wwPDB EM Validation Summary Report (i)

Mar 5, 2024 – 12:59 pm GMT

PDB ID	:	8R6S
EMDB ID	:	EMD-18935
Title	:	Plastid-encoded RNA polymerase (Integrated model)
Authors	:	Webster, M.W.; Pramanick, I.; Vergara-Cruces, A.
Deposited on	:	2023-11-22
Resolution	:	2.49 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

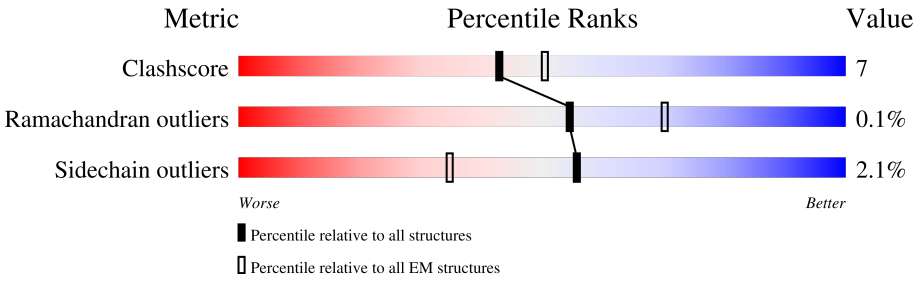
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.49 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	327	17% 76% 15% • 8%
1	B	327	28% 72% 13% 13%
2	C	1072	38% 73% 15% • 10%
3	D	680	25% 70% 14% 16%
4	E	1373	26% 66% 13% • 21%
5	F	911	22% 57% 11% 31%
6	G	862	78% 70% 16% 13%
7	H	675	32% 71% 10% • 19%

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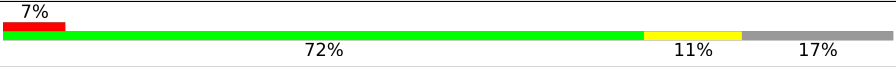
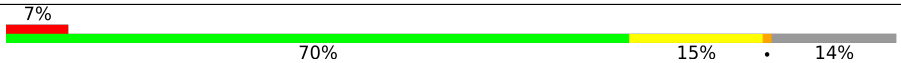
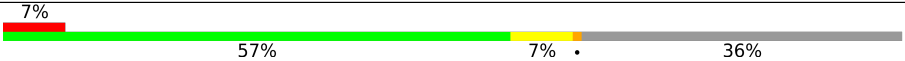
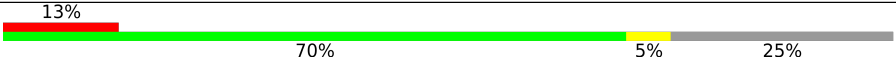
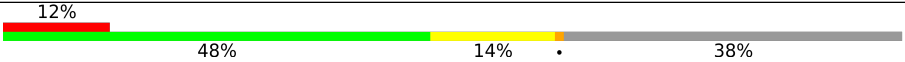
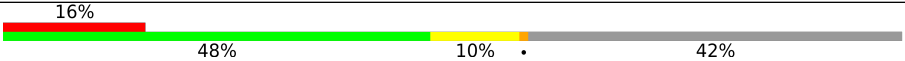
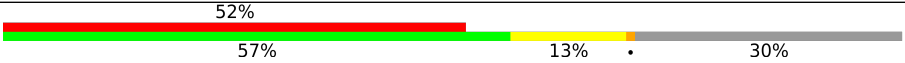
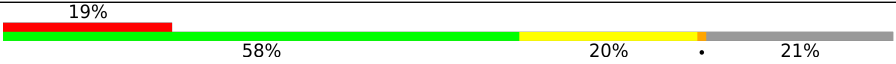
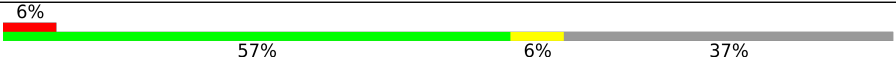
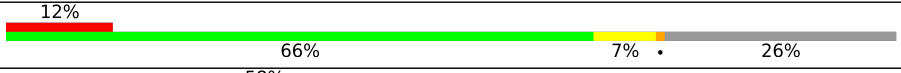
Mol	Chain	Length	Quality of chain
8	I	263	
9	J	529	
10	K	460	
11	L	483	
12	M	334	
13	N	297	
14	O	185	
14	P	185	
15	Q	768	
16	R	162	
17	S	611	
18	T	140	
19	U	187	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 67366 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	301	Total	C	N	O	S	0	0
			2449	1571	422	446	10		
1	B	283	Total	C	N	O	S	0	0
			2292	1461	395	425	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	PHE	SER	conflict	UNP A0A6C0M610
B	67	PHE	SER	conflict	UNP A0A6C0M610

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	961	Total	C	N	O	S	0	0
			7685	4910	1340	1405	30		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	113	PHE	SER	conflict	UNP A0A6C0M5W1
C	657	VAL	ILE	conflict	UNP A0A6C0M5W1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	571	Total	C	N	O	S	0	0
			4664	3006	815	817	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	1091	Total	C	N	O	S	0	0
			8758	5612	1554	1561	31		

- Molecule 5 is a protein called PAP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	629	Total	C	N	O	S	0	0
			5052	3198	879	942	33		

- Molecule 6 is a protein called PAP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	748	Total	C	N	O	S	0	0
			5887	3723	994	1131	39		

- Molecule 7 is a protein called PAP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	549	Total	C	N	O	S	0	0
			4607	2937	799	854	17		

- Molecule 8 is a protein called PAP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	215	Total	C	N	O	S	0	0
			1771	1141	300	324	6		

- Molecule 9 is a protein called PAP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	234	Total	C	N	O	S	0	0
			1970	1247	350	363	10		

- Molecule 10 is a protein called PAP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	384	Total	C	N	O	S	0	0
			3103	1985	520	583	15		

- Molecule 11 is a protein called PAP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	416	Total	C	N	O	S	0	0
			3403	2183	580	620	20		

- Molecule 12 is a protein called PAP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	215	Total	C	N	O	S	0	0
			1803	1142	312	341	8		

- Molecule 13 is a protein called PAP9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	224	Total	C	N	O	S	0	0
			1819	1168	309	338	4		

- Molecule 14 is a protein called PAP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	114	Total	C	N	O	S	0	0
			923	588	148	178	9		
14	P	108	Total	C	N	O	S	0	0
			865	550	139	167	9		

- Molecule 15 is a protein called PAP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	539	Total	C	N	O	S	0	0
			4148	2584	706	833	25		

- Molecule 16 is a protein called PAP12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	128	Total	C	N	O	S	0	0
			1069	672	193	201	3		

- Molecule 17 is a protein called FLN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	386	Total	C	N	O	S	0	0
			3056	1941	516	578	21		

- Molecule 18 is a protein called PTAC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	104	Total	C	N	O	S	0	0
			881	572	148	157	4		

- Molecule 19 is a protein called PRIN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	109	Total	C	N	O	S	0	0
			877	561	144	169	3		

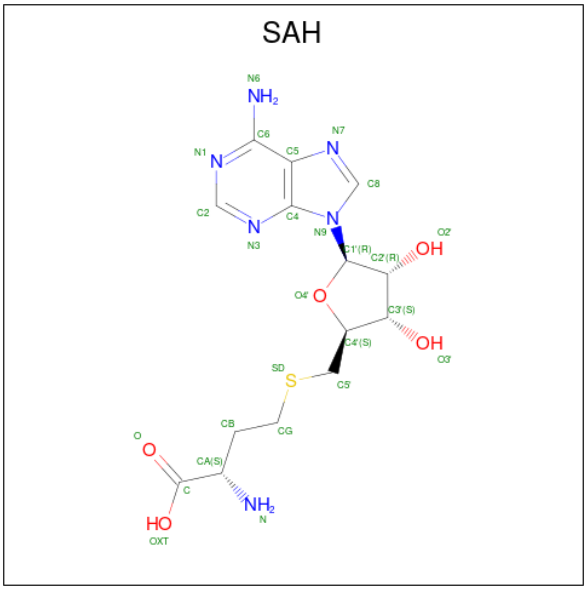
- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	E	1	Total	Zn	0
			1	1	

- Molecule 21 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
21	I	1	Total	Fe	0
			1	1	
21	N	1	Total	Fe	0
			1	1	

- Molecule 22 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
22	L	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 23 is water.

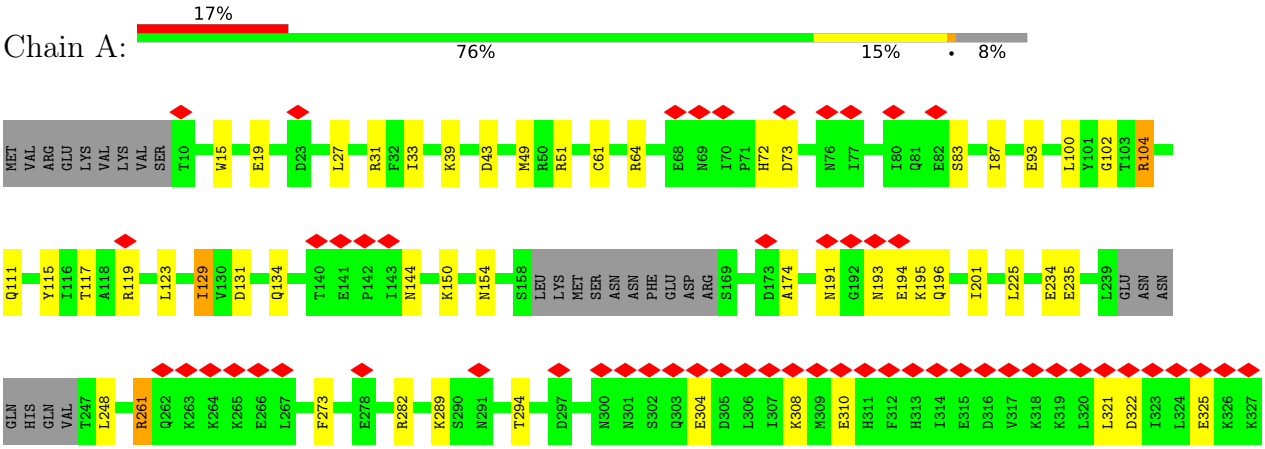
Mol	Chain	Residues	Atoms		AltConf
23	A	18	Total	O	0
			18	18	
23	B	13	Total	O	0
			13	13	
23	C	57	Total	O	0
			57	57	
23	D	21	Total	O	0
			21	21	
23	E	25	Total	O	0
			25	25	
23	F	1	Total	O	0
			1	1	
23	H	6	Total	O	0
			6	6	
23	I	4	Total	O	0
			4	4	
23	J	31	Total	O	0
			31	31	
23	K	15	Total	O	0
			15	15	
23	L	19	Total	O	0
			19	19	
23	M	13	Total	O	0
			13	13	
23	N	3	Total	O	0
			3	3	
23	O	2	Total	O	0
			2	2	
23	P	2	Total	O	0
			2	2	
23	R	2	Total	O	0
			2	2	
23	S	23	Total	O	0
			23	23	

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.

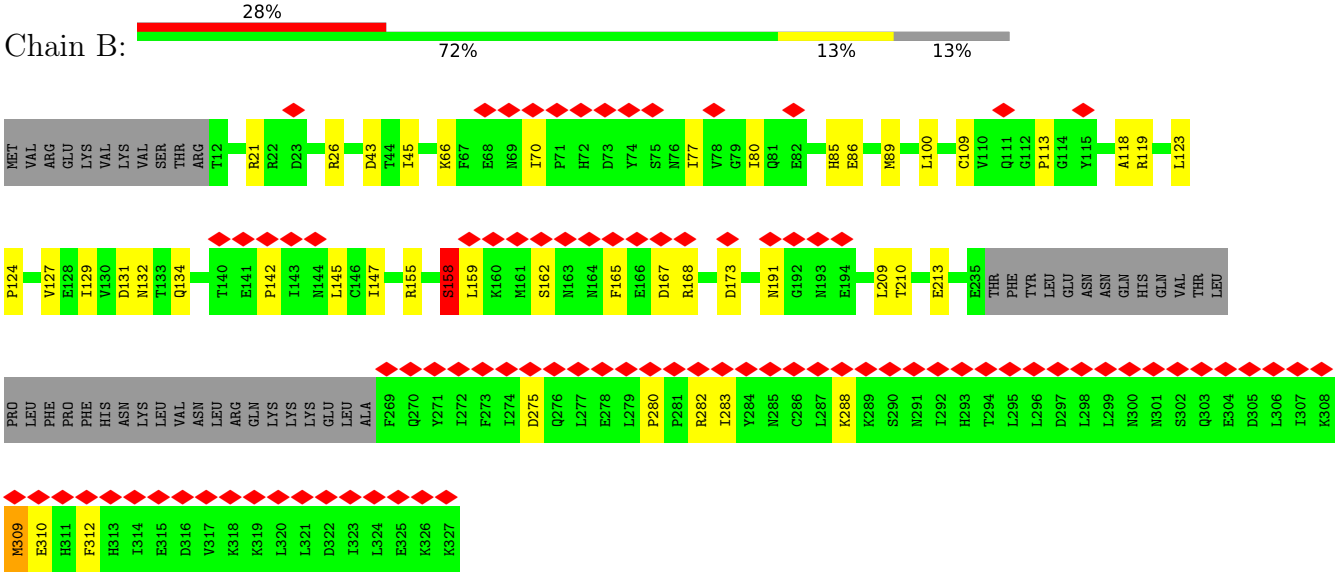
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



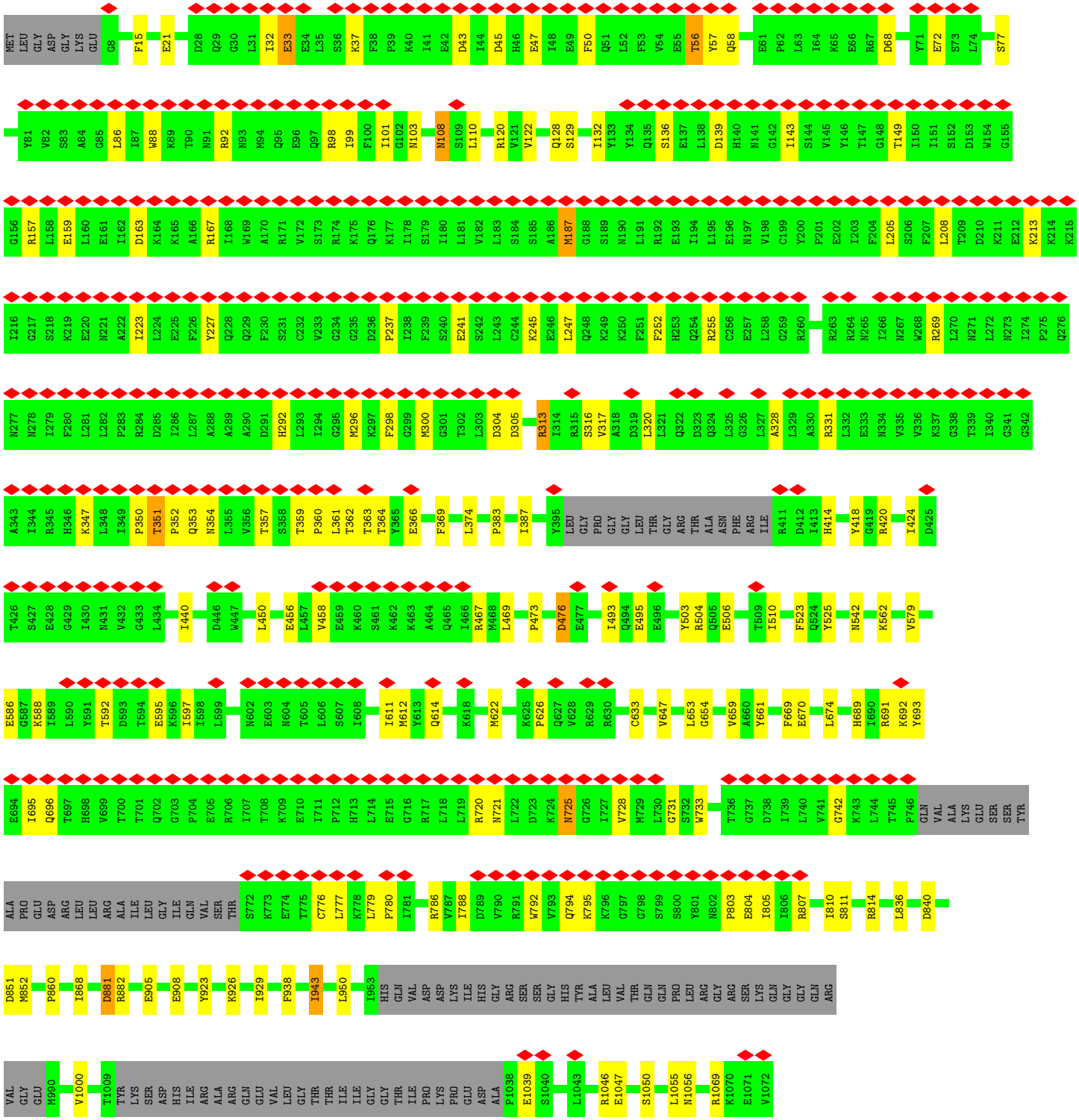
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



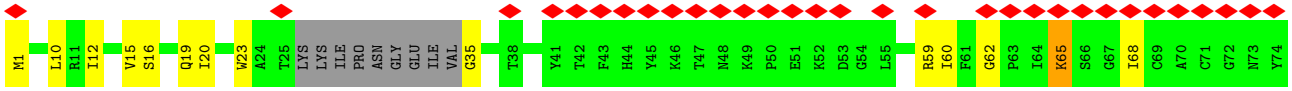
• Molecule 2: DNA-directed RNA polymerase subunit beta

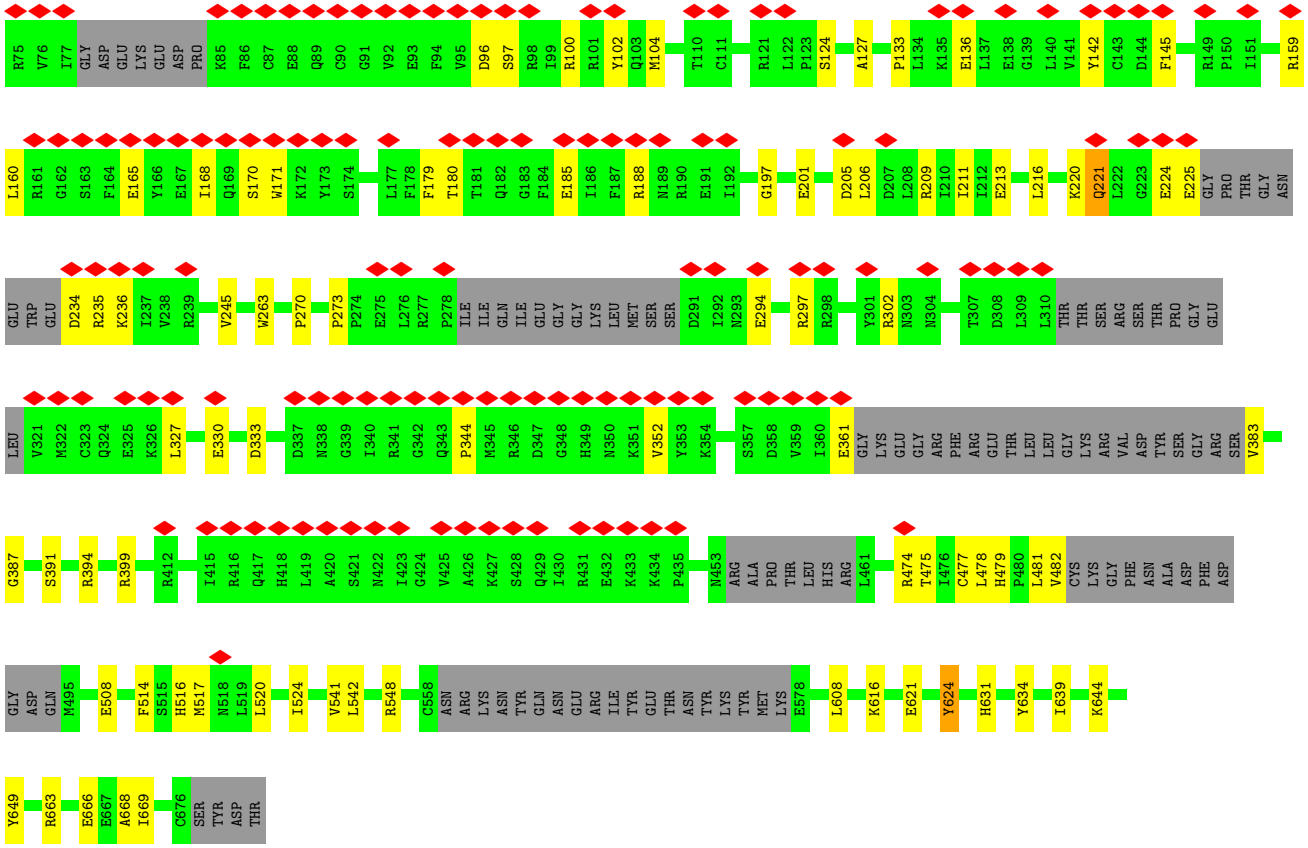
Chain C:



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

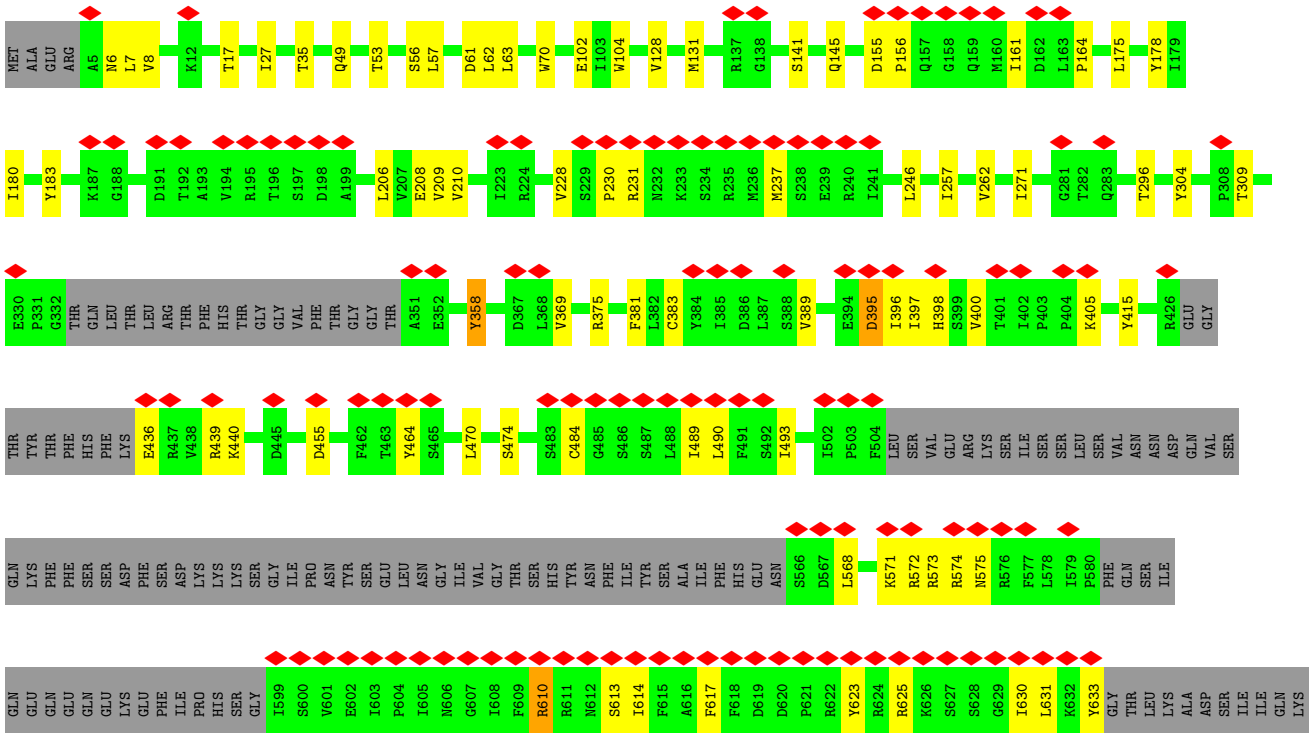
Chain D:

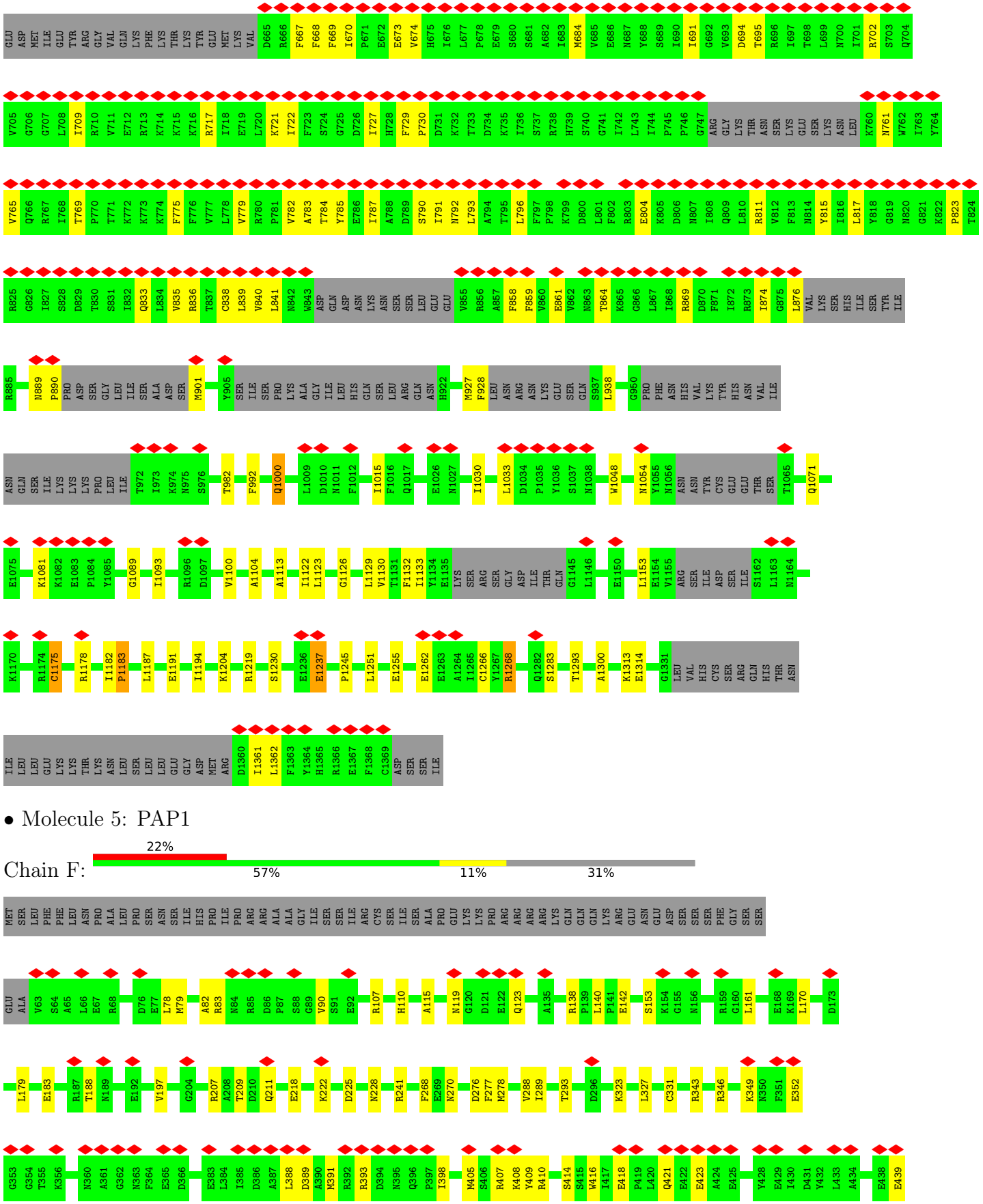




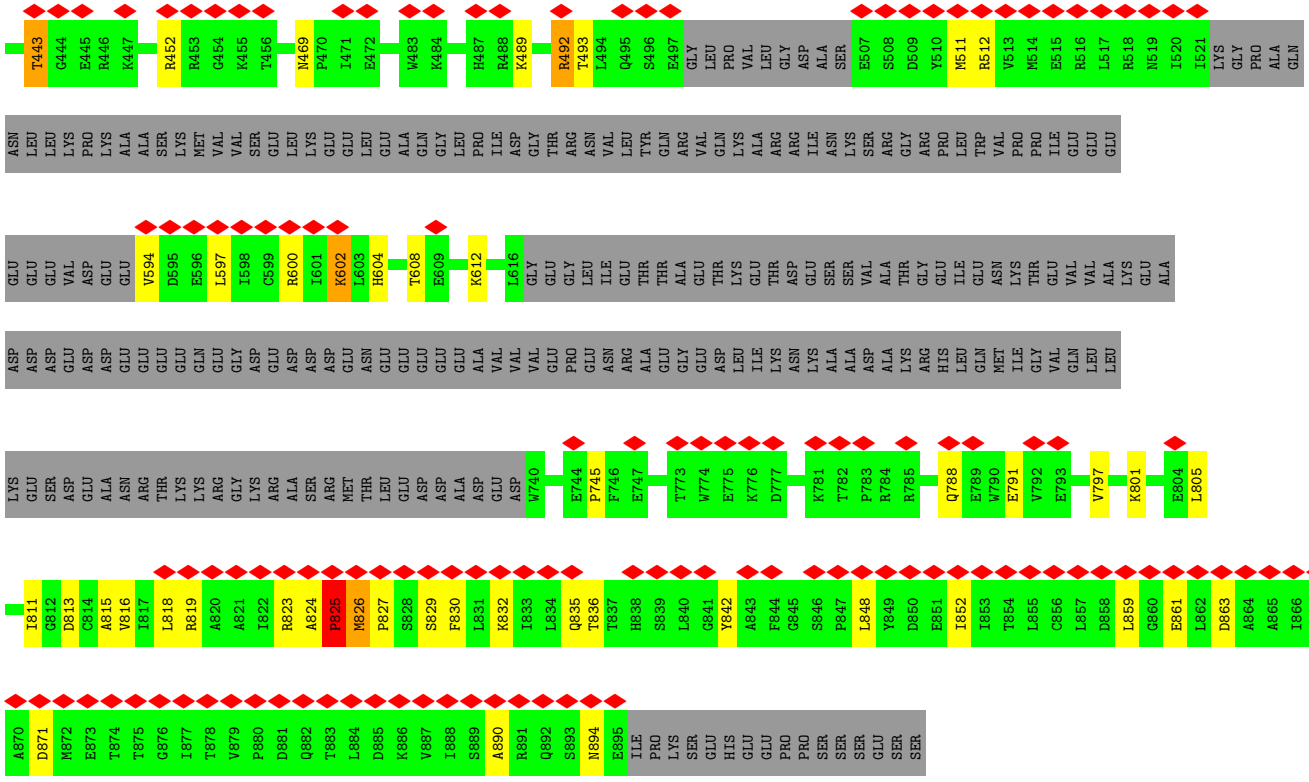
• Molecule 4: DNA-directed RNA polymerase subunit beta"

Chain E:



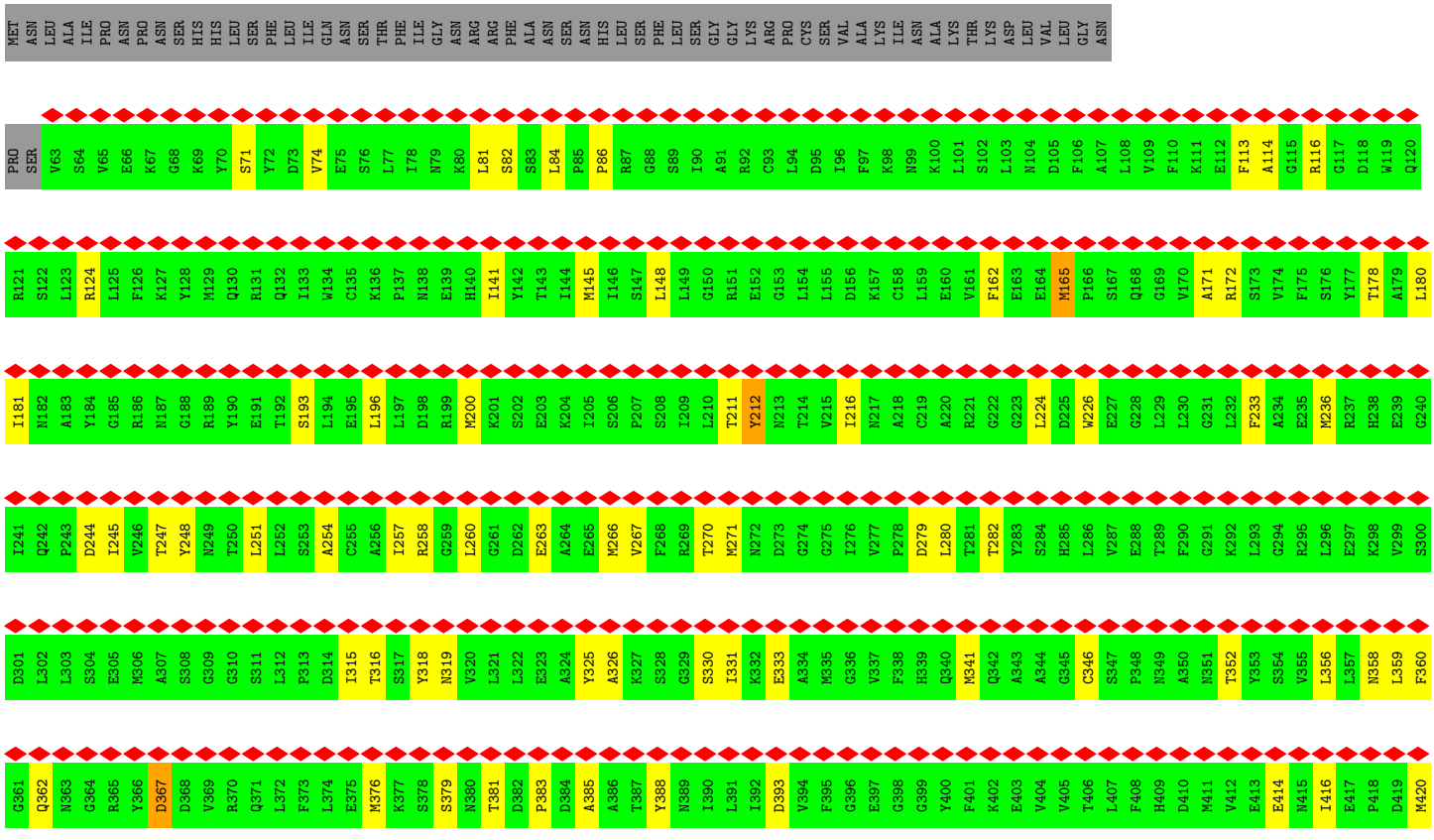


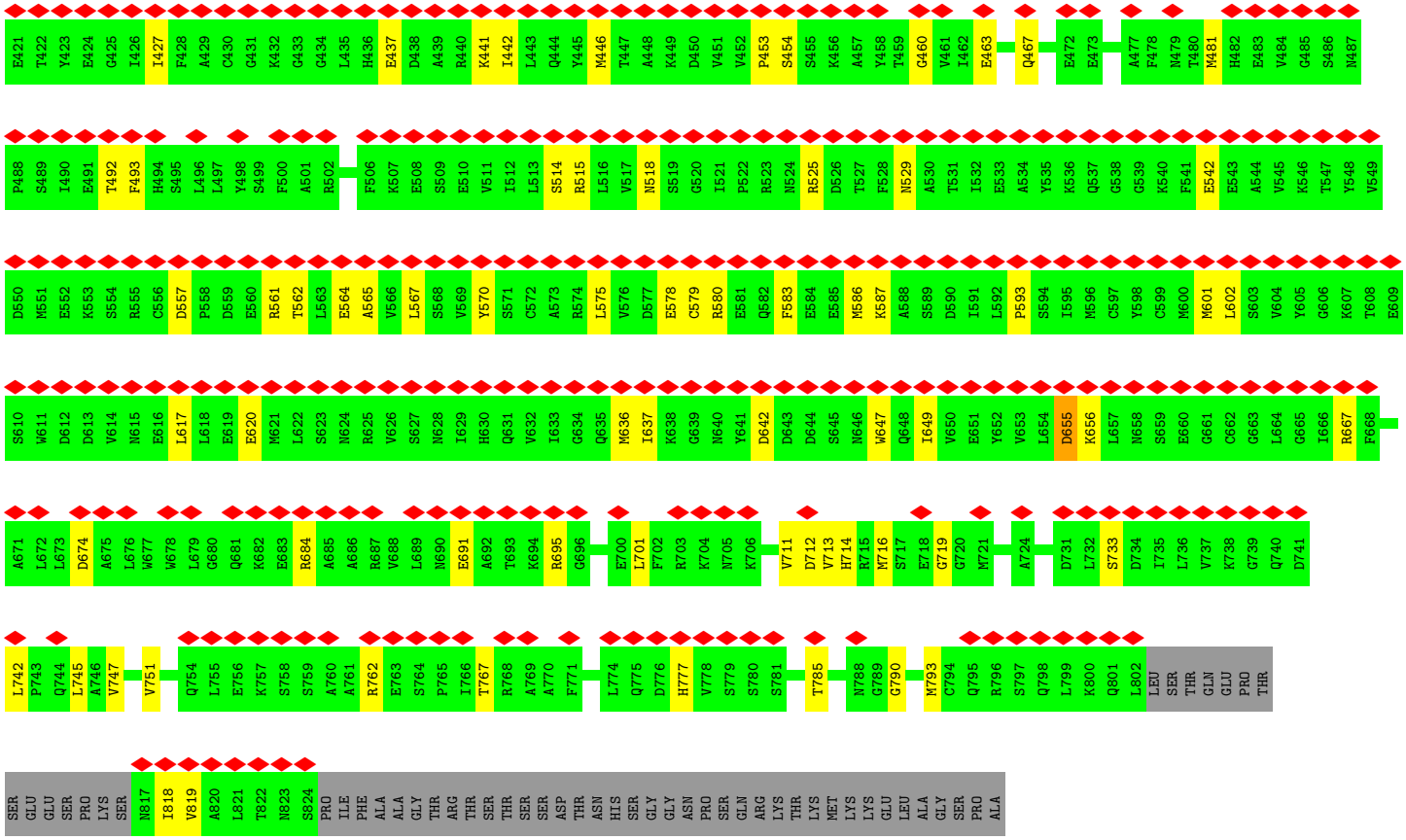
• Molecule 5: PAP1



• Molecule 6: PAP2

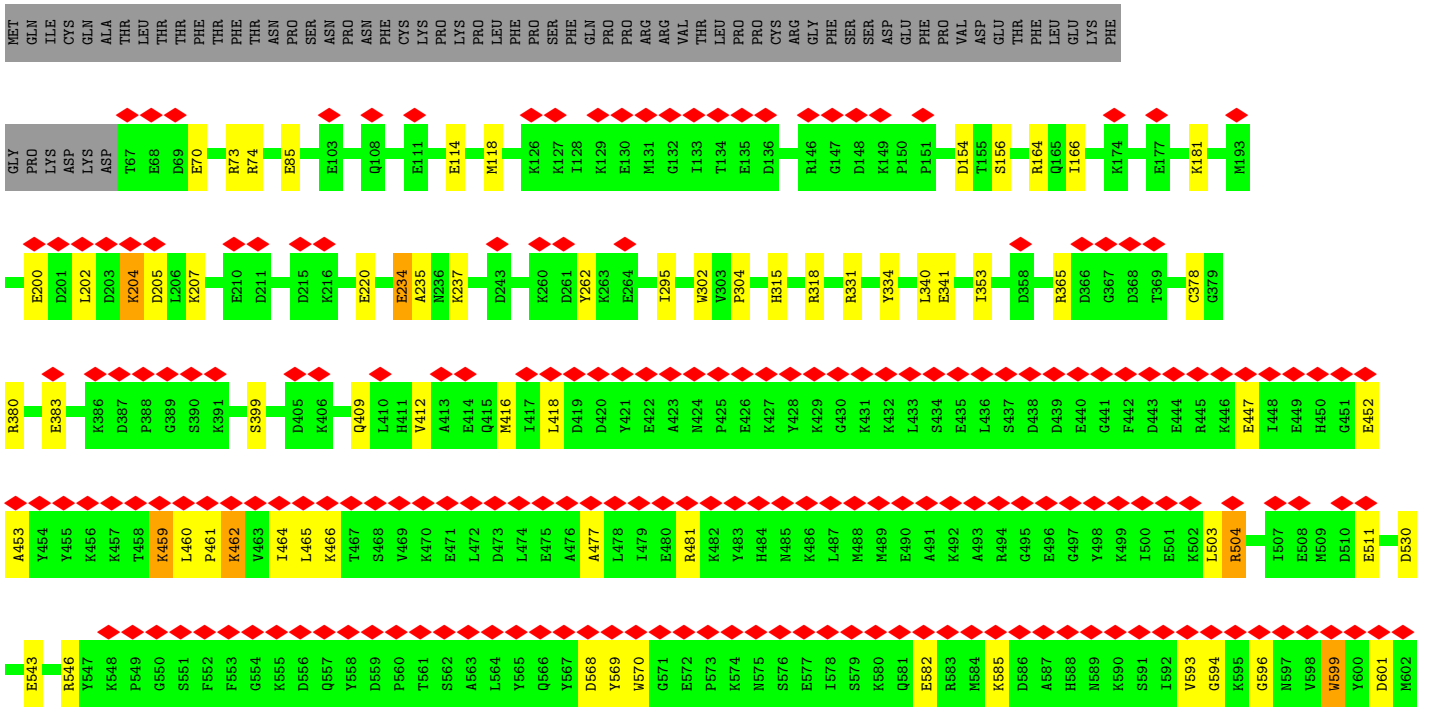
Chain G:

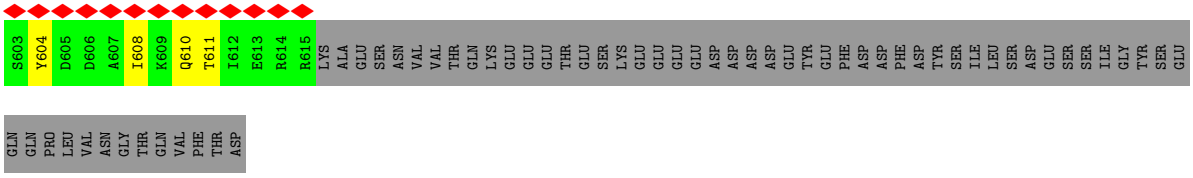




• Molecule 7: PAP3

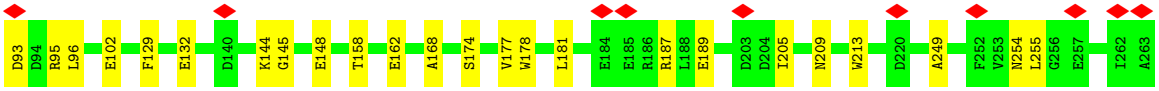
Chain H:





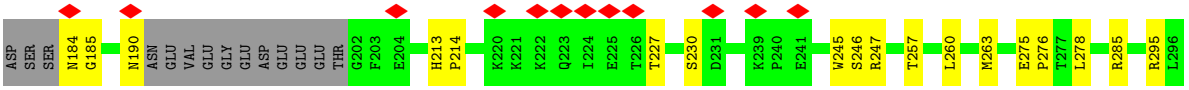
• Molecule 8: PAP4

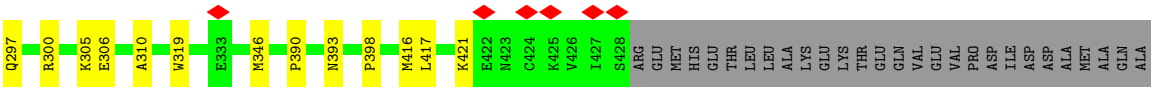
Chain I:



• Molecule 9: PAP5

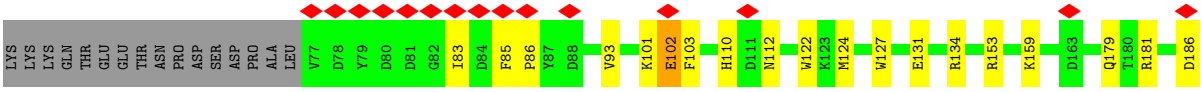
Chain J:

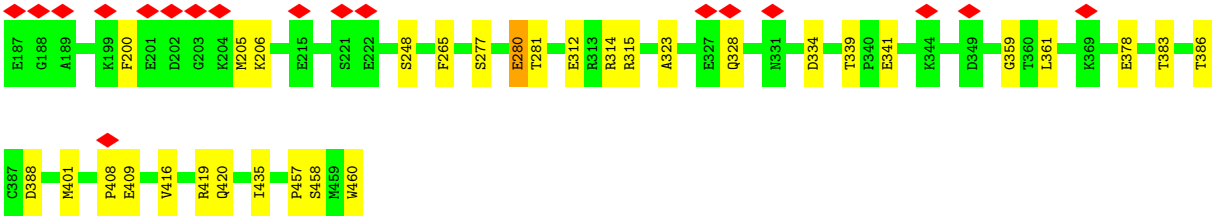




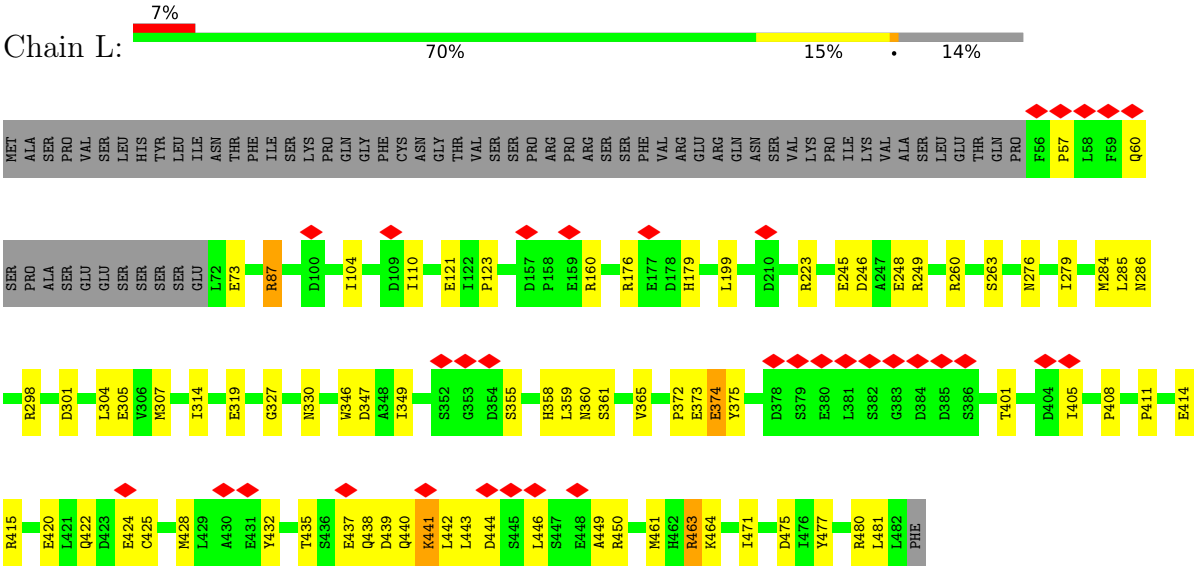
• Molecule 10: PAP6

Chain K:

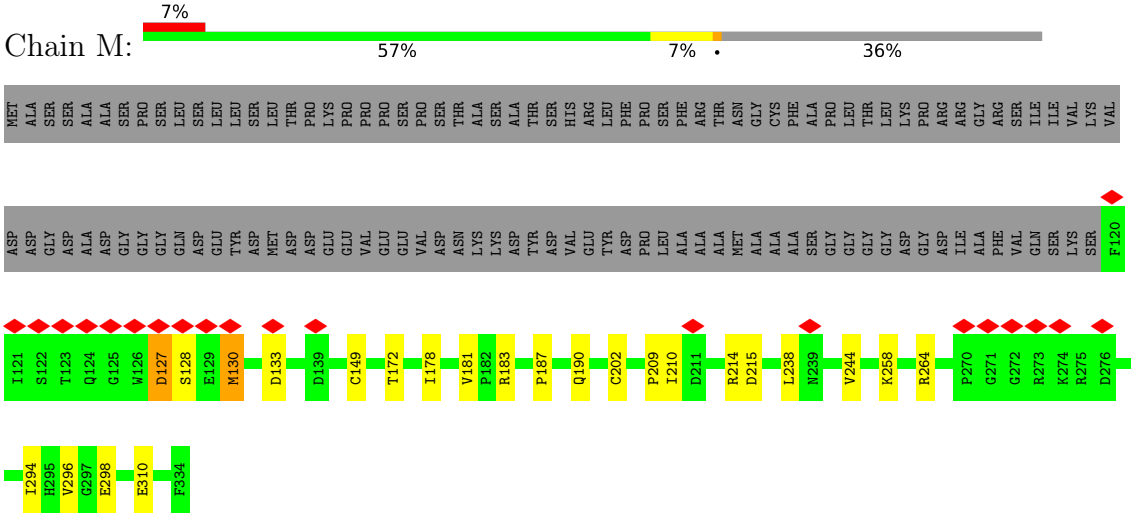




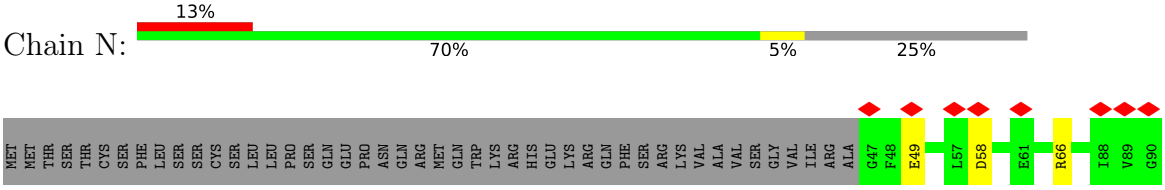
• Molecule 11: PAP7

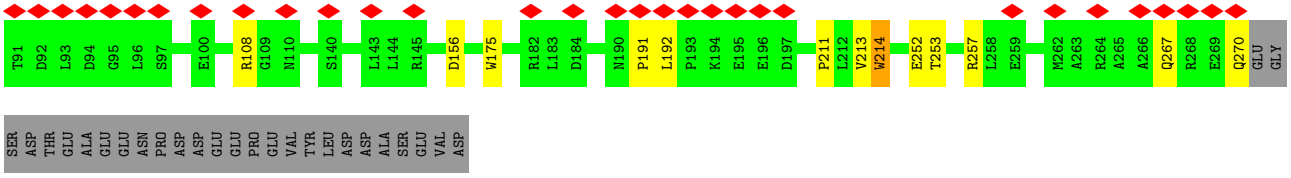


• Molecule 12: PAP8

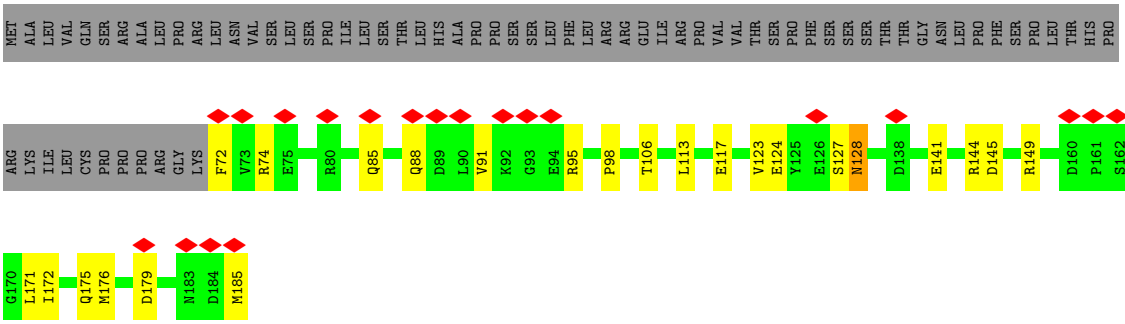


• Molecule 13: PAP9

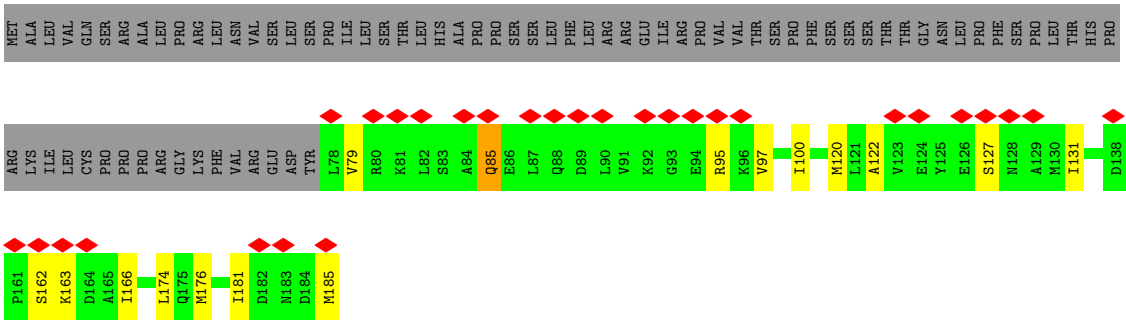




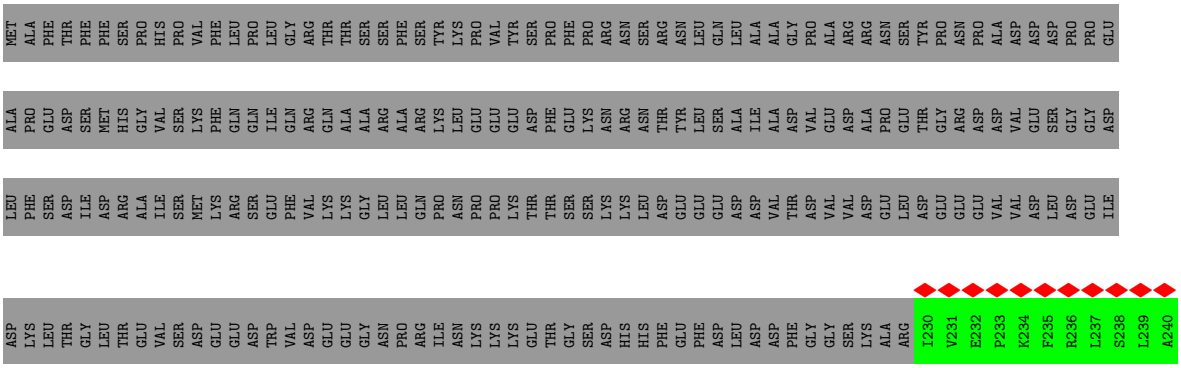
• Molecule 14: PAP10

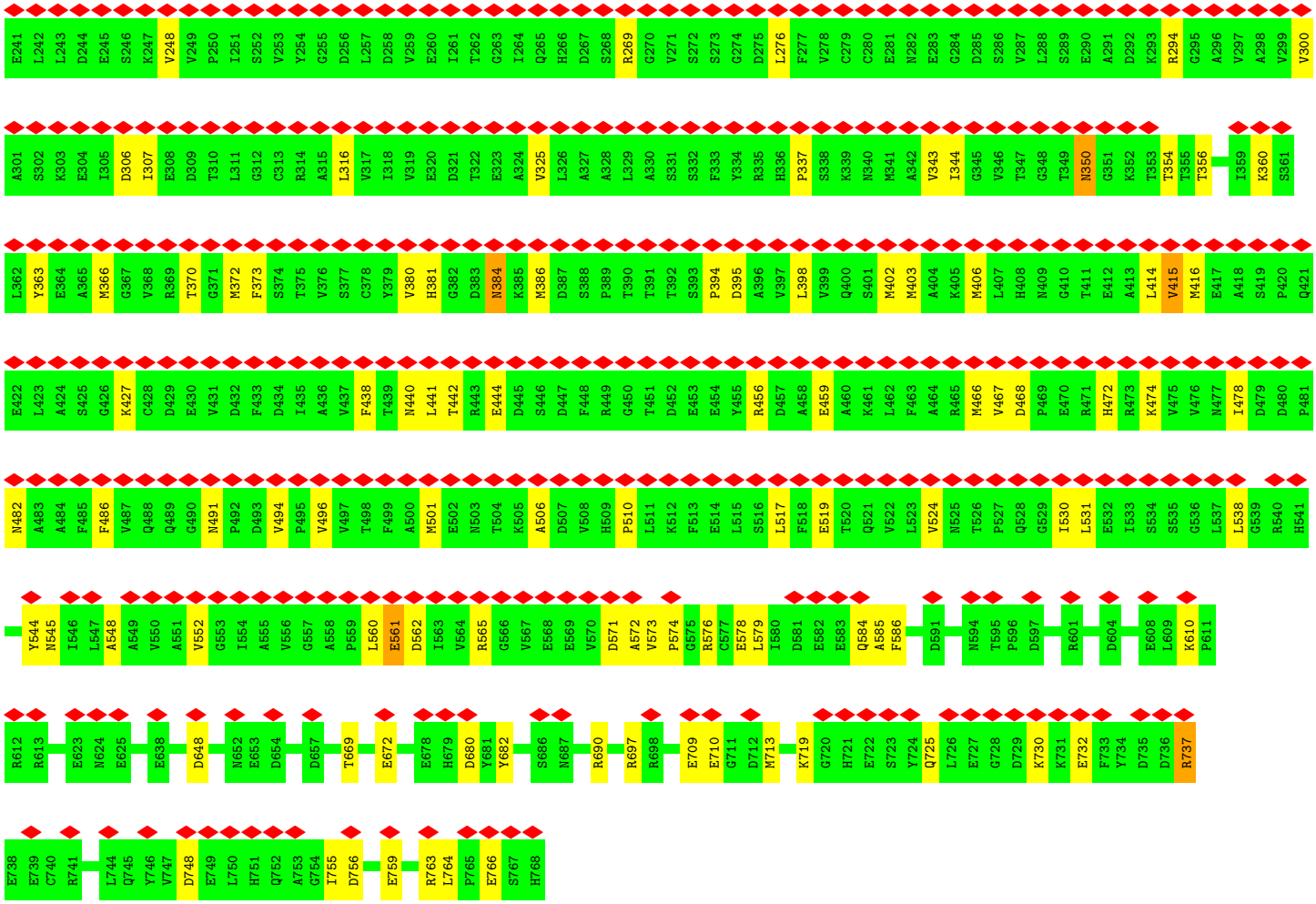


• Molecule 14: PAP10



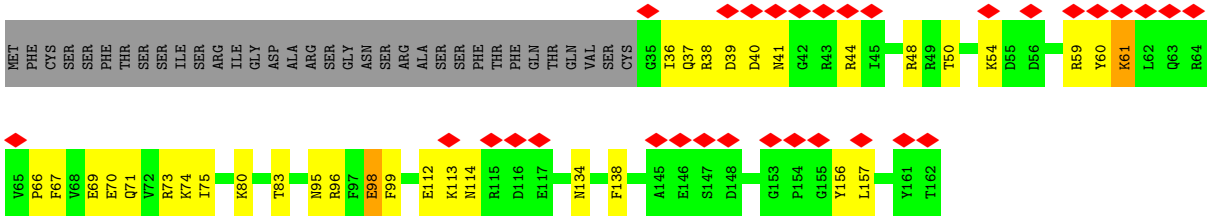
• Molecule 15: PAP11





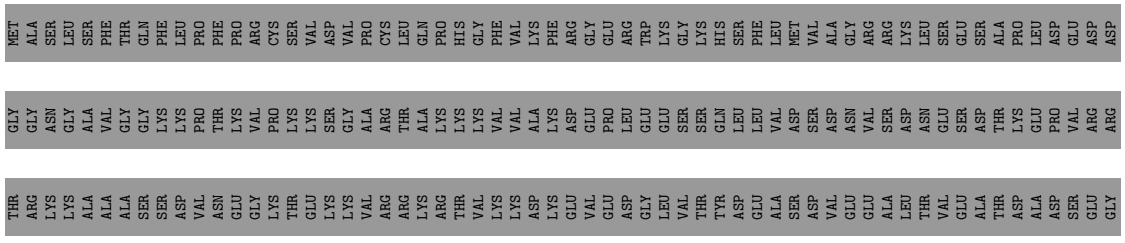
• Molecule 16: PAP12

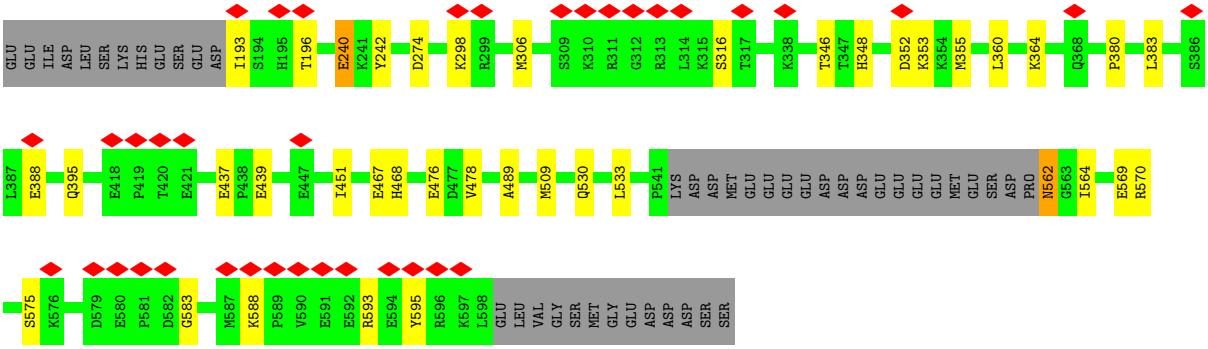
Chain R:



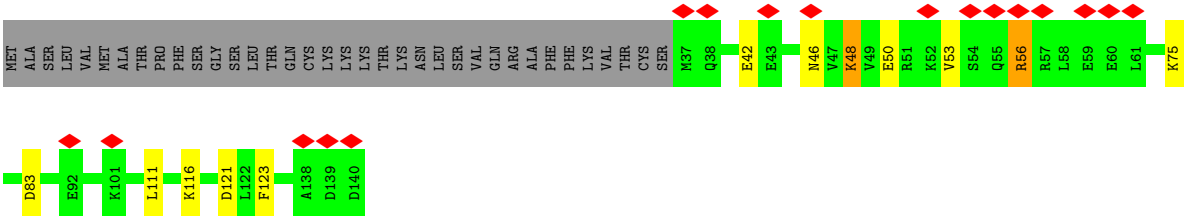
• Molecule 17: FLN2

Chain S:

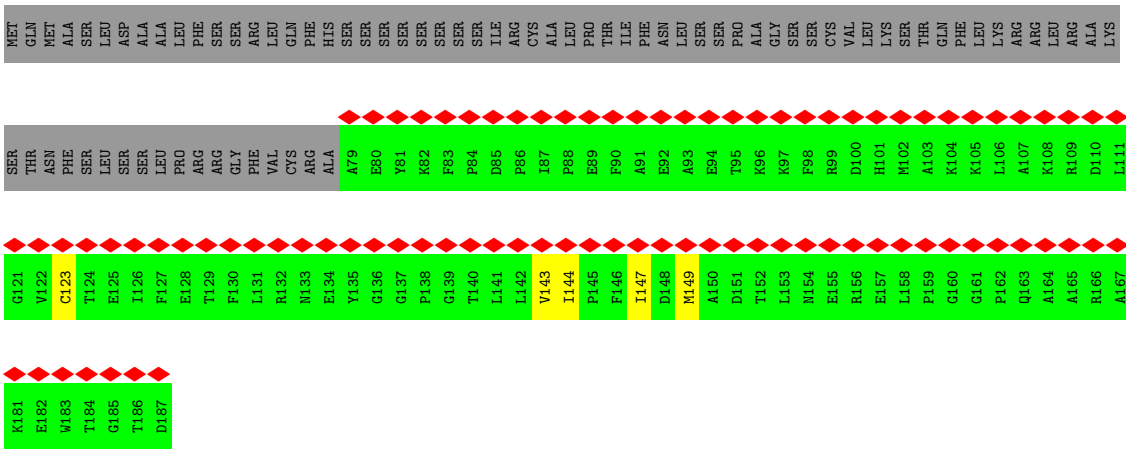




• Molecule 18: PTAC18



• Molecule 19: PRIN2



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	613537	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	300.0, 300.0, 300.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5, 0.5, 0.5	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.27	0/2498	0.50	0/3377
1	B	0.27	0/2336	0.52	0/3159
2	C	0.27	0/7842	0.50	0/10587
3	D	0.28	0/4765	0.50	0/6437
4	E	0.27	0/8932	0.52	1/12058 (0.0%)
5	F	0.27	0/5154	0.48	0/6964
6	G	0.25	0/5997	0.44	0/8096
7	H	0.27	0/4736	0.48	0/6386
8	I	0.28	0/1825	0.47	0/2481
9	J	0.27	0/2021	0.50	0/2724
10	K	0.27	0/3184	0.48	0/4320
11	L	0.29	0/3492	0.48	0/4727
12	M	0.31	0/1848	0.53	0/2502
13	N	0.27	0/1873	0.47	0/2549
14	O	0.27	0/939	0.50	0/1268
14	P	0.30	0/879	0.53	0/1187
15	Q	0.26	0/4218	0.49	0/5720
16	R	0.28	0/1089	0.52	0/1462
17	S	0.28	0/3123	0.49	0/4226
18	T	0.29	0/906	0.51	0/1225
19	U	0.24	0/900	0.40	0/1219
All	All	0.27	0/68557	0.49	1/92674 (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
1	B	0	1
5	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	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})
4	E	890	PRO	CA-N-CD	-8.57	99.50	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	158	SER	Peptide
5	F	418	GLU	Peptide
5	F	825	PRO	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	2449	0	2490	32	0
1	B	2292	0	2311	41	0
2	C	7685	0	7774	125	0
3	D	4664	0	4741	76	0
4	E	8758	0	8895	176	0
5	F	5052	0	5003	77	0
6	G	5887	0	5803	116	0
7	H	4607	0	4464	65	0
8	I	1771	0	1696	19	0
9	J	1970	0	1923	23	0
10	K	3103	0	3026	47	0
11	L	3403	0	3347	59	0
12	M	1803	0	1756	18	0
13	N	1819	0	1746	8	0
14	O	923	0	917	30	0
14	P	865	0	867	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Q	4148	0	4046	86	0
16	R	1069	0	1058	31	0
17	S	3056	0	3042	26	0
18	T	881	0	860	8	0
19	U	877	0	840	32	0
20	E	1	0	0	0	0
21	I	1	0	0	0	0
21	N	1	0	0	0	0
22	L	26	0	19	1	0
23	A	18	0	0	0	0
23	B	13	0	0	0	0
23	C	57	0	0	1	0
23	D	21	0	0	0	0
23	E	25	0	0	0	0
23	F	1	0	0	0	0
23	H	6	0	0	0	0
23	I	4	0	0	0	0
23	J	31	0	0	0	0
23	K	15	0	0	0	0
23	L	19	0	0	1	0
23	M	13	0	0	1	0
23	N	3	0	0	0	0
23	O	2	0	0	0	0
23	P	2	0	0	0	0
23	R	2	0	0	0	0
23	S	23	0	0	0	0
All	All	67366	0	66624	953	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 7.

The worst 5 of 953 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)
4:E:729:PHE:CD1	19:U:143:VAL:HB	1.35	1.58
4:E:729:PHE:CG	19:U:143:VAL:CG2	1.82	1.55
4:E:729:PHE:CE2	19:U:169:ILE:HD11	1.45	1.51
4:E:729:PHE:CG	19:U:143:VAL:HG21	1.40	1.45
4:E:729:PHE:CB	19:U:143:VAL:HG21	0.97	1.43

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	295/327 (90%)	284 (96%)	11 (4%)	0	100	100
1	B	279/327 (85%)	268 (96%)	11 (4%)	0	100	100
2	C	951/1072 (89%)	932 (98%)	19 (2%)	0	100	100
3	D	551/680 (81%)	533 (97%)	18 (3%)	0	100	100
4	E	1057/1373 (77%)	1019 (96%)	36 (3%)	2 (0%)	47	68
5	F	621/911 (68%)	601 (97%)	19 (3%)	1 (0%)	47	68
6	G	744/862 (86%)	725 (97%)	19 (3%)	0	100	100
7	H	547/675 (81%)	533 (97%)	14 (3%)	0	100	100
8	I	213/263 (81%)	205 (96%)	8 (4%)	0	100	100
9	J	230/529 (44%)	222 (96%)	8 (4%)	0	100	100
10	K	382/460 (83%)	369 (97%)	13 (3%)	0	100	100
11	L	412/483 (85%)	403 (98%)	8 (2%)	1 (0%)	47	68
12	M	213/334 (64%)	210 (99%)	3 (1%)	0	100	100
13	N	222/297 (75%)	216 (97%)	6 (3%)	0	100	100
14	O	112/185 (60%)	110 (98%)	2 (2%)	0	100	100
14	P	106/185 (57%)	103 (97%)	3 (3%)	0	100	100
15	Q	537/768 (70%)	527 (98%)	10 (2%)	0	100	100
16	R	126/162 (78%)	119 (94%)	6 (5%)	1 (1%)	19	35
17	S	382/611 (62%)	365 (96%)	17 (4%)	0	100	100
18	T	102/140 (73%)	98 (96%)	4 (4%)	0	100	100
19	U	107/187 (57%)	104 (97%)	3 (3%)	0	100	100
All	All	8189/10831 (76%)	7946 (97%)	238 (3%)	5 (0%)	54	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	1183	PRO
5	F	825	PRO
11	L	405	ILE
16	R	40	ASP
4	E	489	ILE

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	275/301 (91%)	267 (97%)	8 (3%)	42	69
1	B	258/301 (86%)	249 (96%)	9 (4%)	36	62
2	C	843/931 (90%)	826 (98%)	17 (2%)	55	79
3	D	514/608 (84%)	503 (98%)	11 (2%)	53	78
4	E	969/1230 (79%)	953 (98%)	16 (2%)	60	82
5	F	538/782 (69%)	522 (97%)	16 (3%)	41	68
6	G	642/740 (87%)	628 (98%)	14 (2%)	52	77
7	H	488/609 (80%)	478 (98%)	10 (2%)	55	79
8	I	187/230 (81%)	186 (100%)	1 (0%)	88	96
9	J	212/469 (45%)	210 (99%)	2 (1%)	78	92
10	K	338/401 (84%)	334 (99%)	4 (1%)	71	88
11	L	369/431 (86%)	363 (98%)	6 (2%)	62	84
12	M	205/299 (69%)	200 (98%)	5 (2%)	49	74
13	N	192/259 (74%)	188 (98%)	4 (2%)	53	78
14	O	103/169 (61%)	100 (97%)	3 (3%)	42	69
14	P	97/169 (57%)	94 (97%)	3 (3%)	40	67
15	Q	458/661 (69%)	447 (98%)	11 (2%)	49	74
16	R	114/144 (79%)	109 (96%)	5 (4%)	28	52
17	S	336/532 (63%)	332 (99%)	4 (1%)	71	88
18	T	93/126 (74%)	89 (96%)	4 (4%)	29	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	U	91/160 (57%)	91 (100%)	0	100 100
All	All	7322/9552 (77%)	7169 (98%)	153 (2%)	56 78

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	M	130	MET
16	R	96	ARG
13	N	49	GLU
15	Q	350	ASN
18	T	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	1282	GLN
19	U	173	GLN
6	G	777	HIS
15	Q	751	HIS
14	O	88	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	$\#\|Z\| > 2$
22	SAH	L	8001	11	24,28,28	1.19	3 (12%)	25,40,40	1.68	5 (20%)

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
22	SAH	L	8001	11	-	6/11/31/31	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	8001	SAH	C2-N3	3.72	1.38	1.32
22	L	8001	SAH	C2-N1	2.23	1.38	1.33
22	L	8001	SAH	OXT-C	-2.20	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	8001	SAH	N3-C2-N1	-5.27	120.44	128.68
22	L	8001	SAH	C5'-SD-CG	-3.44	91.96	102.27
22	L	8001	SAH	C3'-C2'-C1'	3.05	105.56	100.98
22	L	8001	SAH	OXT-C-O	-2.65	118.08	124.09
22	L	8001	SAH	OXT-C-CA	2.10	120.55	113.38

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

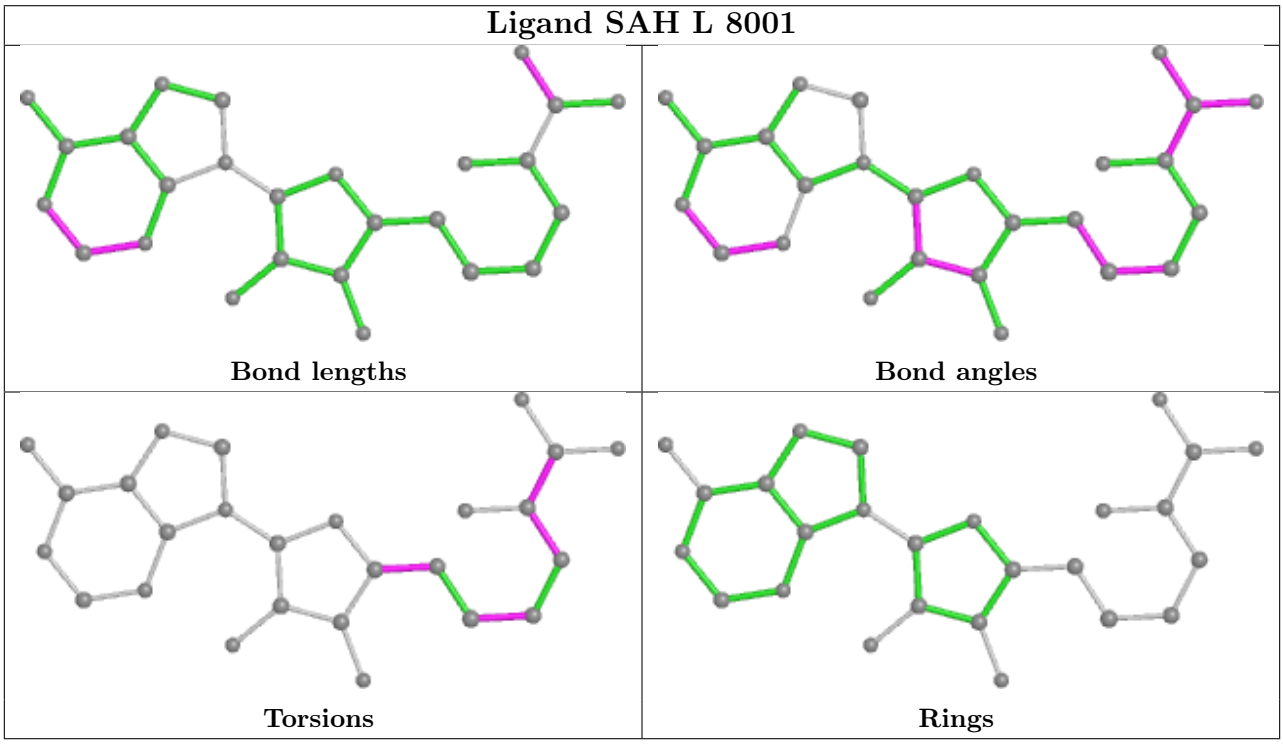
Mol	Chain	Res	Type	Atoms
22	L	8001	SAH	N-CA-CB-CG
22	L	8001	SAH	C-CA-CB-CG
22	L	8001	SAH	C3'-C4'-C5'-SD
22	L	8001	SAH	O-C-CA-CB
22	L	8001	SAH	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	8001	SAH	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.



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.

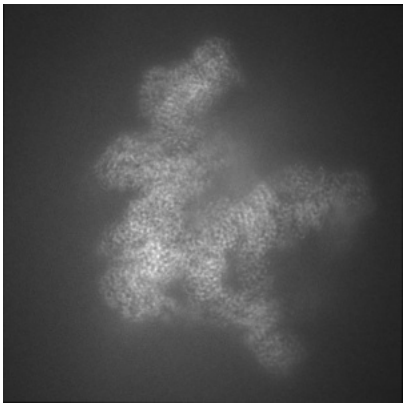
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18935. These allow visual inspection of the internal detail of the map and identification of artifacts.

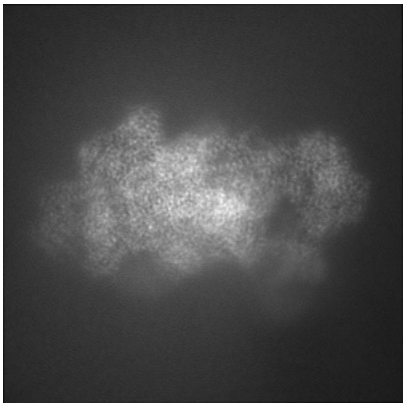
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

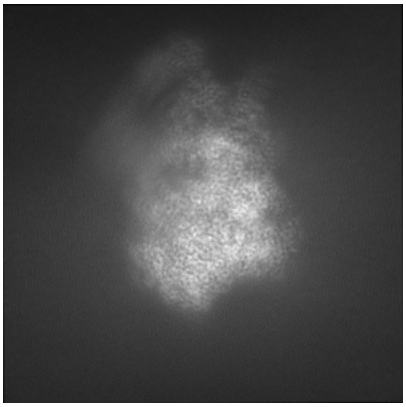
6.1.1 Primary map



X



Y

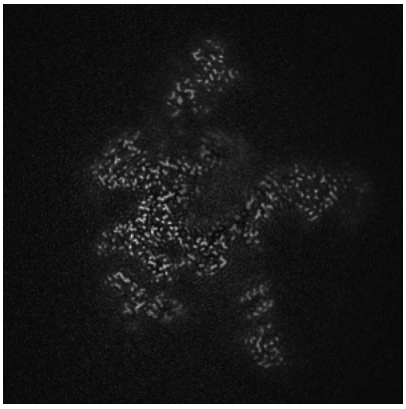


Z

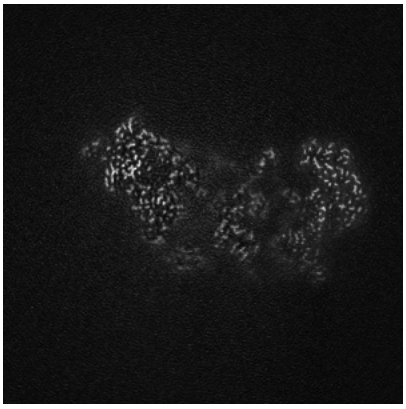
The images above show the map projected in three orthogonal directions.

6.2 Central slices

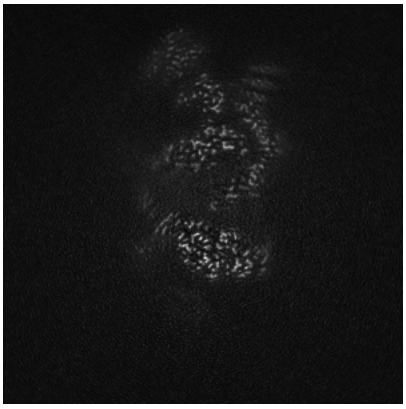
6.2.1 Primary map



X Index: 300



Y Index: 300

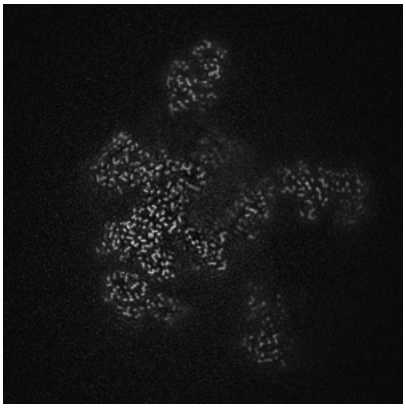


Z Index: 300

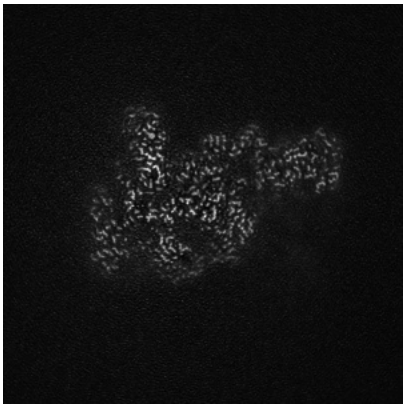
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

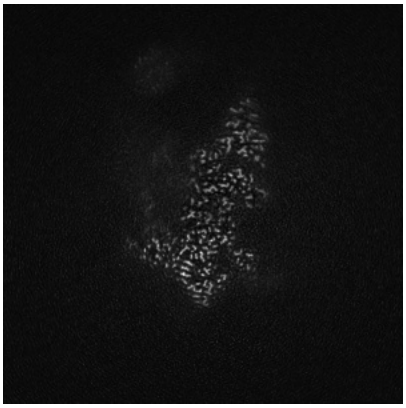
6.3.1 Primary map



X Index: 289



Y Index: 232

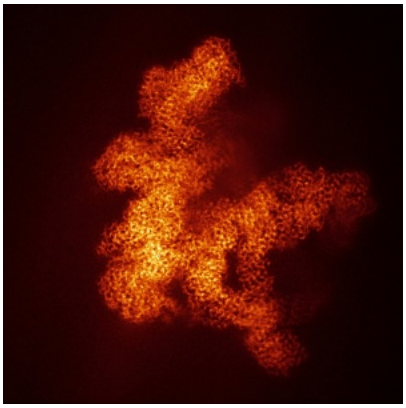


Z Index: 253

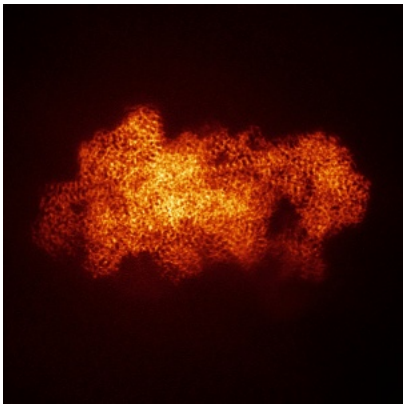
The images above show the largest variance slices of the map in three orthogonal directions.

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

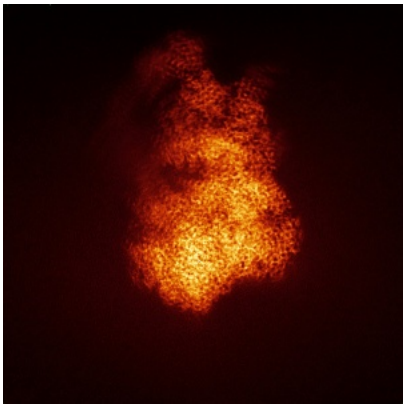
6.4.1 Primary map



X



Y

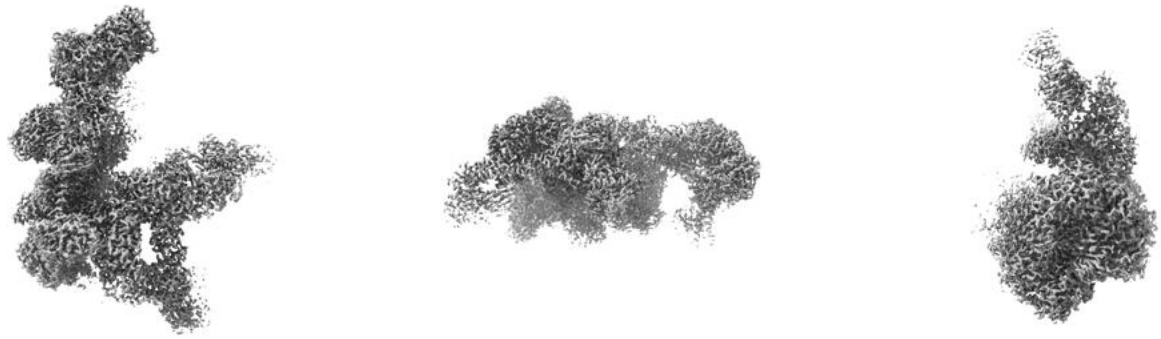


Z

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

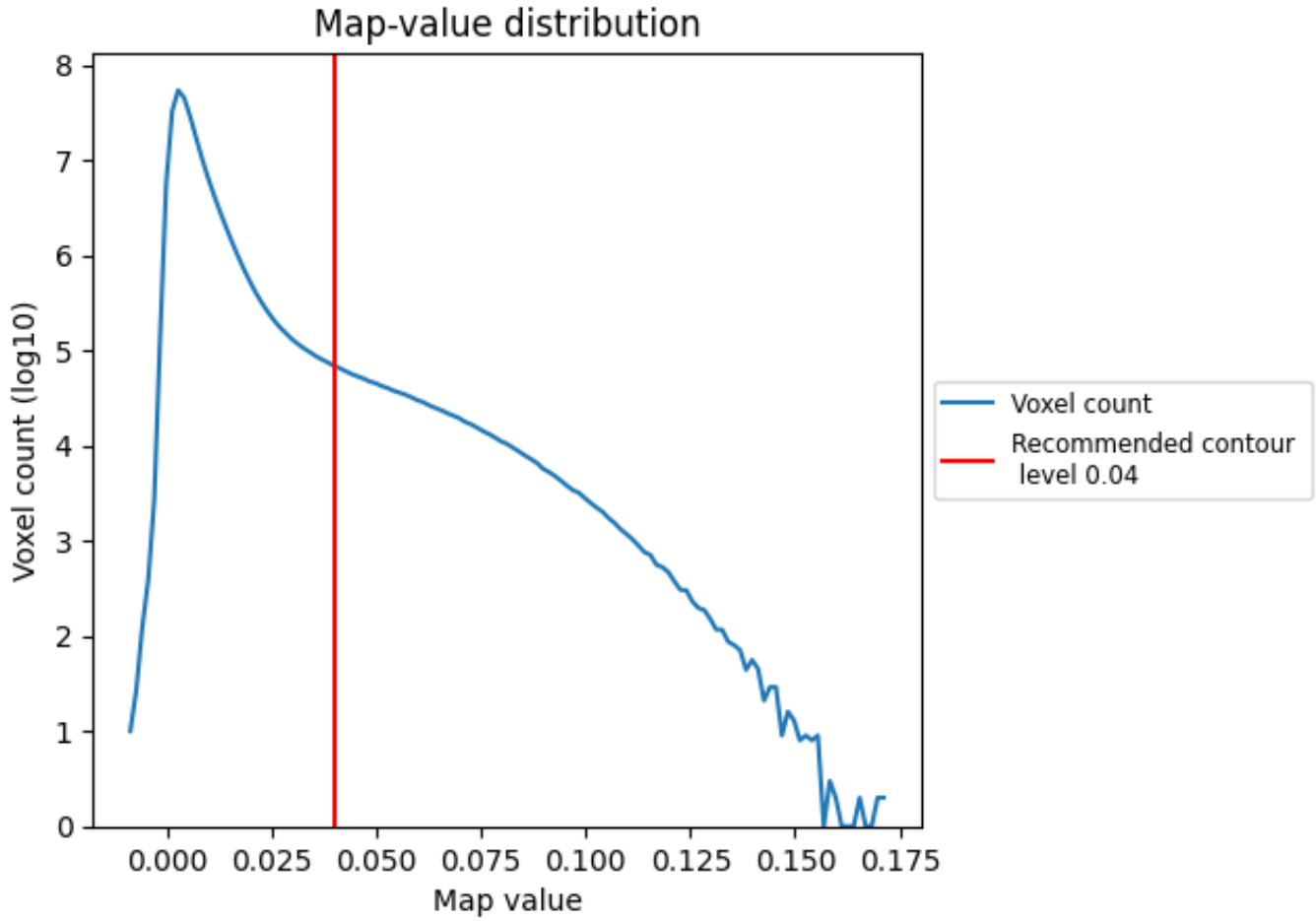
6.6 Mask visualisation (i)

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

7 Map analysis

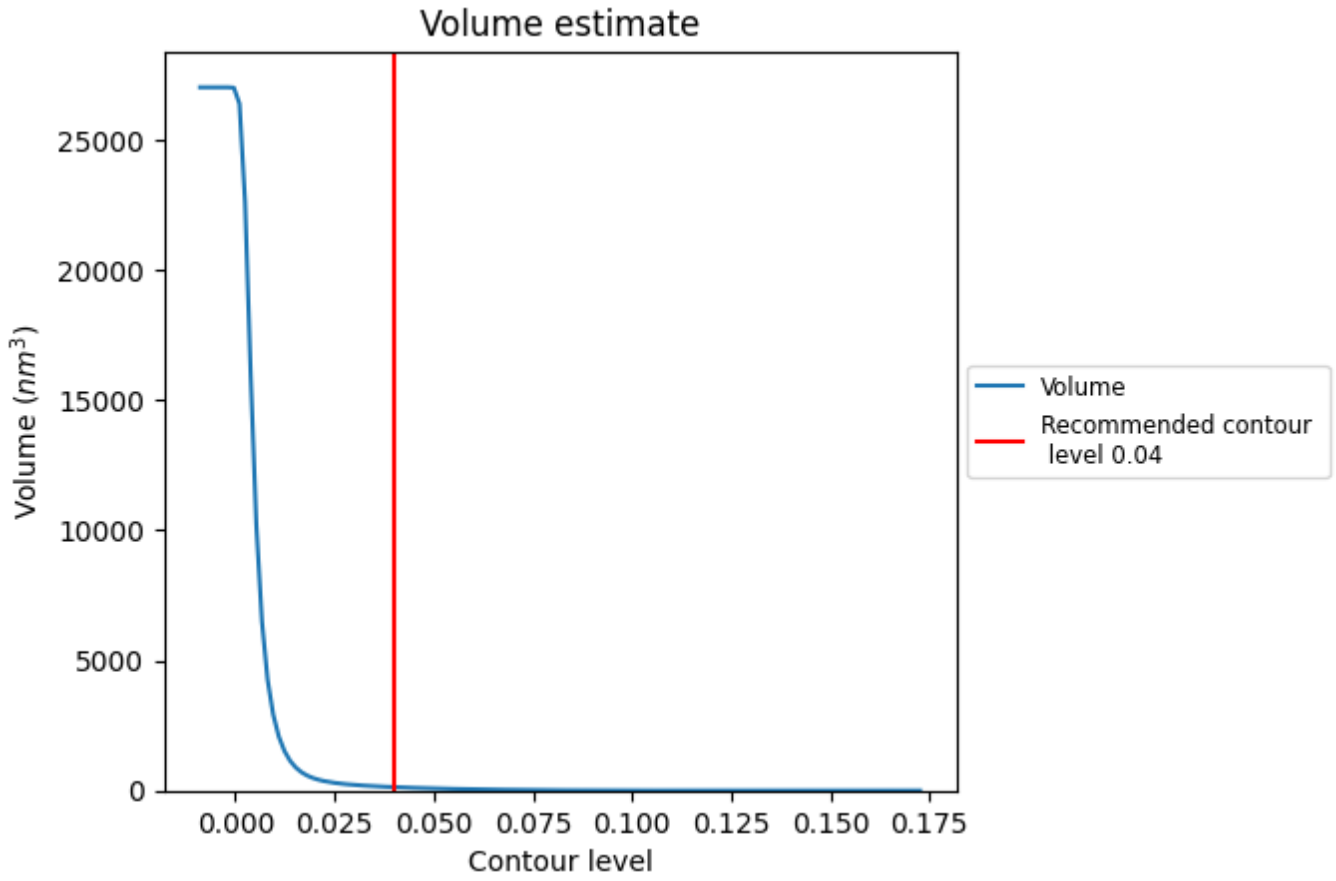
This section contains the results of statistical analysis of the map.

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.

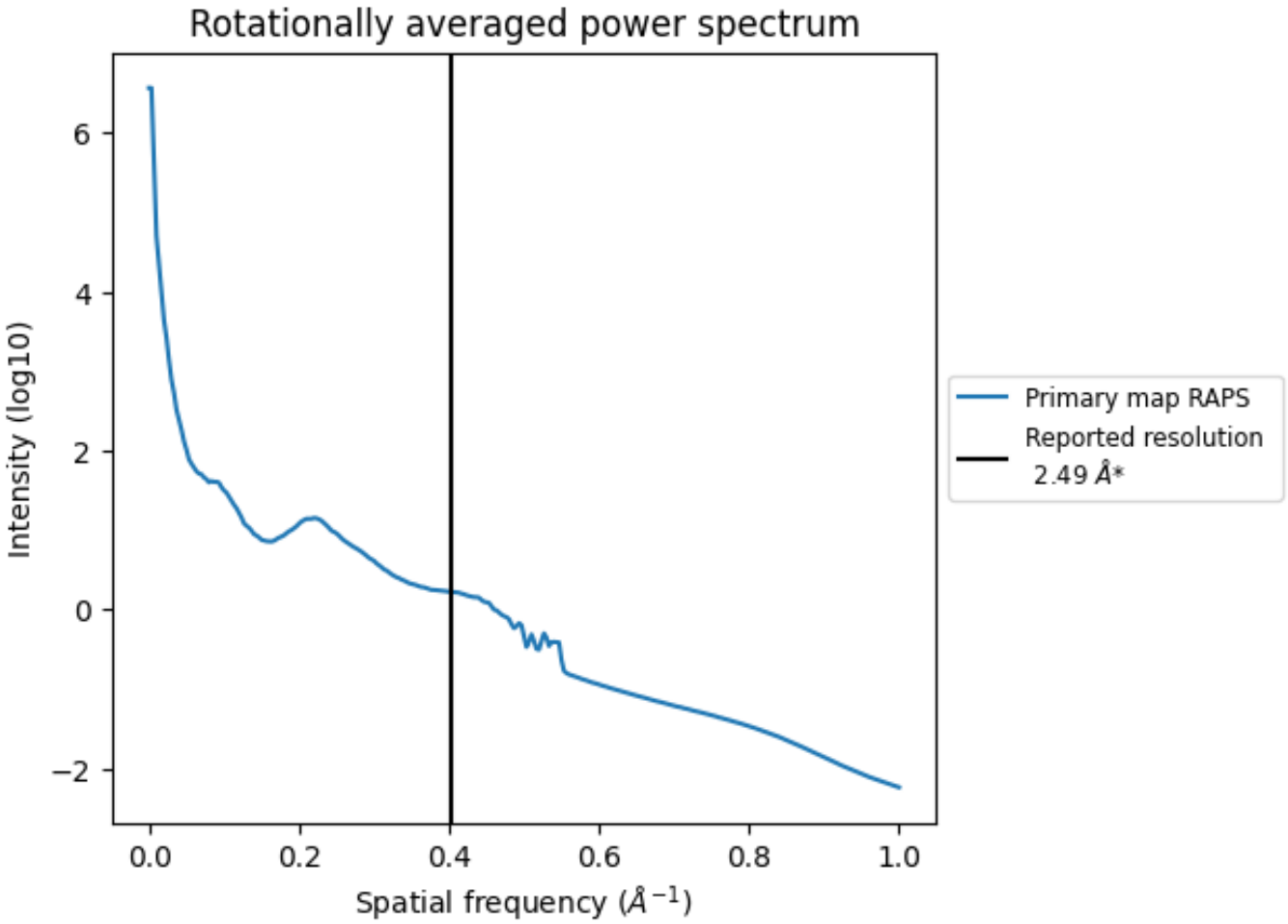
7.2 Volume estimate (i)



The volume at the recommended contour level is 132 nm^3; this corresponds to an approximate mass of 119 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 0.402 Å^{-1}

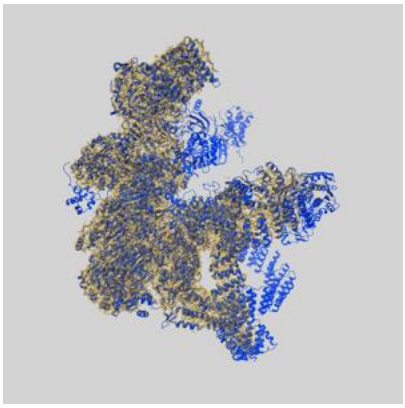
8 Fourier-Shell correlation (i)

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

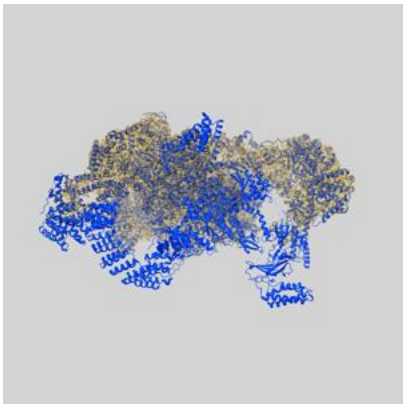
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18935 and PDB model 8R6S. Per-residue inclusion information can be found in section 3 on page 9.

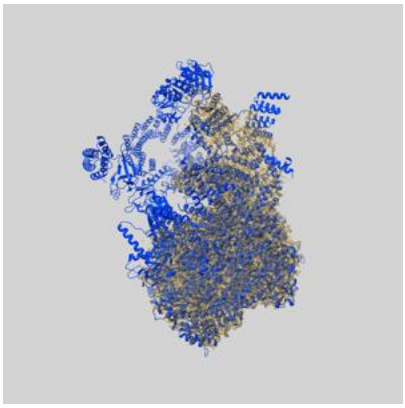
9.1 Map-model overlay



X



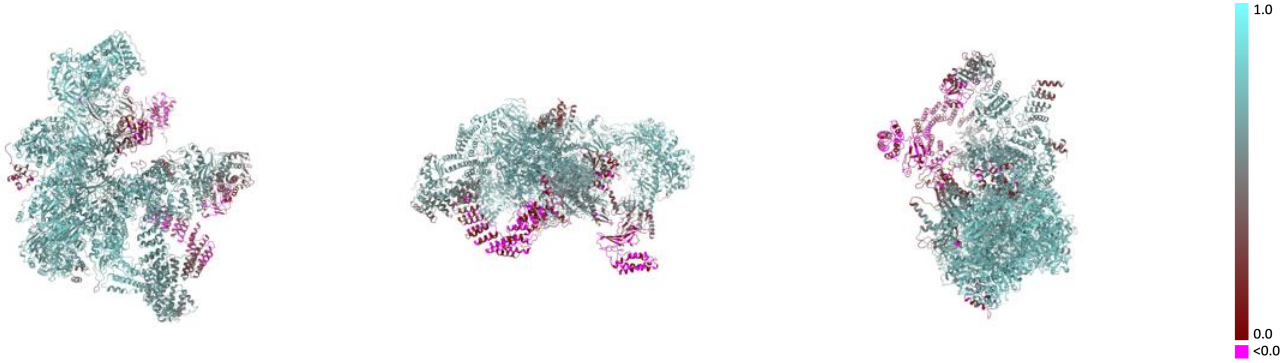
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

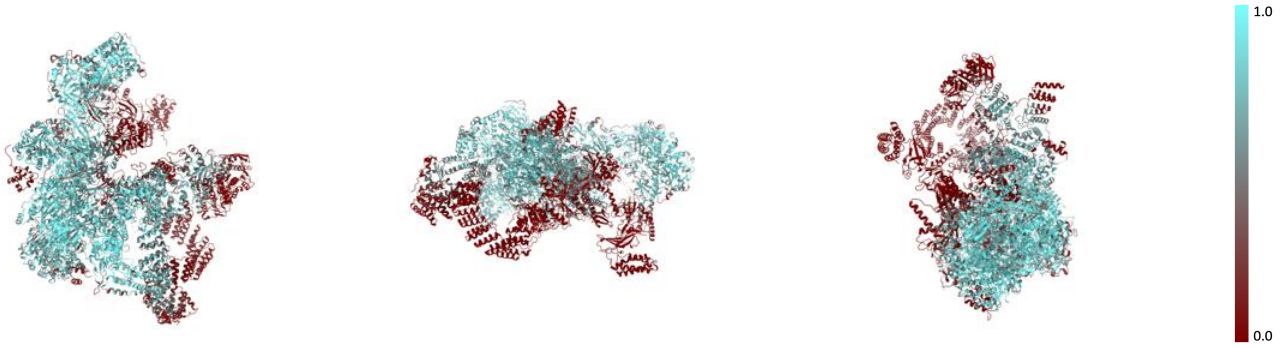
9.2 Q-score mapped to coordinate model



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.

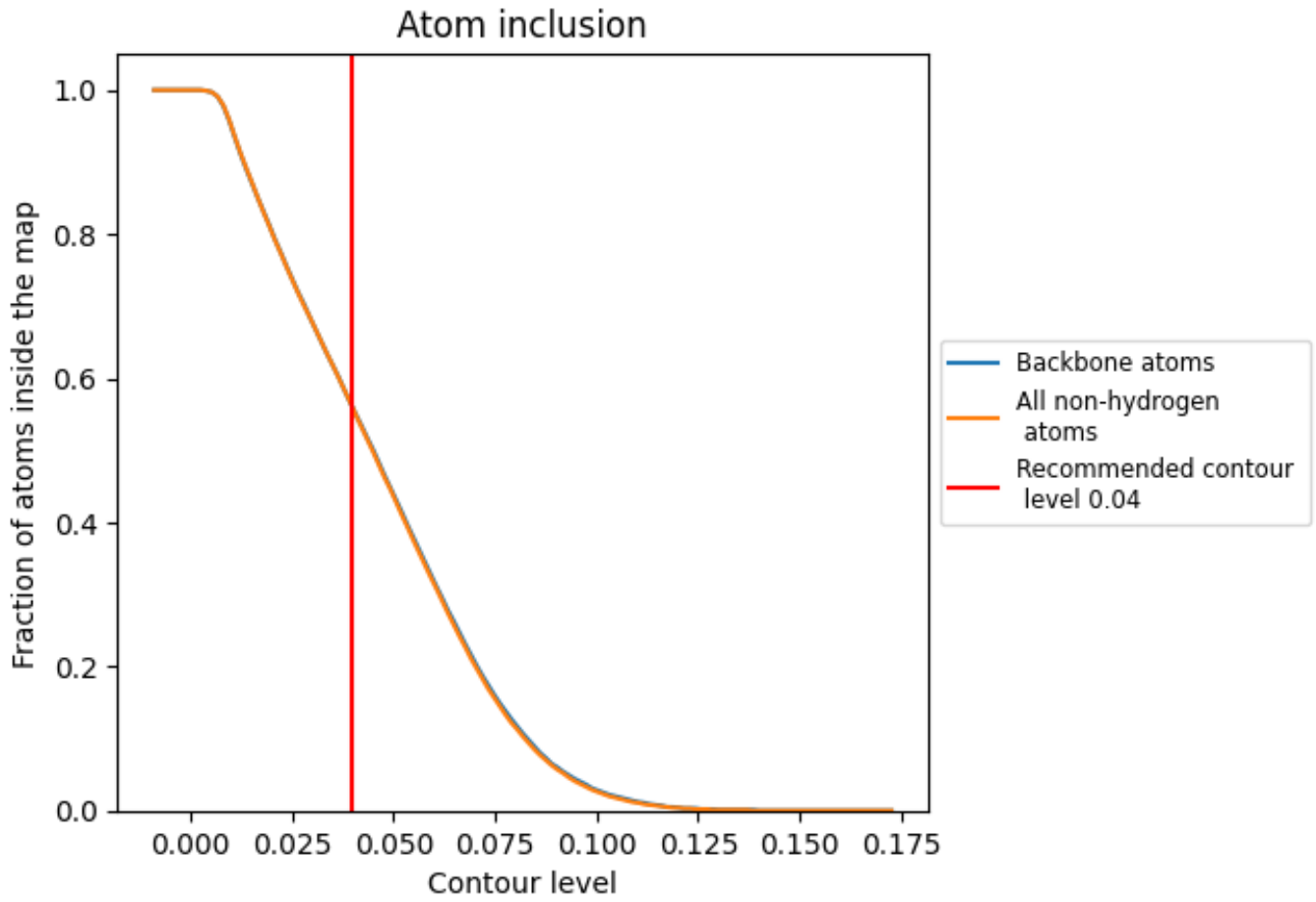
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 56% of all backbone atoms, 56% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5590	0.6030
A	0.7100	0.6970
B	0.5840	0.5800
C	0.5160	0.5900
D	0.6150	0.6510
E	0.5840	0.6060
F	0.5610	0.6250
G	0.1060	0.3550
H	0.5420	0.6210
I	0.8260	0.7430
J	0.8240	0.7410
K	0.7920	0.7240
L	0.8130	0.7120
M	0.7980	0.7110
N	0.7080	0.6890
O	0.6940	0.7100
P	0.6350	0.6800
Q	0.2160	0.4070
R	0.6550	0.6650
S	0.7870	0.7250
T	0.7270	0.7140
U	0.0000	-0.0200