



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:29 PM UTC

PDB ID : 9EPC / pdb_00009epc
EMDB ID : EMD-19877
Title : Cryo-EM structure of the Plastid-encoded RNA polymerase from Sinapis alba
Authors : Effantin, G.; Blanvillain, R.; Cobessi, D.
Deposited on : 2024-03-18
Resolution : 3.00 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:

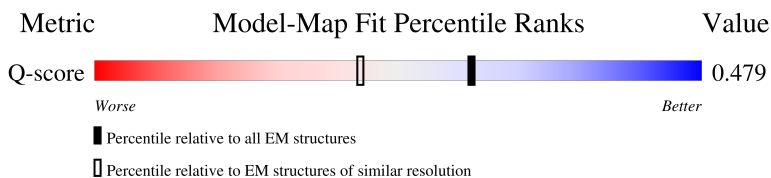
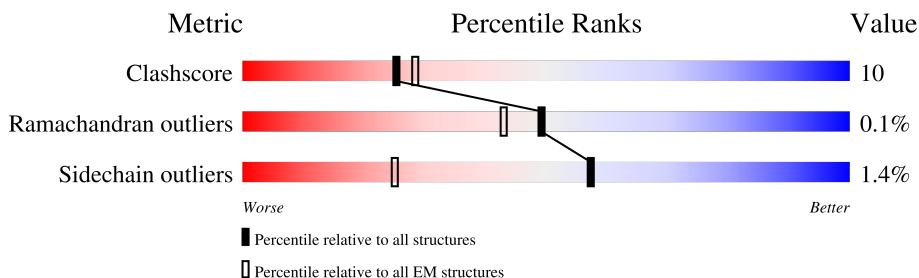
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.00 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.



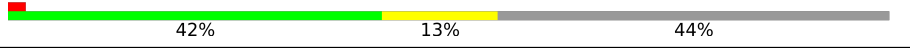
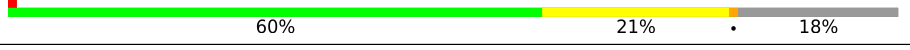
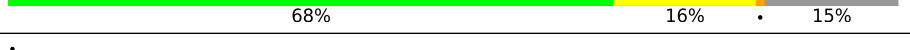
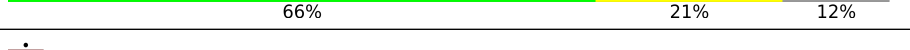
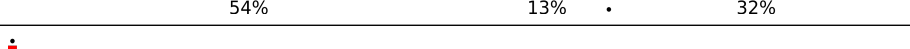
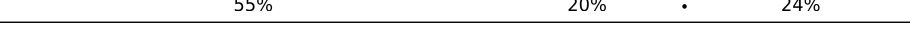
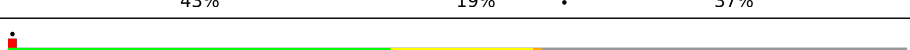
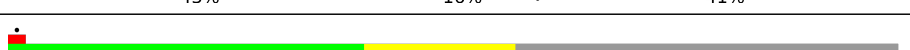
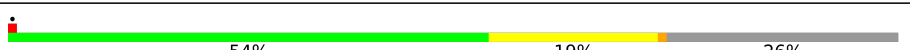
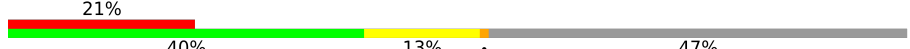
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 $\leq 5\%$. 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	
1	B	327	
2	C	1072	
3	D	680	

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Mol	Chain	Length	Quality of chain
4	E	1373	
5	F	911	
6	G	1174	
7	H	675	
8	I	264	
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

There are 25 unique types of molecules in this entry. The entry contains 65302 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	318	Total	C	N	O	S	0	0
			2595	1657	451	476	11		
1	B	271	Total	C	N	O	S	0	0
			2188	1395	379	404	10		

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 RpoB, subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	950	Total	C	N	O	S	0	0
			7594	4843	1336	1387	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	612	Total	C	N	O	S	0	0
			4992	3202	880	887	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	1027	Total	C	N	O	S	1	0
			8219	5239	1460	1490	30		

- Molecule 5 is a protein called PAP1, pTAC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	643	Total	C	N	O	S	0	0
			5141	3253	894	961	33		

- Molecule 6 is a protein called PAP2, pTAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	652	Total	C	N	O	S	0	0
			4604	2876	806	899	23		

- Molecule 7 is a protein called PAP3, pTAC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	551	Total	C	N	O	S	0	0
			4623	2947	799	860	17		

- Molecule 8 is a protein called PAP4, FSD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	215	Total	C	N	O	S	0	0
			1772	1141	301	324	6		

- Molecule 9 is a protein called PAP5, pTAC12, HEMERA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	250	Total	C	N	O	S	0	0
			2104	1328	373	392	11		

- Molecule 10 is a protein called PAP6, FLN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	393	Total	C	N	O	S	0	0
			3167	2023	530	599	15		

- Molecule 11 is a protein called PAP7, pTAC14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	425	Total	C	N	O	S	0	0
			3467	2222	589	636	20		

- Molecule 12 is a protein called PAP8, pTAC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	226	Total	C	N	O	S	0	0
			1885	1192	325	360	8		

- Molecule 13 is a protein called PAP9, FSD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	226	Total	C	N	O	S	0	0
			1832	1175	311	342	4		

- Molecule 14 is a protein called PAP10, TRXz.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	116	Total	C	N	O	S	0	0
			936	596	151	180	9		
14	P	110	Total	C	N	O	S	0	0
			885	563	141	172	9		

- Molecule 15 is a protein called PAP11, MurE-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	441	Total	C	N	O	S	0	0
			3362	2092	579	670	21		

- Molecule 16 is a protein called PAP12, pTAC7.

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	398	Total	C	N	O	S	0	0
			3153	1995	531	606	21		

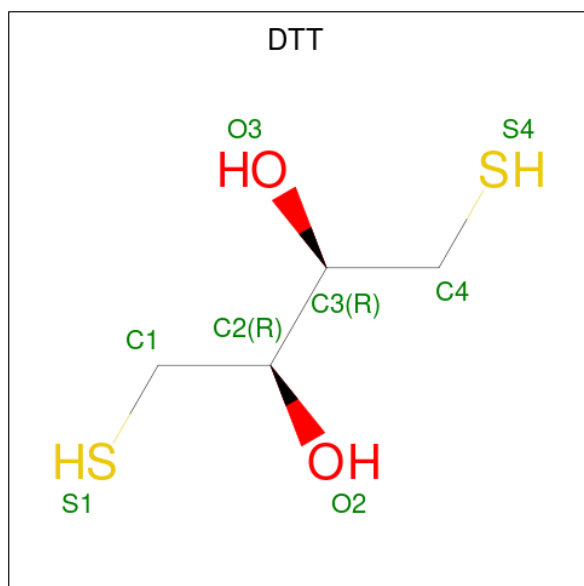
- Molecule 18 is a protein called pTAC18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	104	Total	C	N	O	S	0	0
			881	571	148	158	4		

- Molecule 19 is a protein called PRIN2, PLASTID REDOX INSENSITIVE 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	99	Total	C	N	O	S	0	0
			793	505	133	152	3		

- Molecule 20 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
20	D	1	Total	C	O	S	0
			8	4	2	2	

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest"

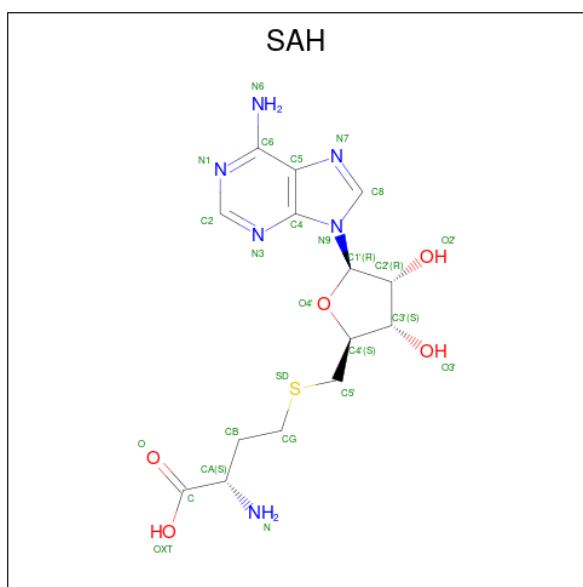
by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	K	1	Total	Ca	0
			1	1	
23	S	1	Total	Ca	0
			1	1	

- Molecule 24 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	K	1	Total	K	0
			1	1	

- Molecule 25 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S) (labeled as "Ligand of Interest" by depositor).

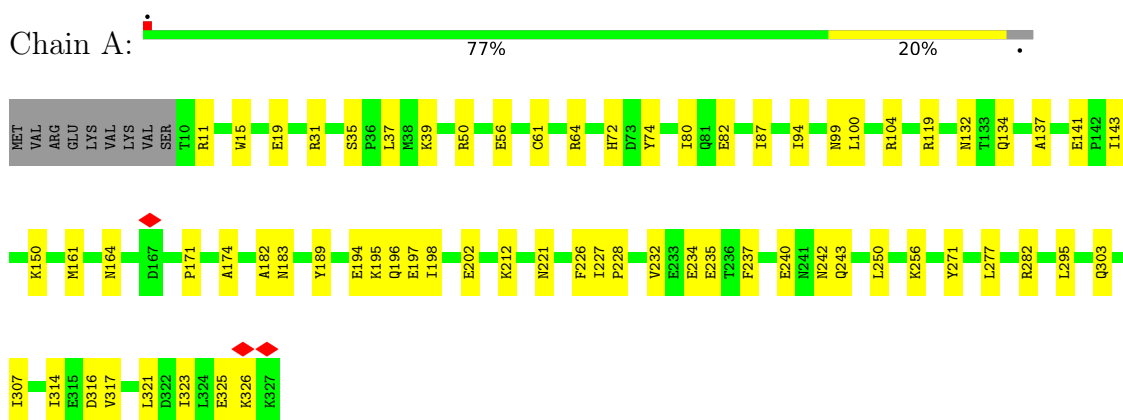


Mol	Chain	Residues	Atoms					AltConf
25	L	1	Total	C	N	O	S	0
			26	14	6	5	1	

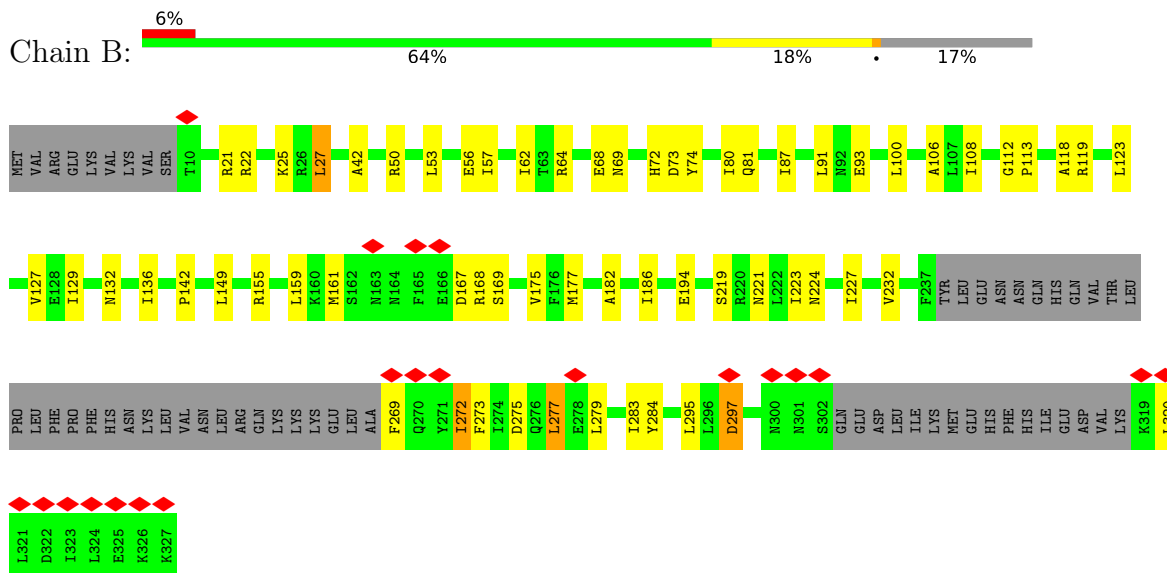
3 Residue-property plots

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

- Molecule 1: DNA-directed RNA polymerase subunit alpha

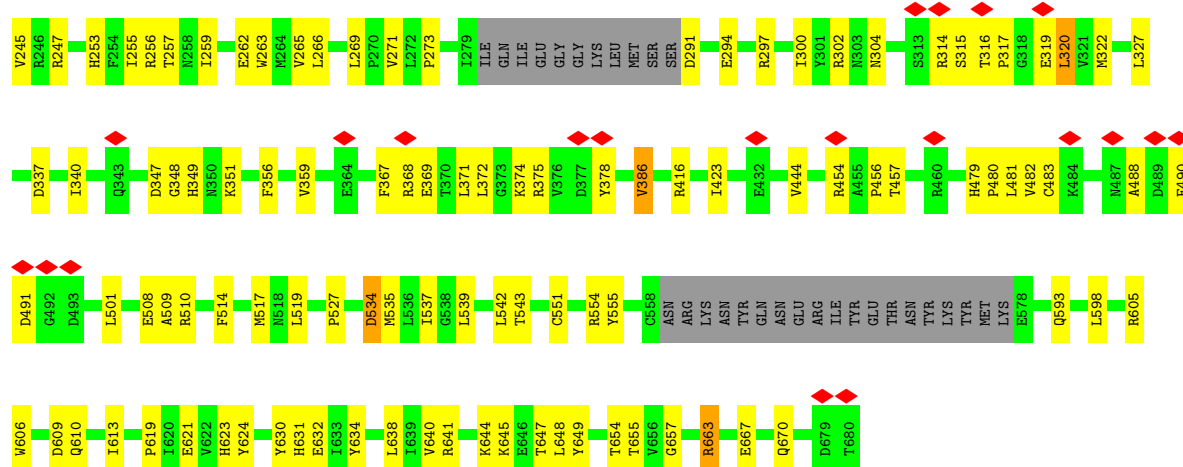


- Molecule 1: DNA-directed RNA polymerase subunit alpha

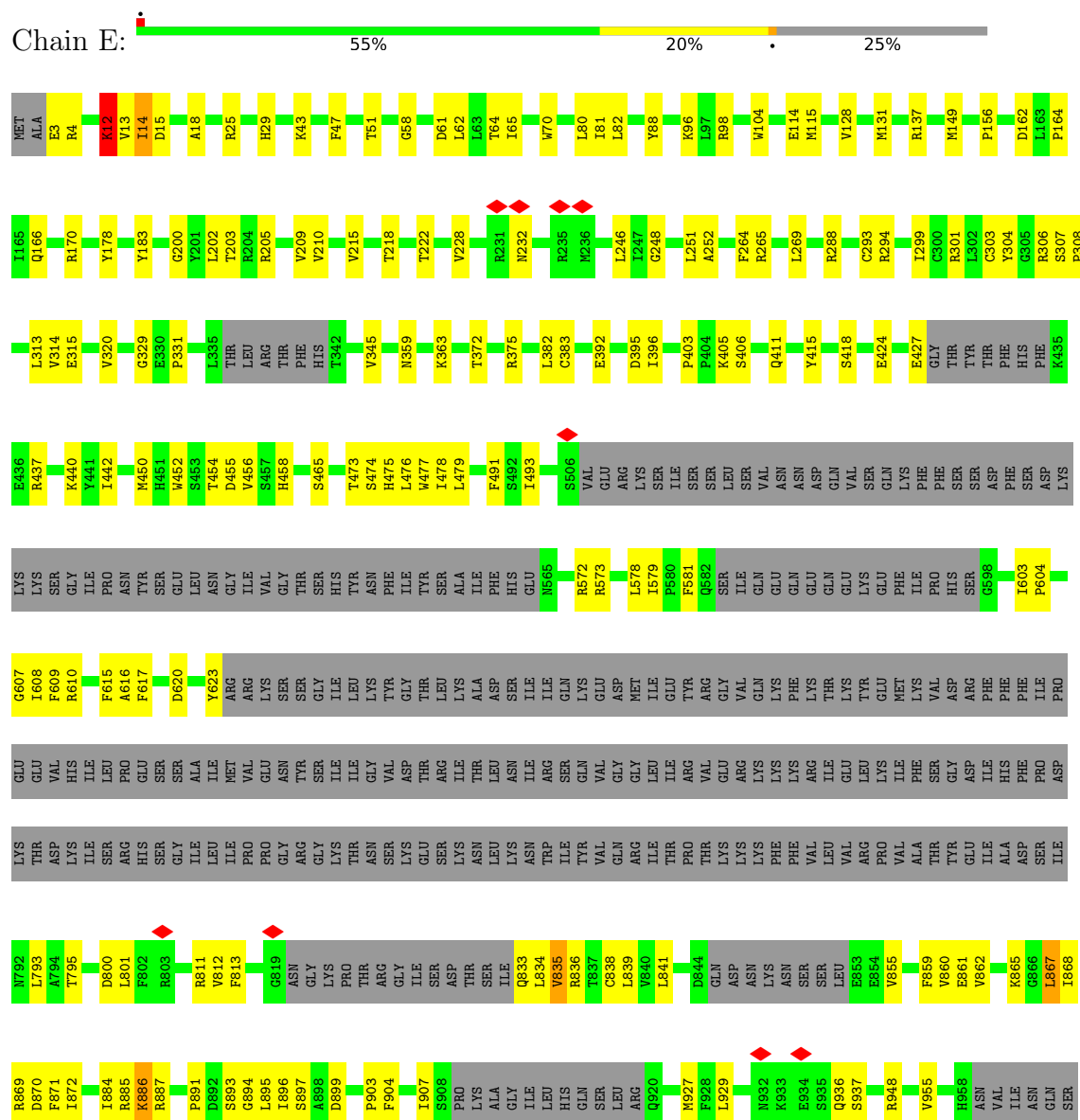


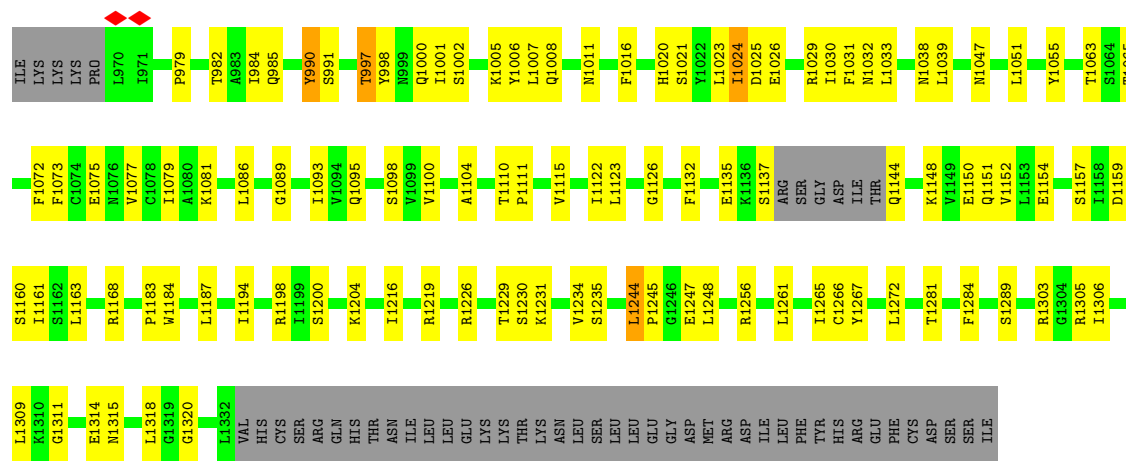
- Molecule 2: RpoB, subunit beta



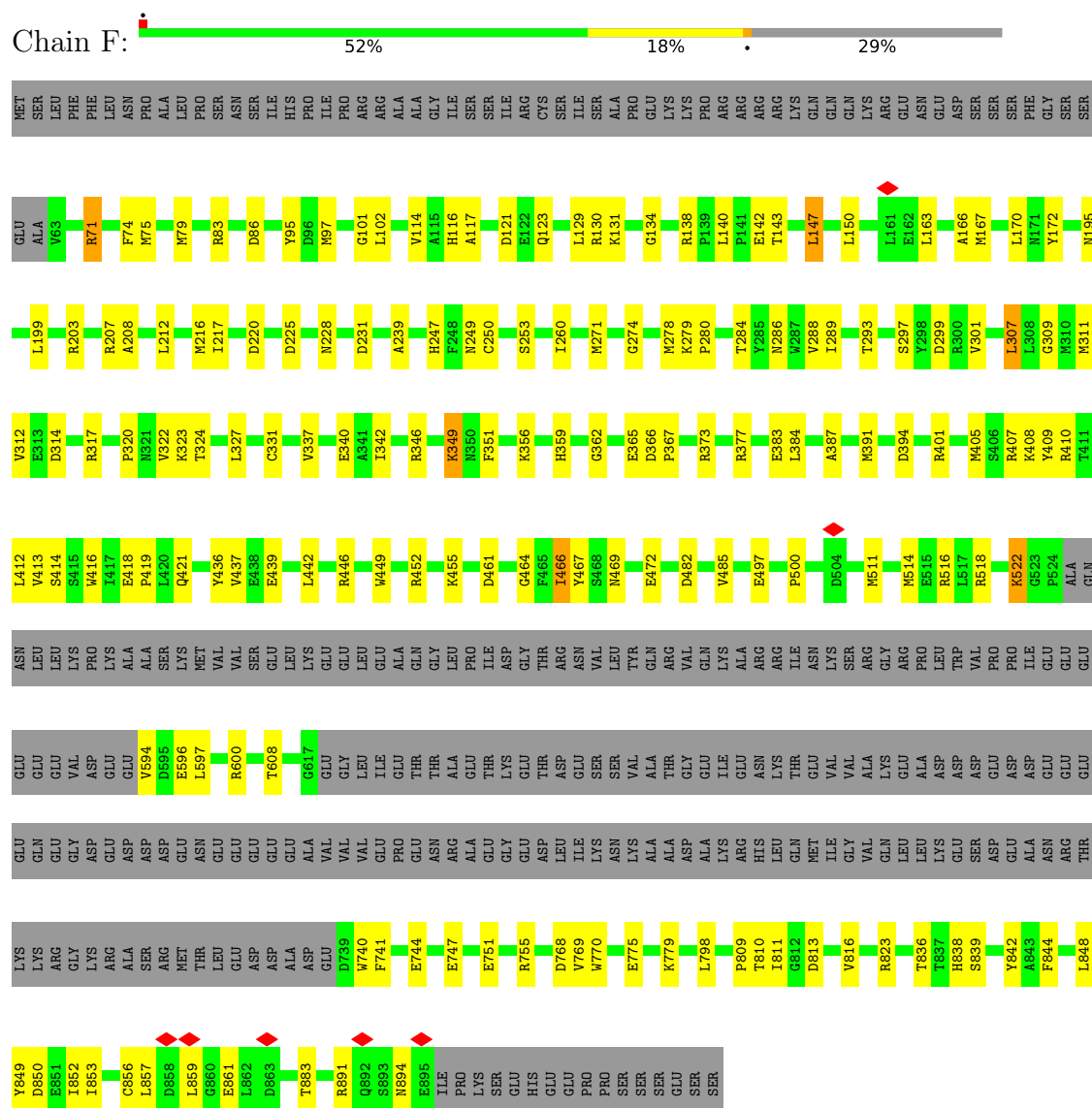


• Molecule 4: DNA-directed RNA polymerase subunit beta”

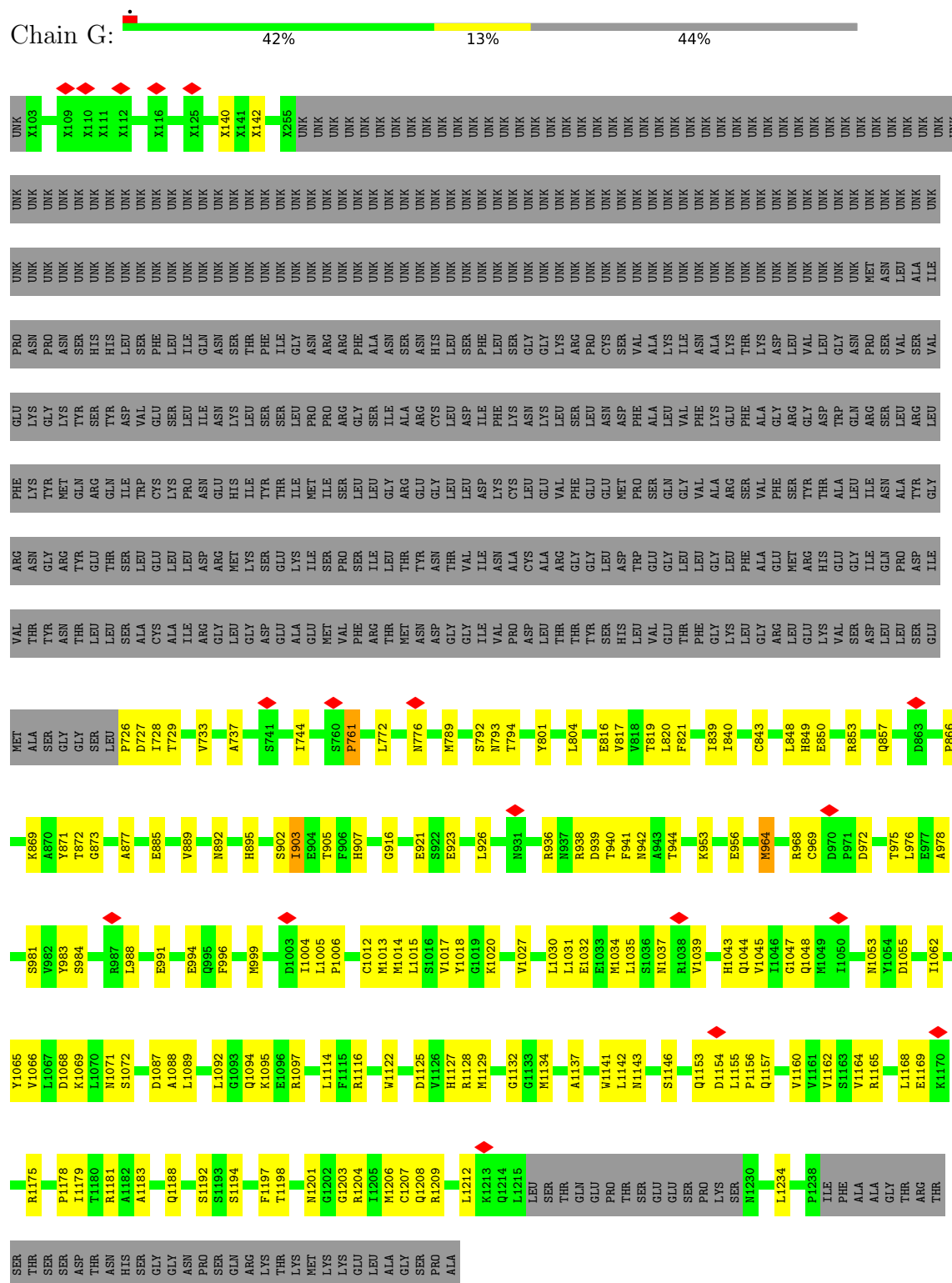


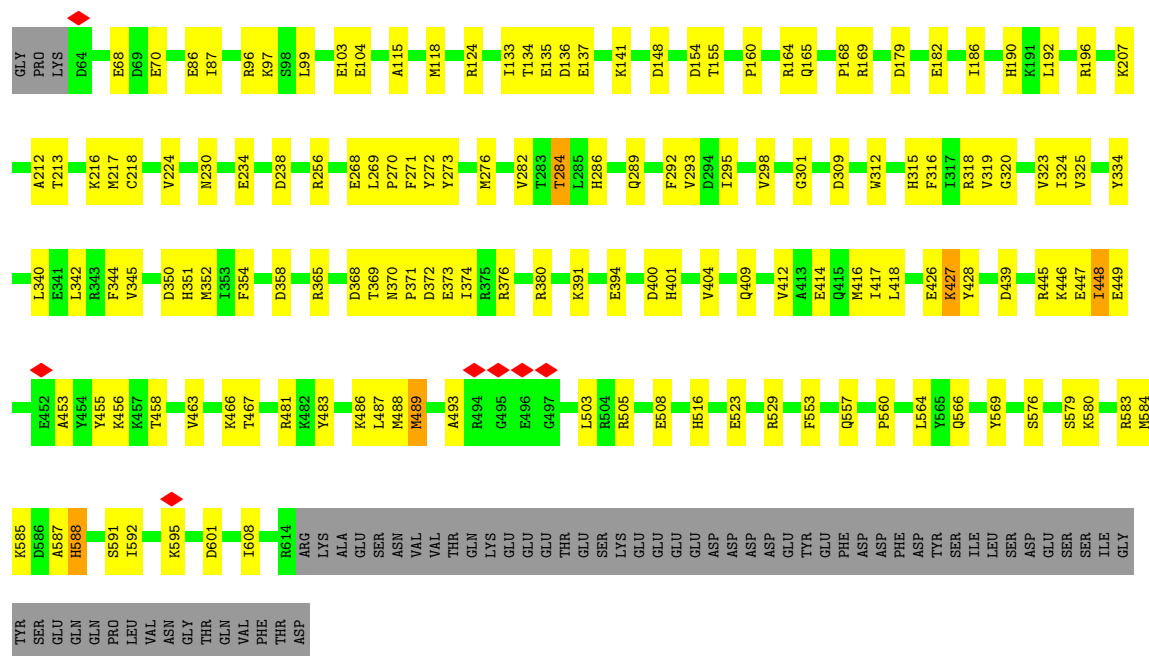


• Molecule 5: PAP1, pTAC3

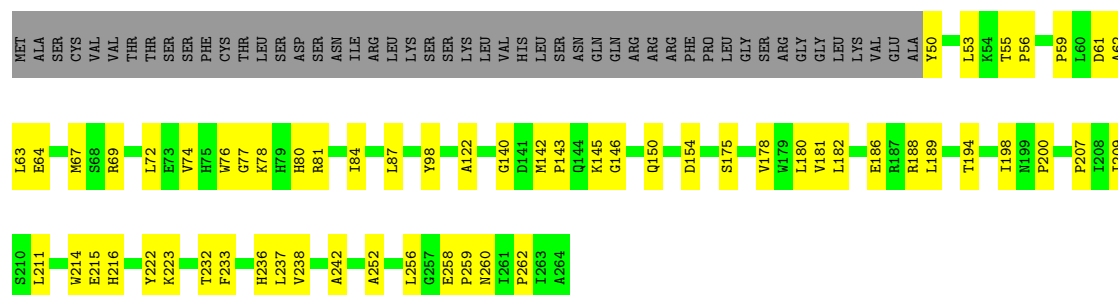


• Molecule 6: PAP2, pTAC2

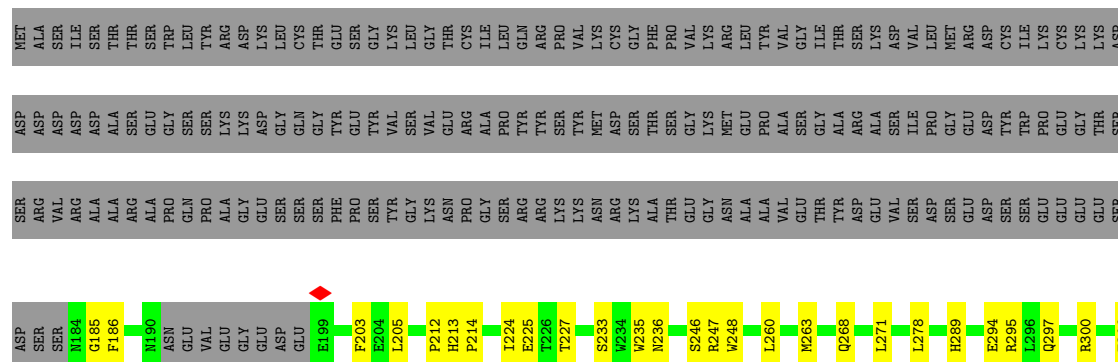
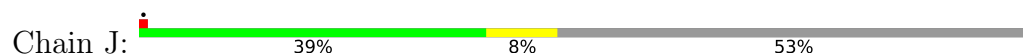


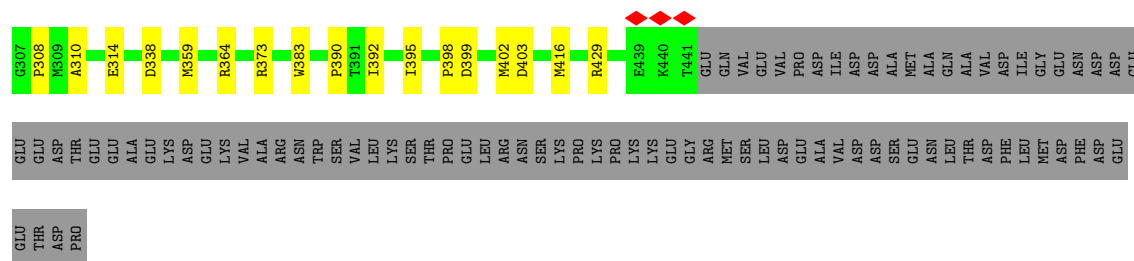


• Molecule 8: PAP4, FSD3

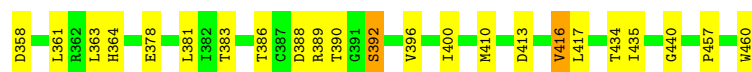
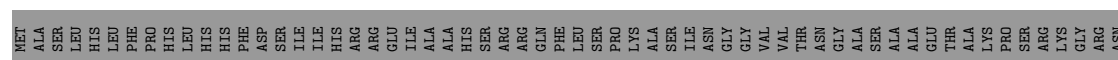


• Molecule 9: PAP5, pTAC12, HEMERA

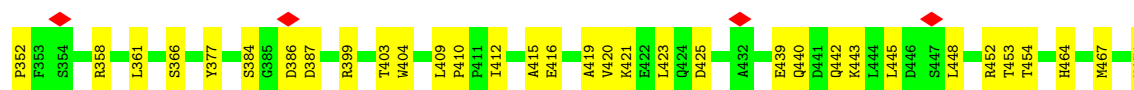
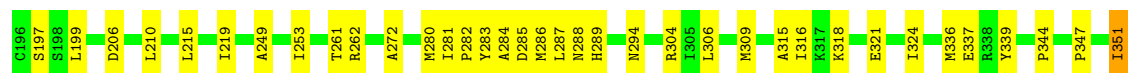
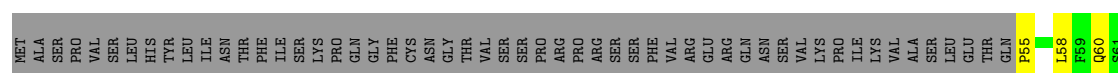




• Molecule 10: PAP6, FLN1



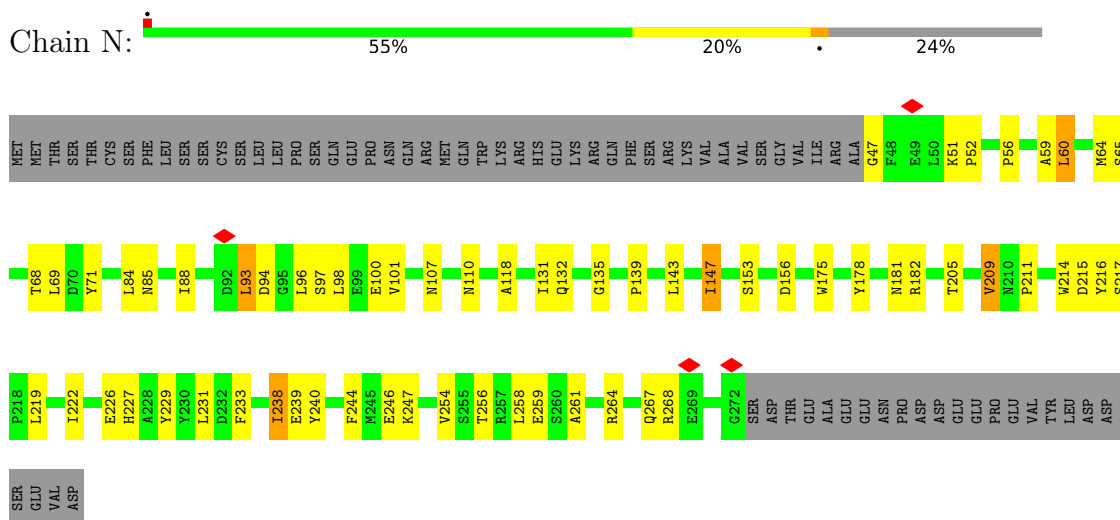
• Molecule 11: PAP7, pTAC14



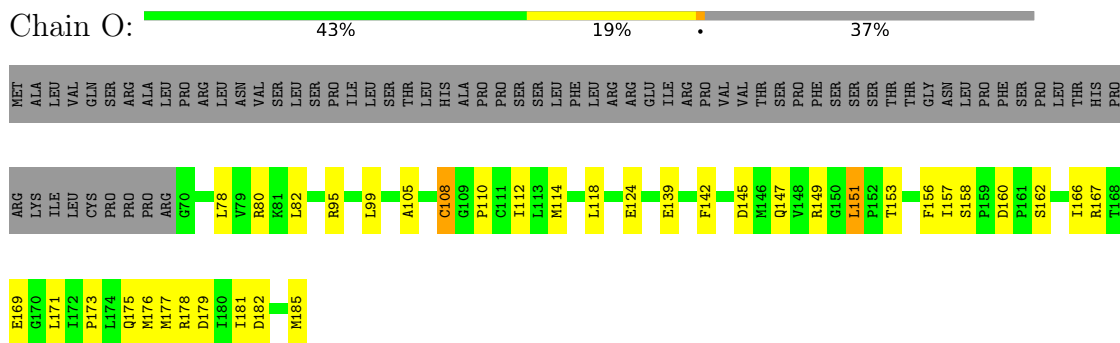
• Molecule 12: PAP8, pTAC6



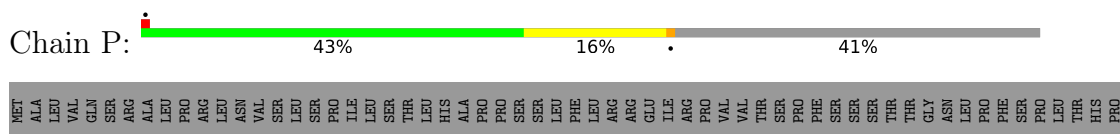
- Molecule 13: PAP9, FSD2

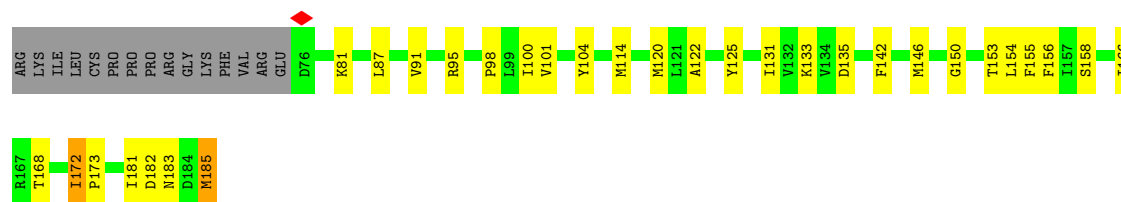


- Molecule 14: PAP10, TRXz

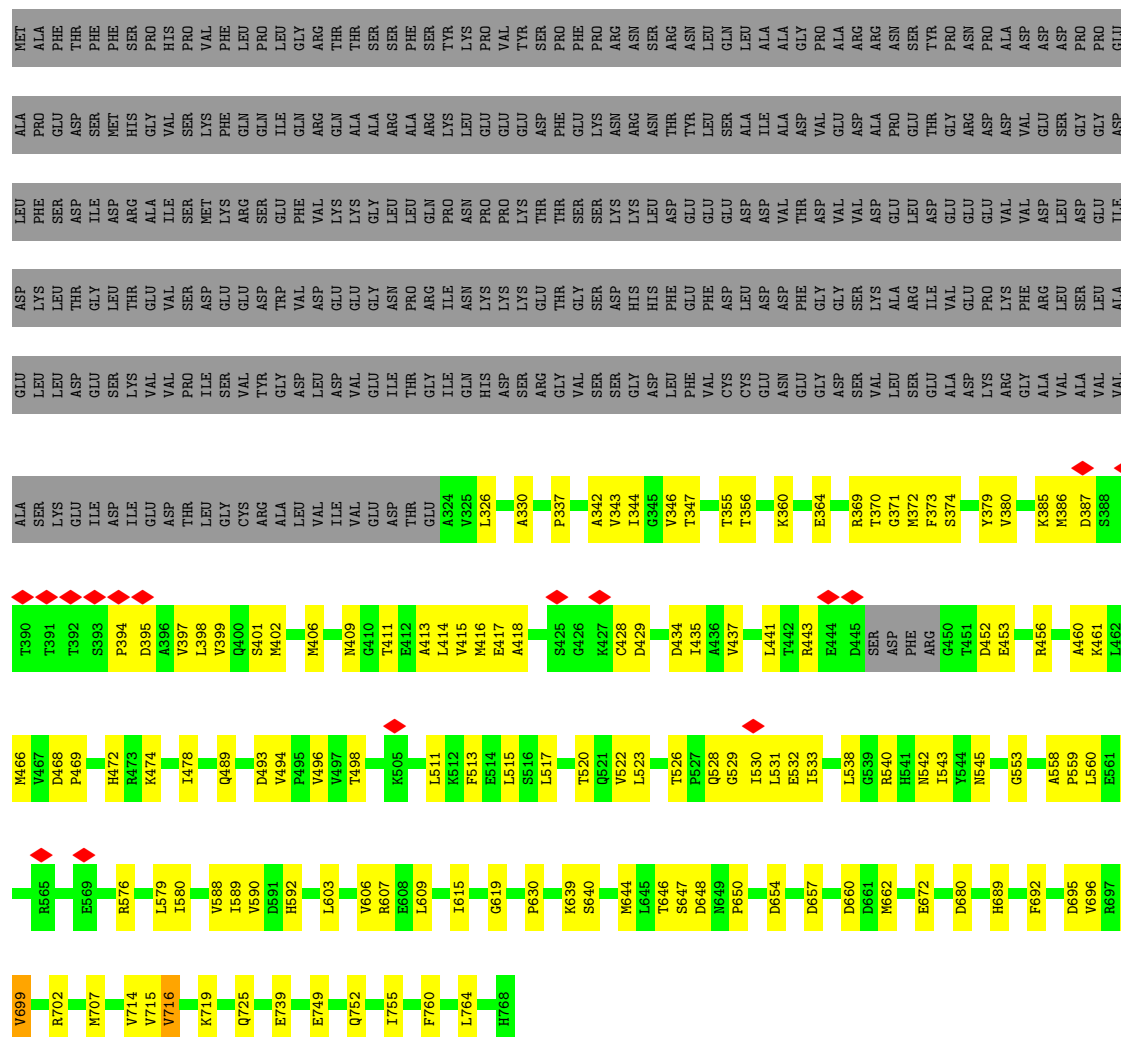


- Molecule 14: PAP10, TRXz

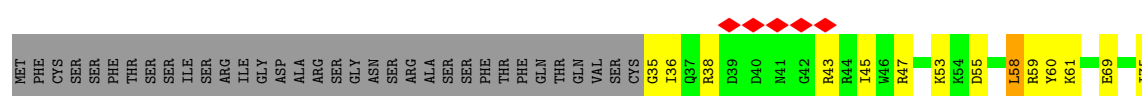




• Molecule 15: PAP11, MurE-like



• Molecule 16: PAP12, pTAC7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105796	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00912	Depositor
Map size (Å)	370.99997, 370.99997, 370.99997	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: DTT, K, CA, 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	0.15	0/2648	0.26	0/3581
1	B	0.14	0/2229	0.24	0/3015
2	C	0.14	0/7746	0.25	0/10464
3	D	0.13	0/5106	0.25	0/6906
4	E	0.15	1/8382 (0.0%)	0.27	0/11327
5	F	0.11	0/5246	0.26	0/7091
6	G	0.11	0/3908	0.31	2/5287 (0.0%)
7	H	0.13	0/4752	0.26	0/6409
8	I	0.11	0/1826	0.24	0/2480
9	J	0.15	0/2156	0.26	0/2904
10	K	0.15	0/3250	0.26	0/4413
11	L	0.11	0/3559	0.24	0/4817
12	M	0.13	0/1931	0.22	0/2614
13	N	0.11	0/1886	0.26	0/2566
14	O	0.15	0/952	0.25	0/1284
14	P	0.13	0/900	0.27	0/1216
15	Q	0.12	0/3421	0.29	2/4643 (0.0%)
16	R	0.11	0/1089	0.24	0/1462
17	S	0.14	0/3222	0.24	0/4360
18	T	0.12	0/906	0.26	0/1226
19	U	0.10	0/812	0.24	0/1097
All	All	0.13	1/65927 (0.0%)	0.26	4/89162 (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	D	0	1
5	F	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	L	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	12	LYS	C-N	-5.28	1.30	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	761	PRO	N-CA-CB	7.90	111.54	103.25
6	G	726	PRO	N-CA-CB	6.76	110.43	103.00
15	Q	337	PRO	N-CA-CB	6.19	110.07	103.39
15	Q	326	LEU	CB-CA-C	-5.62	110.08	116.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	663	ARG	Sidechain
5	F	71	ARG	Sidechain
11	L	141	PHE	Peptide

5.2 Too-close contacts ⓘ

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	2595	0	2624	42	0
1	B	2188	0	2210	51	0
2	C	7594	0	7673	199	0
3	D	4992	0	5050	124	0
4	E	8219	0	8285	228	0
5	F	5141	0	5092	118	0
6	G	4604	0	3835	108	0
7	H	4623	0	4480	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	1772	0	1698	40	0
9	J	2104	0	2056	42	0
10	K	3167	0	3082	58	0
11	L	3467	0	3403	78	0
12	M	1885	0	1832	33	0
13	N	1832	0	1755	51	0
14	O	936	0	931	26	0
14	P	885	0	878	21	0
15	Q	3362	0	3227	101	0
16	R	1069	0	1058	26	0
17	S	3153	0	3113	46	0
18	T	881	0	858	17	0
19	U	793	0	766	15	0
20	D	8	0	9	1	0
21	E	1	0	0	0	0
22	I	1	0	0	0	0
22	N	1	0	0	0	0
23	K	1	0	0	0	0
23	S	1	0	0	0	0
24	K	1	0	0	0	0
25	L	26	0	19	5	0
All	All	65302	0	63934	1338	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 10.

The worst 5 of 1338 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)
5:F:288:VAL:CG1	5:F:307:LEU:HD21	1.84	1.06
14:P:120:MET:HE3	17:S:563:GLY:HA3	1.42	1.01
15:Q:371:GLY:HA3	15:Q:406:MET:HE1	1.42	0.97
10:K:434:THR:HG21	10:K:440:GLY:HA3	1.46	0.95
5:F:288:VAL:HG12	5:F:307:LEU:HD21	1.47	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	316/327 (97%)	300 (95%)	16 (5%)	0	100	100
1	B	265/327 (81%)	255 (96%)	10 (4%)	0	100	100
2	C	936/1072 (87%)	887 (95%)	49 (5%)	0	100	100
3	D	602/680 (88%)	580 (96%)	21 (4%)	1 (0%)	43	76
4	E	1006/1373 (73%)	943 (94%)	62 (6%)	1 (0%)	48	80
5	F	637/911 (70%)	604 (95%)	32 (5%)	1 (0%)	43	76
6	G	495/1174 (42%)	477 (96%)	16 (3%)	2 (0%)	30	65
7	H	549/675 (81%)	523 (95%)	25 (5%)	1 (0%)	43	76
8	I	213/264 (81%)	200 (94%)	13 (6%)	0	100	100
9	J	246/529 (46%)	231 (94%)	15 (6%)	0	100	100
10	K	391/460 (85%)	379 (97%)	12 (3%)	0	100	100
11	L	421/483 (87%)	407 (97%)	13 (3%)	1 (0%)	43	76
12	M	224/334 (67%)	218 (97%)	6 (3%)	0	100	100
13	N	224/297 (75%)	208 (93%)	16 (7%)	0	100	100
14	O	114/185 (62%)	112 (98%)	2 (2%)	0	100	100
14	P	108/185 (58%)	106 (98%)	2 (2%)	0	100	100
15	Q	437/768 (57%)	419 (96%)	18 (4%)	0	100	100
16	R	126/162 (78%)	118 (94%)	8 (6%)	0	100	100
17	S	394/611 (64%)	373 (95%)	21 (5%)	0	100	100
18	T	102/140 (73%)	99 (97%)	3 (3%)	0	100	100
19	U	97/187 (52%)	95 (98%)	2 (2%)	0	100	100
All	All	7903/11144 (71%)	7534 (95%)	362 (5%)	7 (0%)	49	80

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	466	ILE
6	G	728	ILE
6	G	761	PRO
7	H	448	ILE
11	L	142	PRO

5.3.2 Protein sidechains ⓘ

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	292/301 (97%)	292 (100%)	0	100	100
1	B	246/301 (82%)	240 (98%)	6 (2%)	43	73
2	C	828/931 (89%)	818 (99%)	10 (1%)	63	82
3	D	548/608 (90%)	540 (98%)	8 (2%)	57	80
4	E	911/1230 (74%)	896 (98%)	15 (2%)	55	79
5	F	547/782 (70%)	539 (98%)	8 (2%)	57	80
6	G	400/740 (54%)	397 (99%)	3 (1%)	73	86
7	H	491/609 (81%)	484 (99%)	7 (1%)	59	80
8	I	187/231 (81%)	186 (100%)	1 (0%)	81	89
9	J	227/469 (48%)	227 (100%)	0	100	100
10	K	346/401 (86%)	340 (98%)	6 (2%)	53	78
11	L	377/431 (88%)	375 (100%)	2 (0%)	81	89
12	M	214/299 (72%)	211 (99%)	3 (1%)	59	80
13	N	193/259 (74%)	186 (96%)	7 (4%)	31	65
14	O	104/169 (62%)	100 (96%)	4 (4%)	29	63
14	P	99/169 (59%)	96 (97%)	3 (3%)	36	69
15	Q	359/661 (54%)	356 (99%)	3 (1%)	73	86
16	R	114/144 (79%)	110 (96%)	4 (4%)	32	65
17	S	348/532 (65%)	346 (99%)	2 (1%)	78	88
18	T	94/127 (74%)	91 (97%)	3 (3%)	34	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	U	82/160 (51%)	81 (99%)	1 (1%)	63 82
All	All	7007/9554 (73%)	6911 (99%)	96 (1%)	57 80

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	I	236	HIS
13	N	98	LEU
10	K	104	VAL
11	L	351	ILE
13	N	238	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	1241	ASN
17	S	333	ASN
7	H	370	ASN
17	S	210	GLN
13	N	227	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	SAH	L	801	-	27,28,28	0.65	0	36,40,40	0.55	0
20	DTT	D	551(A)	3	7,7,7	0.57	0	4,8,8	0.49	0

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
25	SAH	L	801	-	-	4/15/31/31	0/3/3/3
20	DTT	D	551(A)	3	-	0/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	L	801	SAH	CA-CB-CG-SD
25	L	801	SAH	O-C-CA-CB
25	L	801	SAH	CB-CG-SD-C5'
25	L	801	SAH	OXT-C-CA-CB

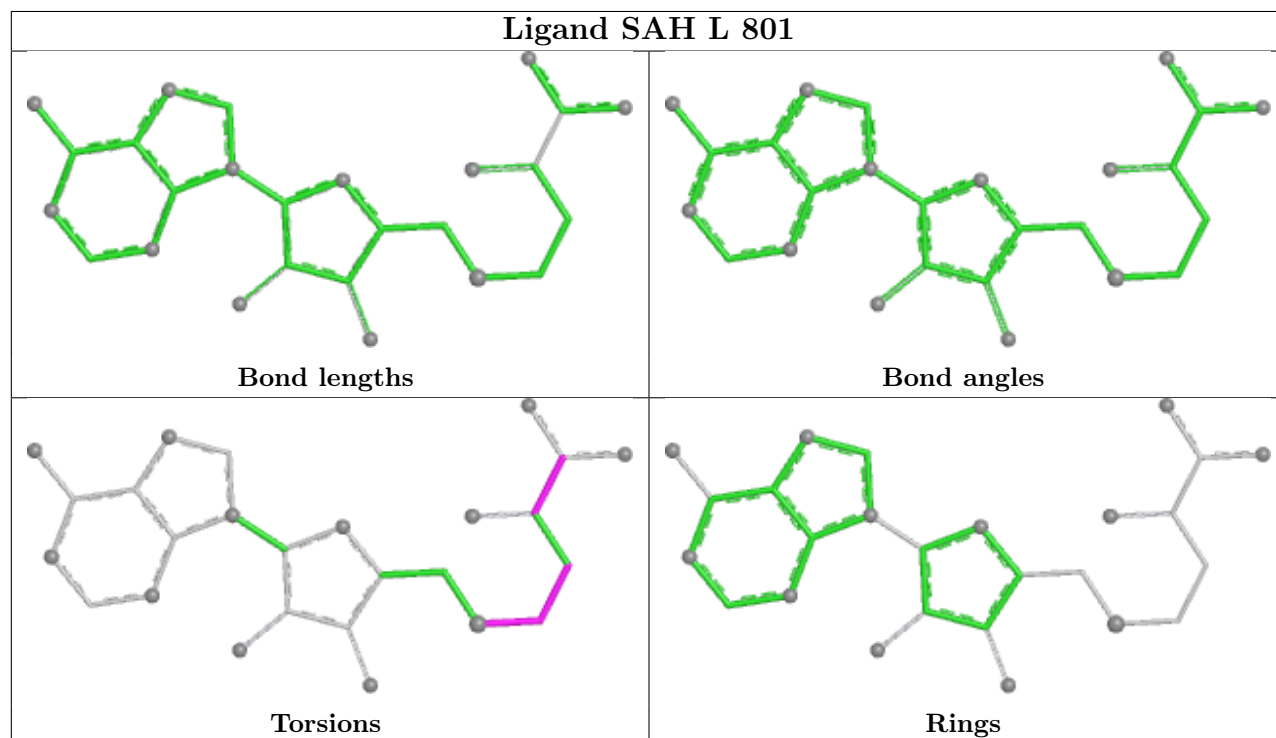
There are no ring outliers.

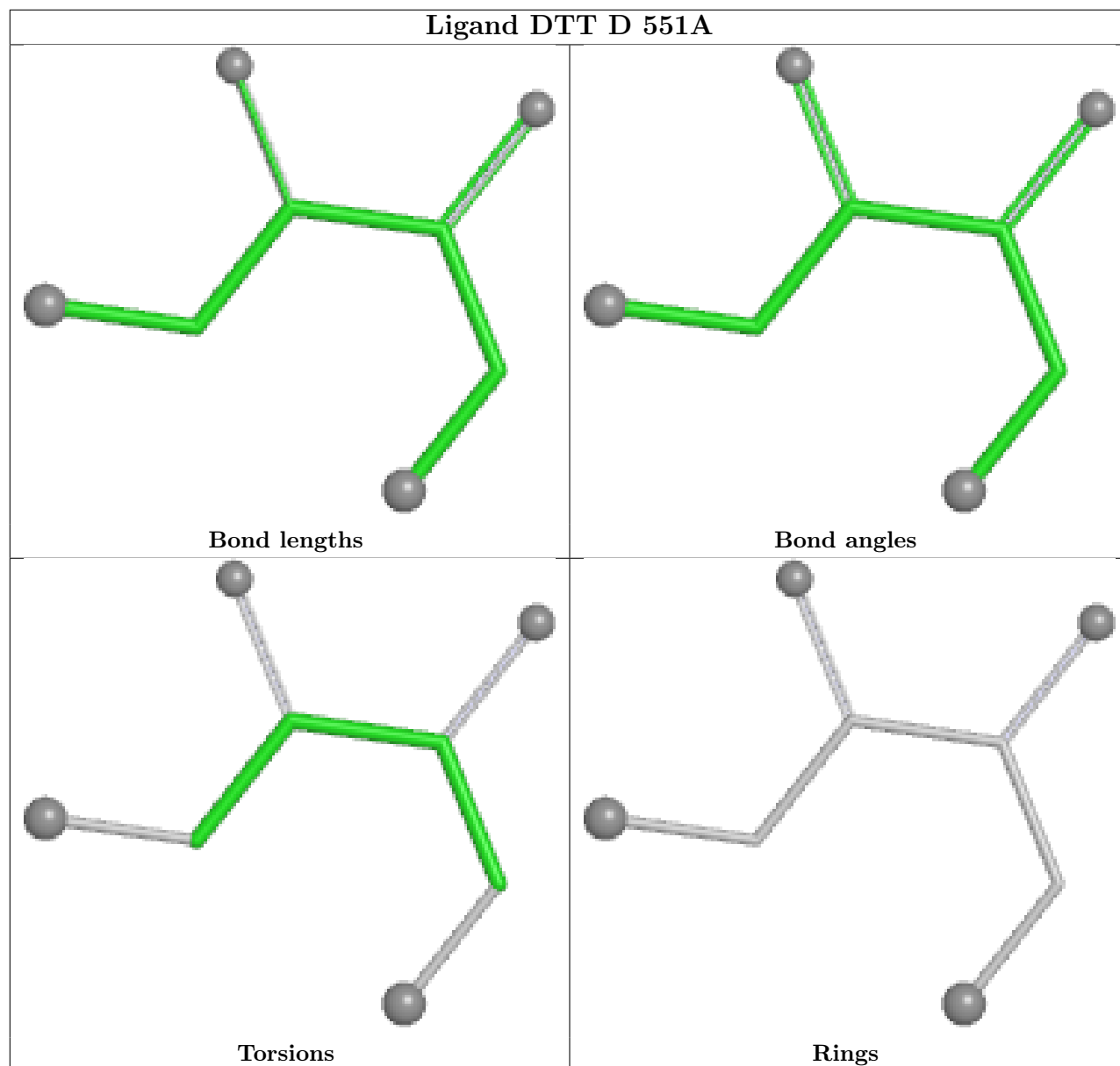
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	L	801	SAH	5	0
20	D	551(A)	DTT	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 than 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	G	9

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	154:UNK	C	155:UNK	N	11.62
1	G	219:UNK	C	220:UNK	N	11.53
1	G	181:UNK	C	182:UNK	N	11.40
1	G	194:UNK	C	195:UNK	N	11.25
1	G	230:UNK	C	231:UNK	N	10.51

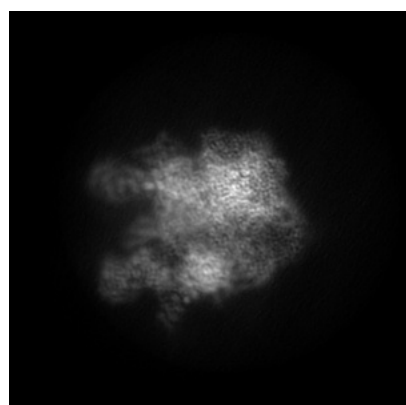
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19877. These allow visual inspection of the internal detail of the map and identification of artifacts.

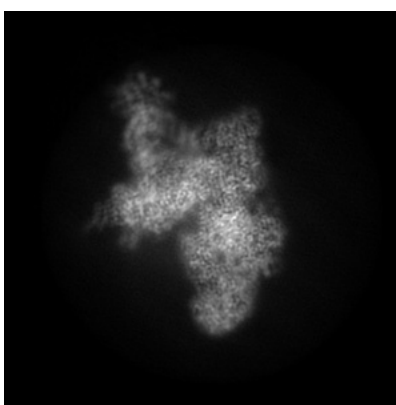
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

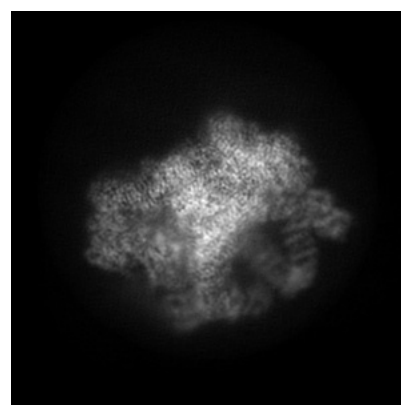
6.1.1 Primary map



X



Y

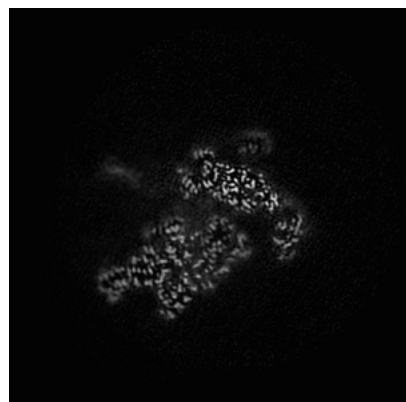


Z

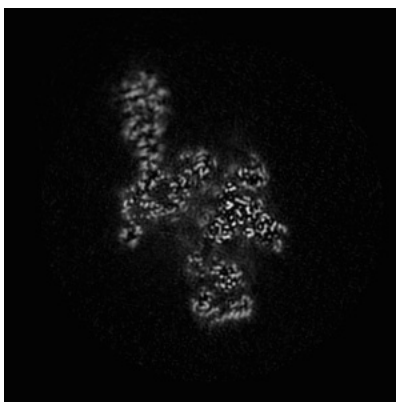
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

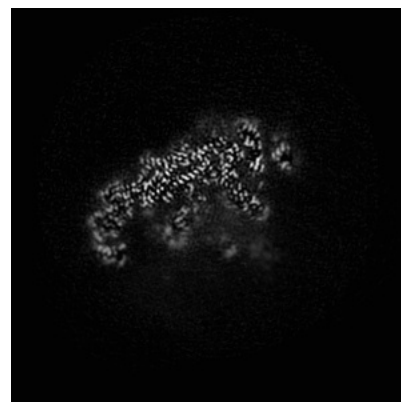
6.2.1 Primary map



X Index: 175



Y Index: 175

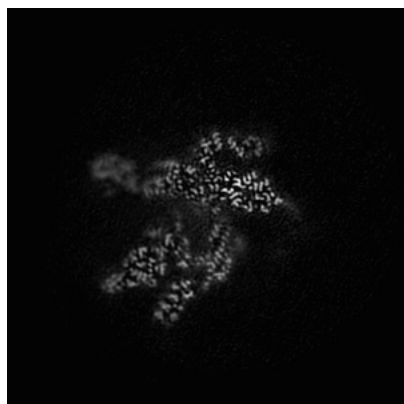


Z Index: 175

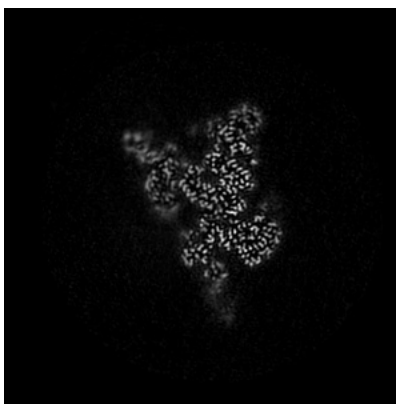
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

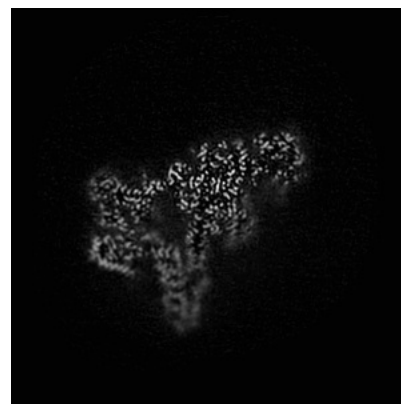
6.3.1 Primary map



X Index: 167



Y Index: 205

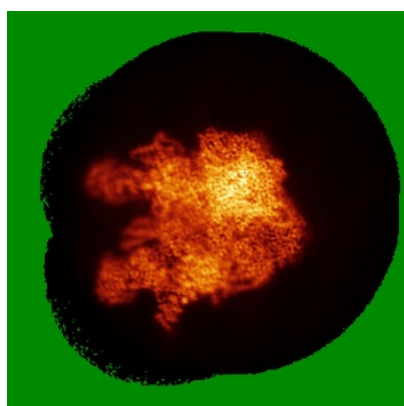


Z Index: 196

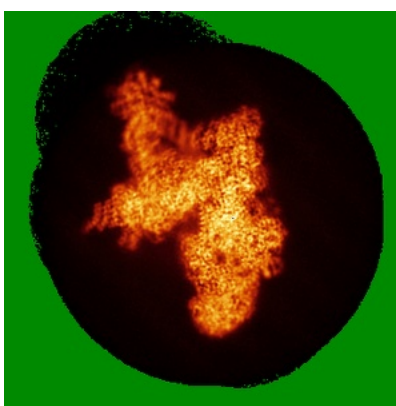
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

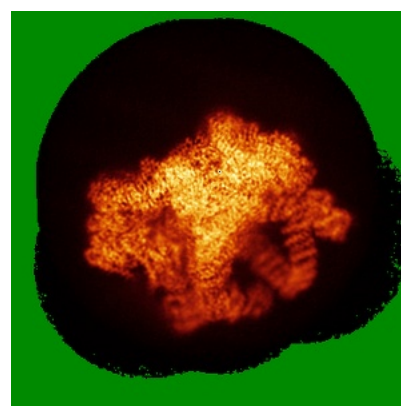
6.4.1 Primary map



X



Y

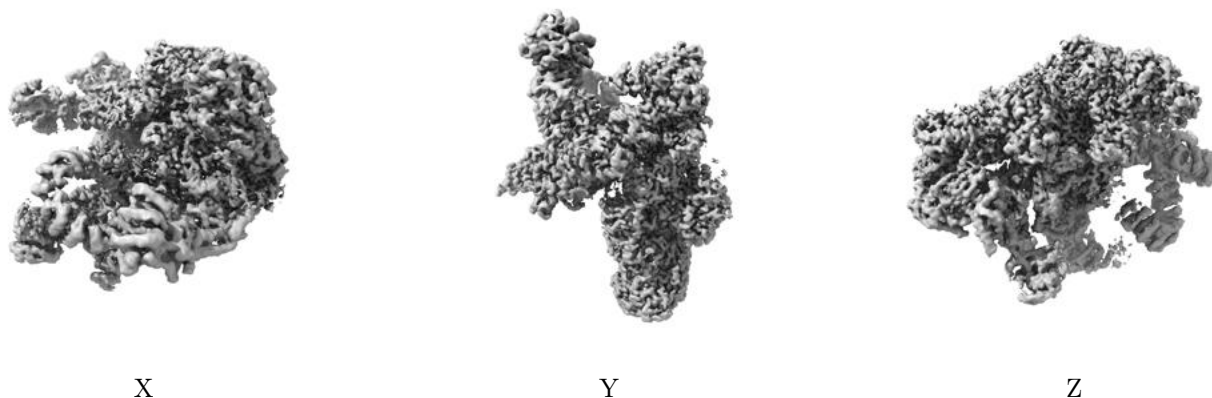


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.00912. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

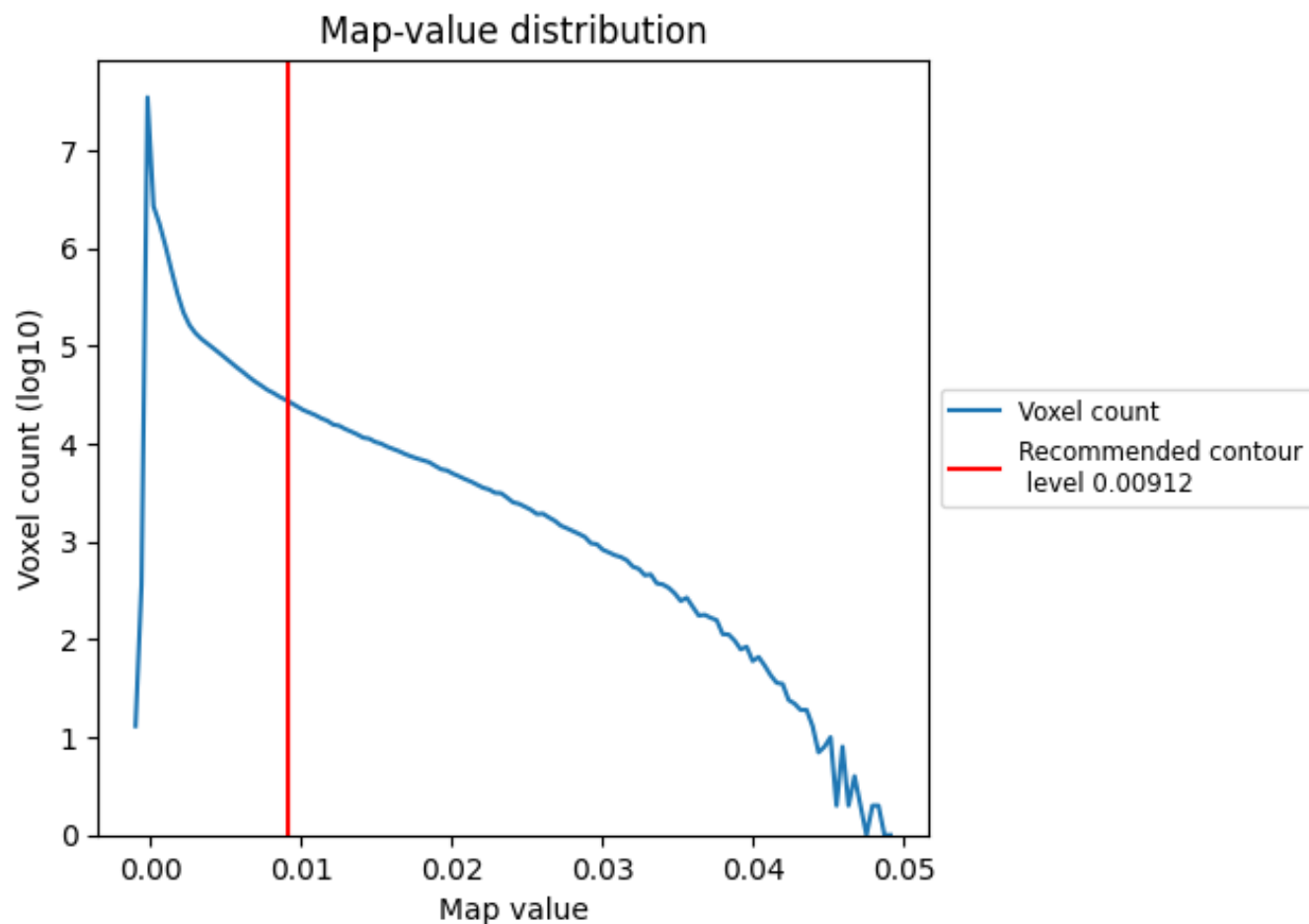
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

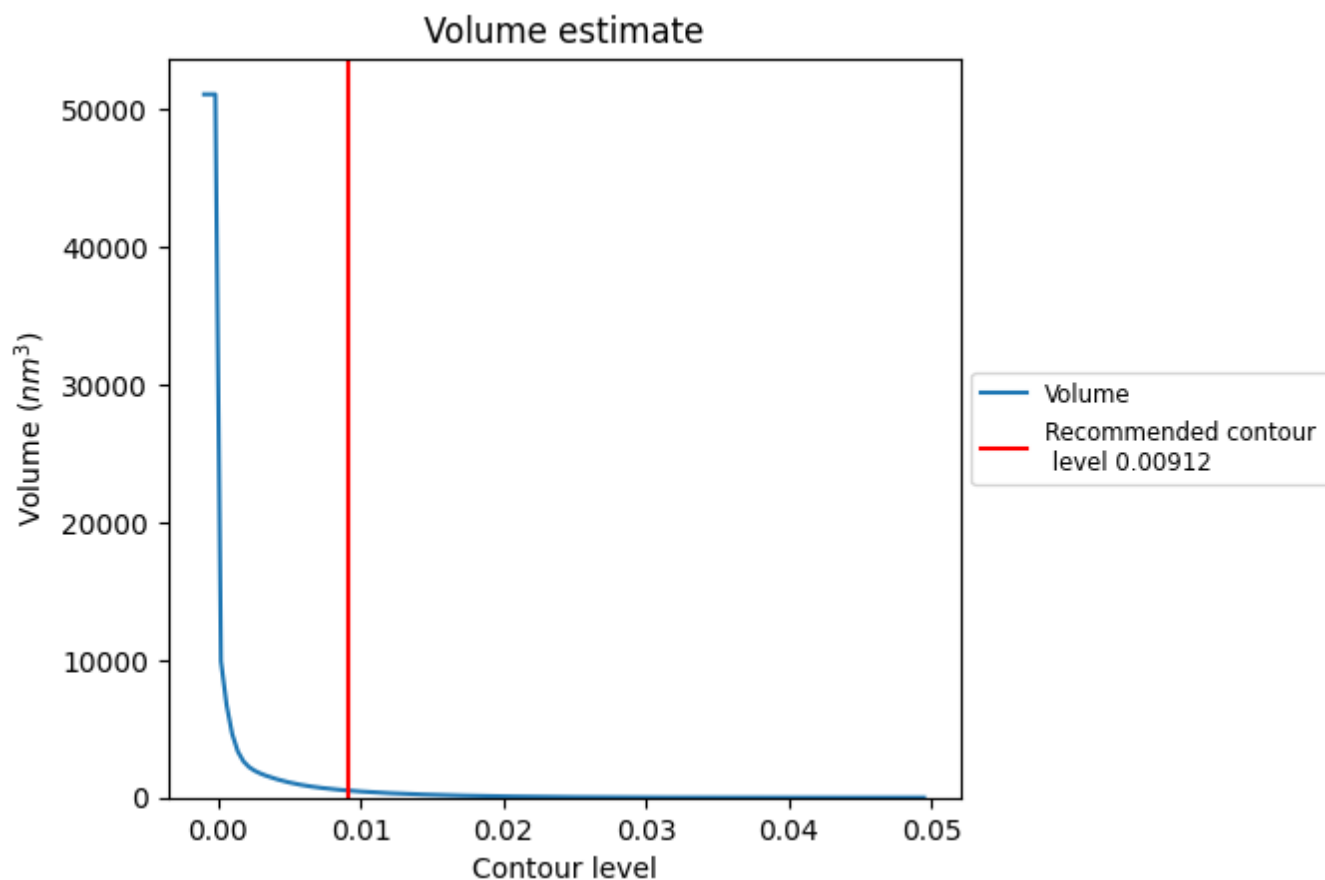
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

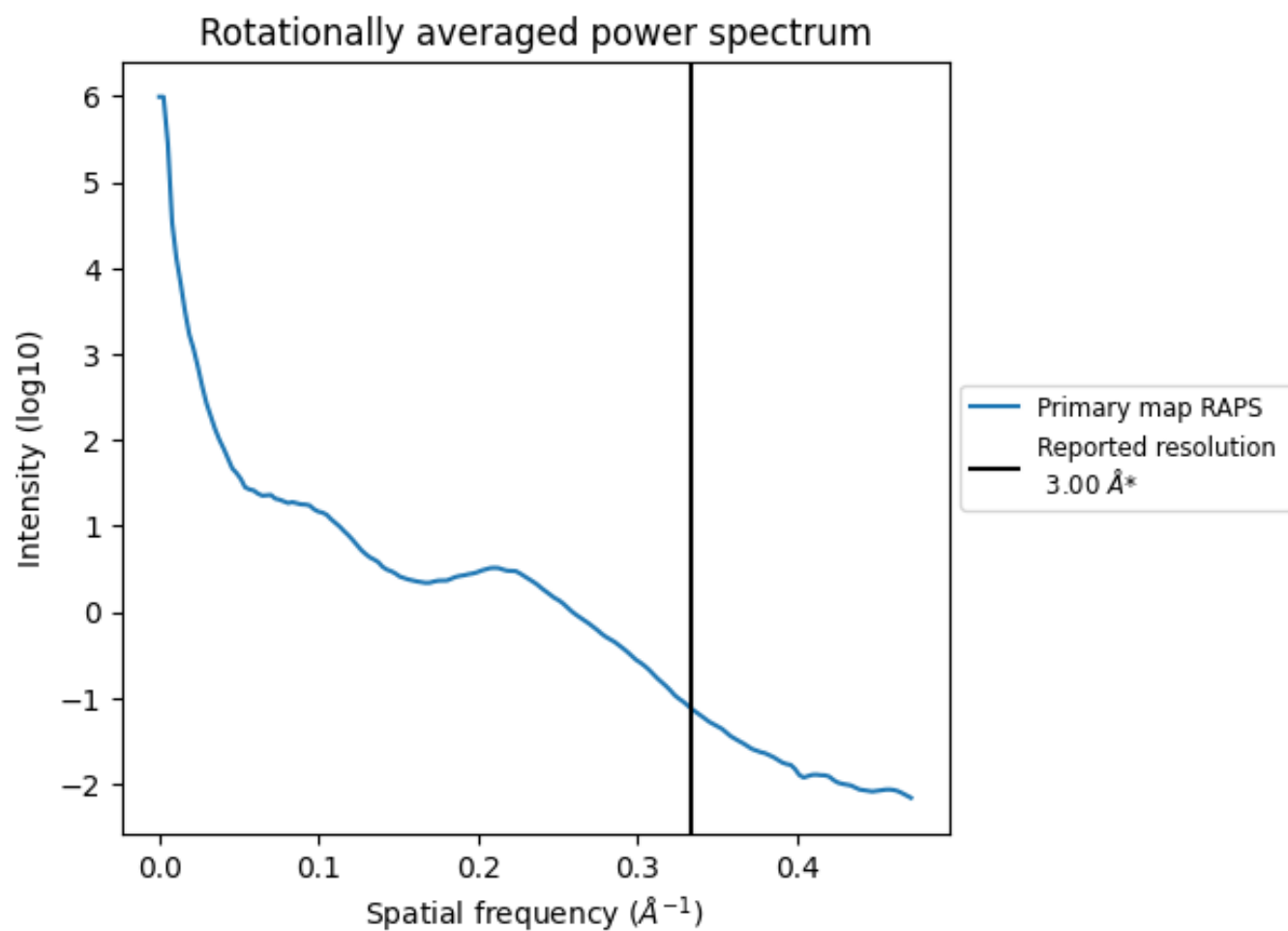
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 511 nm³; this corresponds to an approximate mass of 461 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

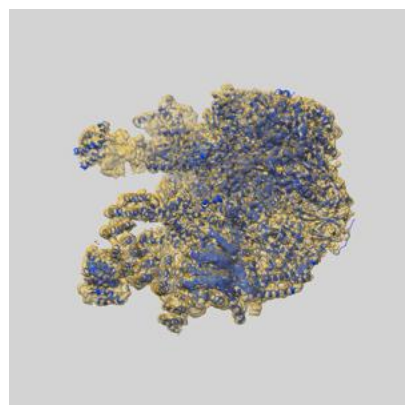
8 Fourier-Shell correlation

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

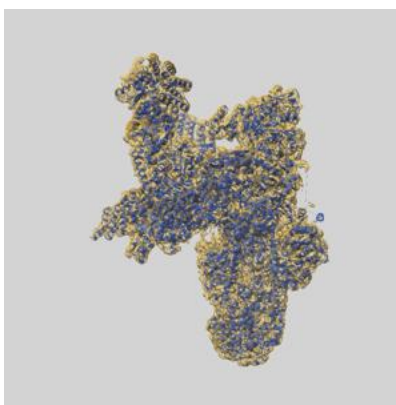
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19877 and PDB model 9EPC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

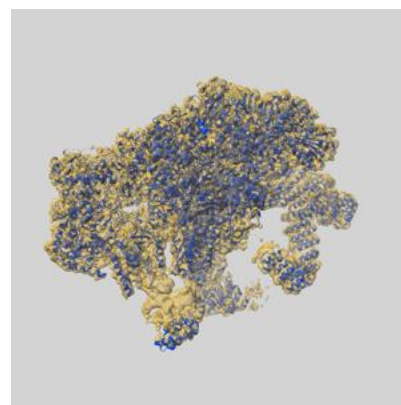
9.1 Map-model overlay [i](#)



X



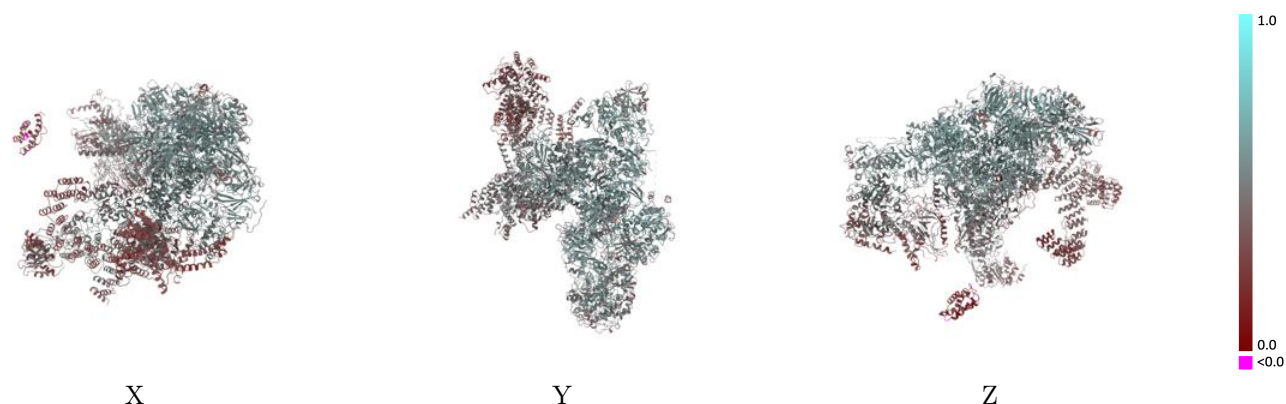
Y



Z

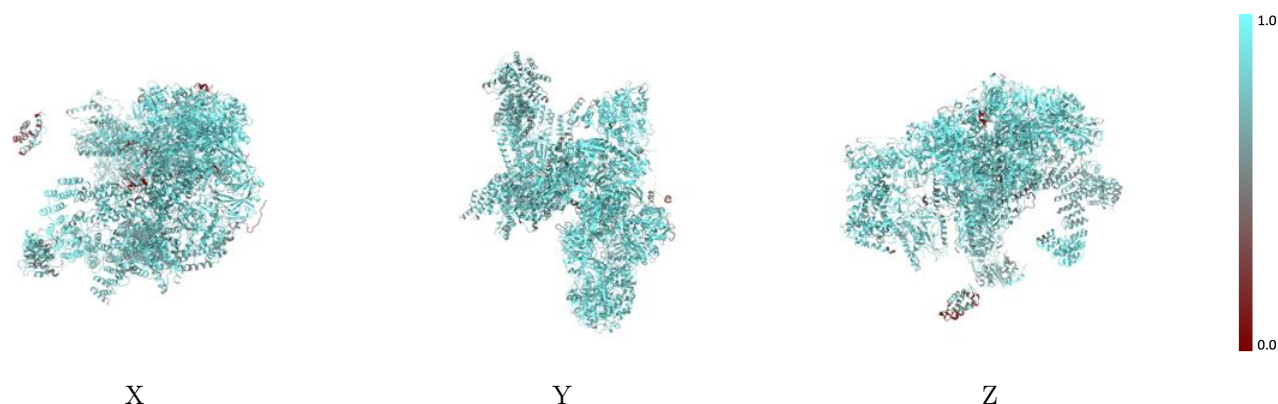
The images above show the 3D surface view of the map at the recommended contour level 0.00912 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



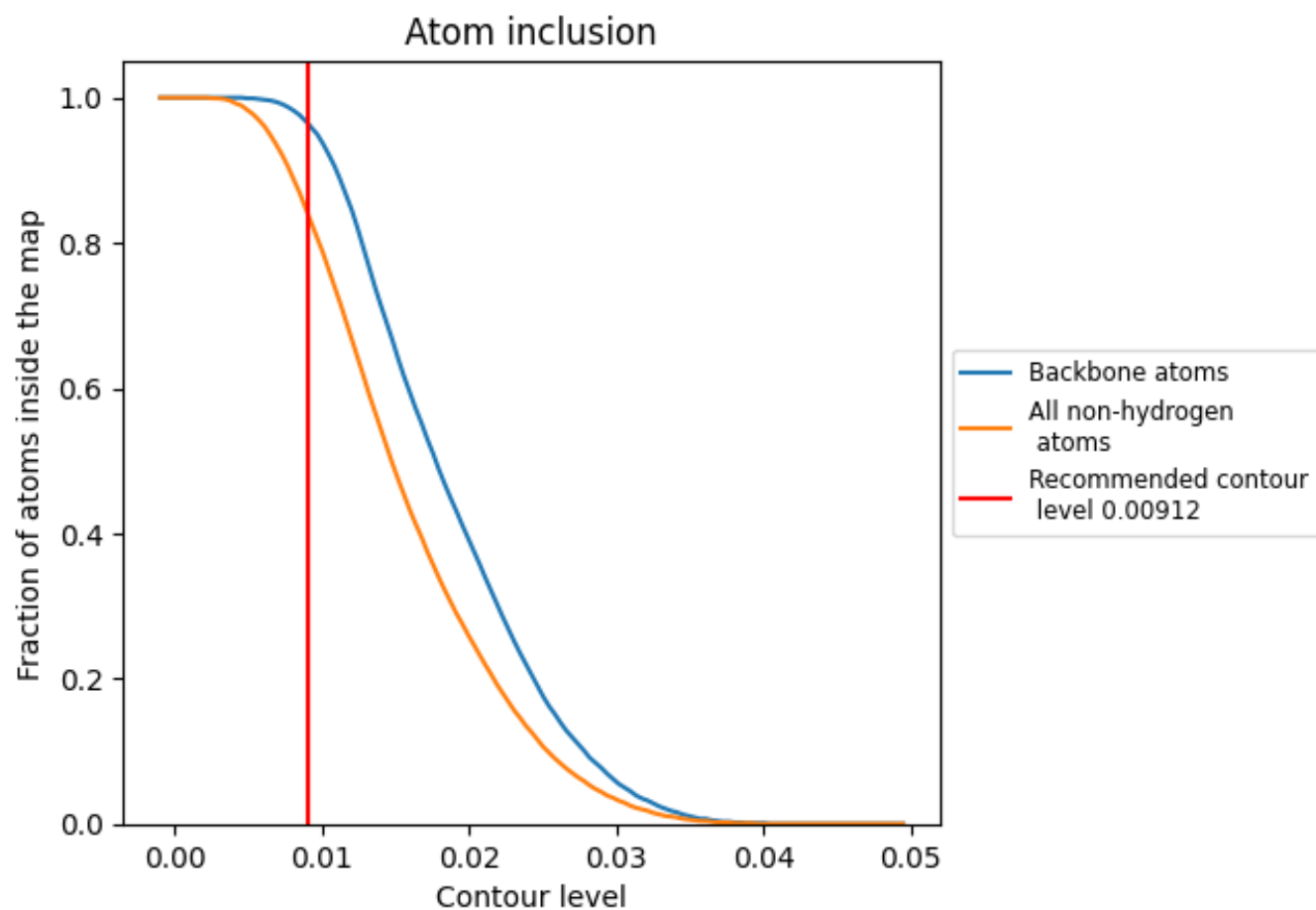
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.00912).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 84% 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 (0.00912) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.4790
A	 0.8730	 0.5350
B	 0.8320	 0.5350
C	 0.8290	 0.5070
D	 0.8400	 0.4890
E	 0.8710	 0.5110
F	 0.8340	 0.4420
G	 0.7500	 0.3160
H	 0.8430	 0.4630
I	 0.8780	 0.4820
J	 0.9100	 0.5650
K	 0.9100	 0.5710
L	 0.8300	 0.4530
M	 0.8440	 0.5420
N	 0.8250	 0.4010
O	 0.9030	 0.5550
P	 0.8320	 0.4980
Q	 0.7480	 0.4240
R	 0.7990	 0.5130
S	 0.8840	 0.5440
T	 0.8610	 0.4630
U	 0.4750	 0.1740

