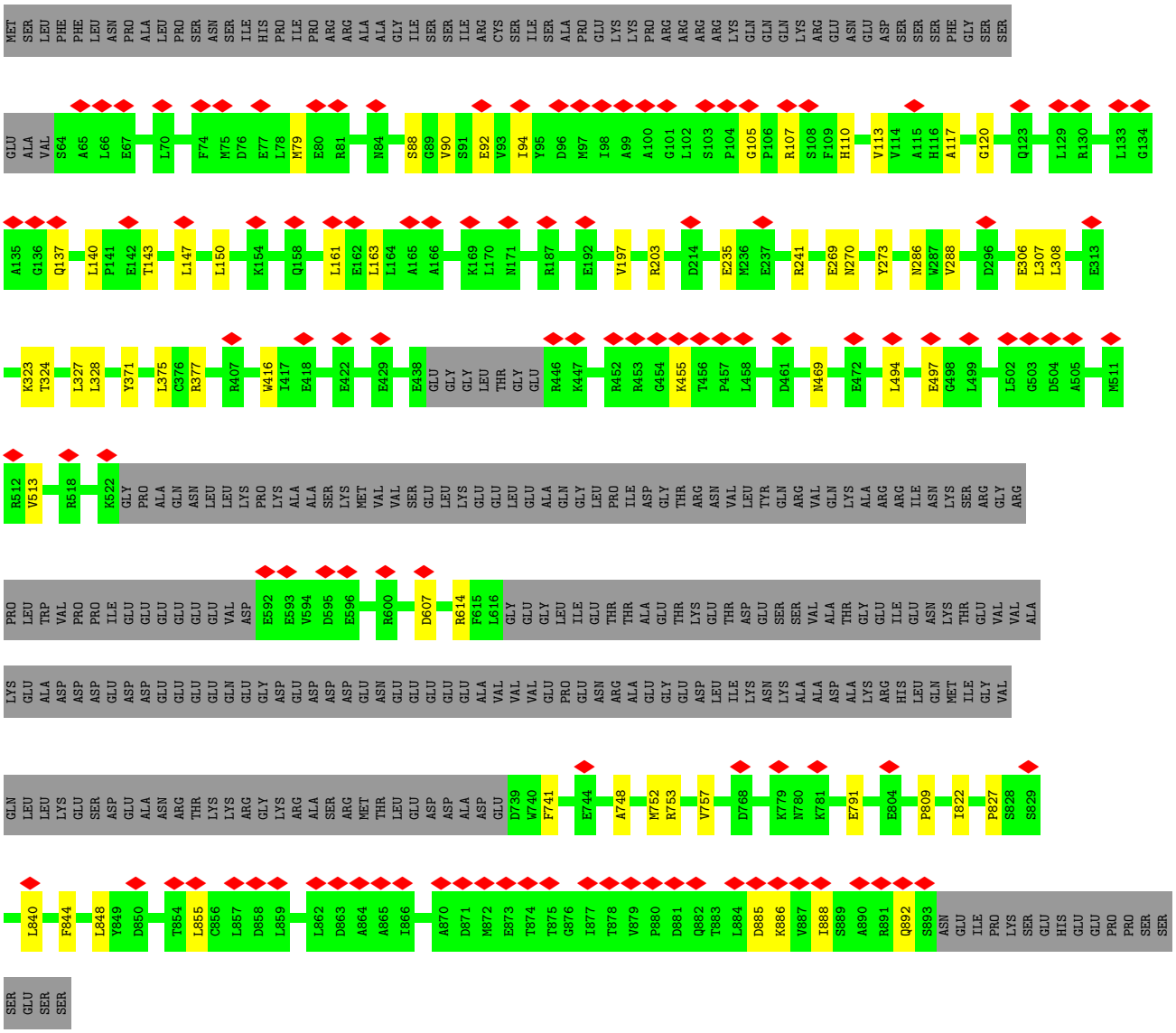
• Molecule 12: DNA-directed RNA polymerase subunit alpha

Chain D:



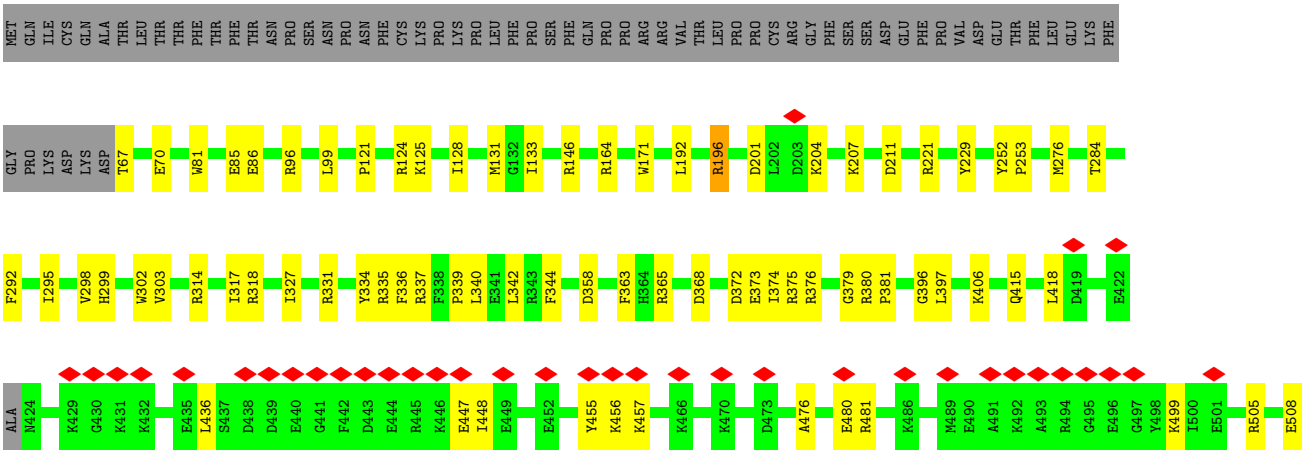
• Molecule 13: PAP1

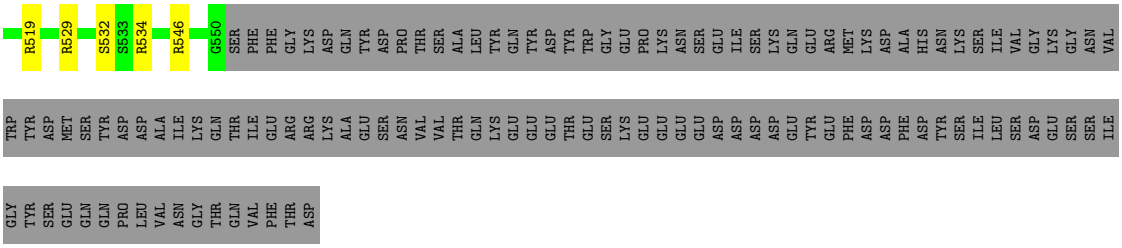
Chain E:



• Molecule 14: PAP3

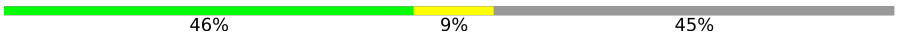
Chain F:

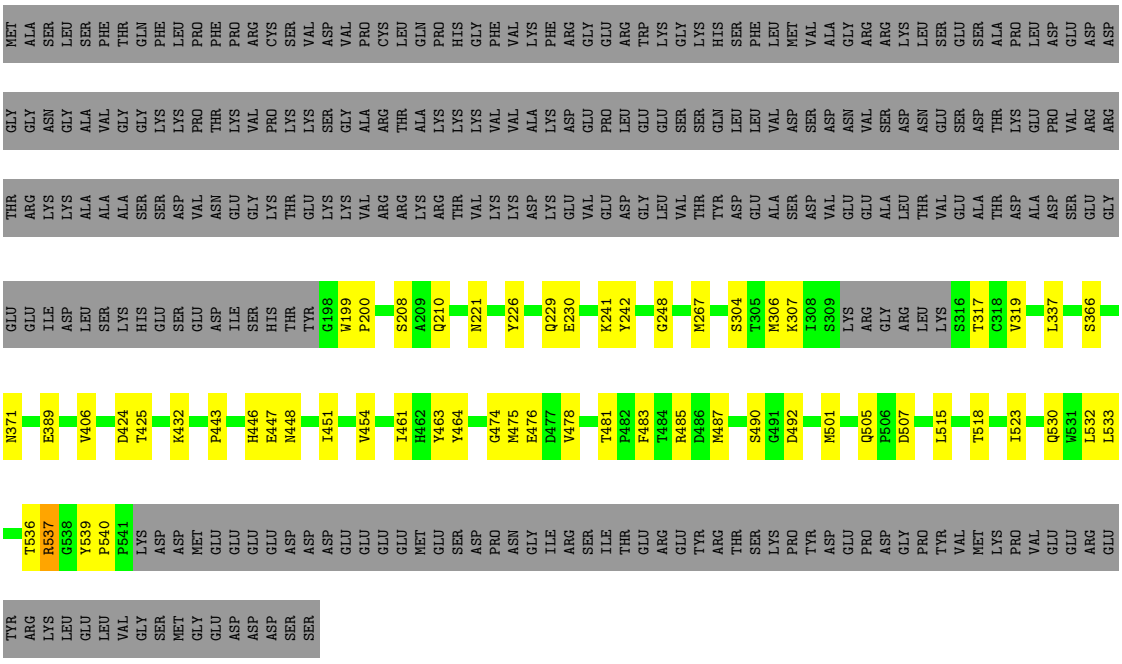




• Molecule 15: FLN2

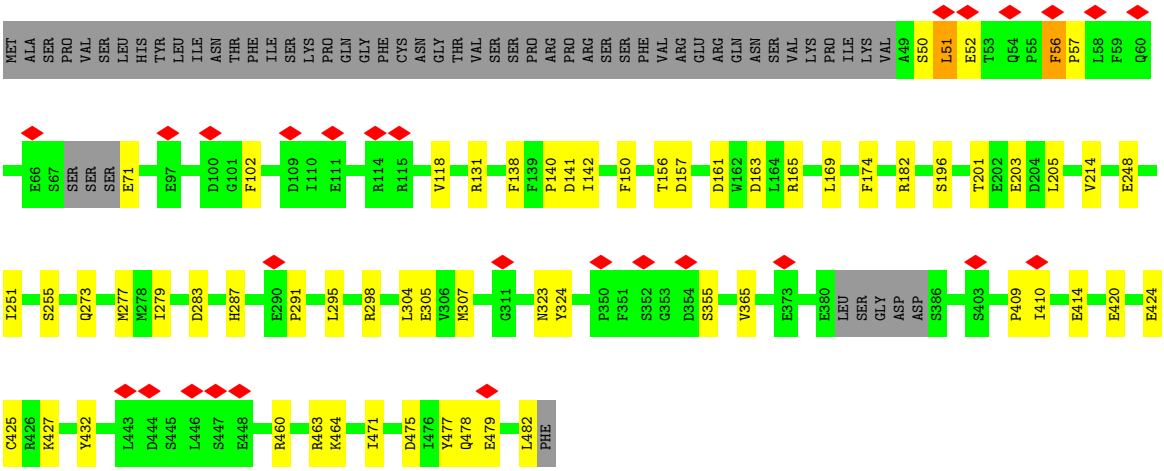
Chain I:





• Molecule 16: PAP7

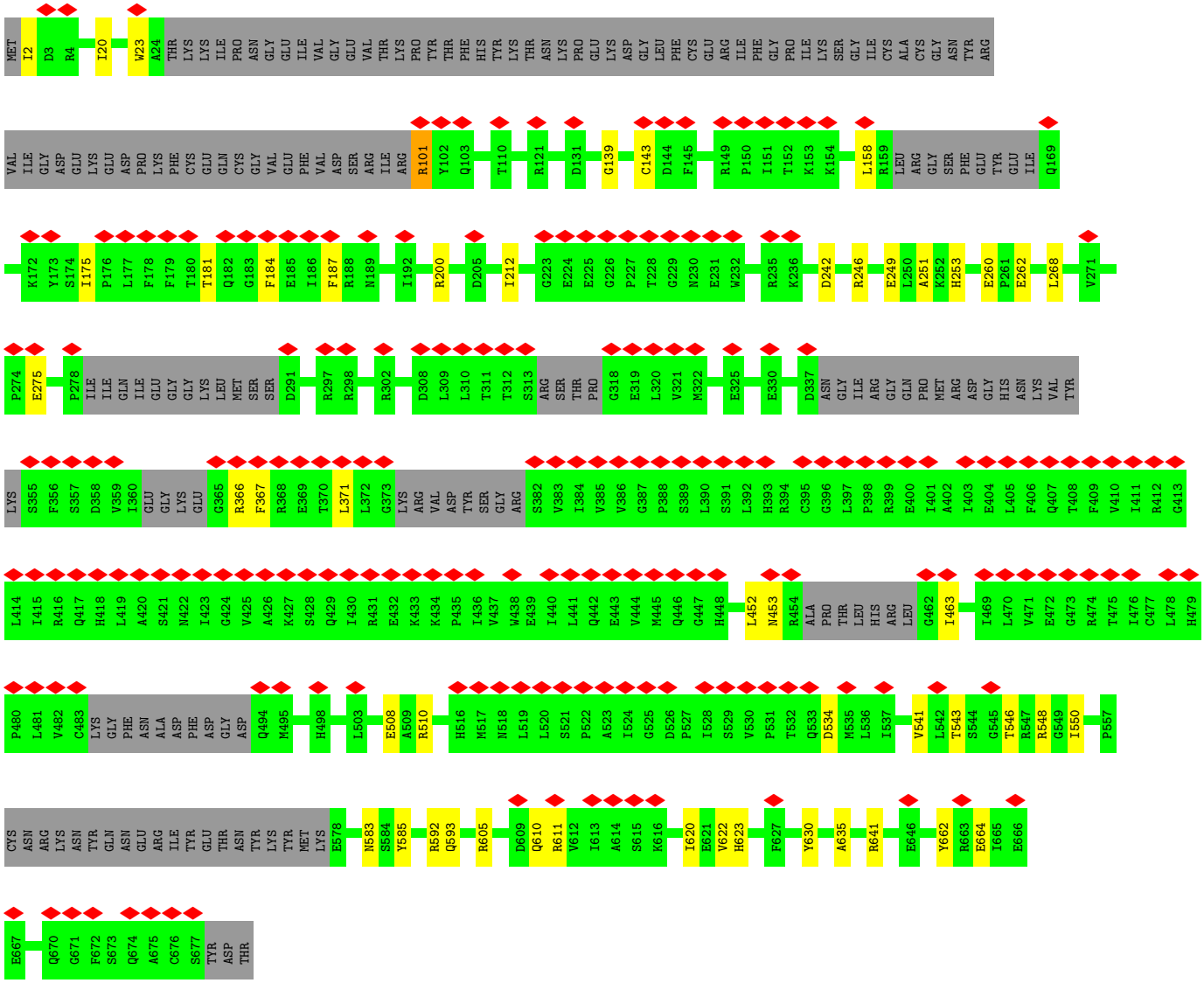
Chain J:



• Molecule 17: DNA-directed RNA polymerase subunit beta'

Chain T:


31%
67%
7%
25%


MET I2 D3 R4 I20 W23 A24 THR LYS LYS ILE PRO ASN GLY GLU ILE VAL GLY GLU VAL THR LYS PRO TYR THR PHE HIS TYR LYS THR ASN LYS PRO GLU LYS ASP GLY LEU PHE CYS GLU ARG ILE PHE GLY PRO ILE LYS SER GLY ILE CYS ALA CYS GLY ASN TYR ARG
VAL ILE GLY ASP GLU LYS GLU ASP PRO LYS PHE CYS GLU GLN CYS GLY VAL GLU PHE VAL ASP SER ARG ILE ARG R101 Y102 Q103 T110 R121 D131 G139 C143 D144 F145 R149 P150 I151 T152 K153 K154 L158 R159 LEU ARG GLY SER PHE GLU TYR GLU ILE Q169
K172 Y173 S174 I175 P176 L177 F178 F179 T180 T181 Q182 G183 F184 E185 I186 F187 R188 N189 I192 R200 D205 I212 G223 E224 E225 G226 P227 T228 G229 N230 E231 W232 R235 K236 D242 R246 E249 L250 A251 K252 H253 E260 P261 E262 L268 V271
P274 E275 P278 ILE ILE GLN ILE GLU GLY GLY LYS LEU MET SER SER D291 R297 R298 R302 D308 L309 L310 T311 T312 S313 ARG SER THR PRO G318 E319 L320 V321 M322 E325 E330 D337 ASN GLY ILE ARG GLY GLN PRO MET ARG ASP GLY HIS ASN LYS VAL TYR
LYS S355 F356 S357 D358 V359 I360 GLU GLY LYS GLU G365 R366 F367 R368 E369 T370 L371 L372 G373 LYS ARG VAL ASP TYR SER GLY ARG S382 V383 I384 V385 V386 G387 P388 S389 L390 S391 L392 H393 R394 C395 G396 L397 P398 R399 E400 I401 A402 I403 E404 L405 F406 Q407 T408 F409 V410 I411 R412 G413
L414 I415 R416 Q417 H418 L419 A420 S421 N422 I423 G424 V425 A426 K427 S428 Q429 I430 R431 E432 K433 K434 P435 I436 V437 W438 E439 I440 L441 Q442 E443 V444 M445 Q446 G447 H448 L452 N453 R454 ALA PRO THR LEU HIS ARG LEU G462 I463 I469 L470 V471 E472 G473 R474 T475 I476 C477 L478 H479
P480 L481 V482 C483 LYS GLY PHE ASN ALA ASP PHE ASP GLY ASP Q494 M495 H498 L503 E508 A509 R510 H516 M517 N518 L519 L520 S521 P522 A523 I524 G525 D526 P527 I528 S529 V530 P531 T532 Q533 D534 M535 L536 I537 V541 L542 T543 S544 G545 T546 R547 R548 G549 I550 P557
CYS ASN ARG LYS ASN TYR GLN ASN GLU ARG ILE TYR GLU THR ASN TYR LYS TYR MET LYS E578 N583 S584 Y585 R592 Q593 R605 D609 Q610 R611 V612 I613 A614 S615 K616 I620 E621 V622 H623 F627 Y630 A635 R641 E646 Y662 R663 E664 I665 E666
E567 Q670 G671 F672 S673 Q674 A675 C676 S677 TYR ASP THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123874	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)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.762	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, FE, SAM

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	0.30	0/1820	0.49	0/2472
2	H	0.28	0/1941	0.56	0/2616
3	K	0.26	0/1722	0.55	0/2329
4	L	0.30	0/1855	0.54	0/2525
5	M	0.29	0/941	0.56	0/1271
5	N	0.28	0/881	0.59	0/1190
6	O	0.24	0/1568	0.54	0/2117
7	P	0.27	0/538	0.53	0/723
8	R	0.34	0/877	0.54	0/1187
9	S	0.31	0/3185	0.53	0/4320
10	A	0.28	0/6435	0.54	0/8690
11	B	0.28	0/7589	0.54	0/10256
12	C	0.26	0/1694	0.54	0/2292
12	D	0.27	0/2294	0.57	2/3107 (0.1%)
13	E	0.25	0/5178	0.53	1/6997 (0.0%)
14	F	0.29	0/4173	0.53	0/5628
15	I	0.27	0/2702	0.50	0/3661
16	J	0.26	0/3567	0.52	1/4829 (0.0%)
17	T	0.25	0/4238	0.51	0/5732
All	All	0.28	0/53198	0.53	4/71942 (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
3	K	0	1
4	L	0	4
6	O	0	1
11	B	0	4

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
12	C	0	1
12	D	0	2
14	F	0	2
15	I	0	1
17	T	0	1
All	All	0	17

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	35	SER	C-N-CD	-11.12	96.14	120.60
13	E	607	ASP	CB-CG-OD1	5.68	123.41	118.30
12	D	248	LEU	CA-CB-CG	-5.55	102.53	115.30
16	J	482	LEU	CA-CB-CG	5.36	127.62	115.30

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	214	ARG	Sidechain
4	L	108	ARG	Sidechain
4	L	160	ARG	Sidechain
4	L	182	ARG	Sidechain
4	L	264	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1766	0	1691	16	0
2	H	1892	0	1857	30	0
3	K	1681	0	1648	24	0
4	L	1801	0	1732	23	0
5	M	925	0	919	23	0
5	N	867	0	867	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	1538	0	1470	21	0
7	P	530	0	510	11	0
8	R	852	0	836	15	0
9	S	3104	0	3026	30	0
10	A	6310	0	6385	84	0
11	B	7445	0	7523	120	0
12	C	1666	0	1685	16	0
12	D	2249	0	2288	20	0
13	E	5075	0	5030	44	0
14	F	4060	0	3959	65	0
15	I	2645	0	2629	46	0
16	J	3477	0	3414	42	0
17	T	4151	0	4219	46	0
18	G	1	0	0	0	0
18	L	1	0	0	0	0
19	B	1	0	0	0	0
20	J	27	0	22	1	0
All	All	52064	0	51710	585	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.

The worst 5 of 585 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)
10:A:99:ILE:HG21	10:A:354:ASN:HB2	1.56	0.88
9:S:184:LYS:HD3	9:S:185:PHE:H	1.38	0.87
17:T:20:ILE:HD13	17:T:23:TRP:HE1	1.44	0.82
11:B:493:ILE:HD11	14:F:374:ILE:HB	1.61	0.82
11:B:1163:LEU:HD13	11:B:1165:LEU:HB3	1.61	0.81

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	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
2	H	222/529 (42%)	211 (95%)	10 (4%)	1 (0%)	29	68
3	K	198/334 (59%)	189 (96%)	8 (4%)	1 (0%)	29	68
4	L	220/297 (74%)	213 (97%)	5 (2%)	2 (1%)	17	56
5	M	112/184 (61%)	109 (97%)	3 (3%)	0	100	100
5	N	106/184 (58%)	99 (93%)	7 (7%)	0	100	100
6	O	192/768 (25%)	181 (94%)	11 (6%)	0	100	100
7	P	63/162 (39%)	61 (97%)	2 (3%)	0	100	100
8	R	98/140 (70%)	95 (97%)	3 (3%)	0	100	100
9	S	382/460 (83%)	367 (96%)	14 (4%)	1 (0%)	41	75
10	A	773/1072 (72%)	740 (96%)	32 (4%)	1 (0%)	51	84
11	B	901/1373 (66%)	860 (95%)	39 (4%)	2 (0%)	47	81
12	C	204/327 (62%)	195 (96%)	8 (4%)	1 (0%)	29	68
12	D	272/327 (83%)	253 (93%)	18 (7%)	1 (0%)	34	72
13	E	624/911 (68%)	602 (96%)	20 (3%)	2 (0%)	41	75
14	F	479/675 (71%)	464 (97%)	15 (3%)	0	100	100
15	I	334/611 (55%)	315 (94%)	18 (5%)	1 (0%)	41	75
16	J	420/483 (87%)	400 (95%)	19 (4%)	1 (0%)	47	81
17	T	487/680 (72%)	470 (96%)	17 (4%)	0	100	100
All	All	6299/9781 (64%)	6031 (96%)	254 (4%)	14 (0%)	50	81

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	212	PRO
4	L	198	LYS
12	D	36	PRO
4	L	186	ALA
15	I	447	GLU

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	187/231 (81%)	186 (100%)	1 (0%)	88	94
2	H	204/469 (44%)	201 (98%)	3 (2%)	65	84
3	K	191/299 (64%)	187 (98%)	4 (2%)	53	79
4	L	190/259 (73%)	187 (98%)	3 (2%)	62	83
5	M	103/168 (61%)	101 (98%)	2 (2%)	57	80
5	N	97/168 (58%)	97 (100%)	0	100	100
6	O	167/661 (25%)	166 (99%)	1 (1%)	86	94
7	P	57/144 (40%)	57 (100%)	0	100	100
8	R	91/127 (72%)	89 (98%)	2 (2%)	52	78
9	S	338/401 (84%)	334 (99%)	4 (1%)	71	87
10	A	688/931 (74%)	685 (100%)	3 (0%)	91	96
11	B	823/1230 (67%)	810 (98%)	13 (2%)	62	83
12	C	185/301 (62%)	185 (100%)	0	100	100
12	D	252/301 (84%)	247 (98%)	5 (2%)	55	79
13	E	541/782 (69%)	540 (100%)	1 (0%)	93	98
14	F	431/609 (71%)	430 (100%)	1 (0%)	93	98
15	I	291/532 (55%)	290 (100%)	1 (0%)	92	97
16	J	378/431 (88%)	377 (100%)	1 (0%)	92	97
17	T	458/608 (75%)	457 (100%)	1 (0%)	93	98
All	All	5672/8652 (66%)	5626 (99%)	46 (1%)	82	91

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	B	187	LYS
11	B	1318	LEU
11	B	195	ARG
11	B	1096	ARG

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Mol	Chain	Res	Type
12	D	103	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
11	B	1196	GLN
17	T	128	ASN
13	E	270	ASN
17	T	610	GLN
15	I	505	GLN

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 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	$\#\|Z\| > 2$
20	SAM	J	501	-	24,29,29	0.67	0	23,42,42	0.88	1 (4%)

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
20	SAM	J	501	-	-	7/12/33/33	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	501	SAM	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

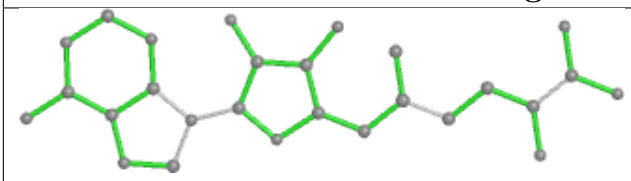
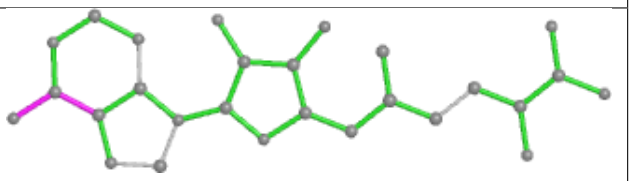
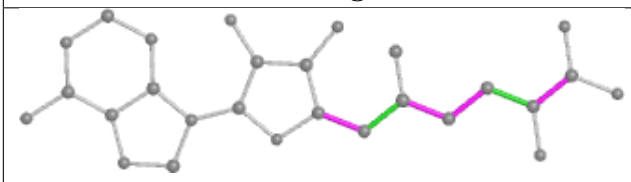
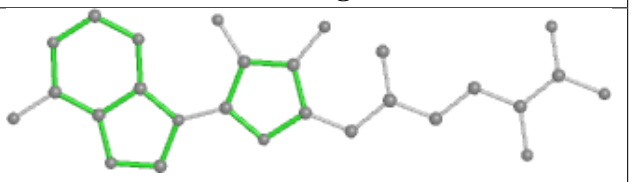
Mol	Chain	Res	Type	Atoms
20	J	501	SAM	O4'-C4'-C5'-SD
20	J	501	SAM	C3'-C4'-C5'-SD
20	J	501	SAM	CB-CG-SD-CE
20	J	501	SAM	CB-CG-SD-C5'
20	J	501	SAM	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	501	SAM	1	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 SAM J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

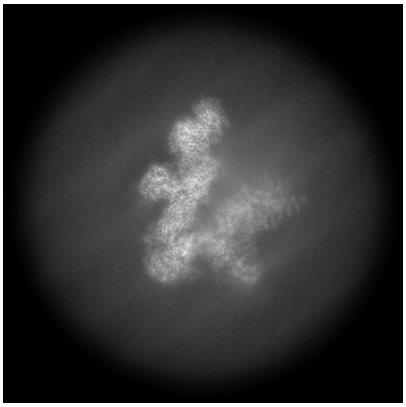
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18496. These allow visual inspection of the internal detail of the map and identification of artifacts.

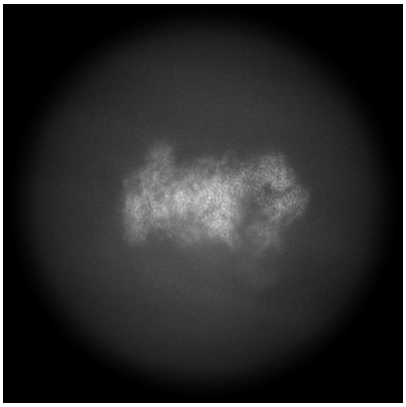
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

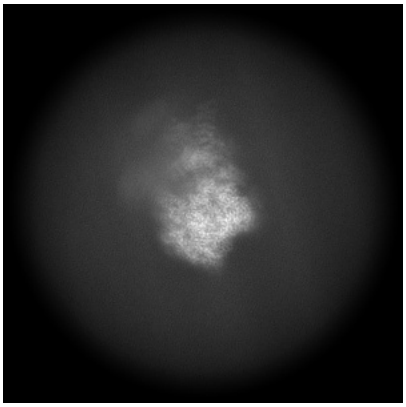
6.1.1 Primary map



X



Y

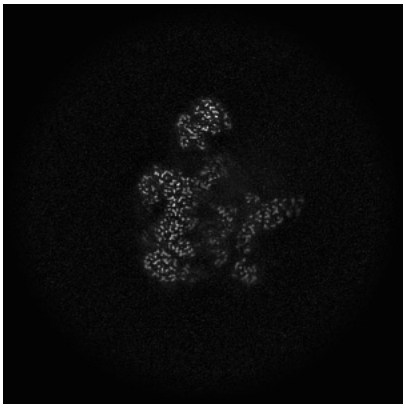


Z

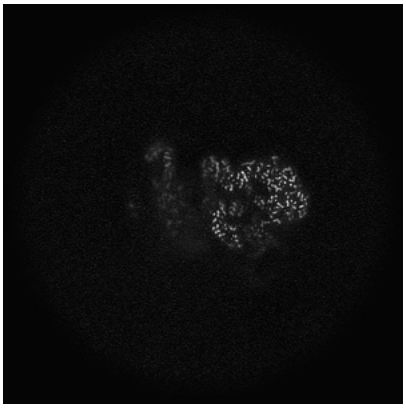
The images above show the map projected in three orthogonal directions.

6.2 Central slices

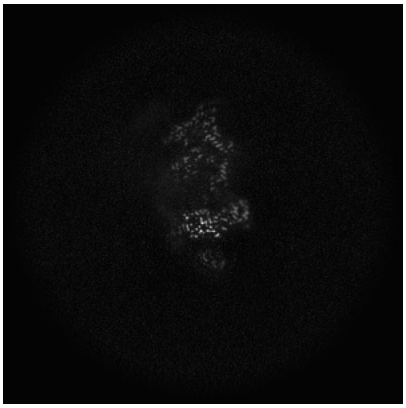
6.2.1 Primary map



X Index: 220



Y Index: 220

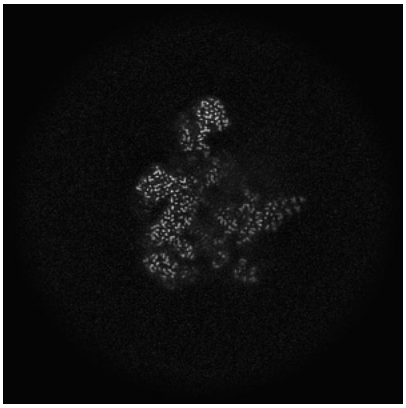


Z Index: 220

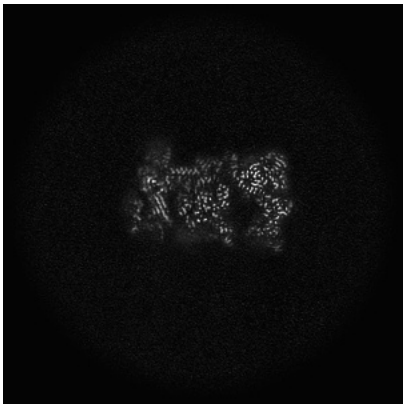
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

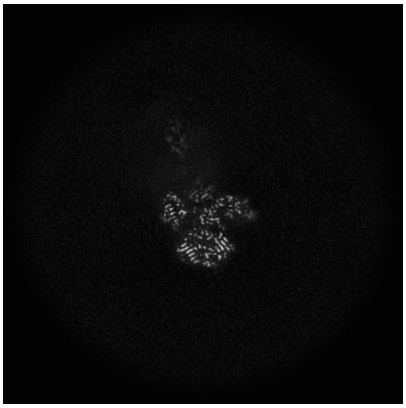
6.3.1 Primary map



X Index: 224



Y Index: 202

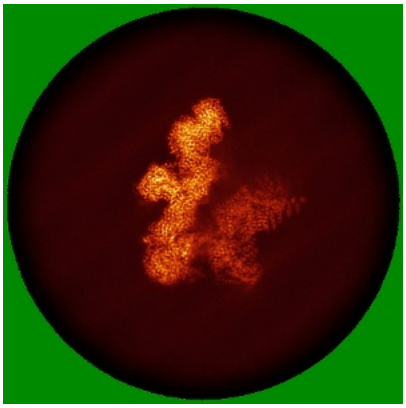


Z Index: 246

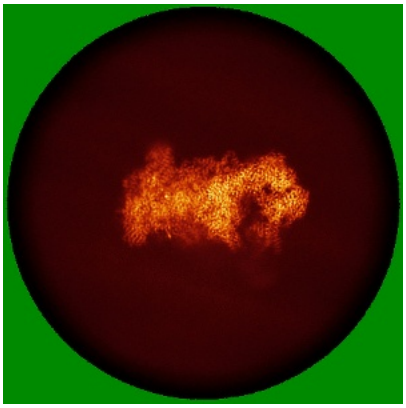
The images above show the largest variance slices of the map in three orthogonal directions.

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

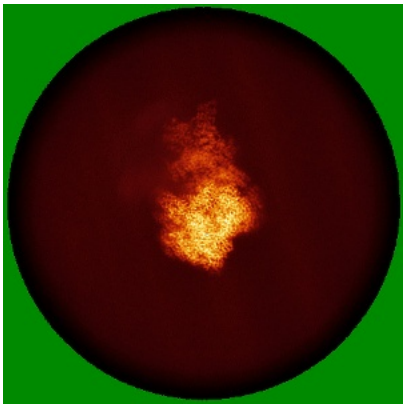
6.4.1 Primary map



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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

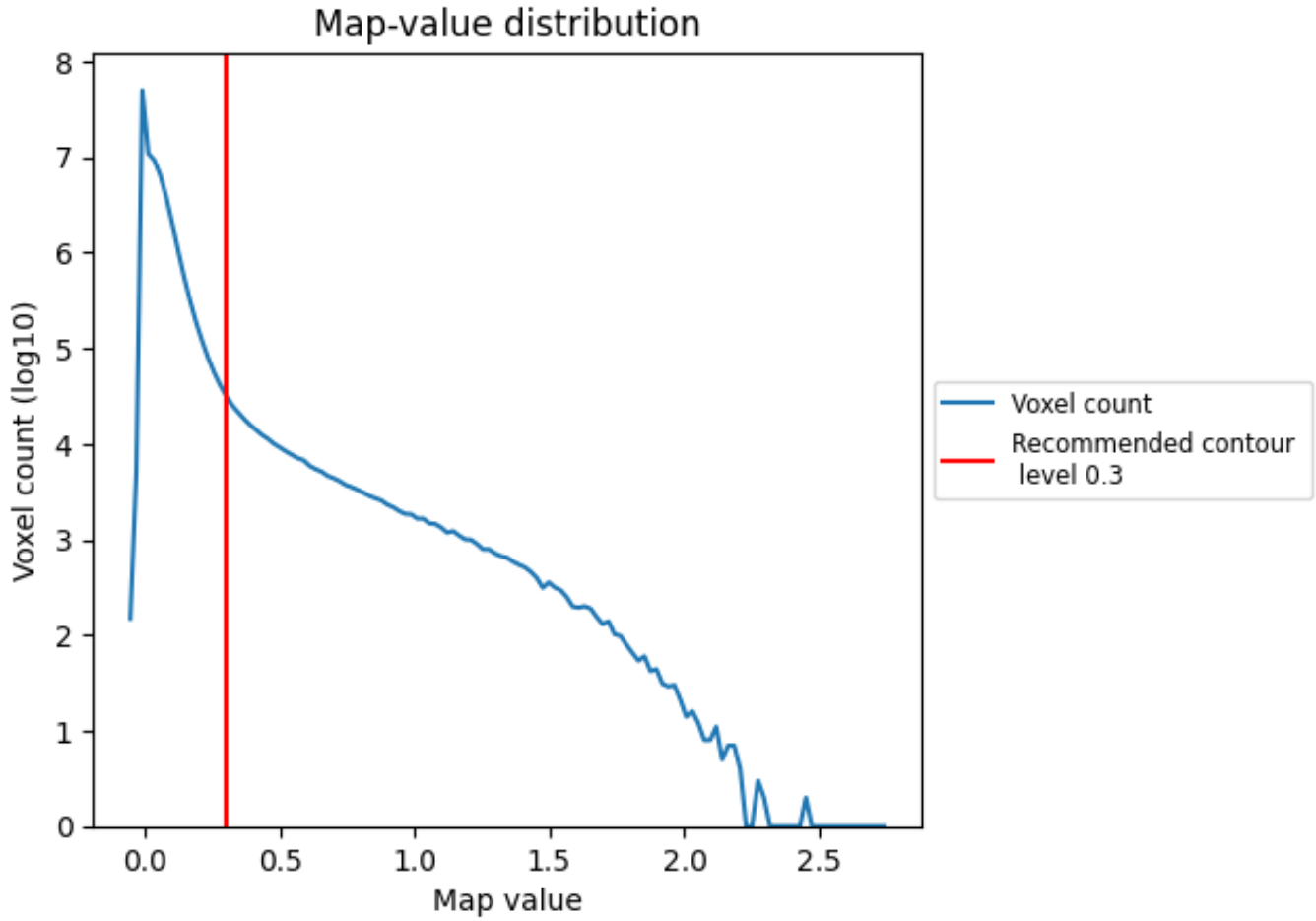
6.6 Mask visualisation (i)

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

7 Map analysis

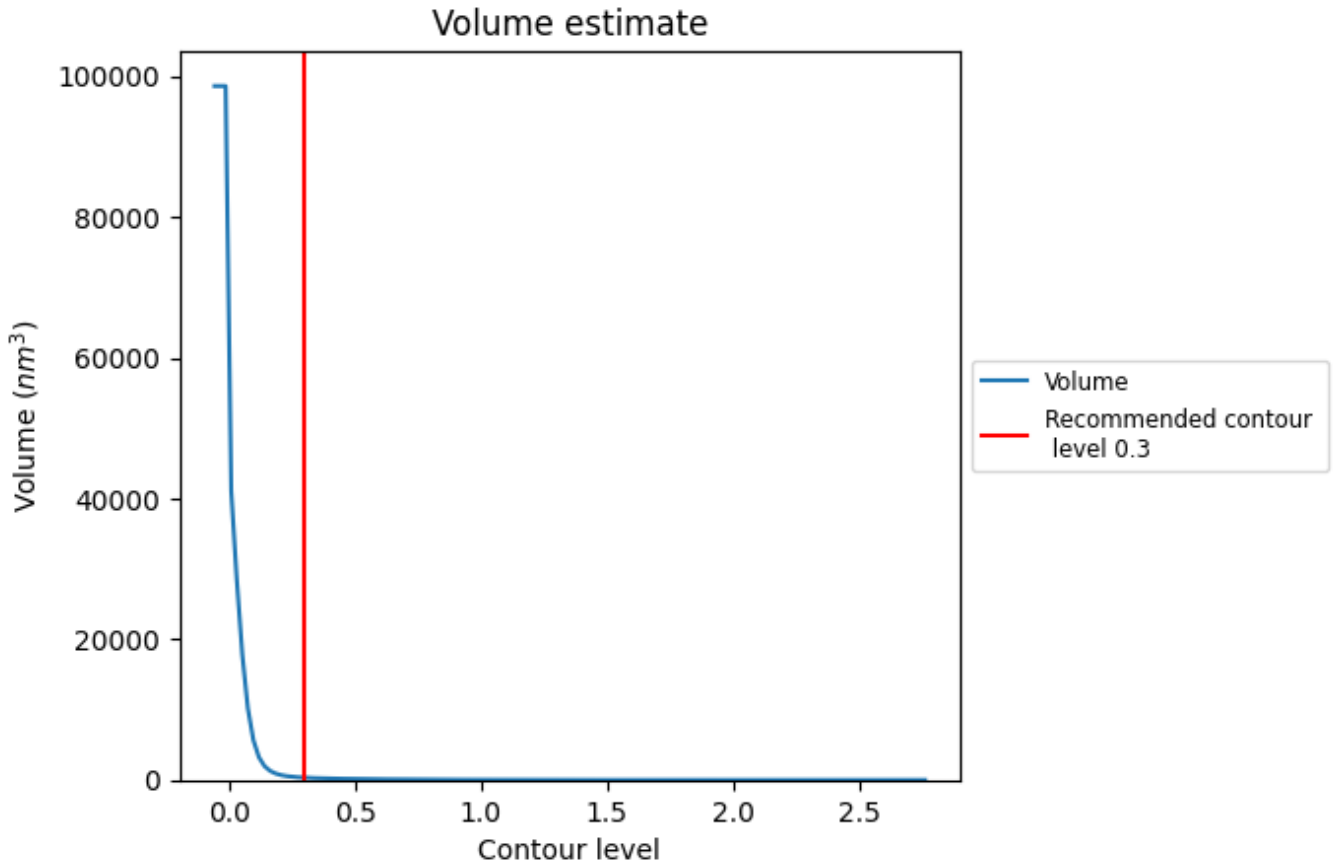
This section contains the results of statistical analysis of the map.

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.

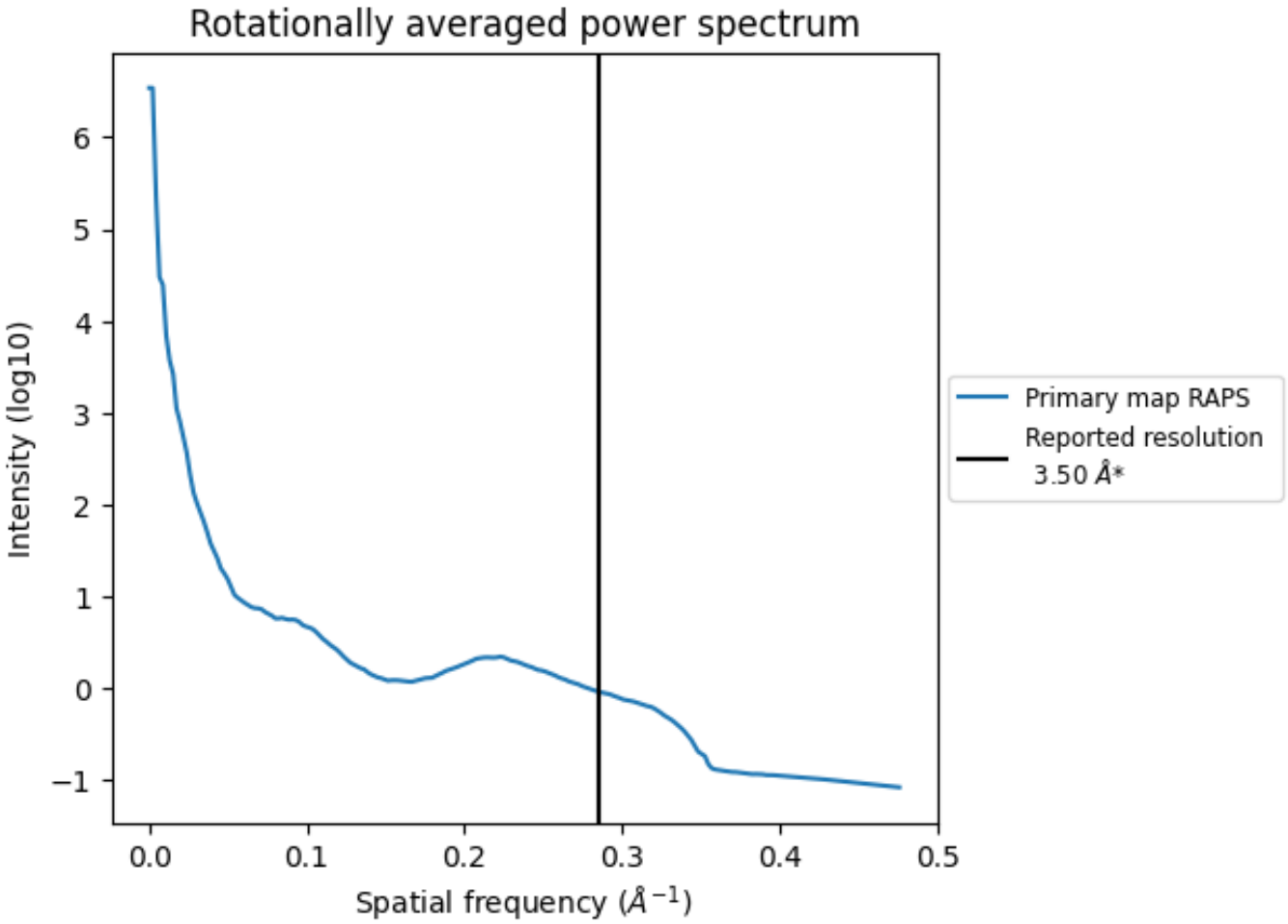
7.2 Volume estimate (i)



The volume at the recommended contour level is 330 nm^3; this corresponds to an approximate mass of 298 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 0.286 Å^{-1}

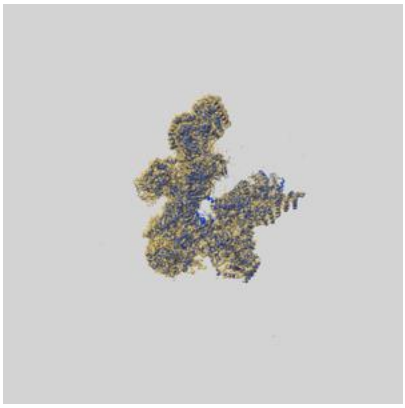
8 Fourier-Shell correlation (i)

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

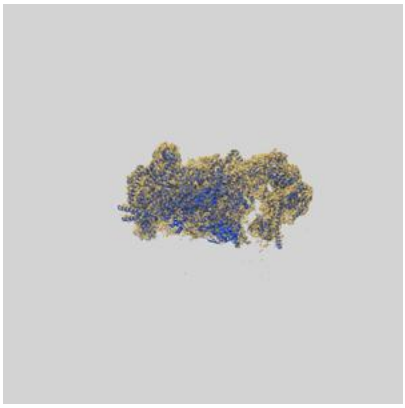
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18496 and PDB model 8QMA. Per-residue inclusion information can be found in section 3 on page 8.

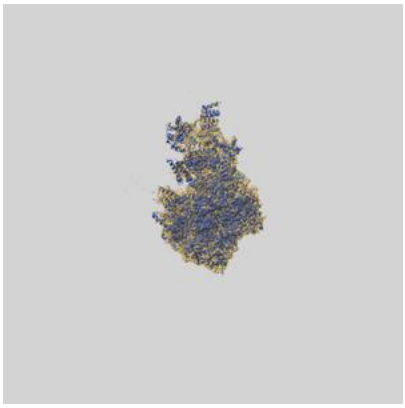
9.1 Map-model overlay



X



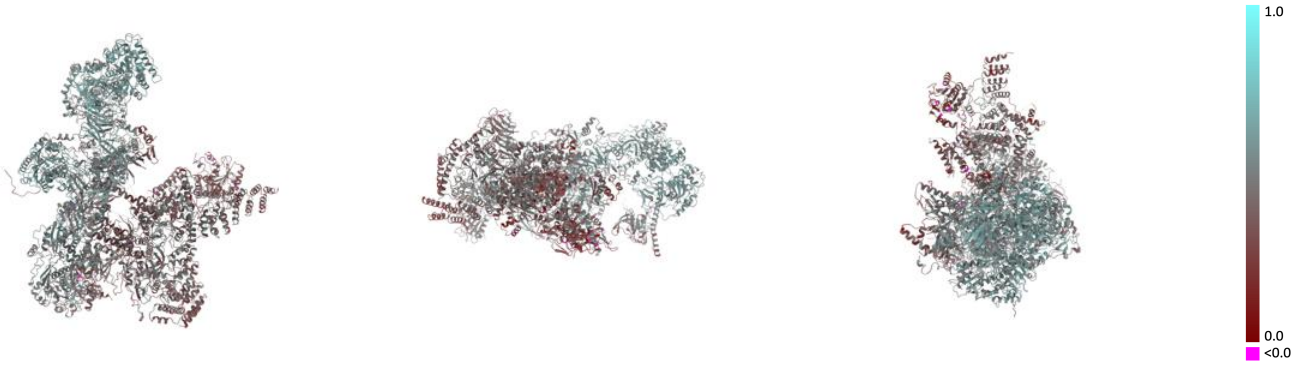
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

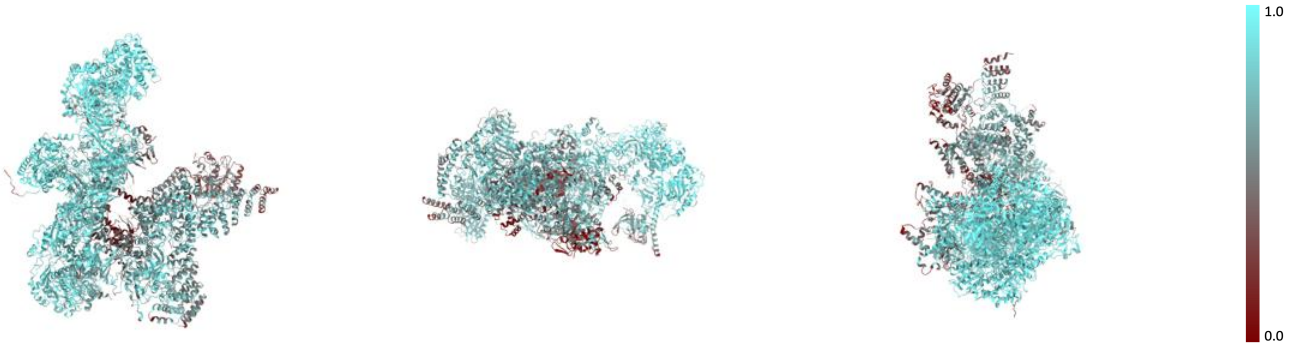
9.2 Q-score mapped to coordinate model



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.

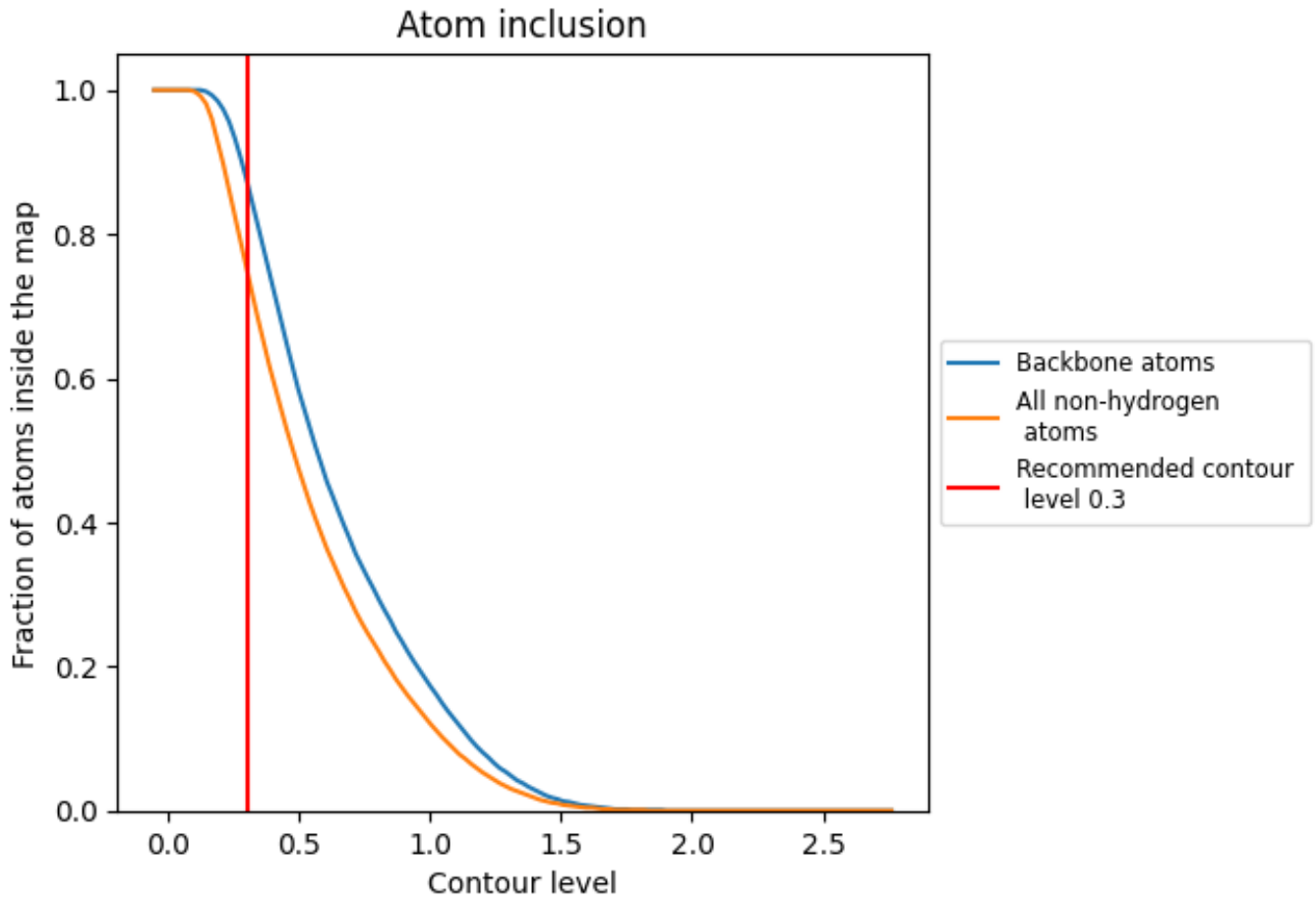
9.3 Atom inclusion mapped to coordinate model



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 75% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7480	0.4610
A	0.7720	0.4740
B	0.7140	0.4630
C	0.8410	0.4650
D	0.7880	0.4570
E	0.6290	0.3910
F	0.8230	0.5210
G	0.9470	0.5820
H	0.8900	0.5200
I	0.8950	0.4900
J	0.7330	0.4160
K	0.6930	0.4000
L	0.9250	0.5620
M	0.9050	0.5460
N	0.7800	0.4330
O	0.3140	0.2910
P	0.4840	0.3120
R	0.9340	0.5890
S	0.9210	0.5640
T	0.4820	0.3490