wwPDB EM Validation Summary Report (i)

Jul 3, 2024 – 03:15 am BST

PDB ID	:	7NW0
EMDB ID	:	EMD-12619
Title	:	RNA polymerase II pre-initiation complex with open promoter DNA
Authors	:	Aibara, S.; Schilbach, S.; Cramer, P.
Deposited on	:	2021-03-16
Resolution	:	6.60 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 (1)) were used in the production of this report:

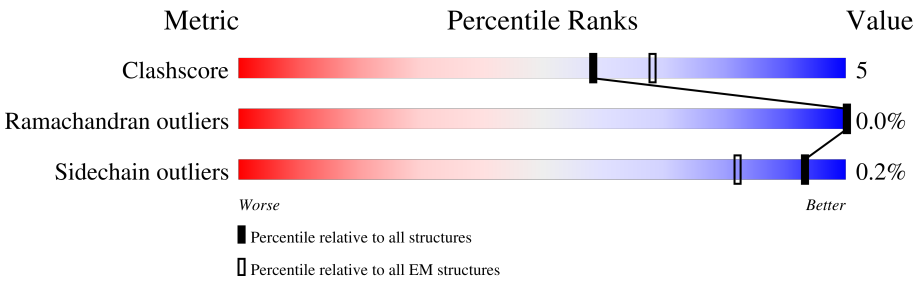
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 6.60 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	0	760	52% 79% 15% 6%
2	1	548	32% 42% 6% 52%
3	2	462	26% 72% 12% 16%
4	3	309	14% 12% • 86%
5	4	308	38% 69% 16% 15%
6	5	71	38% 82% 11% 7%
7	6	395	25% 68% 15% 17%
8	7	782	22% 66% 12% 23%

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Mol	Chain	Length	Quality of chain
9	A	1970	11% 63% 9% 28%
10	B	1174	16% 87% 10%
11	C	275	17% 82% 12% 7%
12	D	142	58% 86% 10%
13	E	210	14% 87% 13%
14	F	127	6% 57% 5% 38%
15	G	172	28% 88% 11%
16	H	150	25% 90% 9%
17	I	125	9% 78% 14% 9%
18	J	67	19% 87% 9%
19	K	117	24% 86% 12%
20	L	58	24% 67% 9% 24%
21	M	316	19% 87% 7% 6%
22	N	106	7% 53% 9% 38%
23	O	339	21% 47% 5% 47%
24	Q	517	12% 24% 73%
25	R	249	36% 80% 10% 11%
26	T	106	10% 54% 10% 36%
27	U	376	30% 28% 70%
28	V	109	90% 82% 9% 9%
29	W	439	23% 39% 7% 54%
30	X	291	31% 52% 7% 41%
31	Y	16	81% 81% 19%
32	Z	8	100% 100%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 66935 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 TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	714	5751	3683	999	1040	29	0	0

- Molecule 2 is a protein called General transcription factor IIH subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	265	2167	1382	378	395	12	0	0

- Molecule 3 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	390	3158	2050	545	551	12	0	0

- Molecule 4 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	3	44	382	245	61	76	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	263	2066	1323	344	380	19	0	0

- Molecule 6 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	66	523	337	83	100	3	0	0

- Molecule 7 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	329	2567	1621	440	479	27	0	0

- Molecule 8 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	605	4890	3127	848	885	30	0	0

- Molecule 9 is a protein called RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	1423	11274	7092	2016	2094	72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	1136	9076	5739	1597	1676	64	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	257	2059	1294	351	408	6	0	0

- Molecule 12 is a protein called RPOL4c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	128	1050	656	178	212	4	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	209	1721	1089	300	324	8	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	79	636	406	108	117	5	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	171	1351	875	219	249	8	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	148	1186	750	194	237	5	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	I	114	928	571	166	180	11	0	0

- Molecule 18 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	64	507	328	86	87	6	0	0

- Molecule 19 is a protein called RNA_pol_L_2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	K	115	920	593	152	173	2	0	0

- Molecule 20 is a protein called RNA polymerase II subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	44	373	231	72	64	6	0	0

- Molecule 21 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	298	2301	1435	409	439	18	0	0

- Molecule 22 is a DNA chain called Non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	N	66	1369	646	260	398	65	0	0

- Molecule 23 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	179	1422	923	251	241	7	0	0

- Molecule 24 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	138	1138	719	208	208	3	0	0

- Molecule 25 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	222	1788	1127	320	338	3	0	0

- Molecule 26 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	T	68	1358	642	246	402	68	0	0

- Molecule 27 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	113	930	585	152	189	4	0	0

- Molecule 28 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	V	99	806	510	142	151	3	0	0

- Molecule 29 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	202	1659	1042	299	307	11	0	0

- Molecule 30 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	X	171	1403	895	243	261	4	0	0

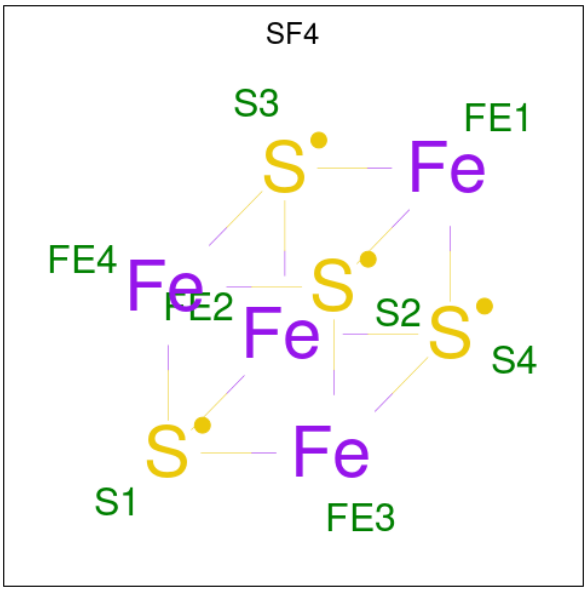
- Molecule 31 is a protein called Unassigned peptide, likely TFIIE-Beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	Y	16	80	48	16	16	0	0

- Molecule 32 is a protein called Unassigned peptide, likely XPB.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	Z	8	40	24	8	8	0	0

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



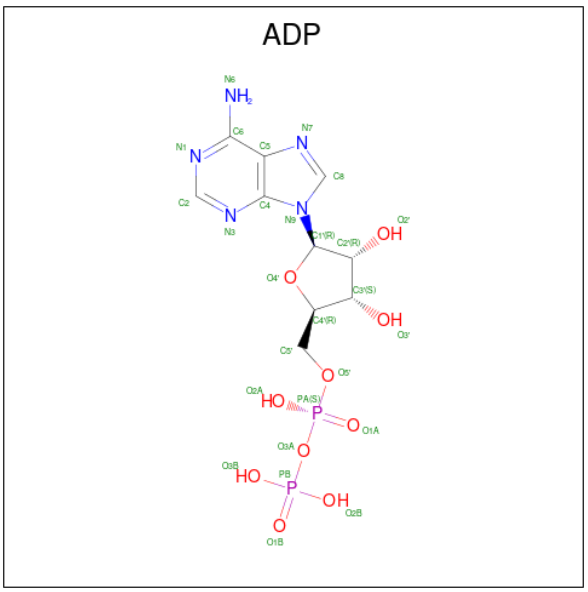
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
33	0	1	8	4	4	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
34	4	2	2	2	0
34	6	3	3	3	0
34	A	2	2	2	0
34	B	1	1	1	0
34	C	1	1	1	0
34	I	2	2	2	0
34	J	1	1	1	0
34	L	1	1	1	0
34	M	1	1	1	0
34	W	1	1	1	0

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).

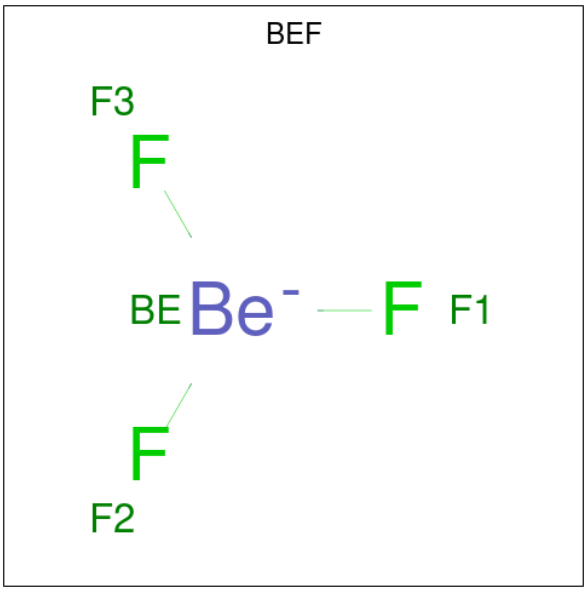


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
35	7	1	27	10	5	10	2	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	7	1	1	1	0
			Total	Mg	
36	A	1	1	1	0

- Molecule 37 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).

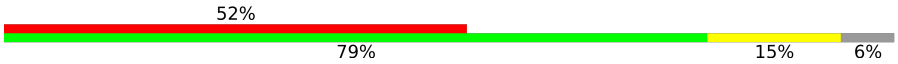


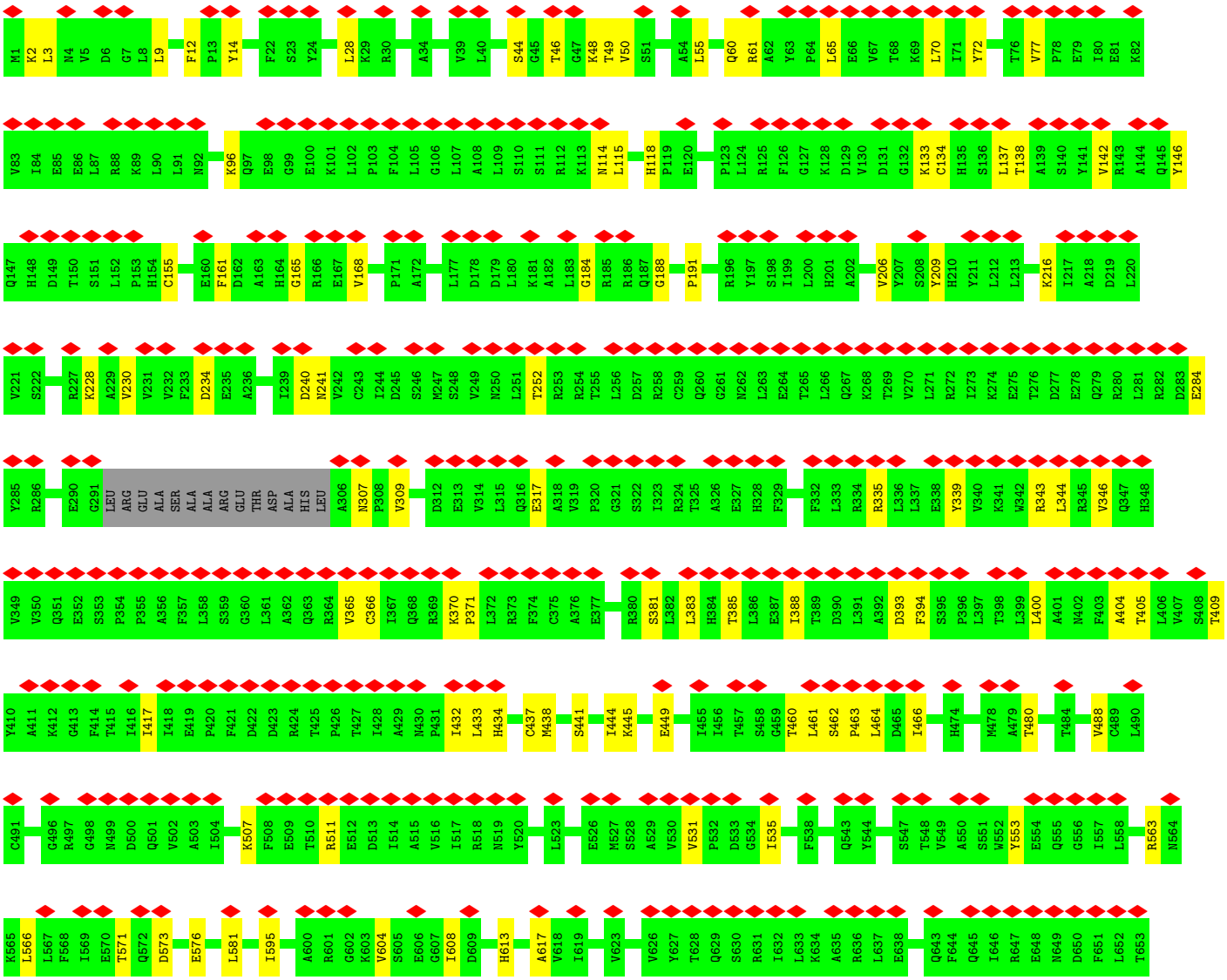
Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
37	7	1	4	1	3	0

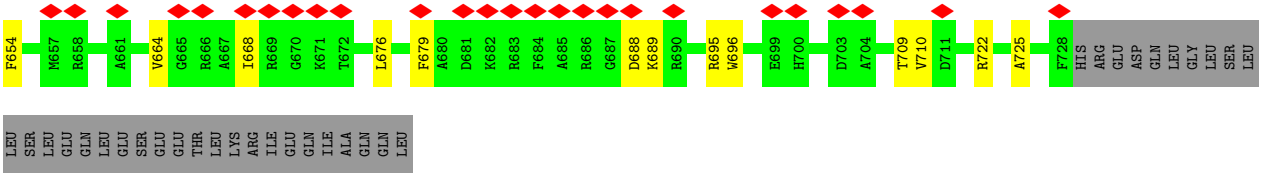
3 Residue-property plots (i)

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

- Molecule 1: TFIIH basal transcription factor complex helicase XPD subunit

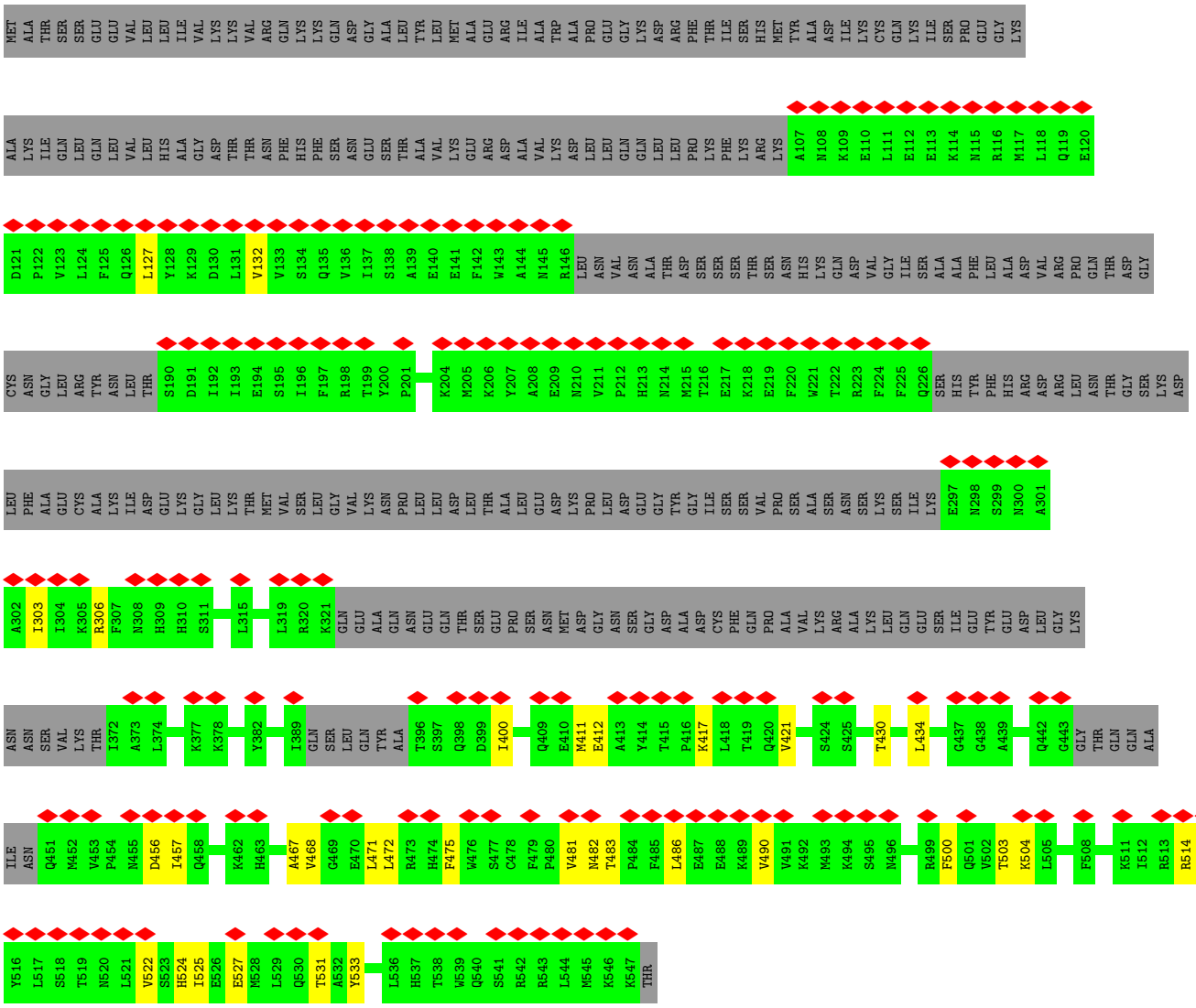
Chain 0: 





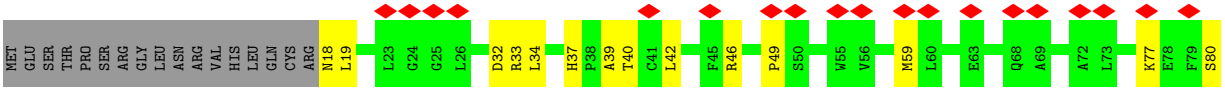
• Molecule 2: General transcription factor IIH subunit 1

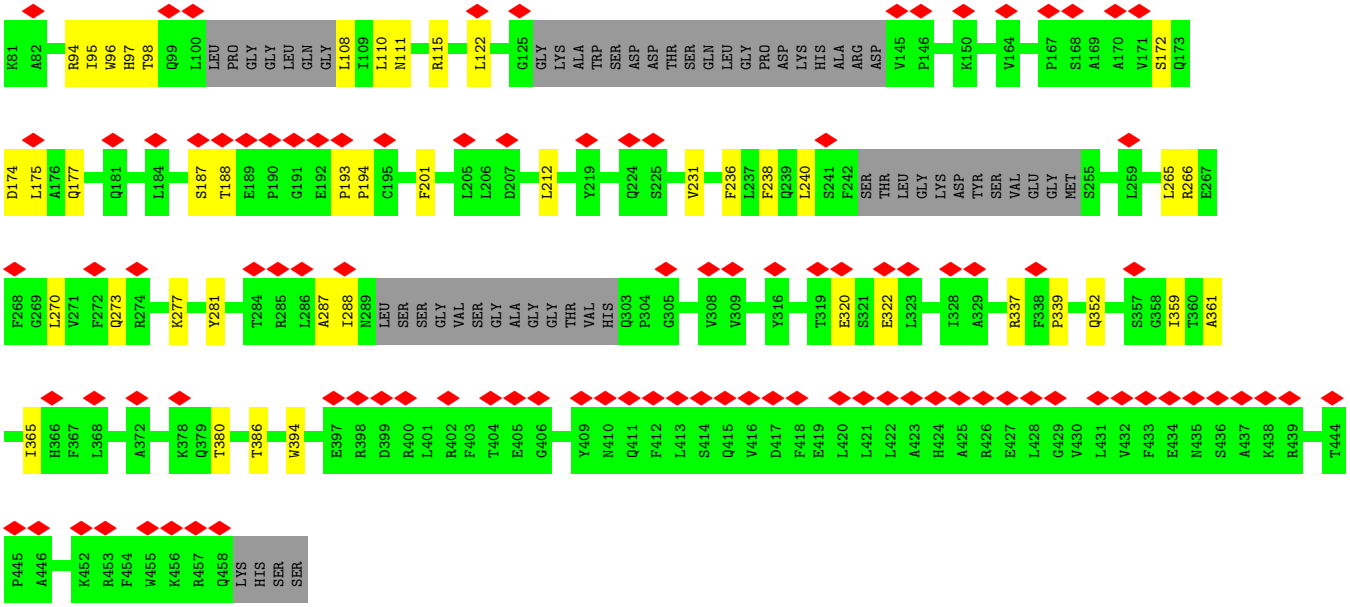
Chain 1:



• Molecule 3: General transcription factor IIH subunit 4

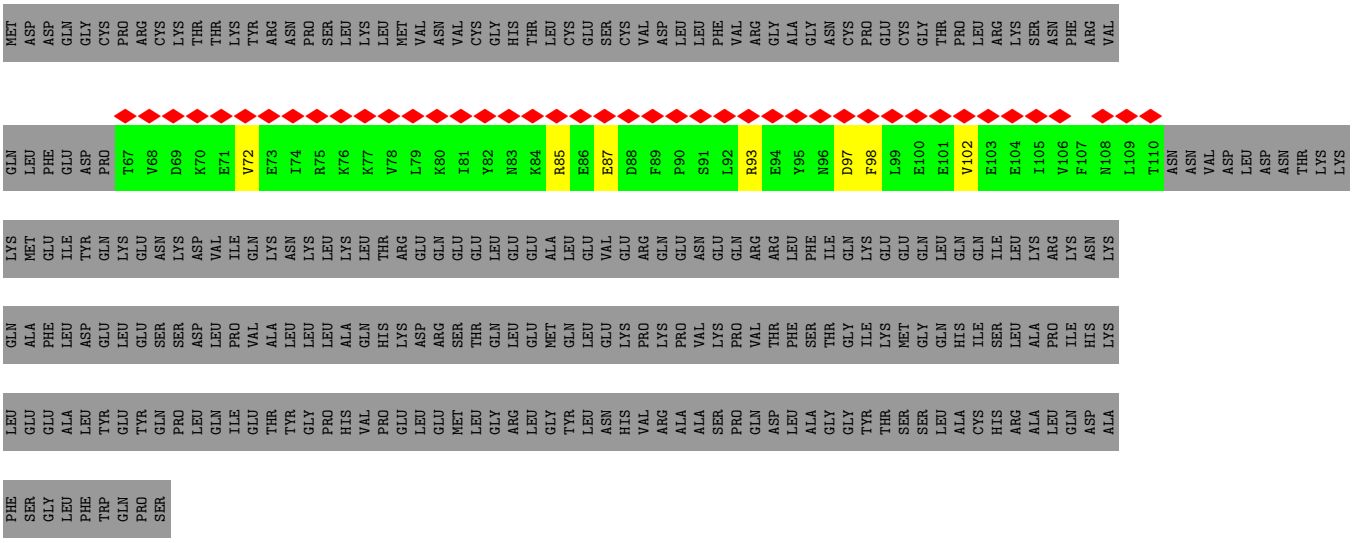
Chain 2:





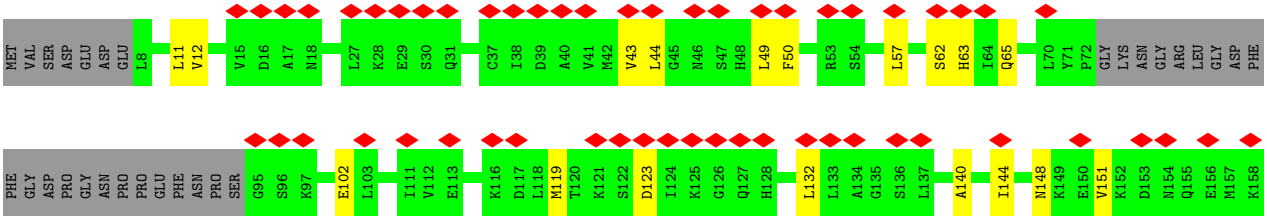
- Molecule 4: CDK-activating kinase assembly factor MAT1

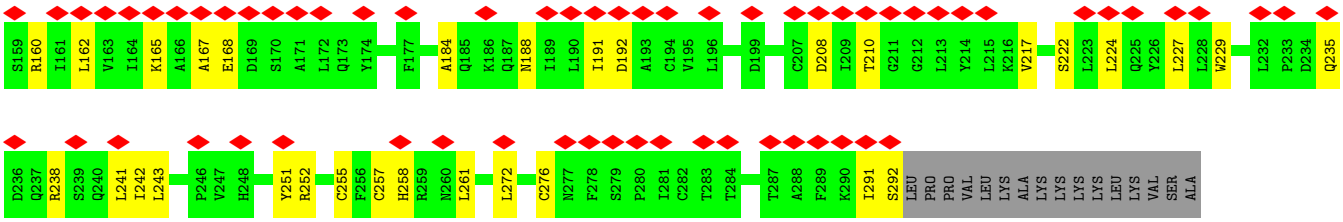
Chain 3:



- Molecule 5: General transcription factor IIH subunit 3

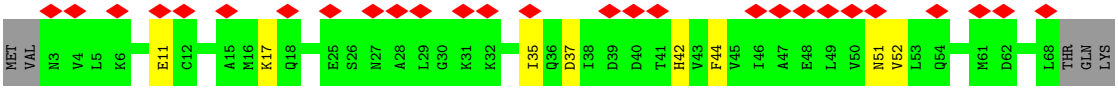
Chain 4:





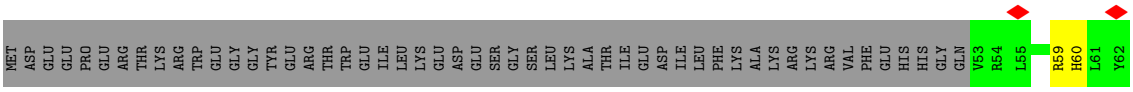
• Molecule 6: General transcription factor IIH subunit 5

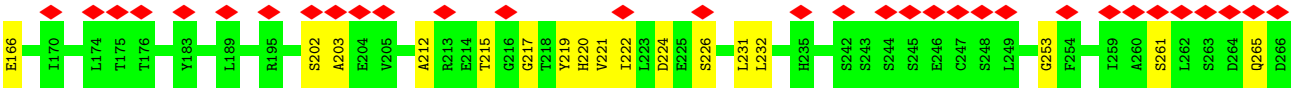
Chain 5:

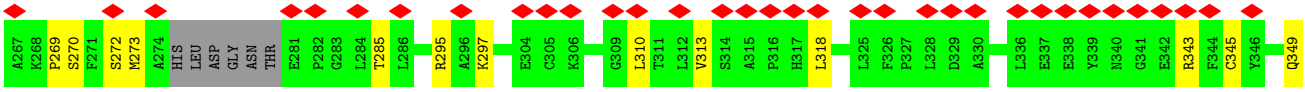


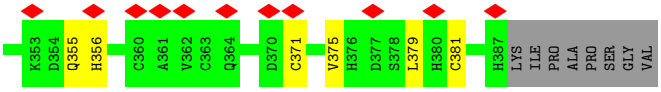
• Molecule 7: General transcription factor IIH subunit 2

Chain 6:



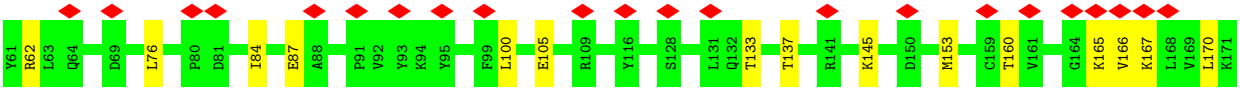


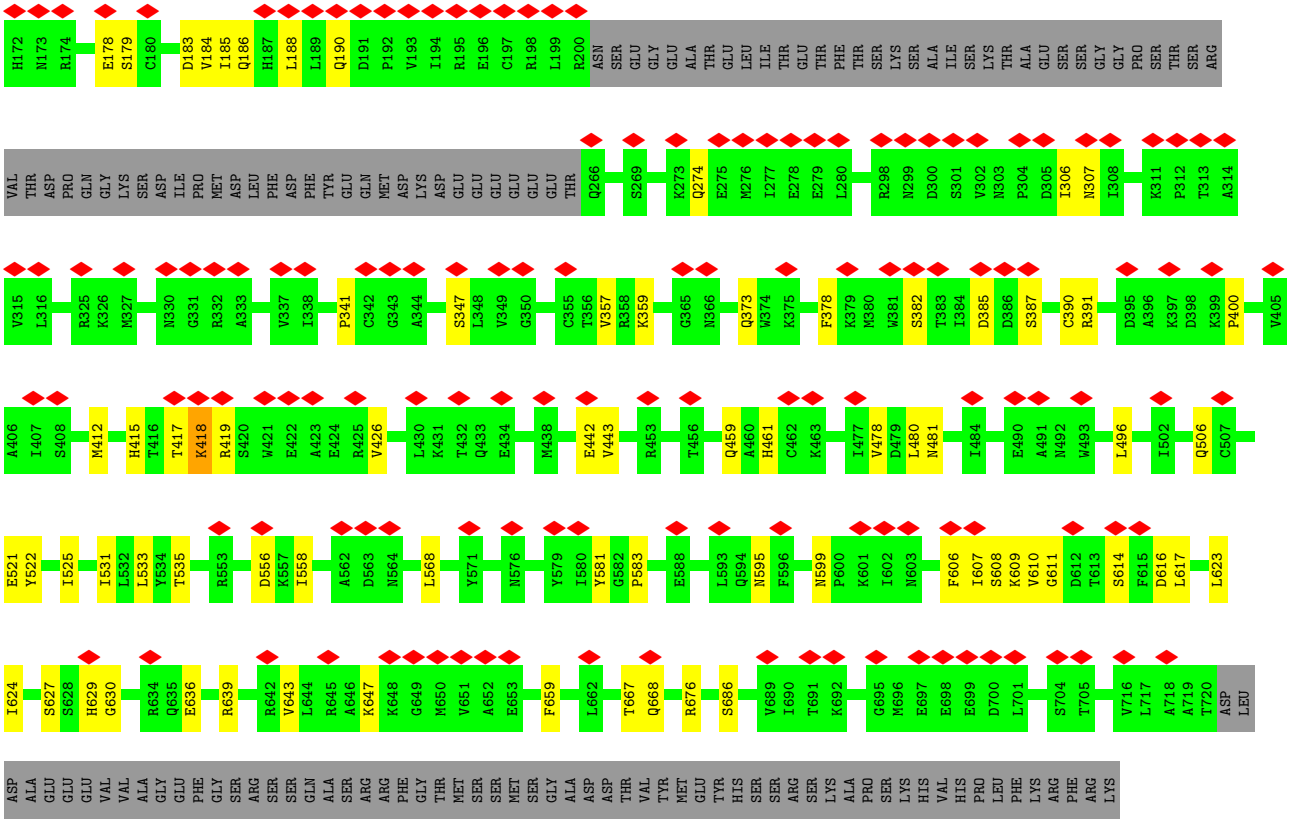




• Molecule 8: General transcription and DNA repair factor IIH helicase subunit XPB

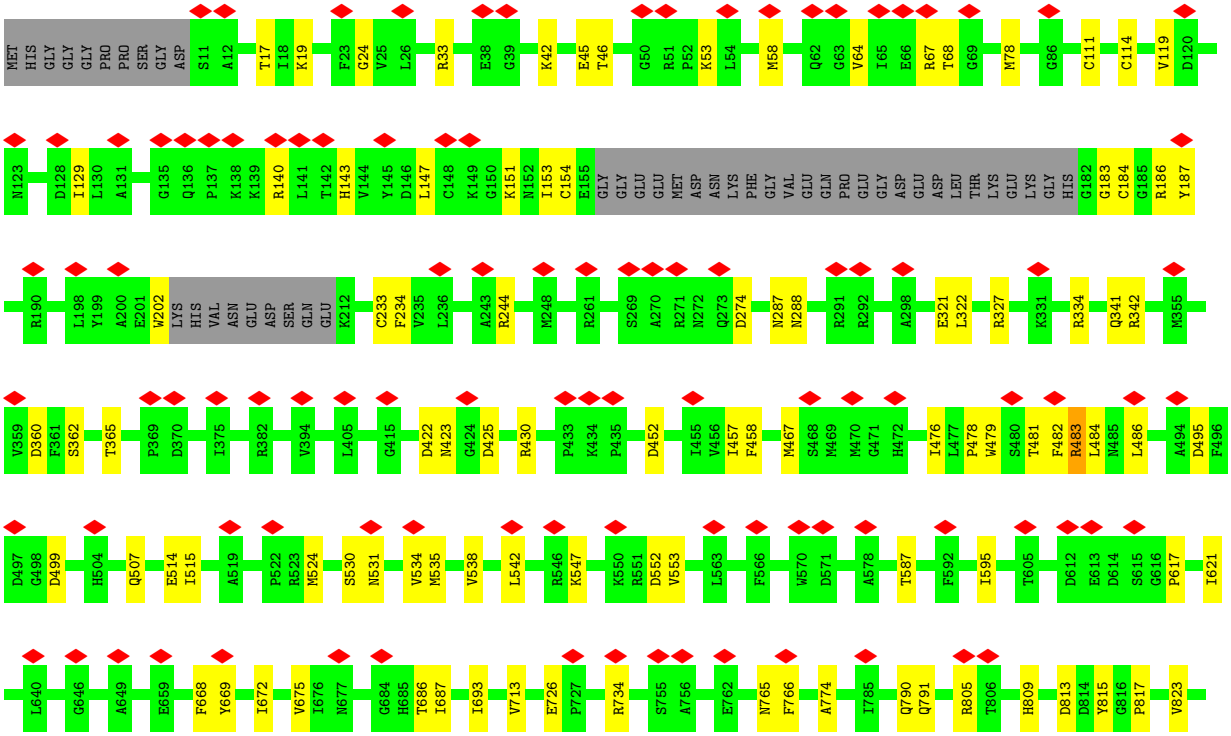
Chain 7:

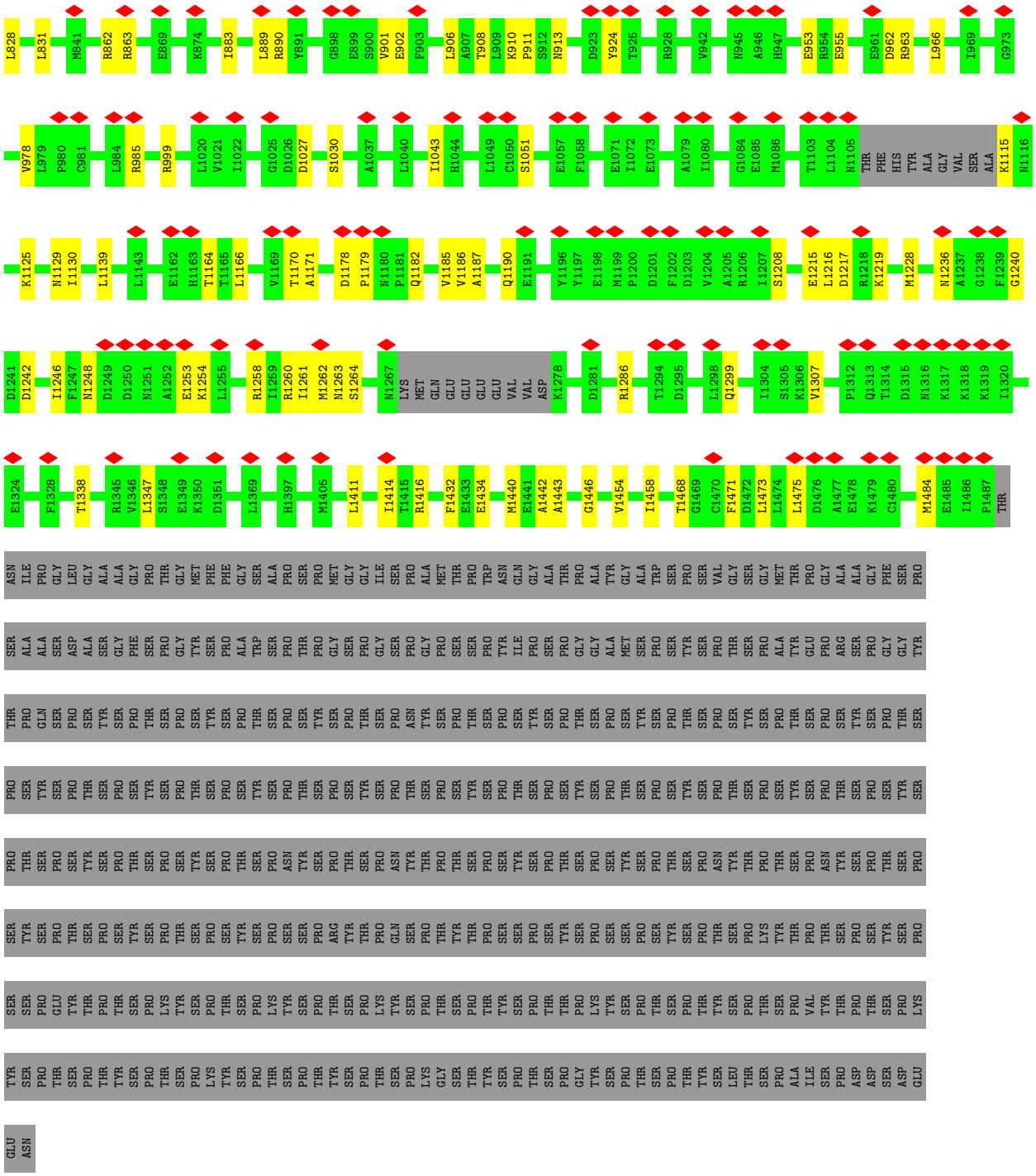




- Molecule 9: RPB1

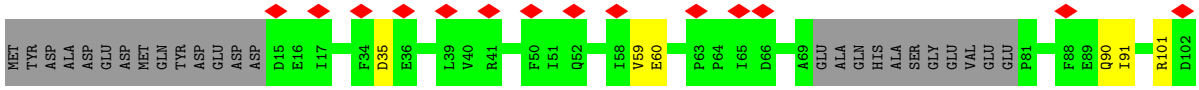
Chain A:

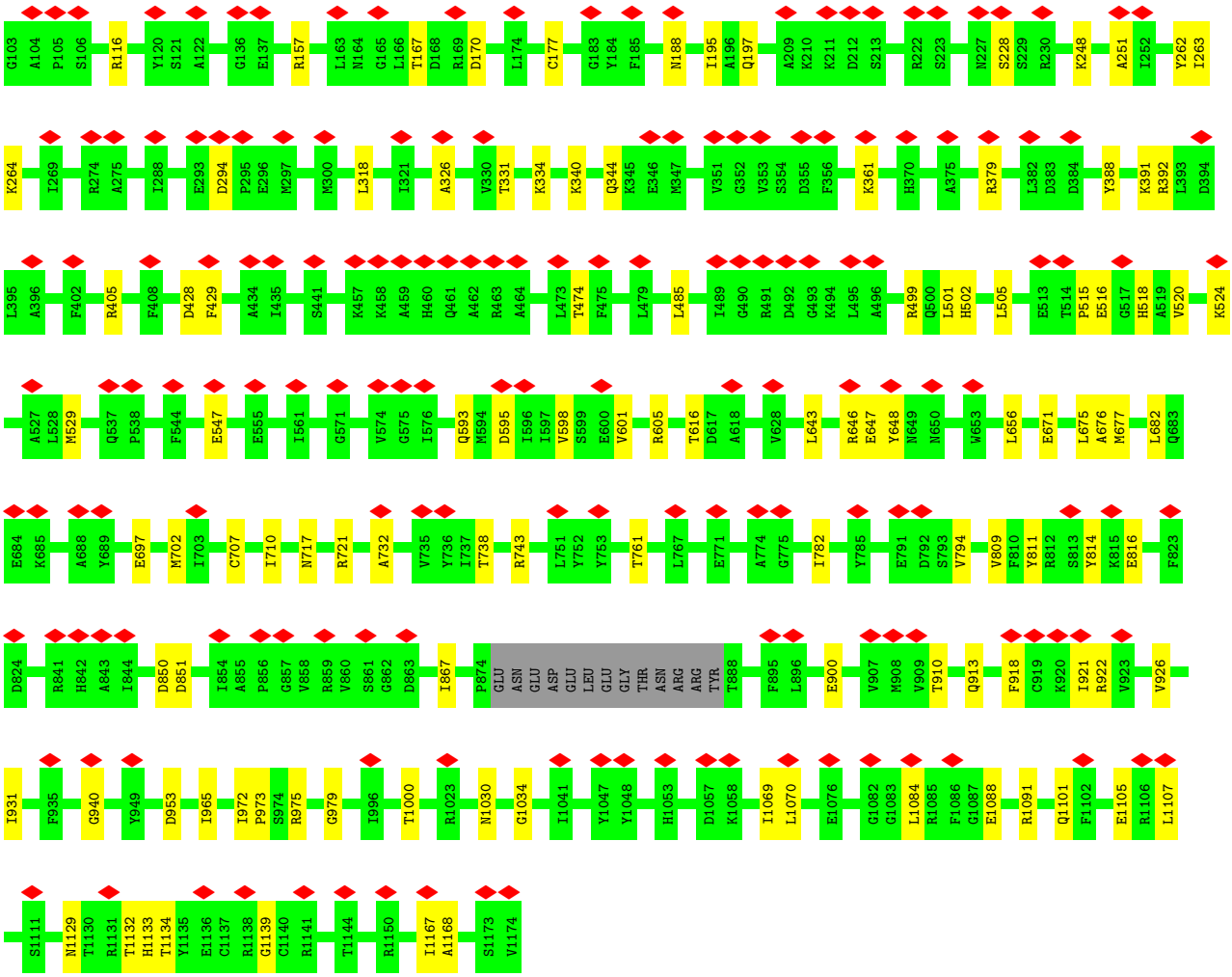




- Molecule 10: DNA-directed RNA polymerase subunit beta

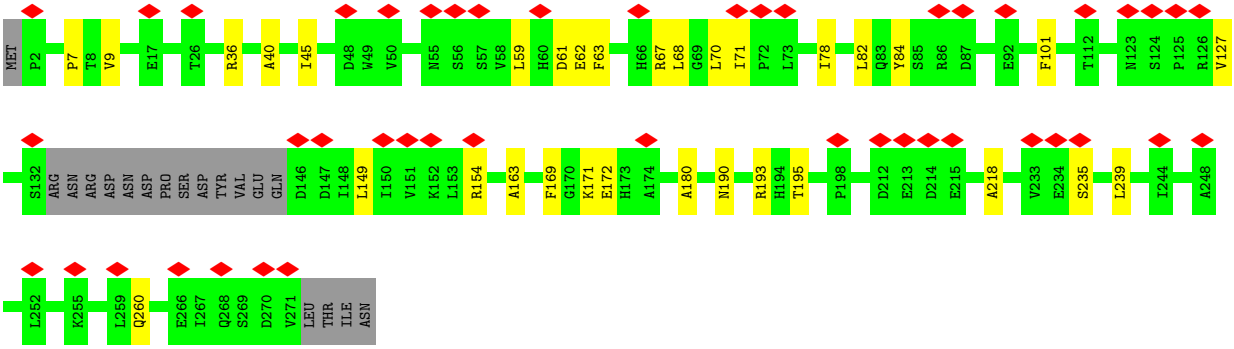
Chain B:





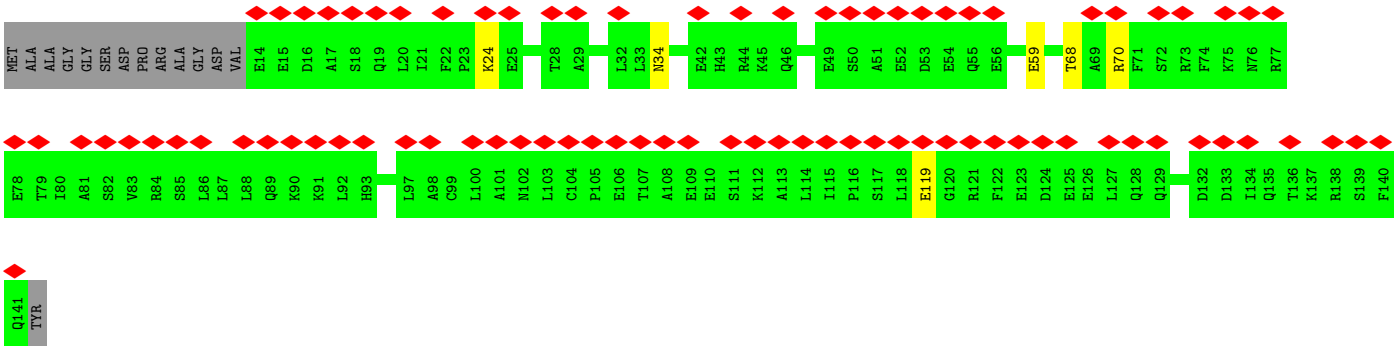
- Molecule 11: DNA-directed RNA polymerase II subunit RPB3

Chain C:



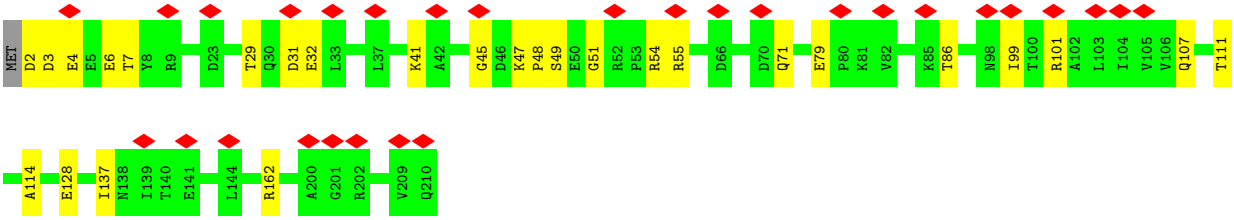
- Molecule 12: RPOL4c domain-containing protein

Chain D:



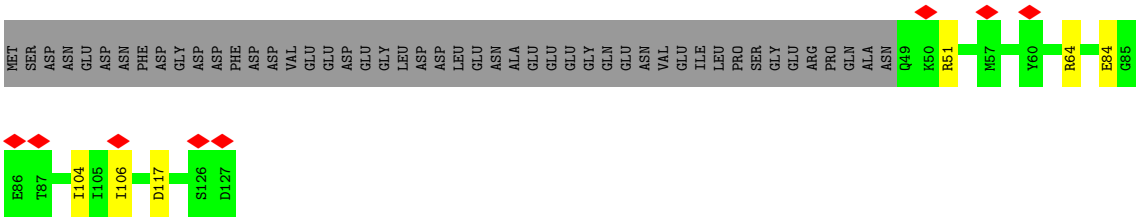
• Molecule 13: DNA-directed RNA polymerase II subunit E

Chain E:



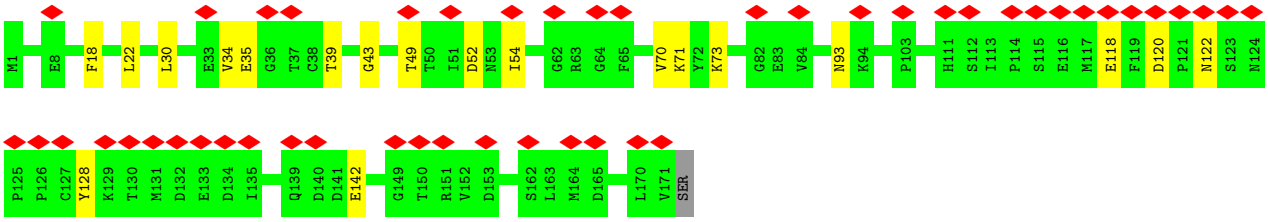
• Molecule 14: DNA-directed RNA polymerase II subunit F

Chain F:



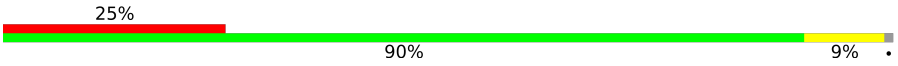
• Molecule 15: DNA-directed RNA polymerase II subunit RPB7

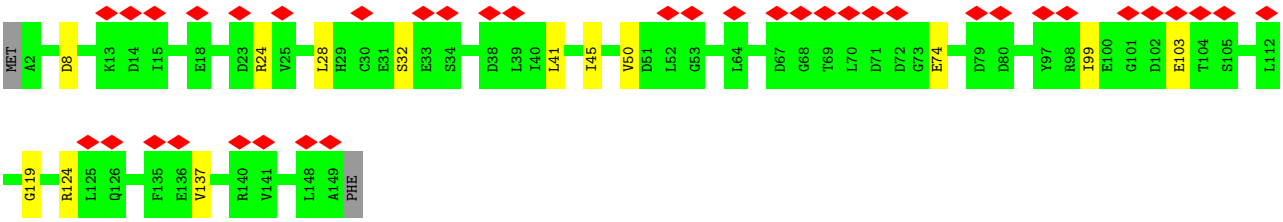
Chain G:



• Molecule 16: DNA-directed RNA polymerases I, II, and III subunit RPABC3

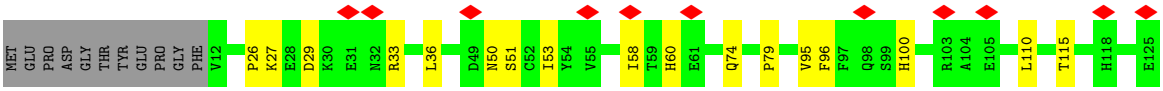
Chain H:





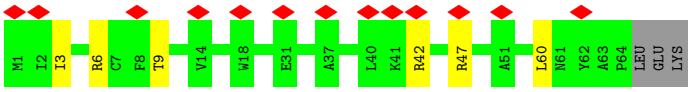
• Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I:



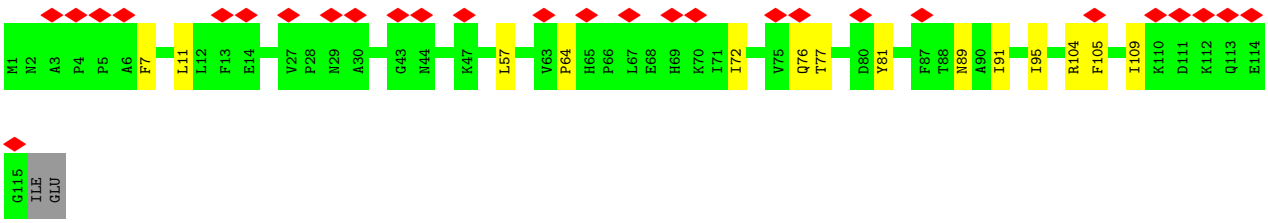
• Molecule 18: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



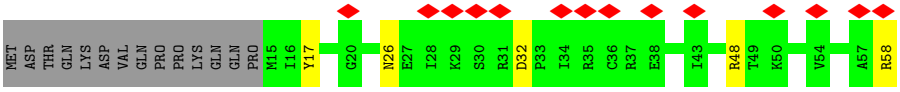
• Molecule 19: RNA_pol_L_2 domain-containing protein

Chain K:



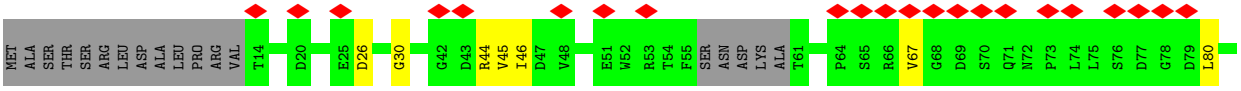
• Molecule 20: RNA polymerase II subunit K

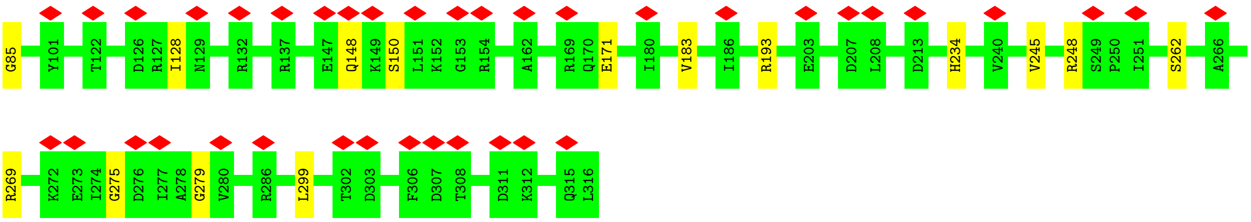
Chain L:



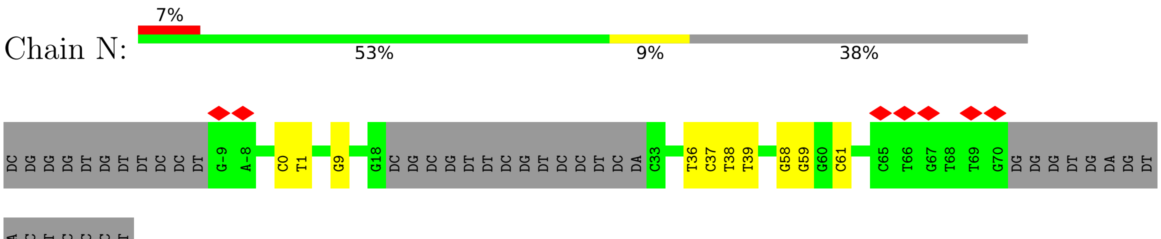
• Molecule 21: Transcription initiation factor IIB

Chain M:

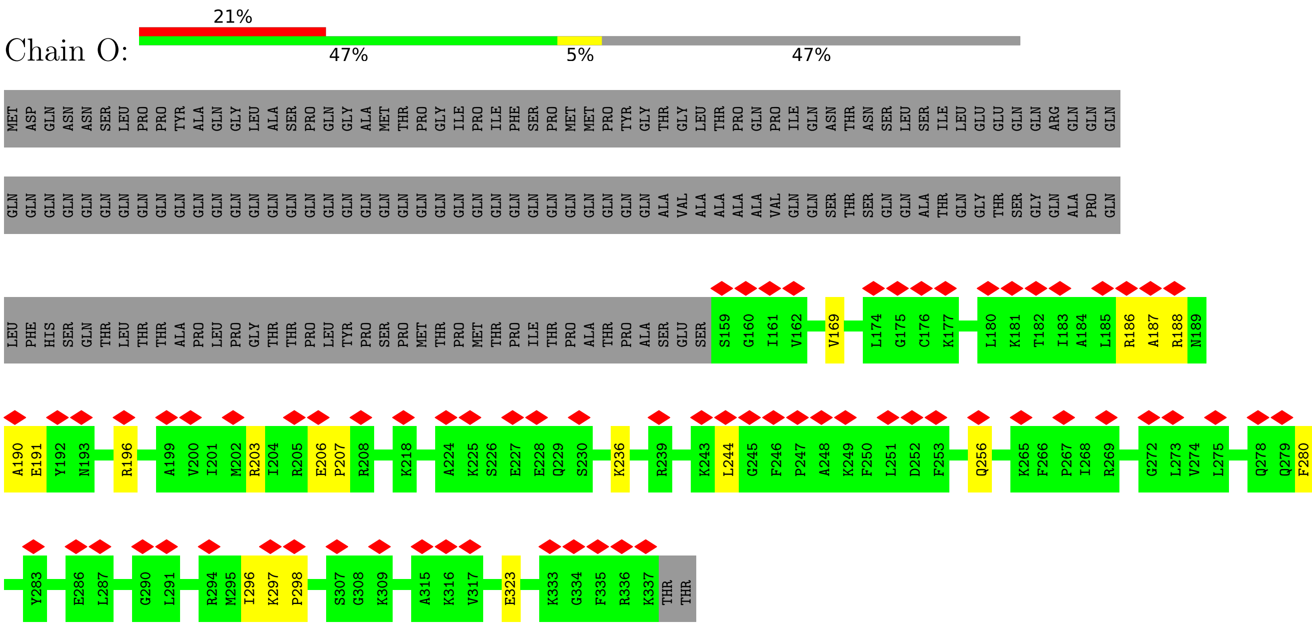




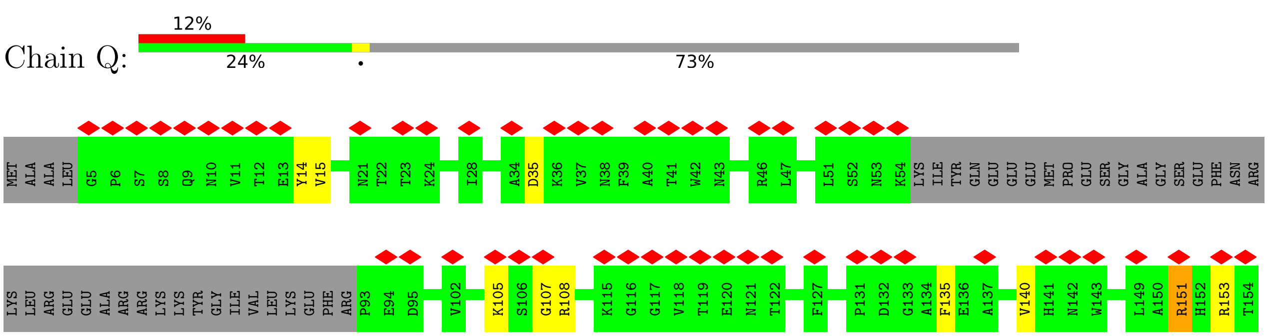
• Molecule 22: Non-template DNA

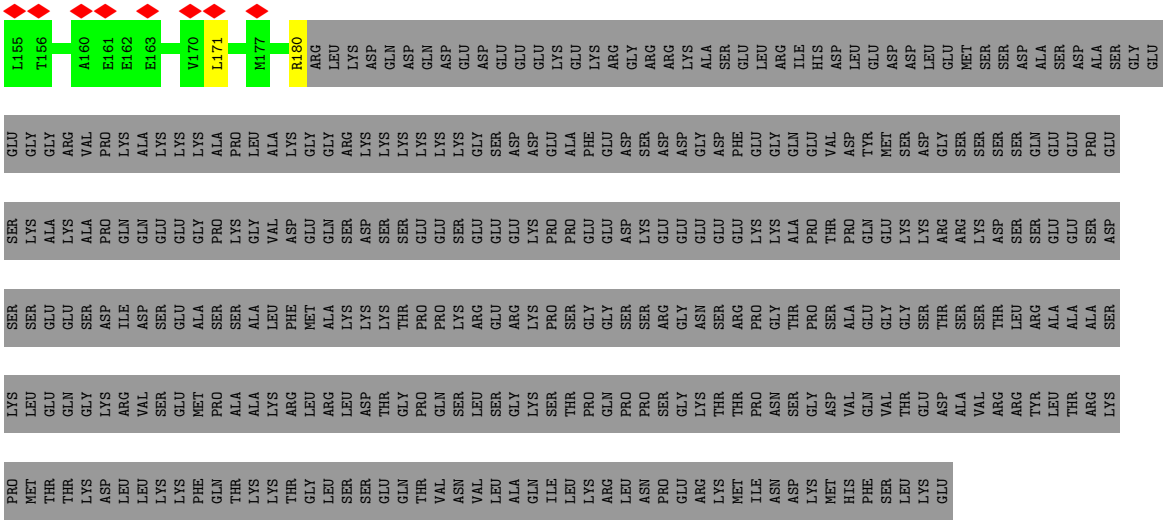


• Molecule 23: TATA-box-binding protein



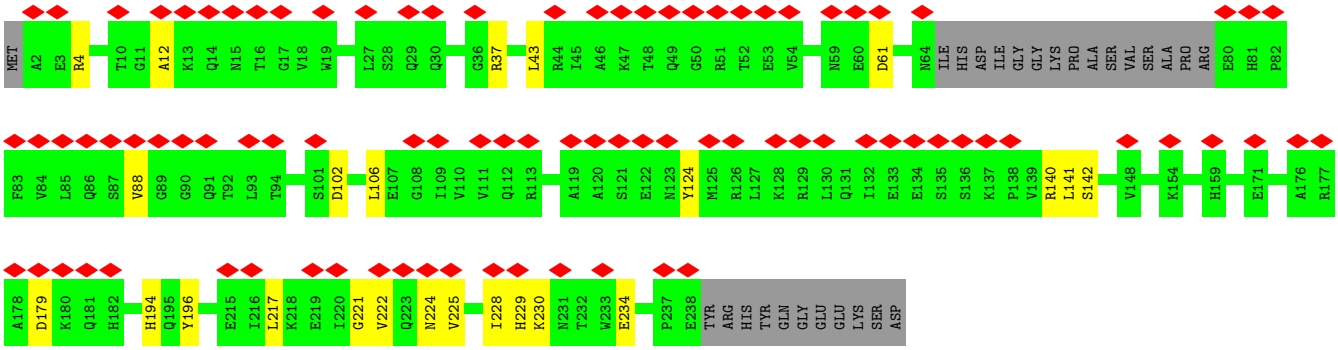
• Molecule 24: General transcription factor IIF subunit 1





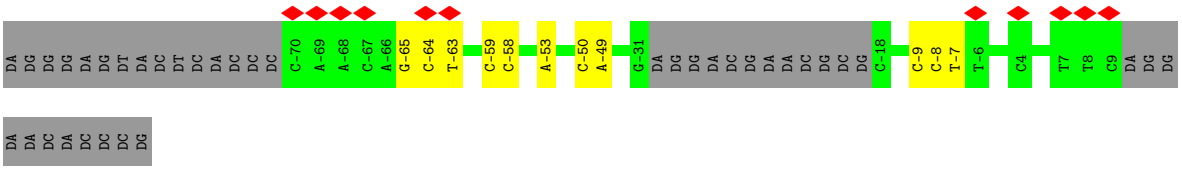
- Molecule 25: General transcription factor IIF subunit 2

Chain R:



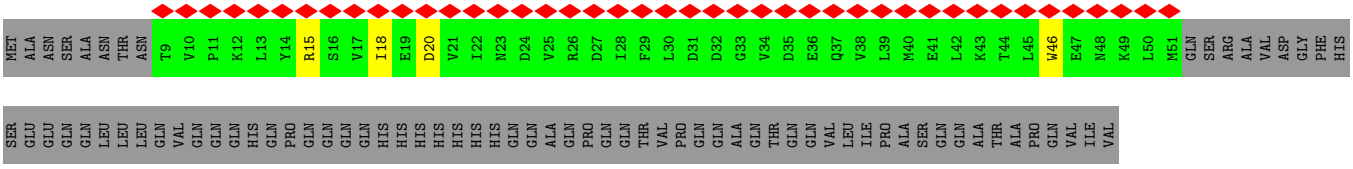
- Molecule 26: Template DNA

Chain T:



- Molecule 27: Transcription initiation factor IIA subunit 1

Chain U:



PRO ASP SER LYS LEU ILE GLN HIS MET ASN ALA SER ASN MET SER ALA ALA ALA THR ALA ALA THR LEU ALA LEU PRO ALA GLY VAL THR PRO VAL GLN GLN ILE LEU THR ASN SER GLY GLN LEU LEU GLN VAL VAL ARG ALA ALA ASN GLY ALA GLN TYR ILE PHE GLN PRO GLN GLN

SER VAL VAL LEU GLN GLN GLN VAL ILE PRO GLN MET GLN PRO GLY GLY VAL GLN ALA PRO VAL ILE GLN GLN VAL LEU ALA PRO LEU PRO GLY GLY ILE SER PRO GLN THR GLY VAL ILE ILE GLN PRO GLN GLN ILE LEU PHE THR GLY ASN LYS THR GLN VAL ILE PRO THR THR VAL

ALA ALA PRO THR PRO ALA GLN ALA GLN ILE THR ALA THR GLY GLN GLN GLN PRO GLN ALA GLN PRO ALA GLN THR GLN ALA PRO LEU VAL LEU GLN VAL ASP GLY THR GLY ASP THR SER SER GLU GLU ASP GLU ASP GLU GLU GLU ASP TYR ASP ASP ASP GLU GLU GLU ASP LYS GLU

LYS ASP GLY ALA GLU ASP G307 Q308 V309 E310 E311 E312 P313 L314 N315 S316 E317 D318 D319 V320 S321 D322 E323 E324 G325 Q326 E327 L328 F329 D330 T331 E332 N333 V334 V335 V336 C337 Q338 Y339 D340 K341 I342 H343 R344 S345 K346 N347 K348 W349 K350 F351 H352 L353 K354 D355 G356 I357 M358 M359 L360

N361 G362 R363 D364 Y365 I366 F367 S368 K369 A370 I371 G372 D373 A374 E375 W376

- Molecule 28: Transcription initiation factor IIA subunit 2

Chain V:

M1 A2 Y3 Q4 L5 Y6 R7 N8 T9 T10 L11 G12 N13 S14 L15 Q16 E17 S18 L19 D20 E21 L22 I23 Q24 S25 Q26 Q27 I28 T29 P30 Q31 L32 A33 L34 Q35 V36 L37 L38 Q39 F40 D41 K42 A43 I44 N45 A46 A47 L48 A49 Q50 R51 V52 R53 N54 R55 V56 N57 F58 R59 G60

S61 L62 N63 T64 Y65 R66 F67 C68 D69 N70 V71 W72 T73 F74 V75 L76 N77 D78 V79 E80 F81 R82 E83 V84 T85 E86 L87 I88 K89 V90 D91 K92 V93 K94 I95 V96 A97 C98 D99 GLY LYS ASN THR GLY SER ASN THR THR GLU

- Molecule 29: General transcription factor IIE subunit 1

Chain W:

MET ALA ASP PRO ASP VAL LEU THR GLU V10 P11 A12 A13 R16 L17 F25 Y26 H30 A33 I36 L37 I38 R39 N40 S41 C42 D47 R56 K57 K70 K73 C74 R75 M76 E79 T80 A81 A82 D83 G84 K85 T86 T87 R88 H89 Y92 F93 I94 N95

Y96 R97 T98 V103 K104 L107 D108 H109 M110 R111 I114 E115 E118 R119 D120 S121 T122 N123 R124 A125 S126 F127 K128 C129 P130 V131 C132 S133 S134 T135 F136 T137 D138 L139 E140 L144 M148 T149 G150 T151 F152 R153 C154 T155 F156 C157 H158 T159 E160 V161 E162 E163 D164 E165

S166 A167 M168 P169 K170 K171 D172 A173 R174 T175 L176 L177 A178 E182 Q183 I184 I187 Y188 R192 E193 T194 E195 D196 VAL ASN LEU ALA TYR GLU ILE LEU GLU PRO GLU PRO THR GLU ILE PRO ALA LEU LYS GLN SER LYS ASP HIS ALA ALA THR THR ALA GLY ALA ALA SER LEU

ALA GLY GLY HIS HIS ARG GLU ALA TRP ALA THR LYS GLY PRO SER TYR GLU ASP LEU TYR THR GLN ASN VAL VAL ILE ASN MET ASP ASP GLN GLU ASP LEU HIS ARG ALA SER LEU GLU GLY LYS SER A274 K275 E276 R277 L281 R282 E283 S284 Q287 G288 ALA TYR GLY SER GLU

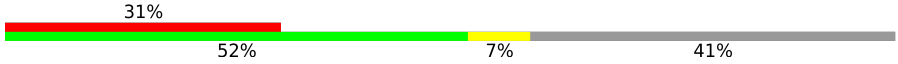
ASP MET LYS GLU GLY GLY ILE ASP MET ASP ALA PHE GLN GLU ARG GLU GLU GLY HIS ALA GLY PRO ASP ASP ASN GLU GLU VAL MET ARG ALA ALA LEU LEU ILE HIS GLU LYS LYS THR SER SER ALA MET ALA GLY SER VAL GLY ALA ALA ALA PRO VAL THR ALA ALA ASN GLY SER ASP

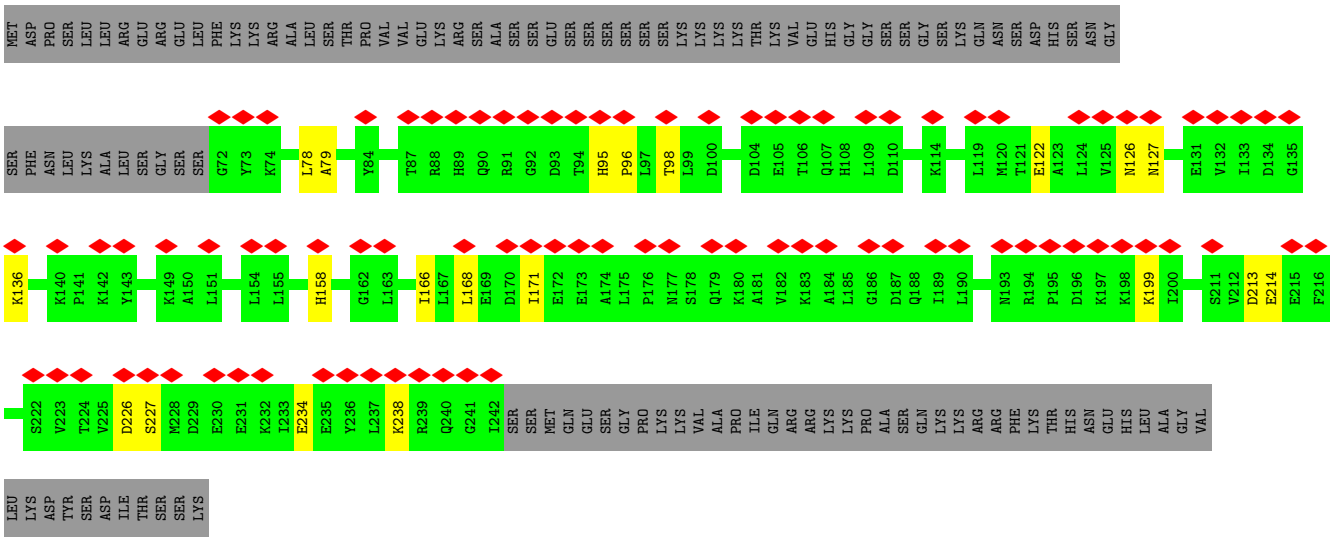
SER GLU SER GLU THR SER GLU SER ASP ASP ASP SER PRO PRO ARG PRO ALA ALA VAL ALA VAL HIS LYS ARG GLU GLU ASP GLU GLU GLU ASP ASP GLU PHE GLU GLU VAL ALA ASP ASP PRO ILE VAL MET VAL ALA GLY ARG PRO PHE SER TYR SER GLU VAL SER GLN ARG PRO GLU

LEU VAL ALA GLN MET THR PRO GLU GLU LYS GLU ALA TYR ILE ALA MET GLY GLN ARG MET PHE GLU ASP LEU PHE GLU

• Molecule 30: Transcription initiation factor IIE subunit beta

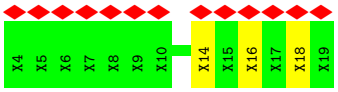
Chain X:





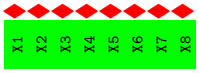
• Molecule 31: Unassigned peptide, likely TFIIE-Beta

Chain Y:



• Molecule 32: Unassigned peptide, likely XPB

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26146	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 ($e^-/Å^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	31.233	Depositor
Minimum map value	-16.532	Depositor
Average map value	-0.005	Depositor
Map value standard deviation	0.967	Depositor
Recommended contour level	6.4	Depositor
Map size (Å)	472.49997, 472.49997, 472.49997	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: MG, SF4, ADP, BEF, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.24	0/5875	0.39	0/7955
2	1	0.24	0/2210	0.38	0/2975
3	2	0.24	0/3230	0.37	0/4376
4	3	0.24	0/387	0.36	0/519
5	4	0.25	0/2103	0.43	0/2846
6	5	0.24	0/529	0.36	0/714
7	6	0.24	0/2624	0.40	0/3555
8	7	0.24	0/4994	0.39	0/6745
9	A	0.24	0/11479	0.40	0/15496
10	B	0.25	0/9257	0.41	0/12493
11	C	0.24	0/2102	0.41	0/2857
12	D	0.24	0/1064	0.34	0/1428
13	E	0.25	0/1752	0.40	0/2366
14	F	0.24	0/646	0.39	0/871
15	G	0.25	0/1382	0.41	0/1874
16	H	0.24	0/1207	0.42	0/1628
17	I	0.24	0/949	0.42	0/1284
18	J	0.25	0/516	0.39	0/696
19	K	0.25	0/939	0.38	0/1271
20	L	0.24	0/378	0.41	0/500
21	M	0.24	0/2337	0.39	0/3154
22	N	0.47	0/1537	0.86	0/2374
23	O	0.24	0/1448	0.41	0/1948
24	Q	0.24	0/1167	0.39	0/1576
25	R	0.23	0/1817	0.39	0/2445
26	T	0.50	0/1518	0.87	0/2333
27	U	0.23	0/945	0.39	0/1274
28	V	0.24	0/816	0.39	0/1105
29	W	0.23	0/1686	0.37	0/2266
30	X	0.23	0/1427	0.37	0/1916
All	All	0.26	0/68321	0.43	0/92840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	5751	0	5794	73	0
2	1	2167	0	2175	27	0
3	2	3158	0	3213	42	0
4	3	382	0	380	4	0
5	4	2066	0	2098	44	0
6	5	523	0	530	5	0
7	6	2567	0	2539	45	0
8	7	4890	0	4949	59	0
9	A	11274	0	11406	129	0
10	B	9076	0	9116	82	0
11	C	2059	0	2007	26	0
12	D	1050	0	1033	4	0
13	E	1721	0	1737	17	0
14	F	636	0	665	5	0
15	G	1351	0	1358	13	0
16	H	1186	0	1147	9	0
17	I	928	0	859	12	0
18	J	507	0	523	5	0
19	K	920	0	942	12	0
20	L	373	0	378	5	0
21	M	2301	0	2316	17	0
22	N	1369	0	743	7	0
23	O	1422	0	1514	14	0
24	Q	1138	0	1103	7	0
25	R	1788	0	1819	16	0
26	T	1358	0	749	8	0
27	U	930	0	888	5	0
28	V	806	0	818	7	0
29	W	1659	0	1666	17	0
30	X	1403	0	1428	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Y	80	0	19	2	0
32	Z	40	0	11	0	0
33	0	8	0	0	0	0
34	4	2	0	0	0	0
34	6	3	0	0	0	0
34	A	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	I	2	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	W	1	0	0	0	0
35	7	27	0	12	1	0
36	7	1	0	0	0	0
36	A	1	0	0	0	0
37	7	4	0	0	0	0
All	All	66935	0	65935	647	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 5.

The worst 5 of 647 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)
5:4:255:CYS:SG	5:4:258:HIS:ND1	2.35	0.99
11:C:67:ARG:NH2	18:J:3:ILE:O	1.97	0.97
7:6:109:THR:HG1	7:6:148:SER:HG	1.18	0.89
16:H:8:ASP:OD2	16:H:32:SER:OG	1.95	0.85
9:A:1208:SER:O	9:A:1260:ARG:NH1	2.10	0.85

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	0	710/760 (93%)	680 (96%)	30 (4%)	0	100	100
2	1	253/548 (46%)	243 (96%)	10 (4%)	0	100	100
3	2	380/462 (82%)	369 (97%)	10 (3%)	1 (0%)	41	76
4	3	42/309 (14%)	41 (98%)	1 (2%)	0	100	100
5	4	259/308 (84%)	251 (97%)	8 (3%)	0	100	100
6	5	64/71 (90%)	64 (100%)	0	0	100	100
7	6	325/395 (82%)	312 (96%)	13 (4%)	0	100	100
8	7	601/782 (77%)	578 (96%)	23 (4%)	0	100	100
9	A	1413/1970 (72%)	1378 (98%)	35 (2%)	0	100	100
10	B	1130/1174 (96%)	1101 (97%)	29 (3%)	0	100	100
11	C	253/275 (92%)	247 (98%)	6 (2%)	0	100	100
12	D	126/142 (89%)	124 (98%)	2 (2%)	0	100	100
13	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
14	F	77/127 (61%)	77 (100%)	0	0	100	100
15	G	169/172 (98%)	168 (99%)	1 (1%)	0	100	100
16	H	146/150 (97%)	141 (97%)	5 (3%)	0	100	100
17	I	112/125 (90%)	106 (95%)	6 (5%)	0	100	100
18	J	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
19	K	113/117 (97%)	111 (98%)	2 (2%)	0	100	100
20	L	42/58 (72%)	39 (93%)	3 (7%)	0	100	100
21	M	294/316 (93%)	291 (99%)	3 (1%)	0	100	100
23	O	177/339 (52%)	176 (99%)	1 (1%)	0	100	100
24	Q	134/517 (26%)	132 (98%)	2 (2%)	0	100	100
25	R	218/249 (88%)	215 (99%)	3 (1%)	0	100	100
27	U	109/376 (29%)	102 (94%)	7 (6%)	0	100	100
28	V	97/109 (89%)	95 (98%)	2 (2%)	0	100	100
29	W	198/439 (45%)	195 (98%)	3 (2%)	0	100	100
30	X	169/291 (58%)	166 (98%)	3 (2%)	0	100	100
All	All	7880/10858 (73%)	7667 (97%)	212 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	2	49	PRO

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	0	624/664 (94%)	623 (100%)	1 (0%)	93	96
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	342/399 (86%)	342 (100%)	0	100	100
4	3	44/283 (16%)	44 (100%)	0	100	100
5	4	234/272 (86%)	234 (100%)	0	100	100
6	5	59/64 (92%)	59 (100%)	0	100	100
7	6	295/352 (84%)	294 (100%)	1 (0%)	92	95
8	7	536/688 (78%)	535 (100%)	1 (0%)	93	96
9	A	1254/1749 (72%)	1253 (100%)	1 (0%)	93	97
10	B	994/1027 (97%)	994 (100%)	0	100	100
11	C	234/252 (93%)	234 (100%)	0	100	100
12	D	118/126 (94%)	117 (99%)	1 (1%)	81	89
13	E	191/192 (100%)	191 (100%)	0	100	100
14	F	69/111 (62%)	69 (100%)	0	100	100
15	G	152/153 (99%)	152 (100%)	0	100	100
16	H	129/131 (98%)	129 (100%)	0	100	100
17	I	103/112 (92%)	103 (100%)	0	100	100
18	J	53/56 (95%)	53 (100%)	0	100	100
19	K	104/106 (98%)	104 (100%)	0	100	100
20	L	41/55 (74%)	41 (100%)	0	100	100
21	M	253/268 (94%)	252 (100%)	1 (0%)	91	94
23	O	154/293 (53%)	154 (100%)	0	100	100
24	Q	121/448 (27%)	119 (98%)	2 (2%)	60	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	R	196/218 (90%)	195 (100%)	1 (0%)	88	93
27	U	105/324 (32%)	105 (100%)	0	100	100
28	V	90/98 (92%)	89 (99%)	1 (1%)	73	84
29	W	182/373 (49%)	180 (99%)	2 (1%)	73	84
30	X	154/261 (59%)	154 (100%)	0	100	100
All	All	7072/9559 (74%)	7060 (100%)	12 (0%)	93	96

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	Q	151	ARG
25	R	230	LYS
29	W	153	ARG
28	V	82	ARG
9	A	483	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 20 ligands modelled in this entry, 17 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
37	BEF	7	903	35	0,3,3	-	-	-		
33	SF4	0	1000	1	0,12,12	-	-	-		
35	ADP	7	901	36,37	24,29,29	0.69	0	29,45,45	0.78	1 (3%)

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
33	SF4	0	1000	1	-	-	0/6/5/5
35	ADP	7	901	36,37	-	1/12/32/32	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})
35	7	901	ADP	C5-C6-N6	2.24	123.76	120.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	7	901	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

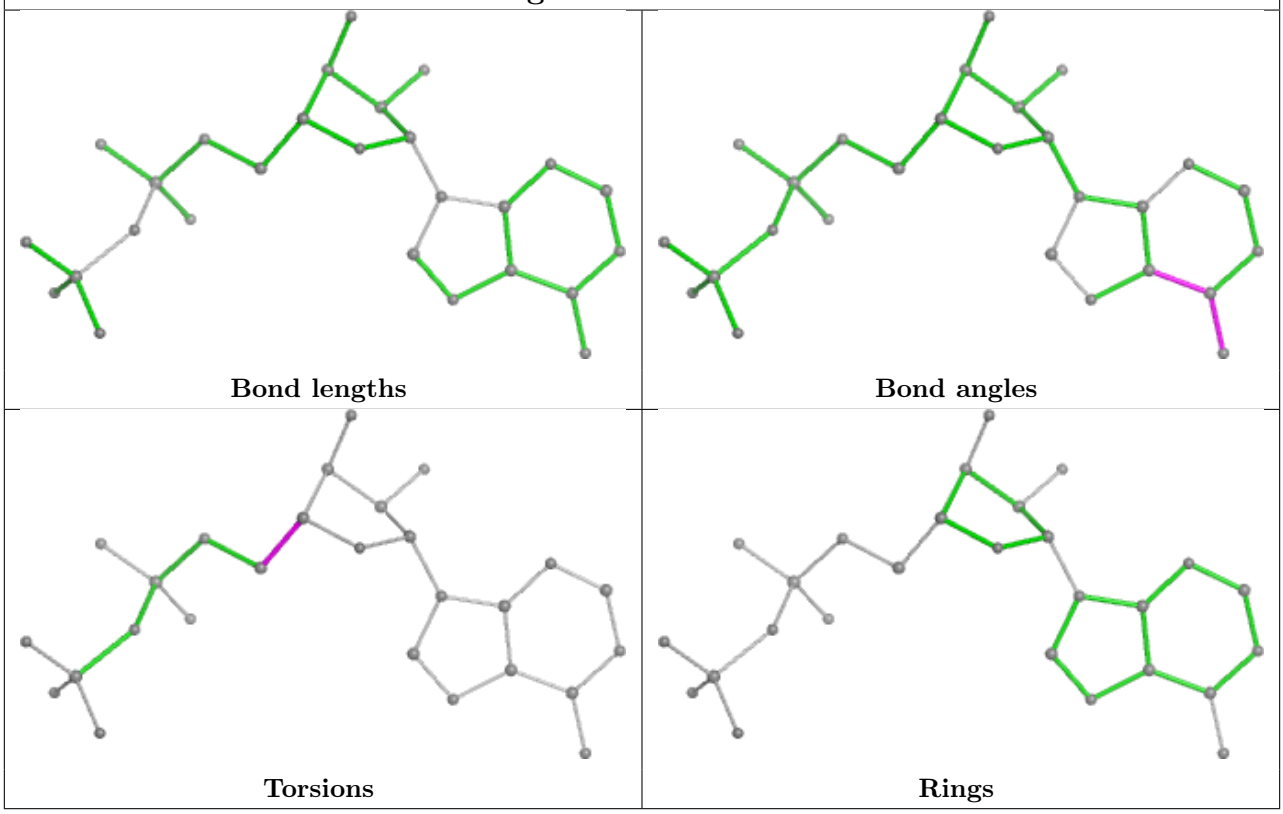
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	7	901	ADP	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 ADP 7 901



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.

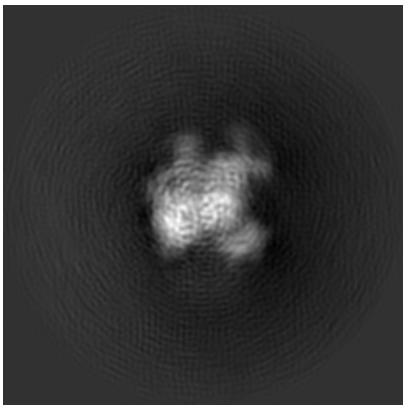
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12619. These allow visual inspection of the internal detail of the map and identification of artifacts.

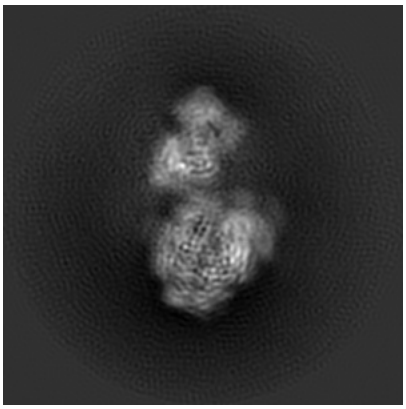
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

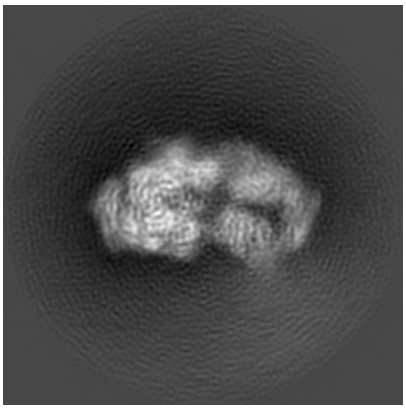
6.1.1 Primary map



X

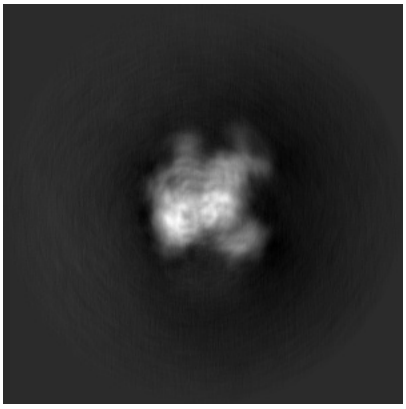


Y

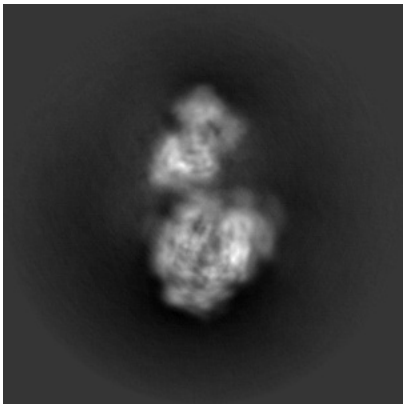


Z

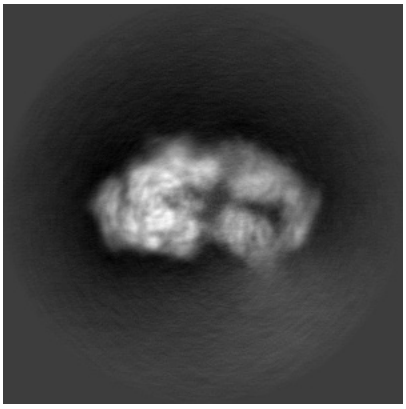
6.1.2 Raw map



X



Y

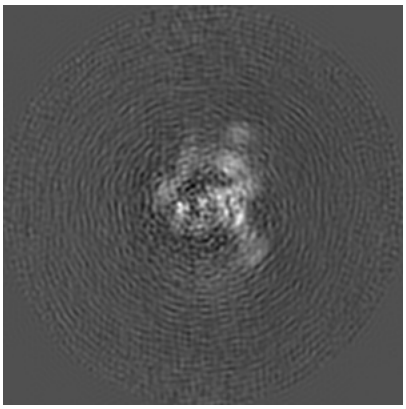


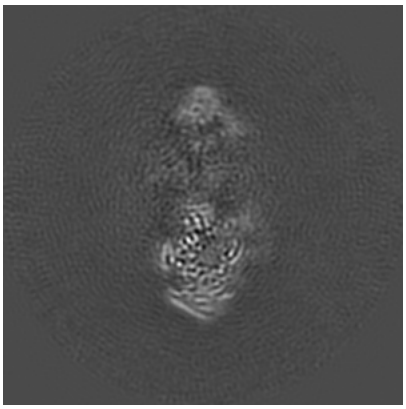
Z

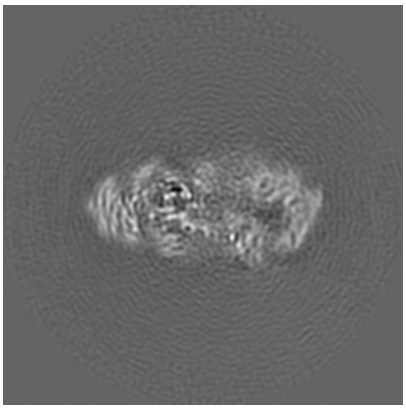
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

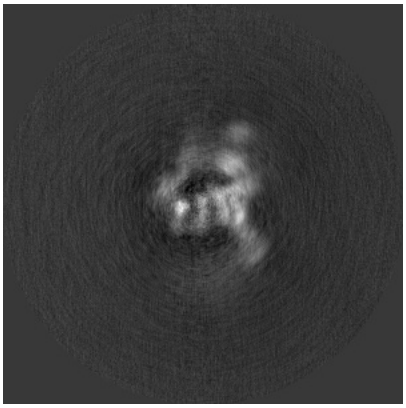
6.2.1 Primary map

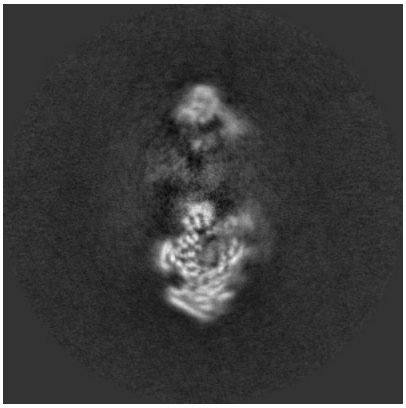

X Index: 225

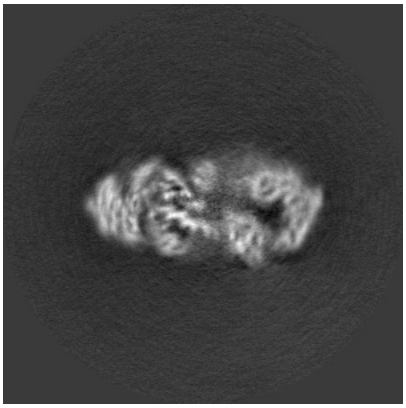

Y Index: 225


Z Index: 225

6.2.2 Raw map


X Index: 225

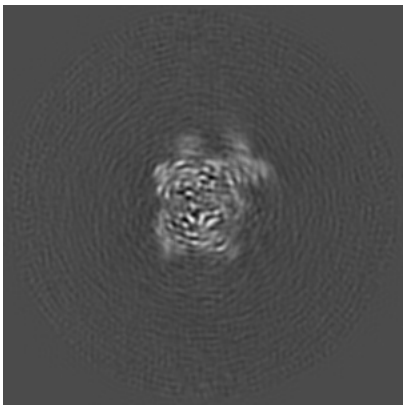

Y Index: 225

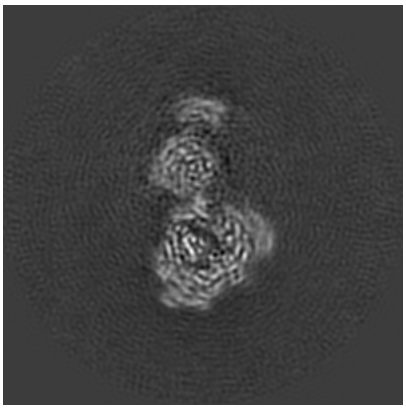

Z Index: 225

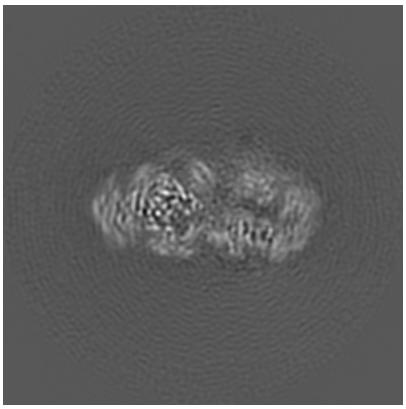
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

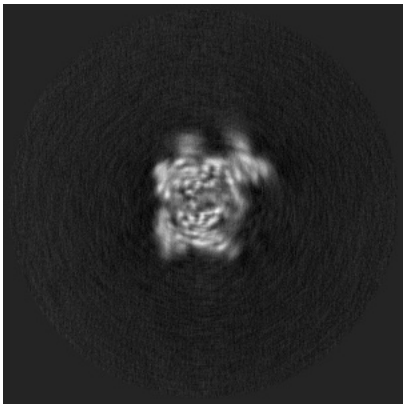
6.3.1 Primary map

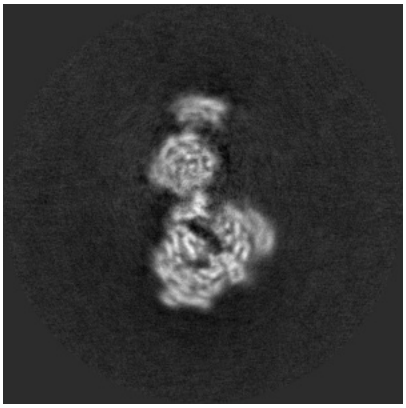

X Index: 168

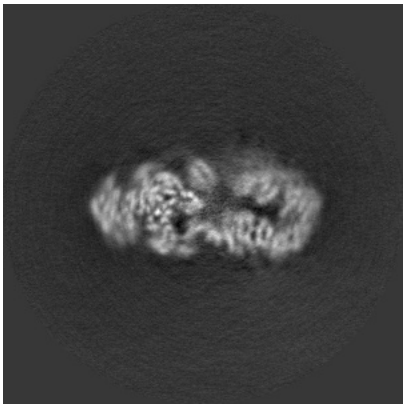

Y Index: 199


Z Index: 213

6.3.2 Raw map


X Index: 168

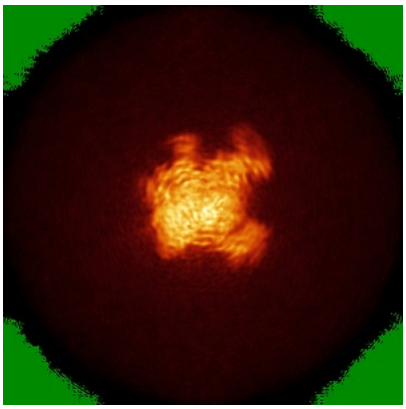

Y Index: 198

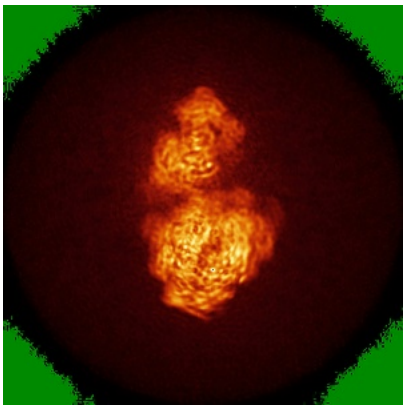

Z Index: 215

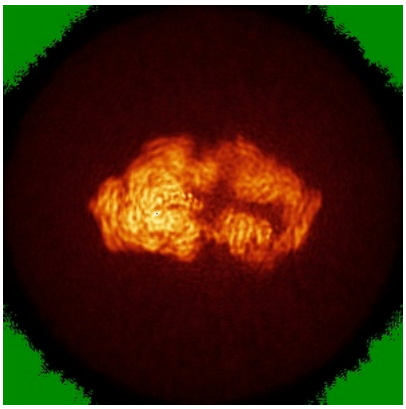
The images above show the largest variance slices of the map in three orthogonal directions.

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

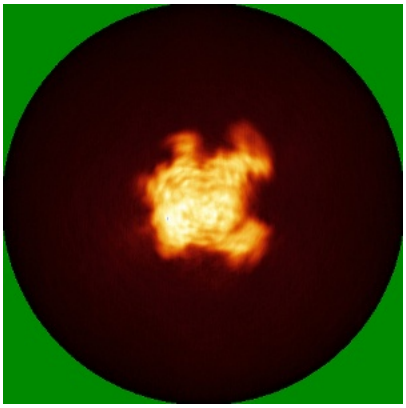
6.4.1 Primary map

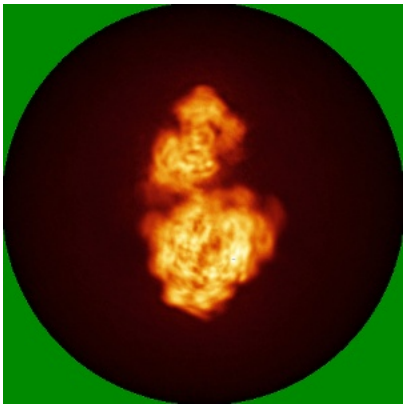

X

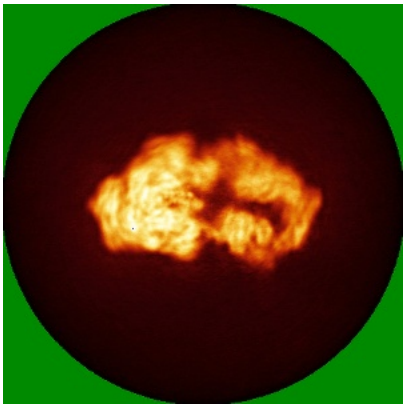

Y


Z

6.4.2 Raw map


X

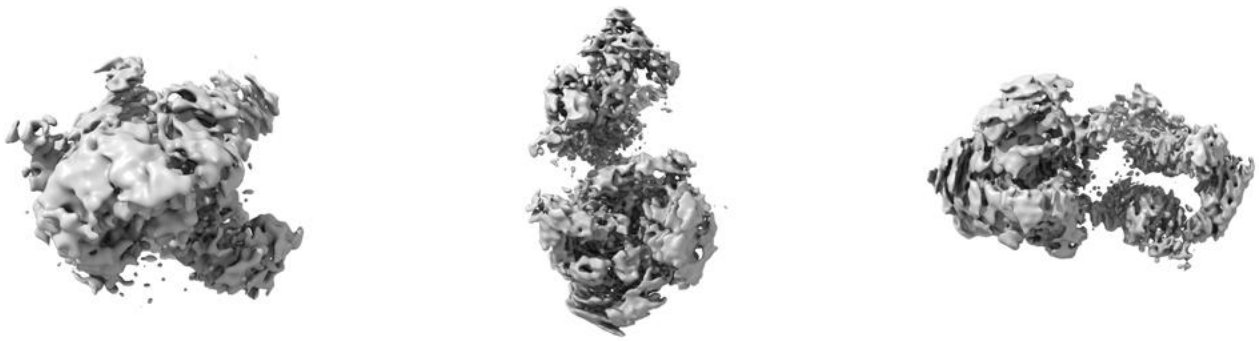

Y


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)

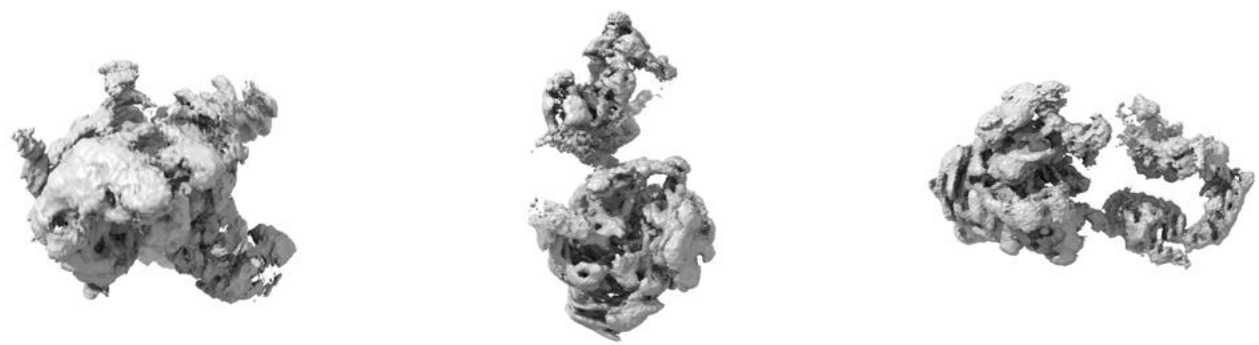
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 6.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

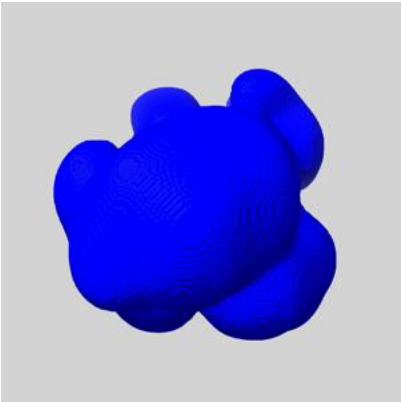
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

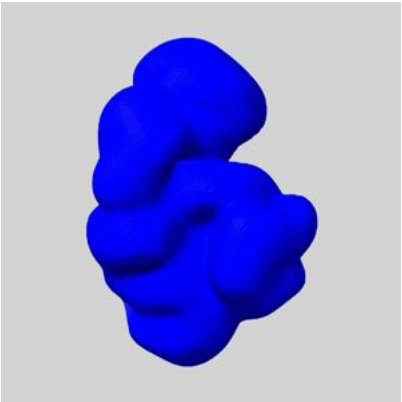
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

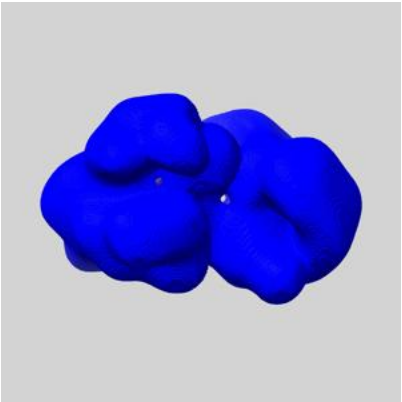
6.6.1 emd_12619_msk_1.map (i)



X



Y

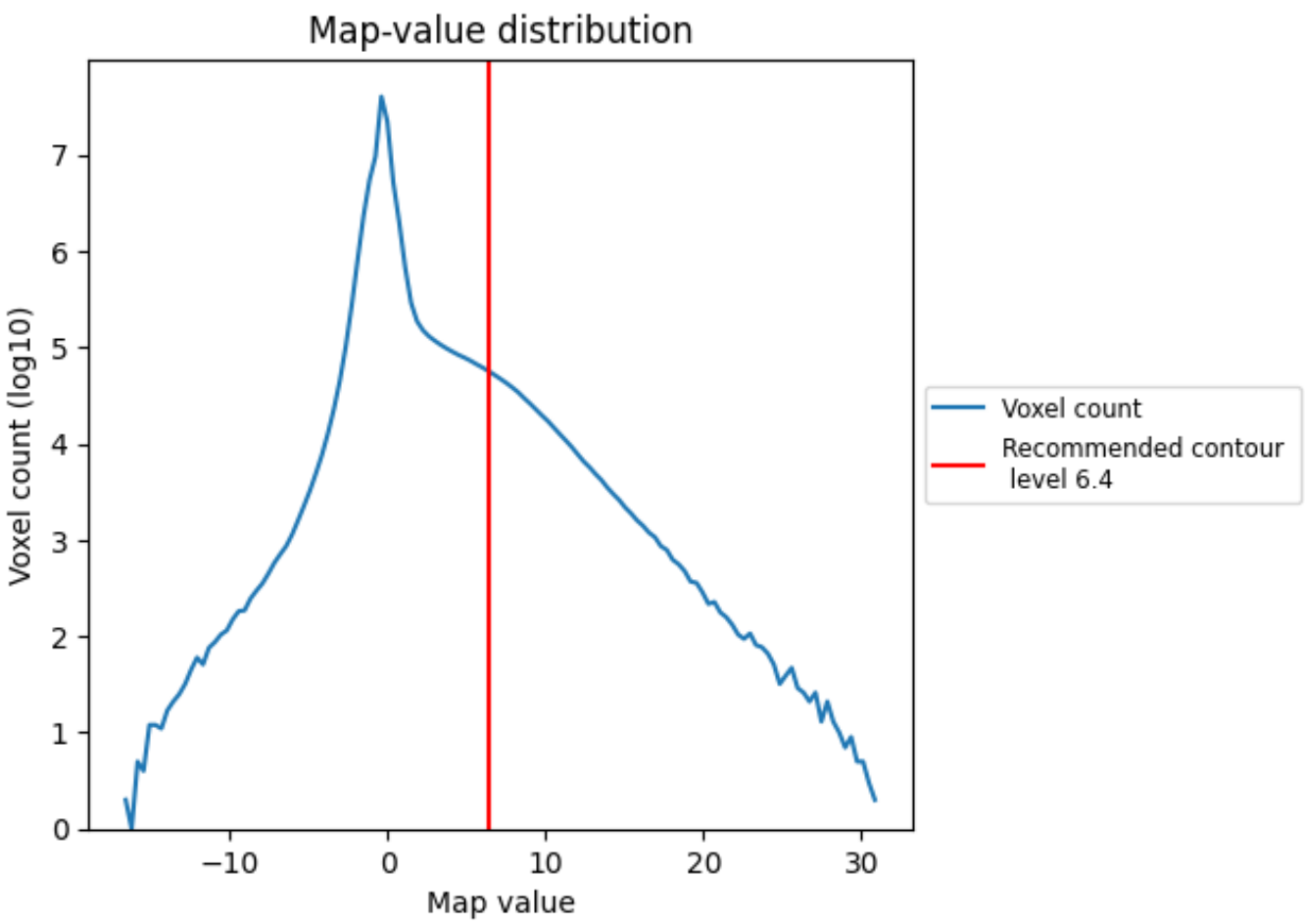


Z

7 Map analysis (i)

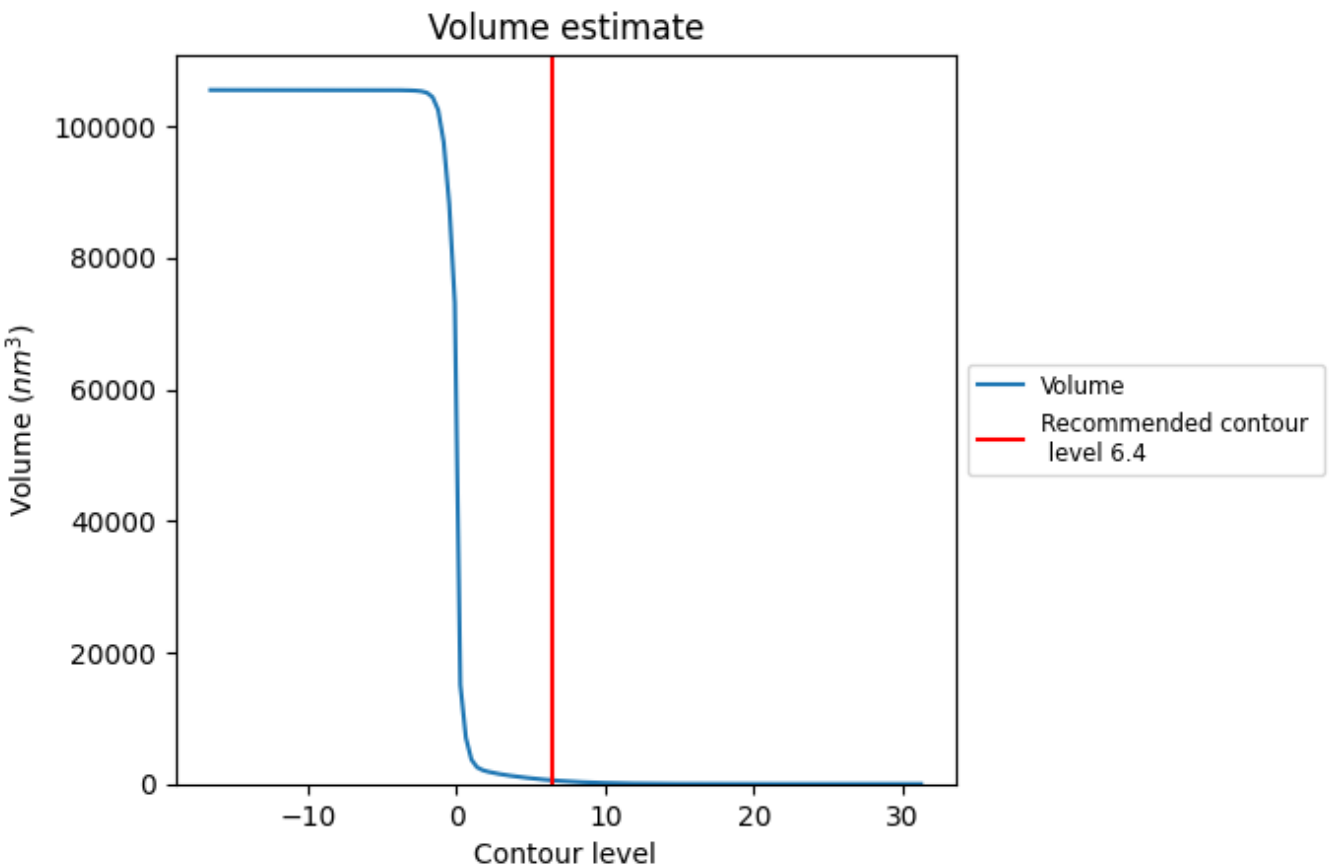
This section contains the results of statistical analysis of the map.

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.

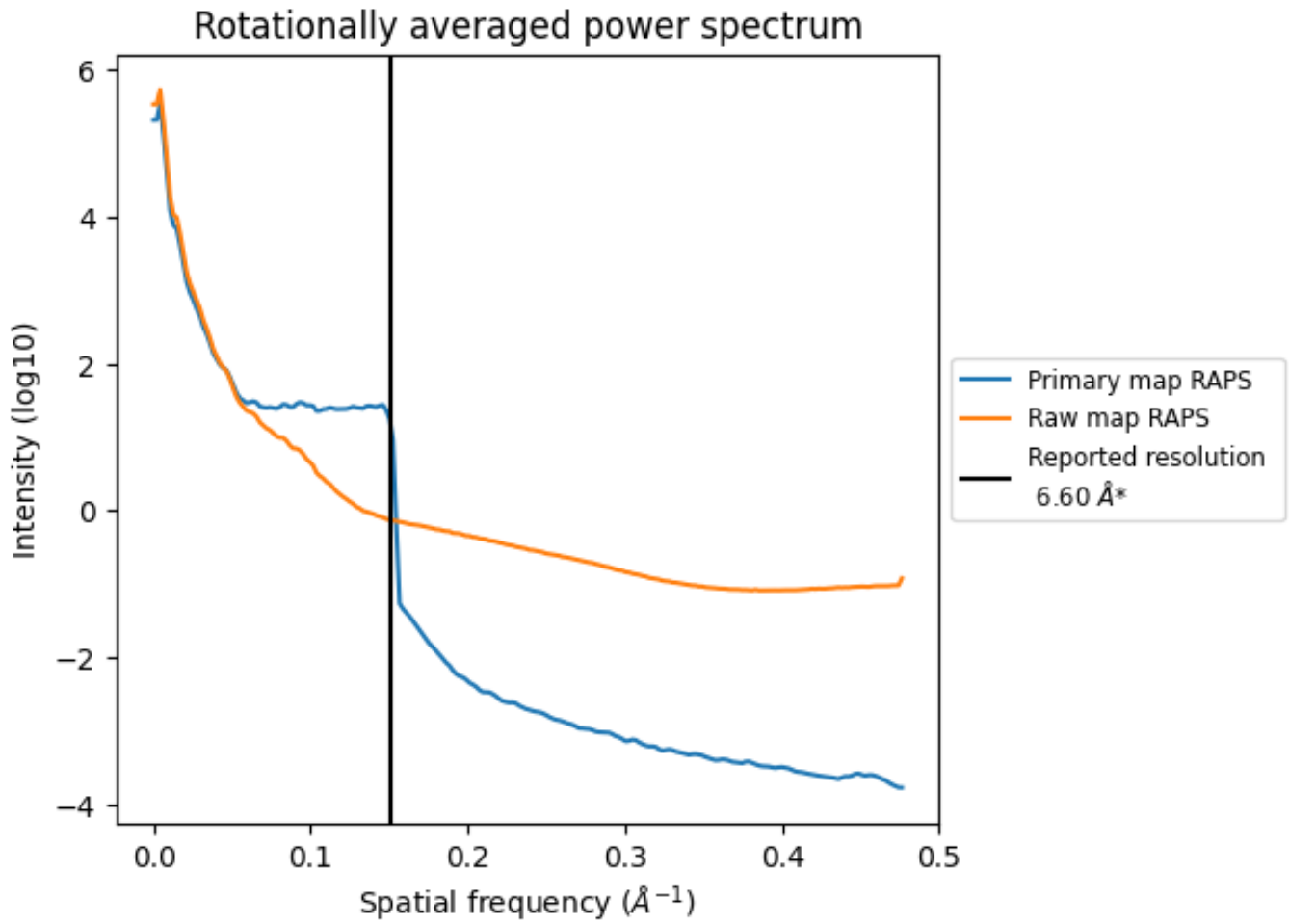
7.2 Volume estimate (i)



The volume at the recommended contour level is 567 nm^3; this corresponds to an approximate mass of 512 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)

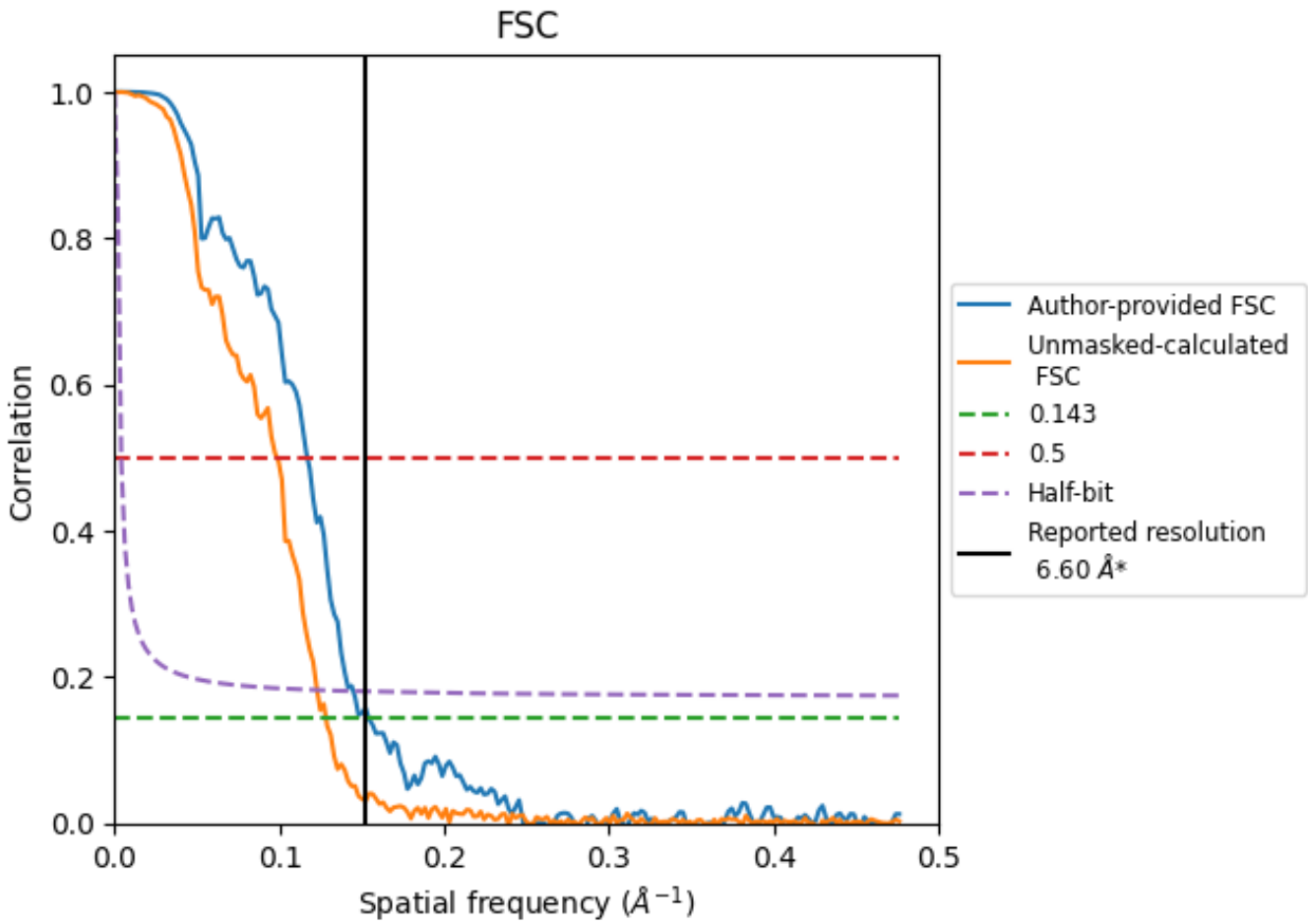


*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8.2 Resolution estimates (i)

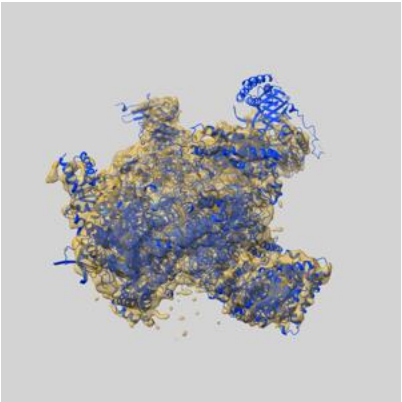
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.48	8.55	6.90
Unmasked-calculated*	7.79	10.15	8.14

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.79 differs from the reported value 6.6 by more than 10 %

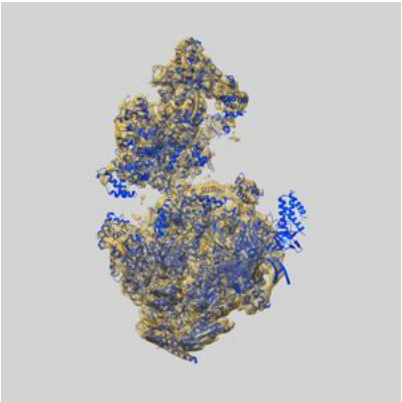
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12619 and PDB model 7NW0. Per-residue inclusion information can be found in section 3 on page 12.

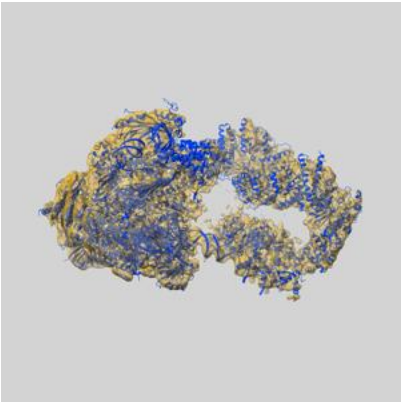
9.1 Map-model overlay (i)



X



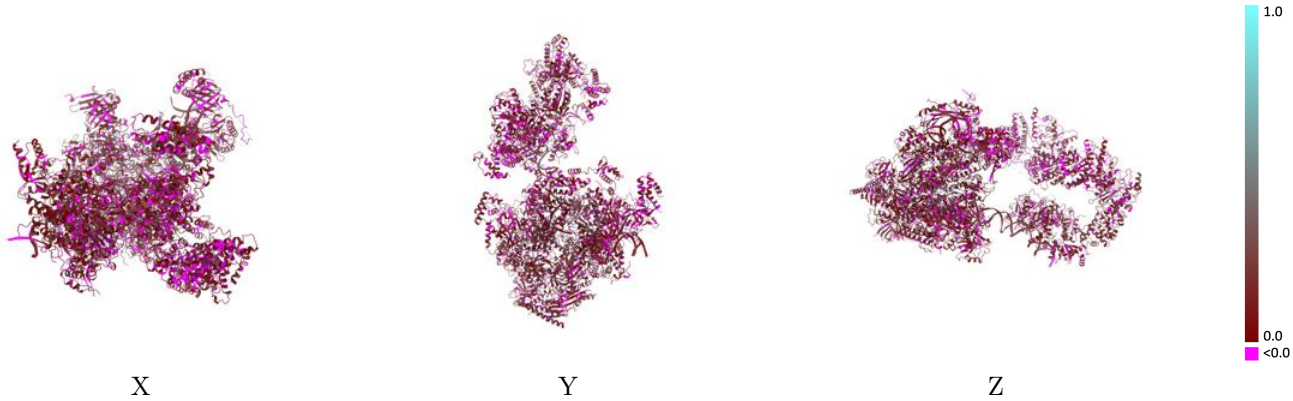
Y



Z

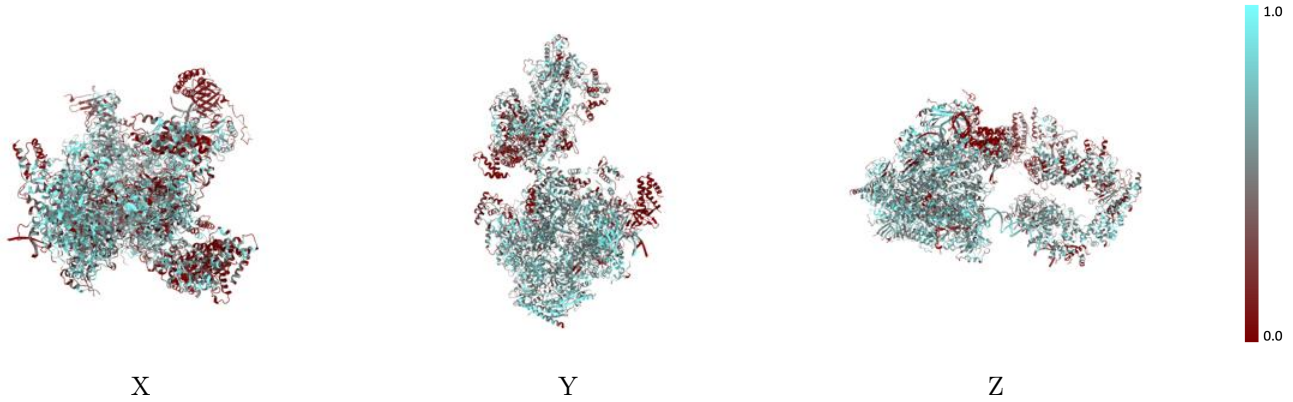
The images above show the 3D surface view of the map at the recommended contour level 6.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



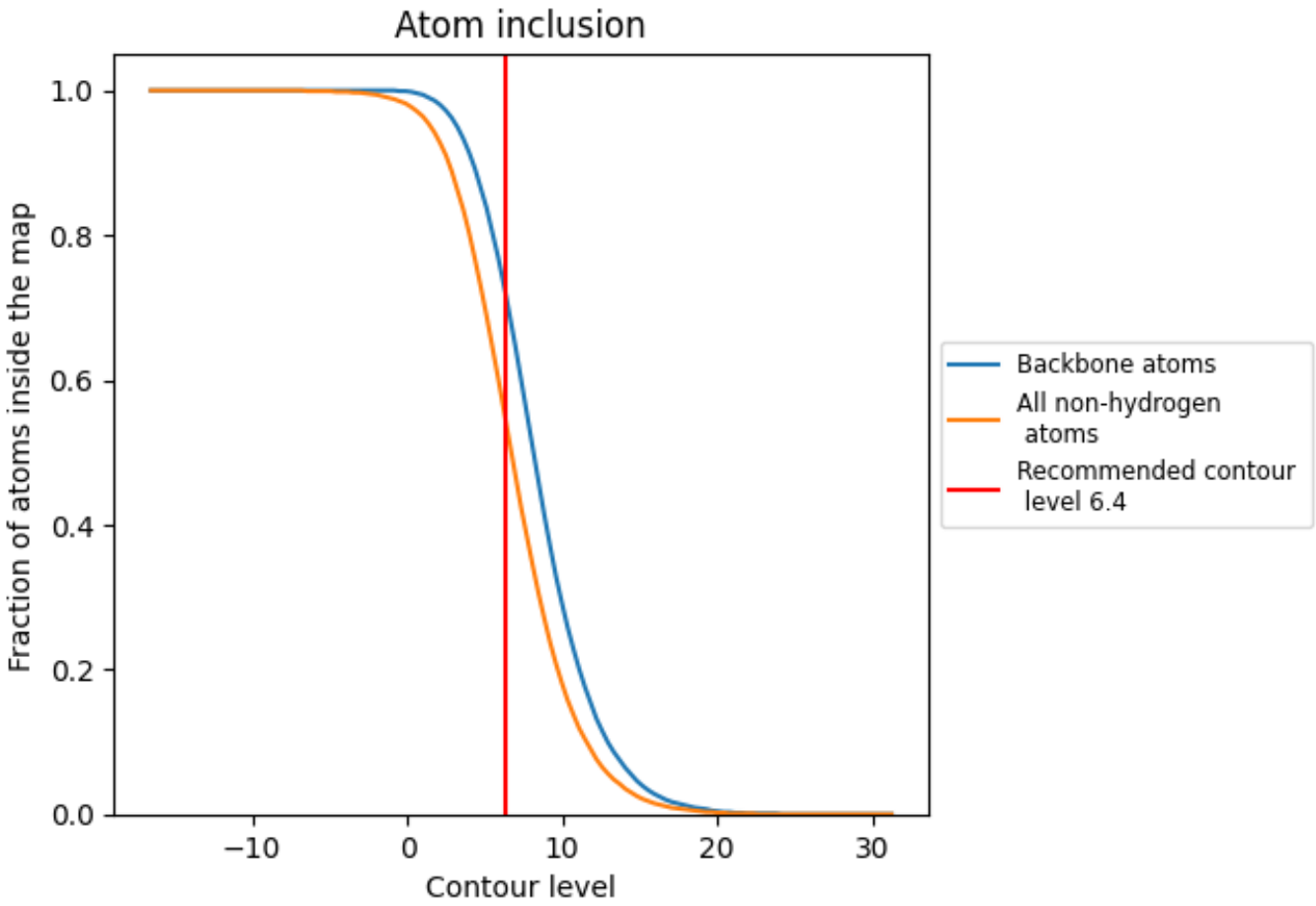
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.4).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (6.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5380	0.1190
0	0.3790	0.0690
1	0.2840	0.0610
2	0.5610	0.1240
3	0.0480	0.0990
4	0.4570	0.0970
5	0.5020	0.1280
6	0.5630	0.1050
7	0.5440	0.1050
A	0.6290	0.1460
B	0.6230	0.1400
C	0.6720	0.1270
D	0.3100	0.1270
E	0.6600	0.1490
F	0.6900	0.1510
G	0.5860	0.1060
H	0.5900	0.1150
I	0.7110	0.1380
J	0.6440	0.1180
K	0.5890	0.1370
L	0.6220	0.1440
M	0.6000	0.1580
N	0.7170	0.1890
O	0.5100	0.1000
Q	0.4760	0.0860
R	0.4780	0.1140
T	0.7090	0.1820
U	0.0040	0.0340
V	0.0220	0.0620
W	0.4340	0.0880
X	0.4000	0.0880
Y	0.1880	0.1140
Z	0.0750	0.0260