Full wwPDB EM Validation Report ⓘ

Dec 26, 2023 – 12:03 PM JST

PDB ID	:	8WAO
EMDB ID	:	EMD-37399
Title	:	Structure of transcribing complex 5 (TC5), the initially transcribing complex with Pol II positioned 5nt downstream of TSS.
Authors	:	Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on	:	2023-09-07
Resolution	:	6.40 Å(reported)

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

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

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

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

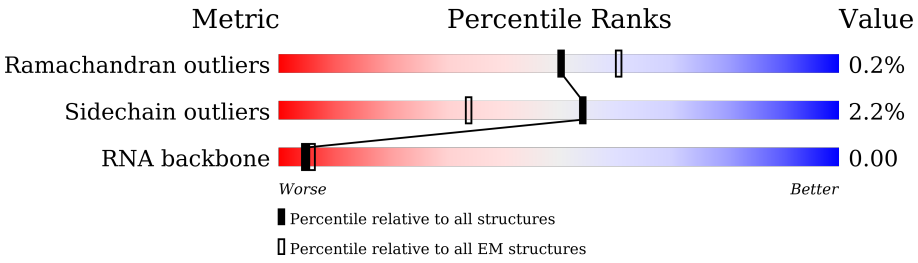
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.40 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	309	43% 53% · 45%
2	1	548	14% 48% 52%
3	2	395	6% 83% · 17%
4	3	308	5% 85% · 15%
5	4	462	8% 84% · 15%
6	5	71	6% 70% 6% 24%
7	6	782	22% 77% · 23%
8	7	760	16% 94% 6%

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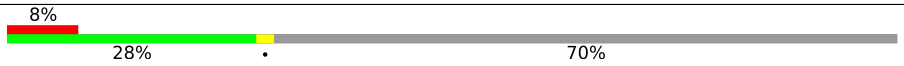
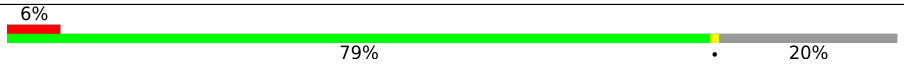
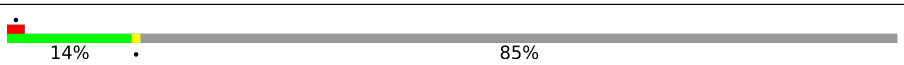
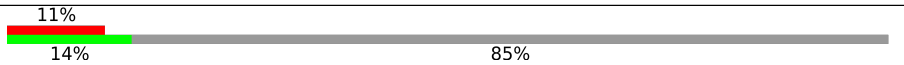
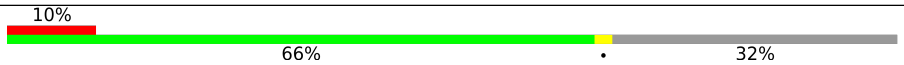
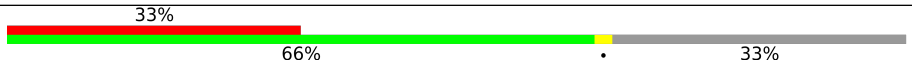
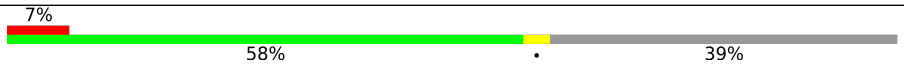
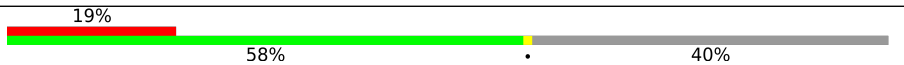
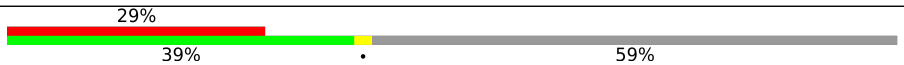
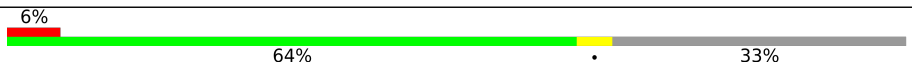
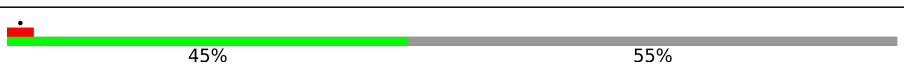
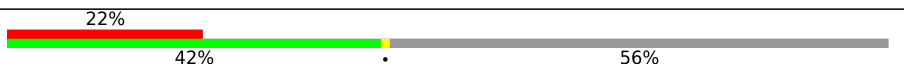
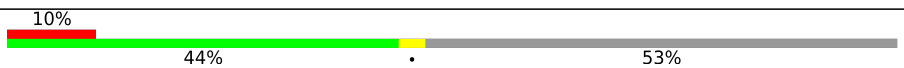
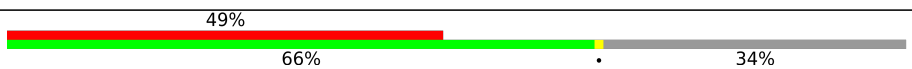
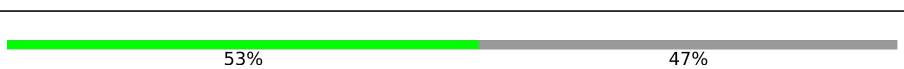
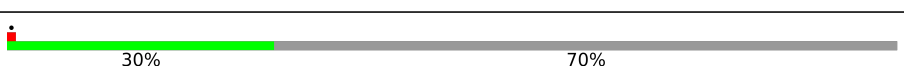
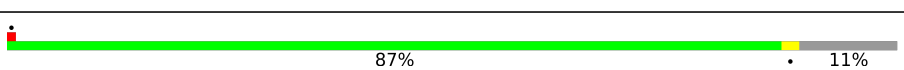
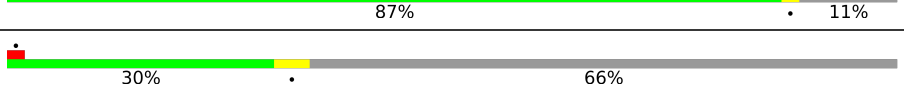
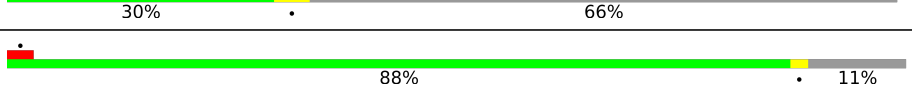
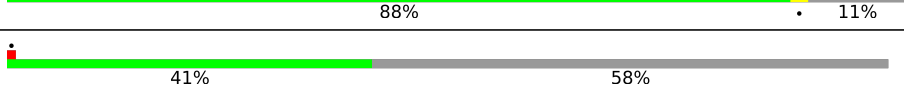
Mol	Chain	Length	Quality of chain
9	N	8	
10	Z	5	
11	A	1872	
12	B	1199	
13	D	1085	
13	d	1085	
14	E	800	
14	e	800	
15	F	677	
15	f	677	
16	G	349	
17	H	310	
18	I	264	
18	i	264	
19	J	218	
19	j	218	
20	L	161	
20	l	161	
21	O	109	
22	P	339	
23	Q	376	
24	R	316	
25	S	517	
26	T	249	
27	U	439	

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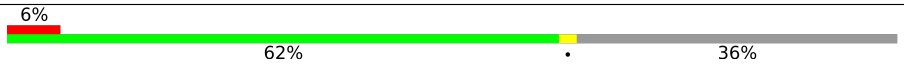
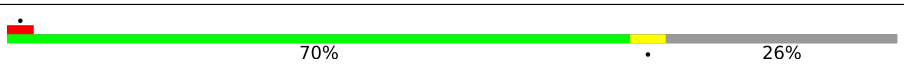
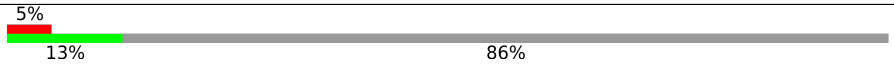
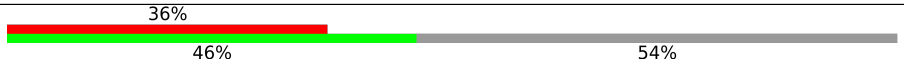
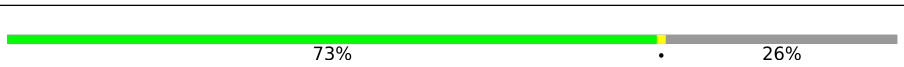
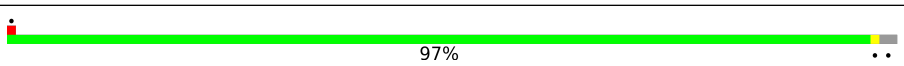
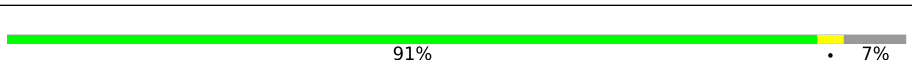
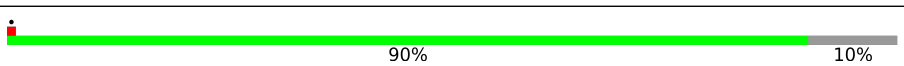
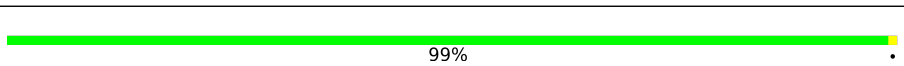
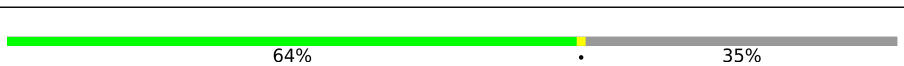
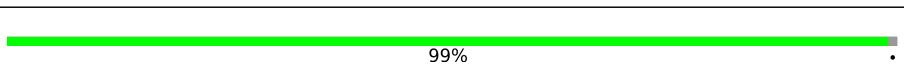
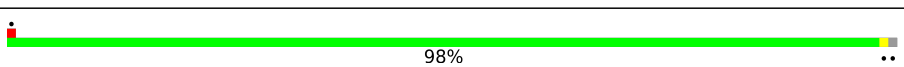
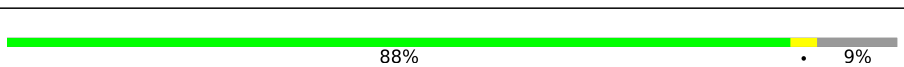
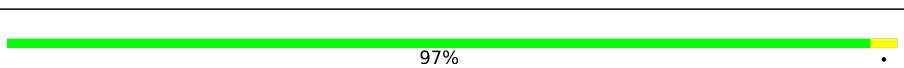
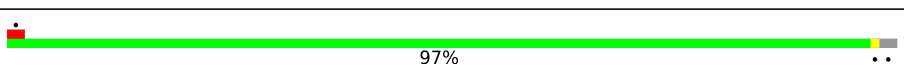
Mol	Chain	Length	Quality of chain
28	V	291	
29	X	99	
30	Y	99	
31	c	929	
32	k	211	
33	m	124	
34	o	1970	
35	p	1174	
36	q	275	
37	r	142	
38	s	210	
39	t	127	
40	u	172	
41	v	150	
42	w	125	
43	x	67	
44	y	117	
45	z	58	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 108622 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 CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	171	1420	882	249	279	10	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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	329	2567	1621	440	479	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	263	2066	1323	344	380	19	0	0

- Molecule 5 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	394	3189	2068	552	557	12	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	54	428	277	67	82	2	0	0

- Molecule 7 is a protein called General transcription and DNA repair factor IIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	605	Total	C	N	O	S	0	0
			4890	3127	848	885	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	714	Total	C	N	O	S	0	0
			5751	3683	999	1040	29		

- Molecule 9 is a protein called Alpha-amanitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	8	Total	C	N	O	S	0	0
			64	39	10	14	1		

- Molecule 10 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Z	5	Total	C	N	O	P	0	0
			117	49	20	41	7		

- Molecule 11 is a protein called Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	559	Total	C	N	O	S	0	0
			4580	2924	795	834	27		

- Molecule 12 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 13 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	164	Total	C	N	O	S	0	0
			1366	851	256	255	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	d	158	Total	C	N	O	S	0	0
			1307	814	238	252	3		

- Molecule 14 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	547	Total	C	N	O	S	0	0
			4376	2774	759	822	21		
14	e	539	Total	C	N	O	S	0	0
			4327	2746	748	814	19		

- Molecule 15 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	412	Total	C	N	O	S	0	0
			3143	1994	548	583	18		
15	f	403	Total	C	N	O	S	0	0
			3081	1954	533	576	18		

- Molecule 16 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	144	Total	C	N	O	S	0	0
			1171	742	215	210	4		

- Molecule 17 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	209	Total	C	N	O	S	0	0
			1633	1034	283	311	5		

- Molecule 18 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	120	Total	C	N	O	S	0	0
			959	610	166	177	6		
18	i	121	Total	C	N	O	S	0	0
			967	615	167	178	7		

- Molecule 19 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	90	Total	C	N	O	S	0	0
			720	466	115	135	4		
19	j	95	Total	C	N	O	S	0	0
			759	488	124	143	4		

- Molecule 20 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	76	Total	C	N	O	S	0	0
			622	388	109	122	3		
20	l	107	Total	C	N	O	S	0	0
			876	547	158	166	5		

- Molecule 21 is a protein called Transcription initiation factor IIA subunit 2.

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

- Molecule 22 is a protein called TATA-box-binding protein.

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

- Molecule 23 is a protein called Transcription initiation factor IIA beta chain.

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

- Molecule 24 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	282	Total	C	N	O	S	0	0
			2167	1353	384	412	18		

- Molecule 25 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	176	Total	C	N	O	S	0	0
			1461	921	268	268	4		

- Molecule 26 is a protein called General transcription factor IIF subunit 2.

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

- Molecule 27 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	184	Total	C	N	O	S	0	0
			1520	957	272	280	11		

- Molecule 28 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 29 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	63	Total	C	N	O	P	0	0
			1302	616	245	378	63		

- Molecule 30 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	73	Total	C	N	O	P	0	0
			1488	707	271	437	73		

- Molecule 31 is a protein called Transcription initiation factor TFIID subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	127	Total	C	N	O	S	0	0
			1011	638	174	193	6		

- Molecule 32 is a protein called Transcription initiation factor TFIID subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	98	Total	C	N	O	S	0	0
			785	499	142	139	5		

- Molecule 33 is a protein called Transcription initiation factor TFIID subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	m	87	Total	C	N	O	S	0	0
			724	456	131	131	6		

- Molecule 34 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	o	1452	Total	C	N	O	S	0	0
			11510	7235	2056	2146	73		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	1835	ALA	THR	conflict	UNP A0A8D1DPV6

- Molecule 35 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	p	1149	Total	C	N	O	S	0	0
			9175	5796	1614	1701	64		

- Molecule 36 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB4.

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

- Molecule 38 is a protein called DNA-directed RNA polymerase II subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	s	209	Total	C	N	O	S	0	0
			1720	1089	300	323	8		

- Molecule 39 is a protein called DNA-directed RNA polymerase II subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	t	82	Total	C	N	O	S	0	0
			657	418	113	121	5		

- Molecule 40 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 41 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 42 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	114	Total	C	N	O	S	0	0
			927	571	166	179	11		

- Molecule 43 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	x	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 44 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

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

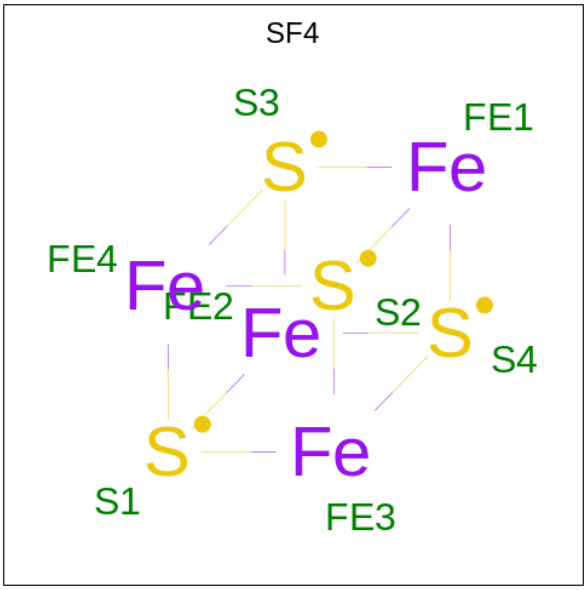
- Molecule 45 is a protein called RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z	44	Total	C	N	O	S	0	0
			372	231	72	63	6		

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
46	0	2	Total Zn 2 2	0
46	2	3	Total Zn 3 3	0
46	3	2	Total Zn 2 2	0
46	R	1	Total Zn 1 1	0
46	U	1	Total Zn 1 1	0
46	o	2	Total Zn 2 2	0
46	p	1	Total Zn 1 1	0
46	q	1	Total Zn 1 1	0
46	w	2	Total Zn 2 2	0
46	x	1	Total Zn 1 1	0
46	z	1	Total Zn 1 1	0

- Molecule 47 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

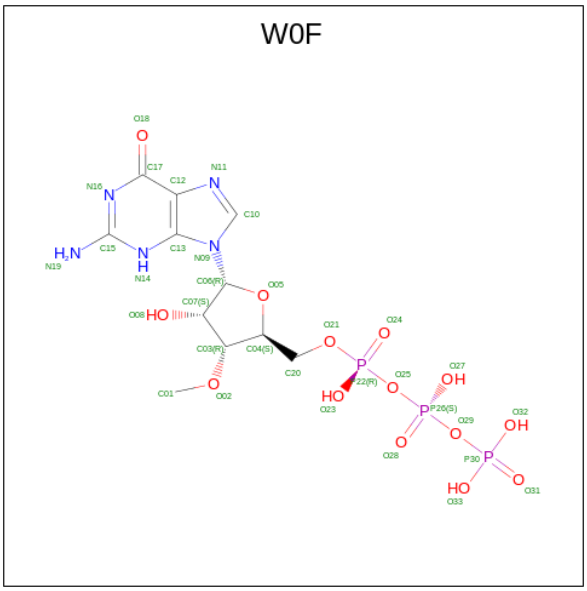


Mol	Chain	Residues	Atoms	AltConf
47	7	1	Total Fe S 8 4 4	0

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
48	o	1	Total Mg 1 1	0

- Molecule 49 is [[(2 {S},3 {R},4 {S},5 {R})-5-(2-azanyl-6-oxidanylidene-3 {H}-purin-9-yl)-3-methoxy-4-oxidanyl-oxolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: W0F) (formula: $C_{11}H_{18}N_5O_{14}P_3$).



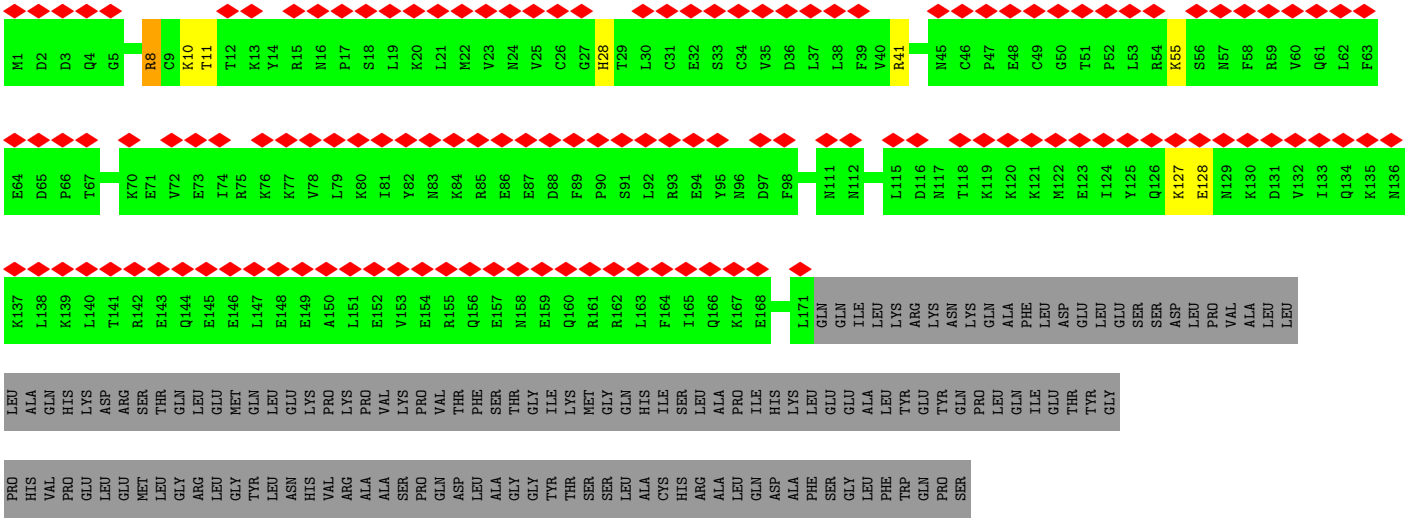
Mol	Chain	Residues	Atoms	AltConf
49	p	1	Total C N O P 33 11 5 14 3	0

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.

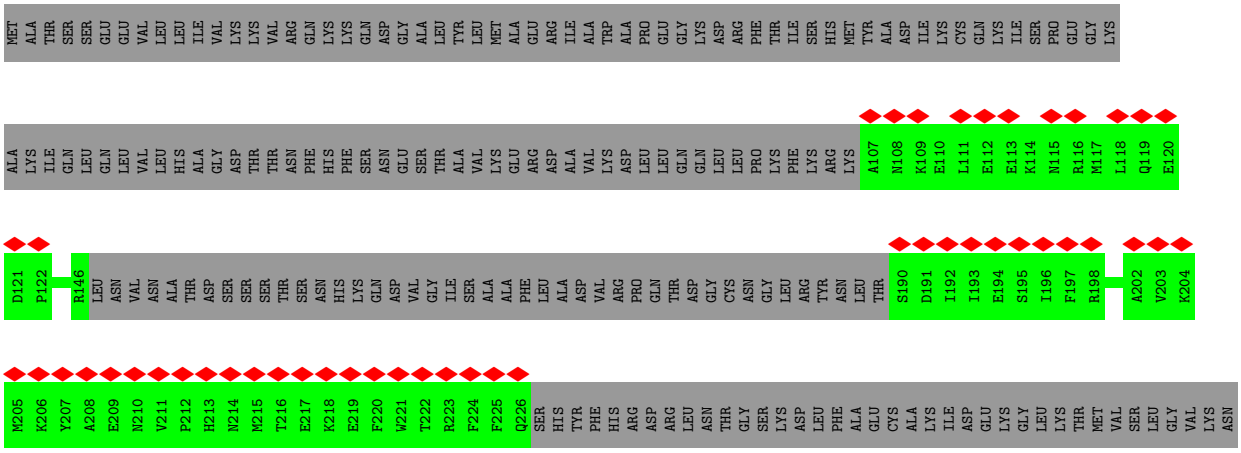
• Molecule 1: CDK-activating kinase assembly factor MAT1

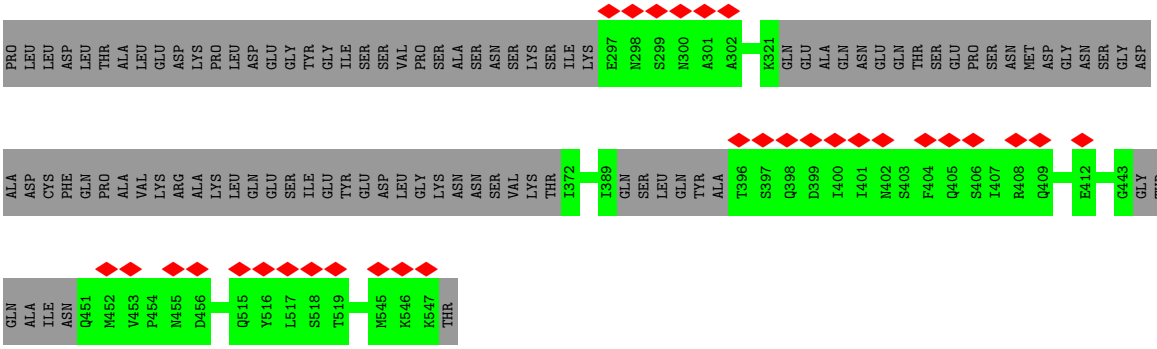
Chain 0:



• Molecule 2: General transcription factor IIH subunit 1

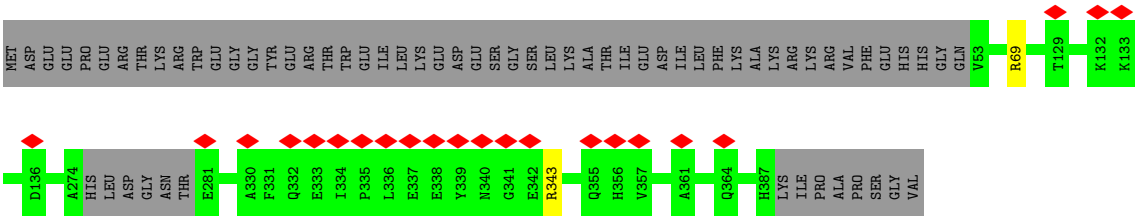
Chain 1:





• Molecule 3: General transcription factor IIH subunit 2

Chain 2:

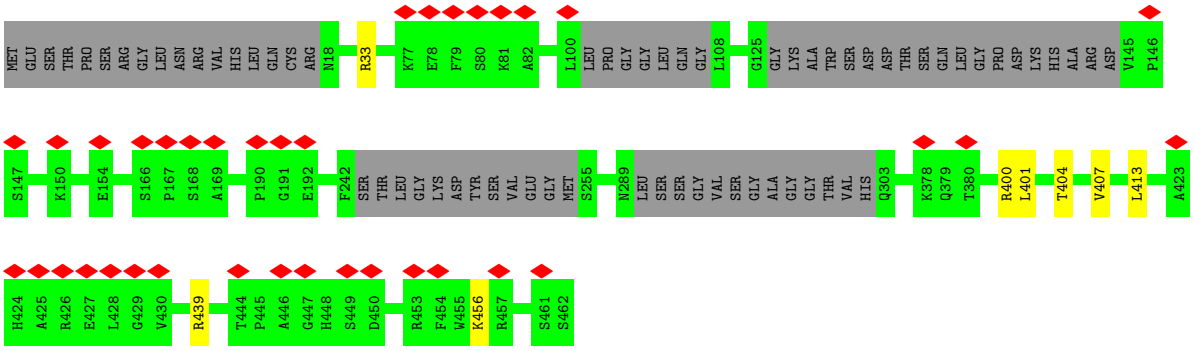


• Molecule 4: General transcription factor IIH subunit 3

Chain 3:

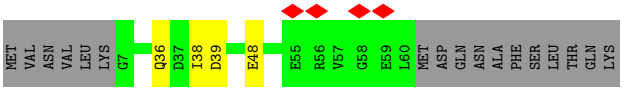
• Molecule 5: General transcription factor IIH subunit 4

Chain 4:



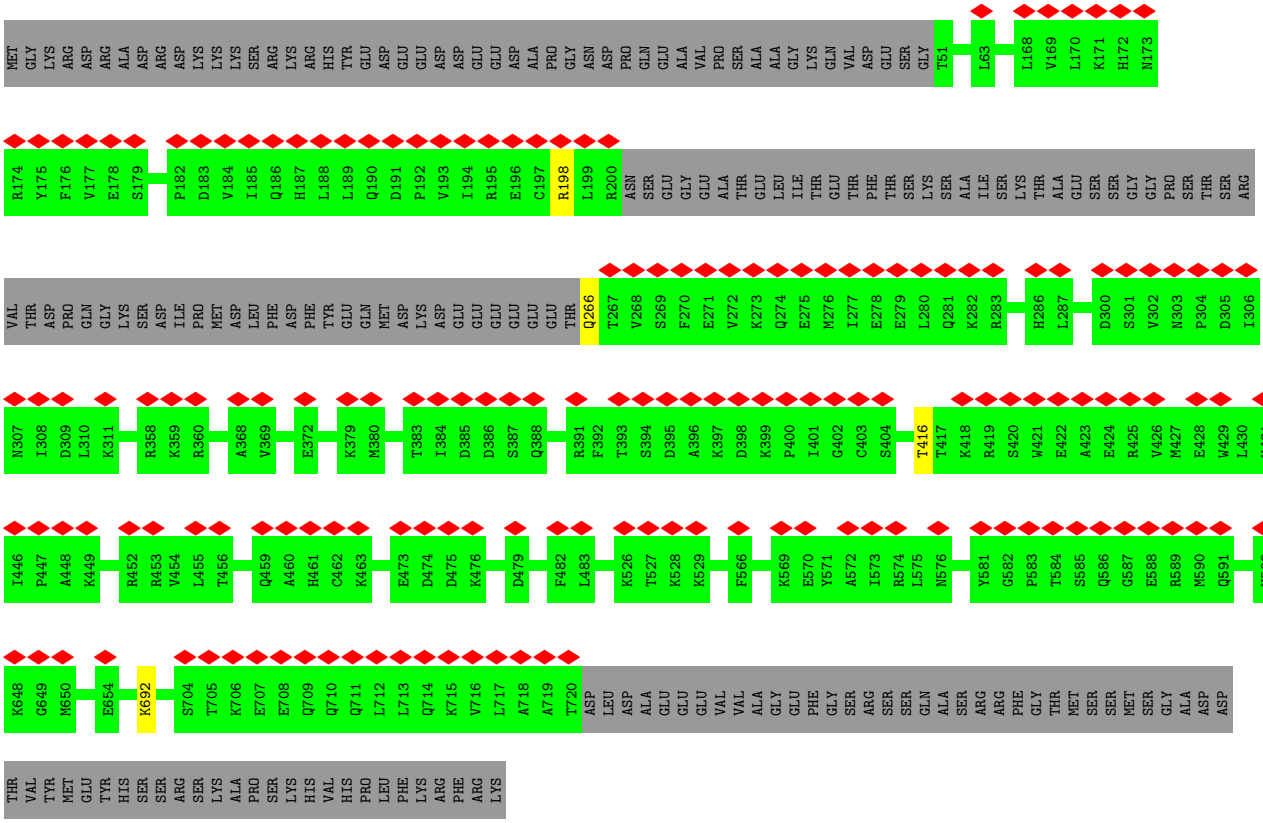
• Molecule 6: General transcription factor IIH subunit 5

Chain 5:



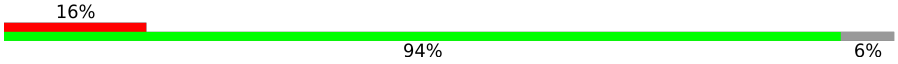
• Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB

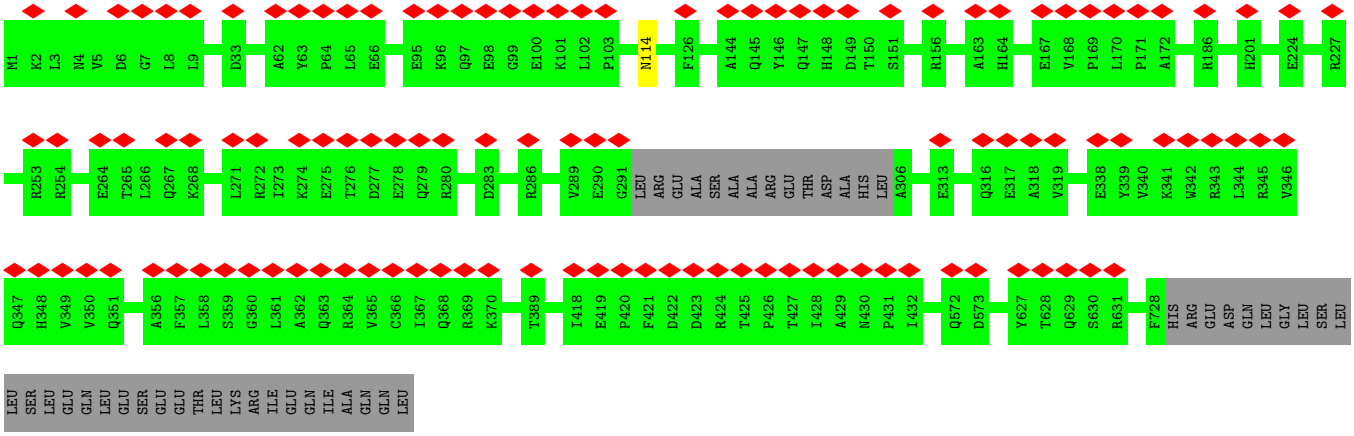
Chain 6:



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

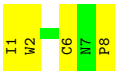
Chain 7:





• Molecule 9: Alpha-amanitin

Chain N:

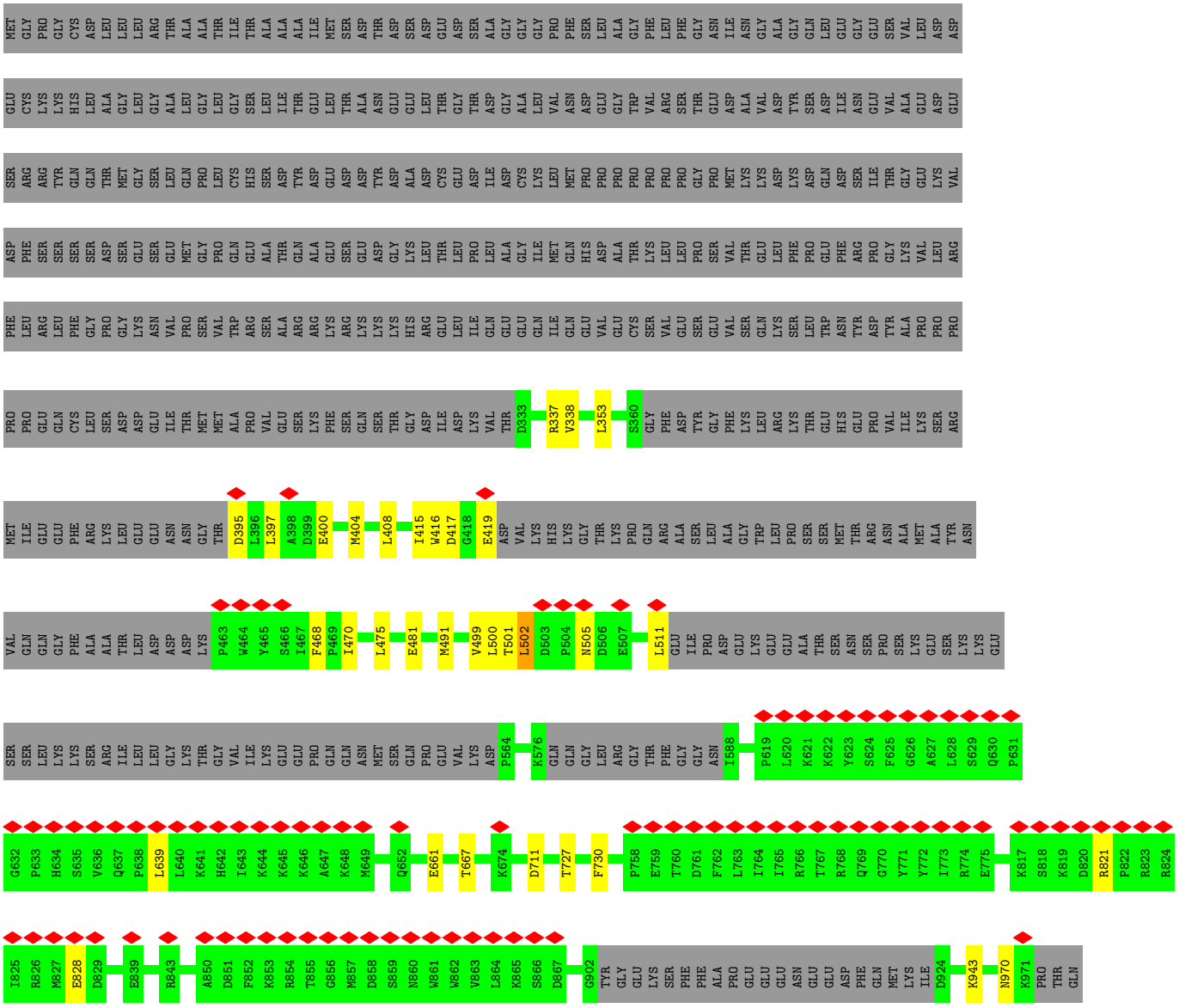


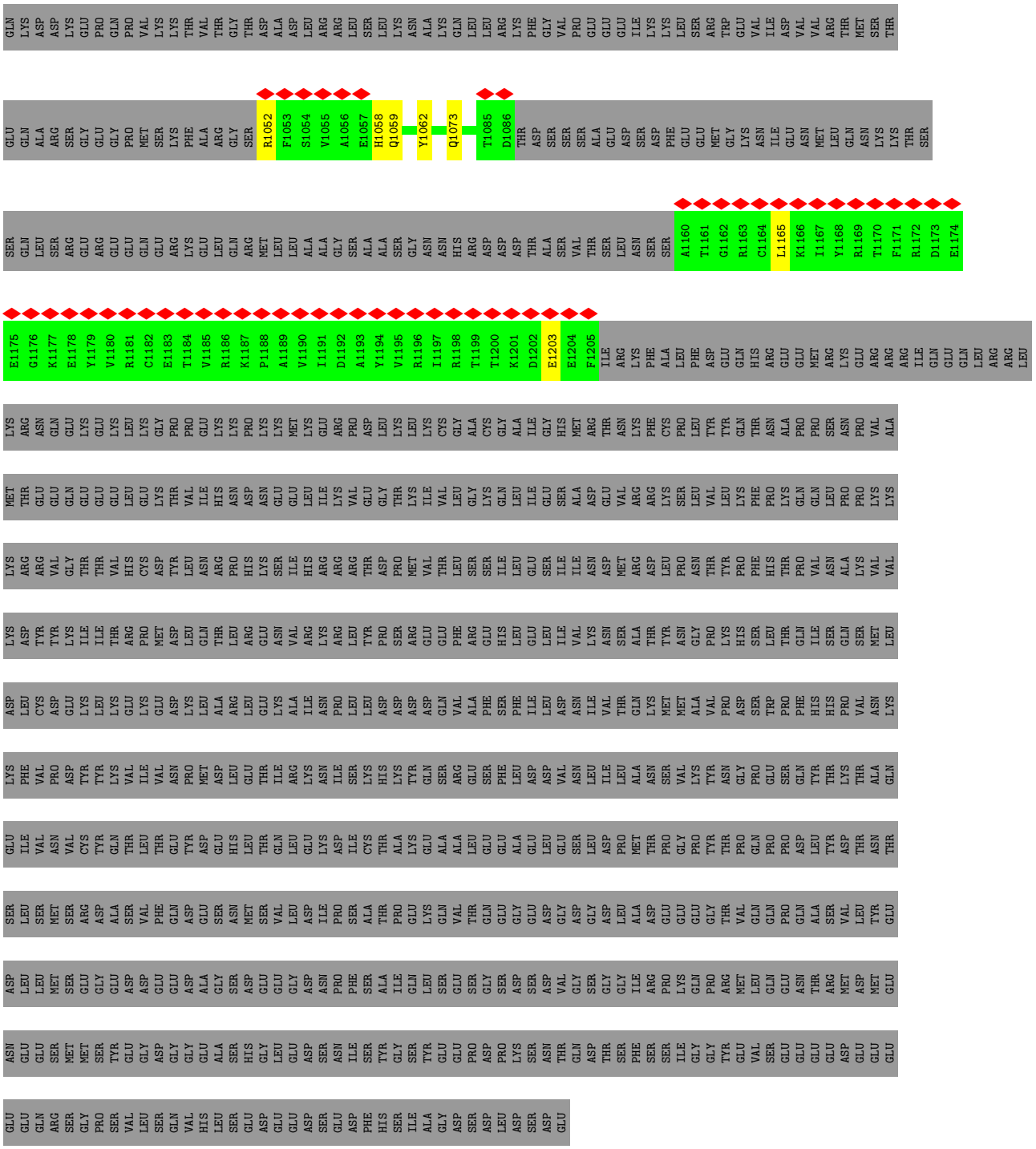
• Molecule 10: RNA

Chain Z:

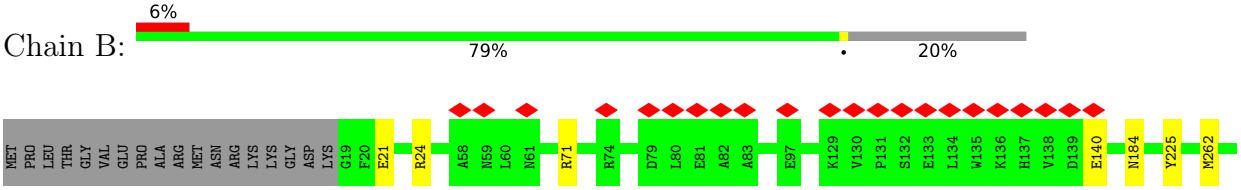
• Molecule 11: Transcription initiation factor TFIID subunit 1

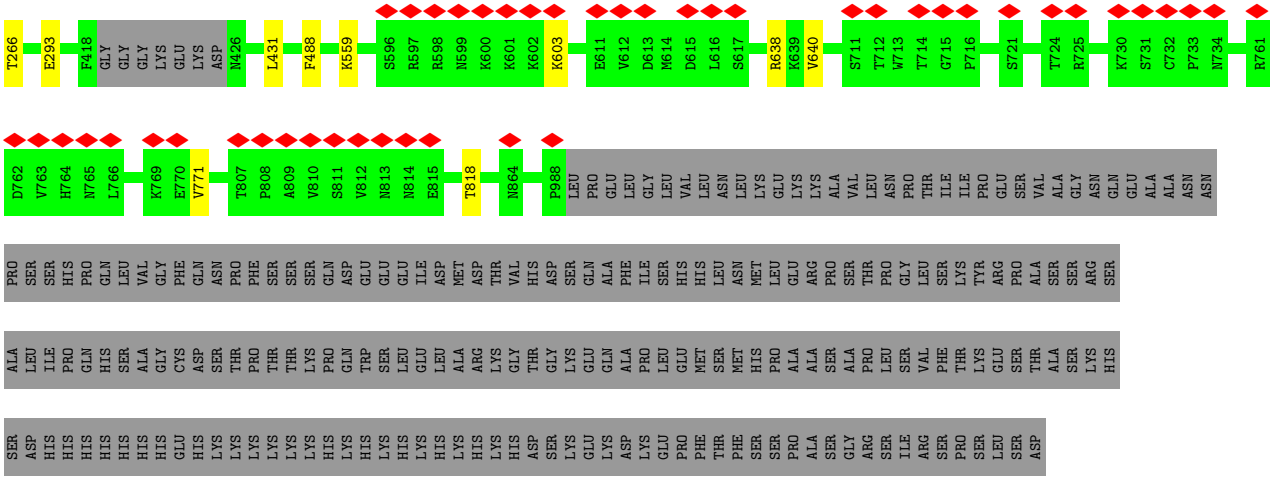
Chain A:





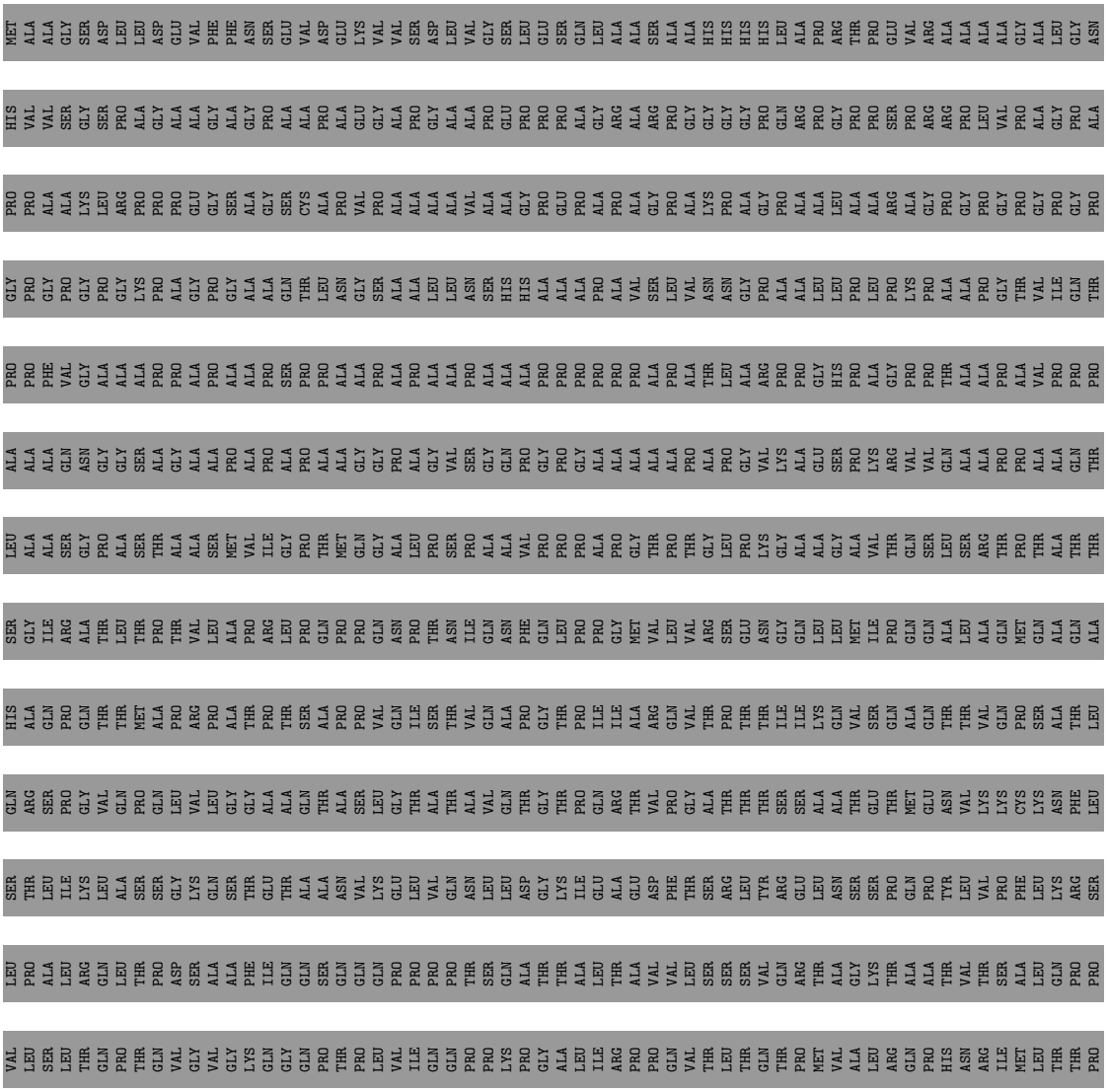
• Molecule 12: Transcription initiation factor TFIID subunit 2

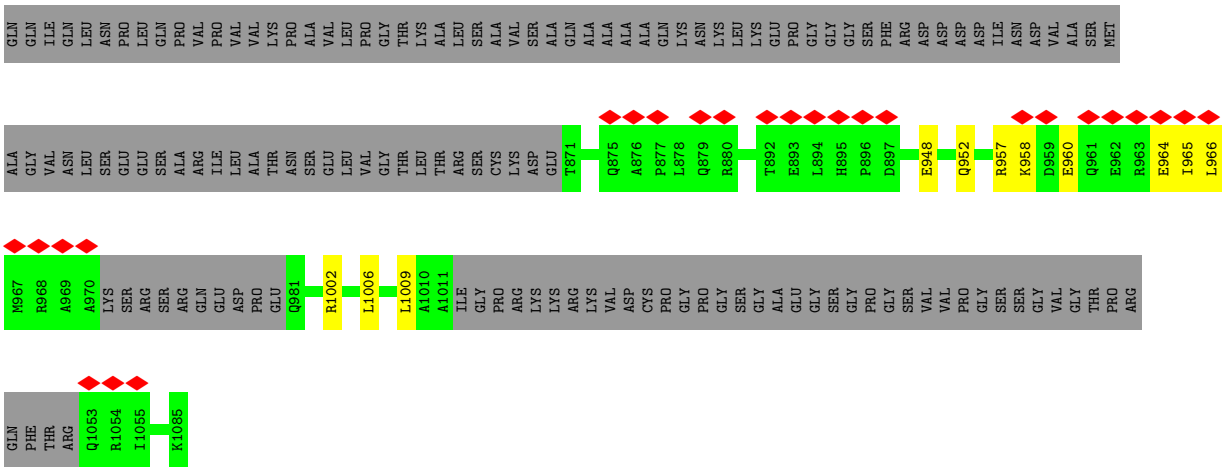




• Molecule 13: Transcription initiation factor TFIID subunit 4

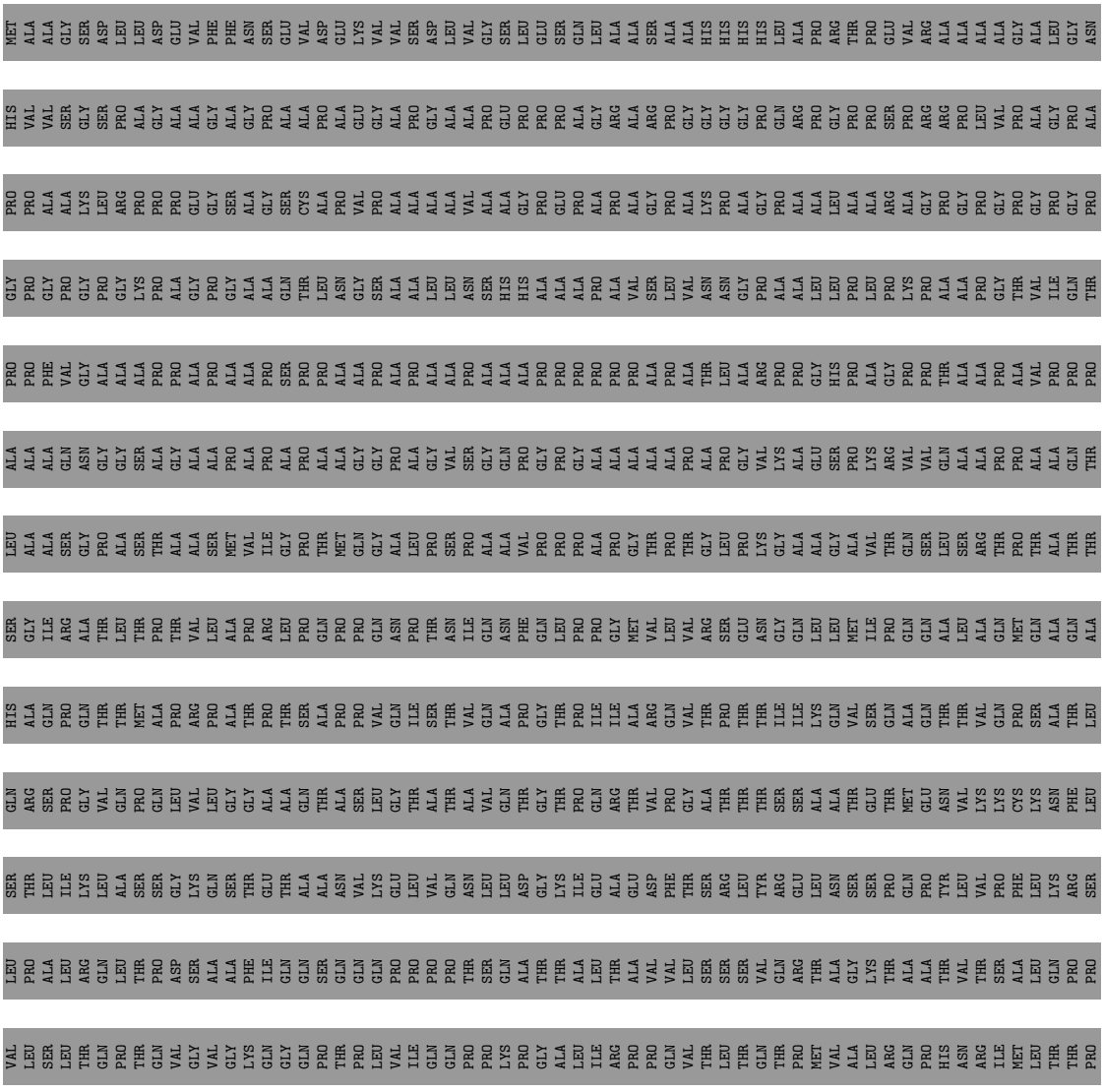
Chain D:

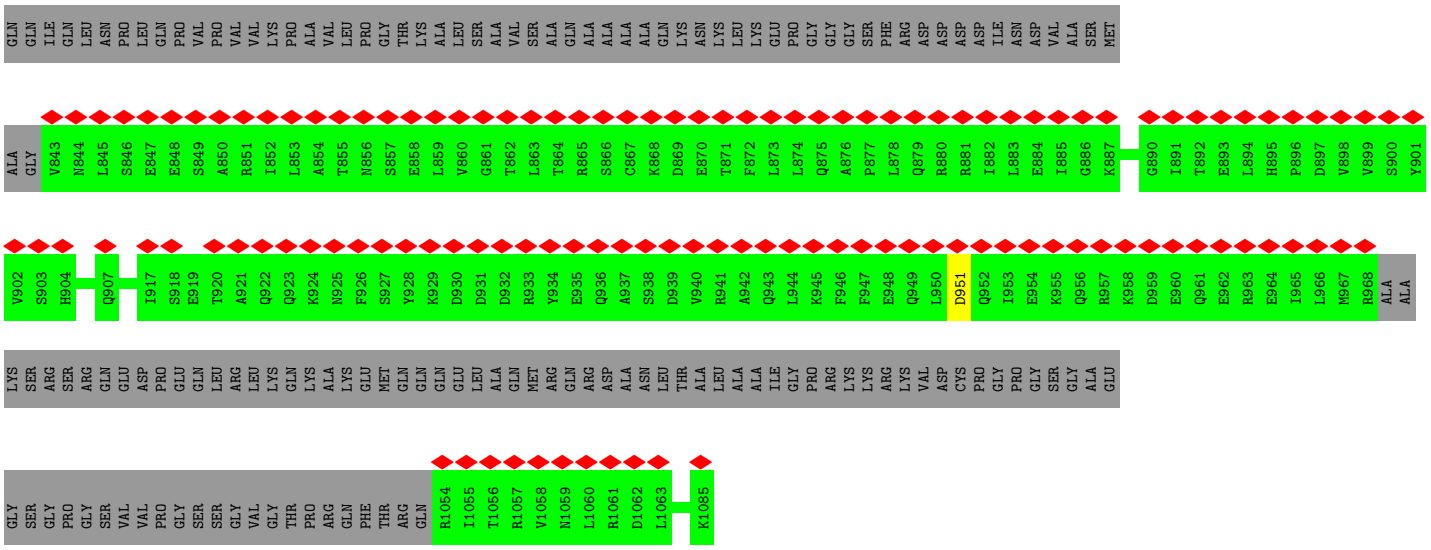




• Molecule 13: Transcription initiation factor TFIID subunit 4

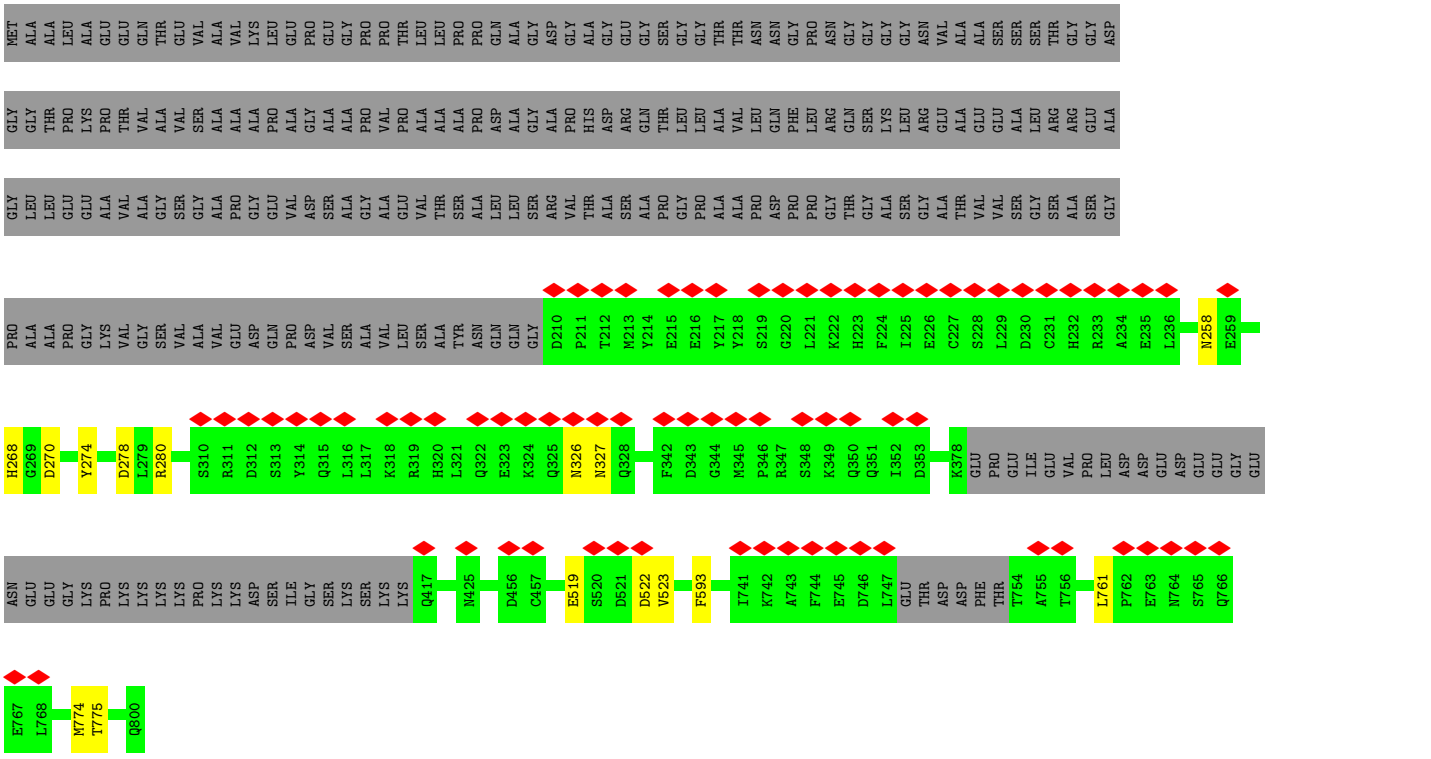
Chain d:





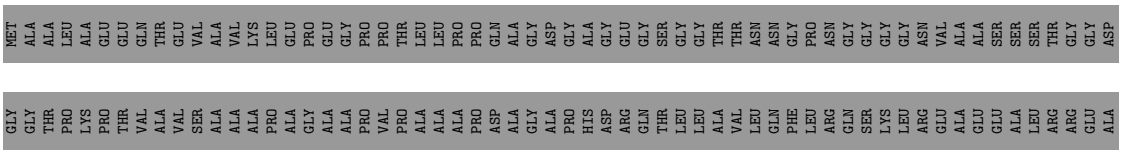
• Molecule 14: Transcription initiation factor TFIID subunit 5

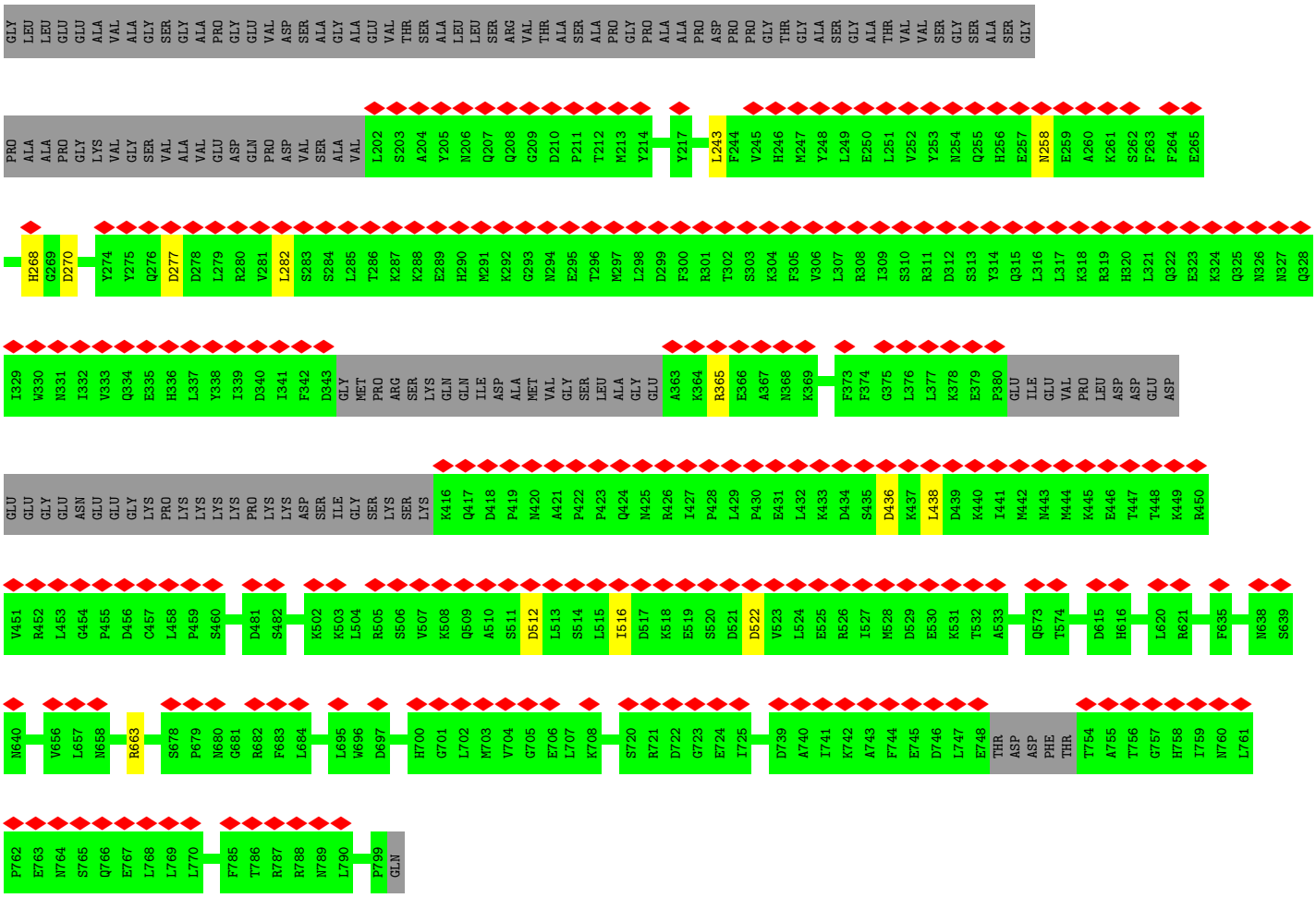
Chain E:



• Molecule 14: Transcription initiation factor TFIID subunit 5

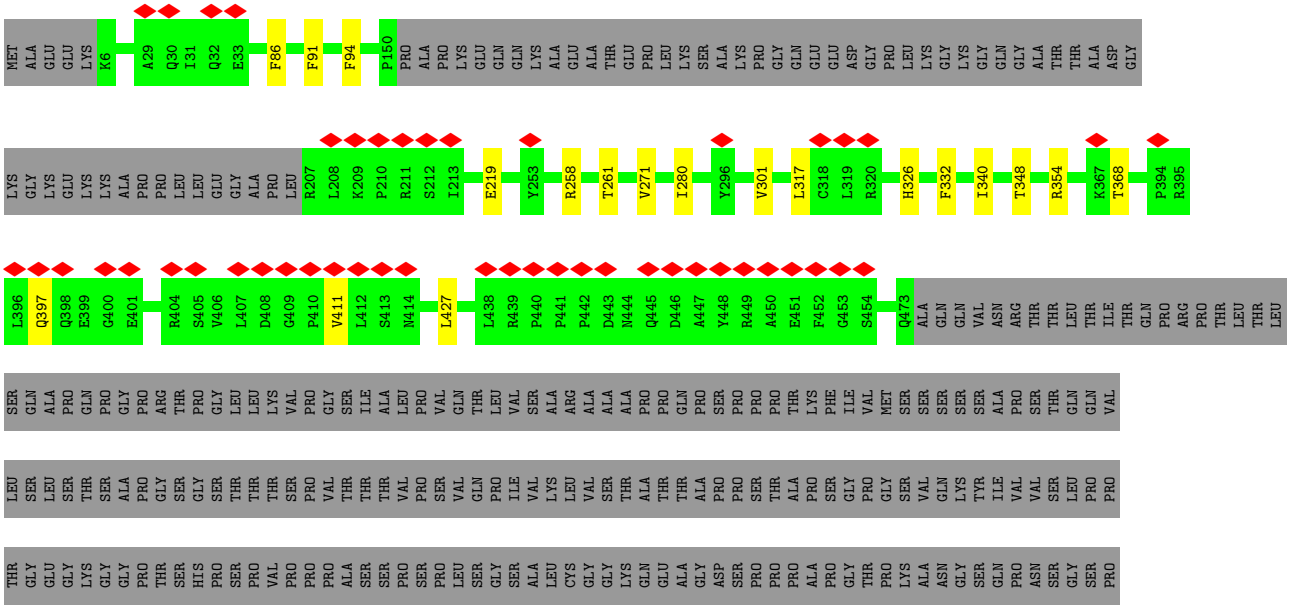
Chain e:





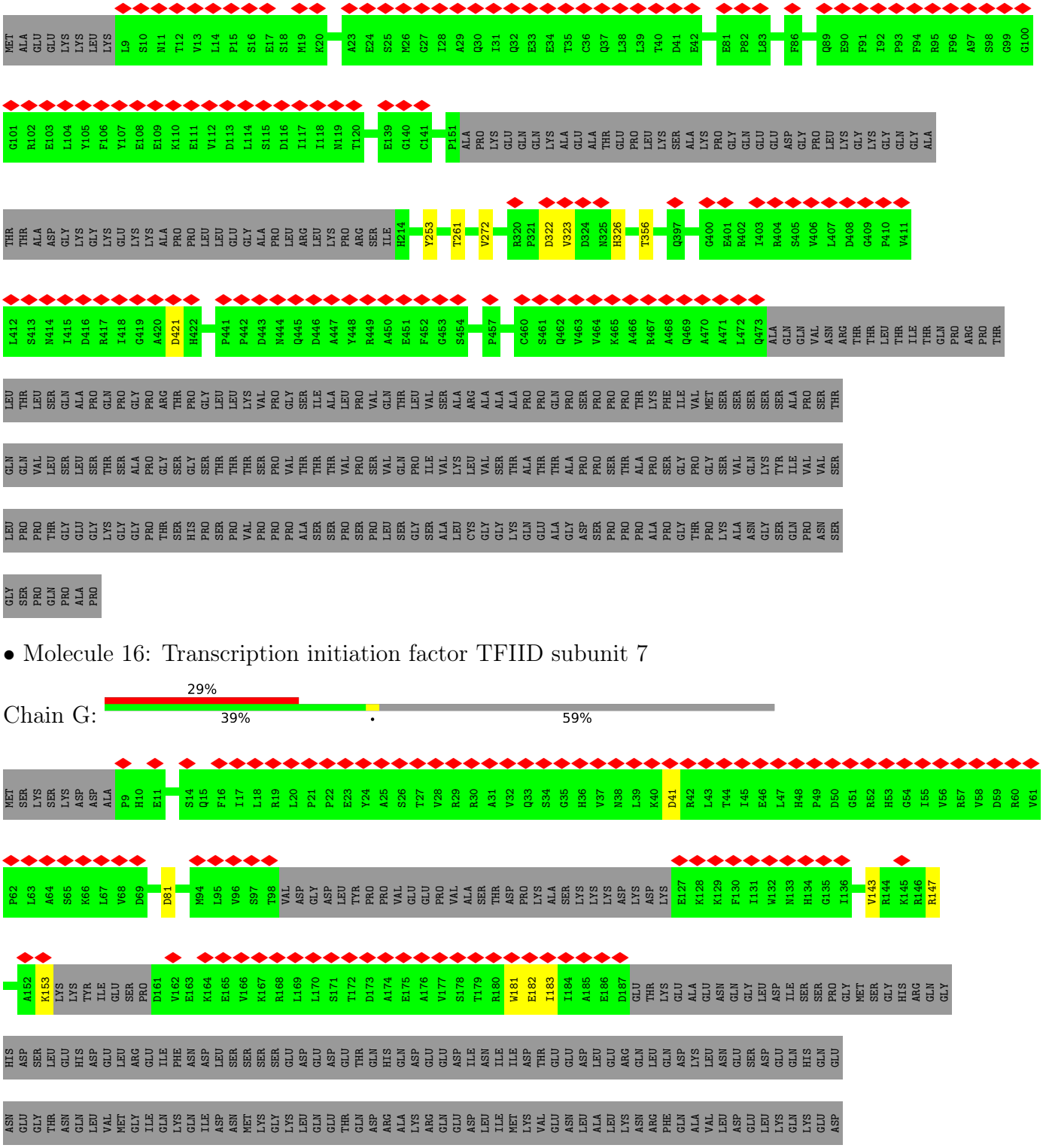
• Molecule 15: Transcription initiation factor TFIID subunit 6

Chain F:



• Molecule 15: Transcription initiation factor TFIID subunit 6

Chain f:

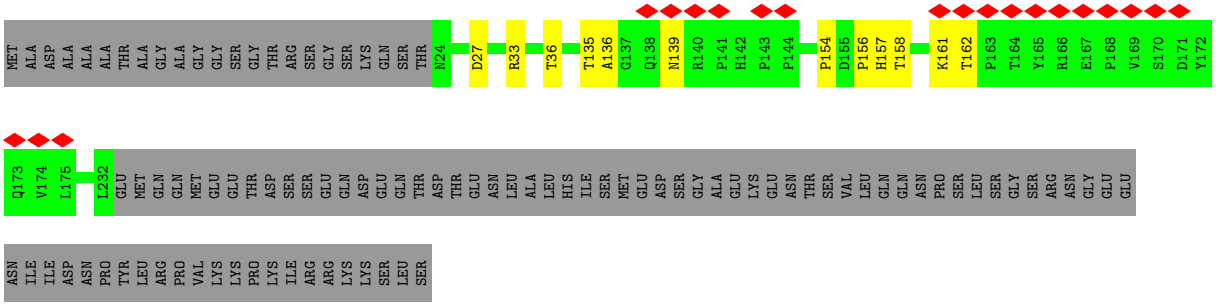


• Molecule 16: Transcription initiation factor TFIID subunit 7

Chain G:

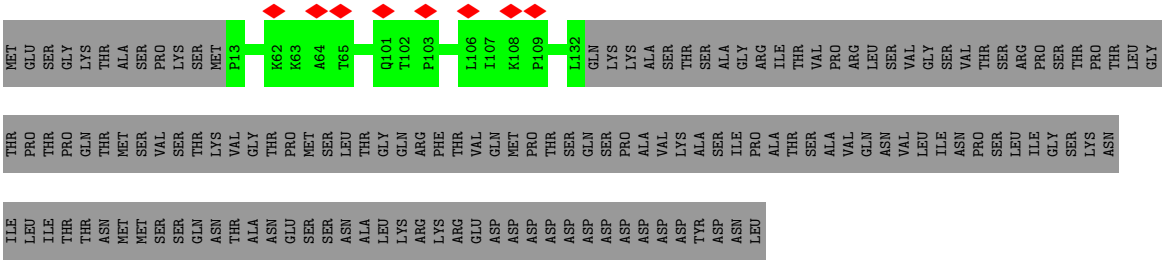
• Molecule 17: Transcription initiation factor TFIID subunit 8

Chain H:



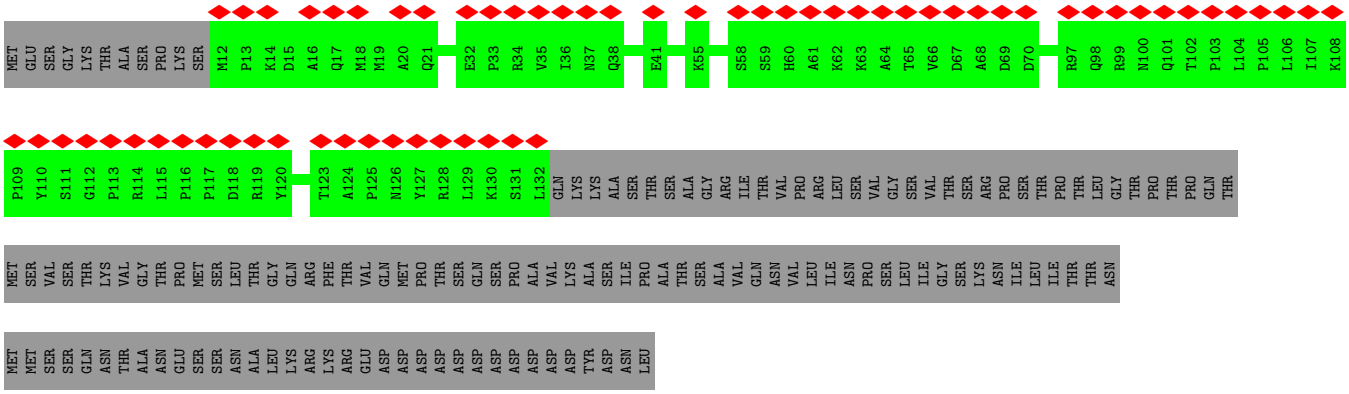
• Molecule 18: Transcription initiation factor TFIID subunit 9

Chain I:



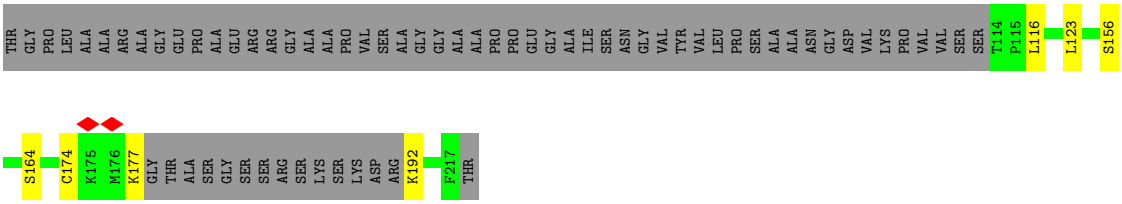
• Molecule 18: Transcription initiation factor TFIID subunit 9

Chain i:

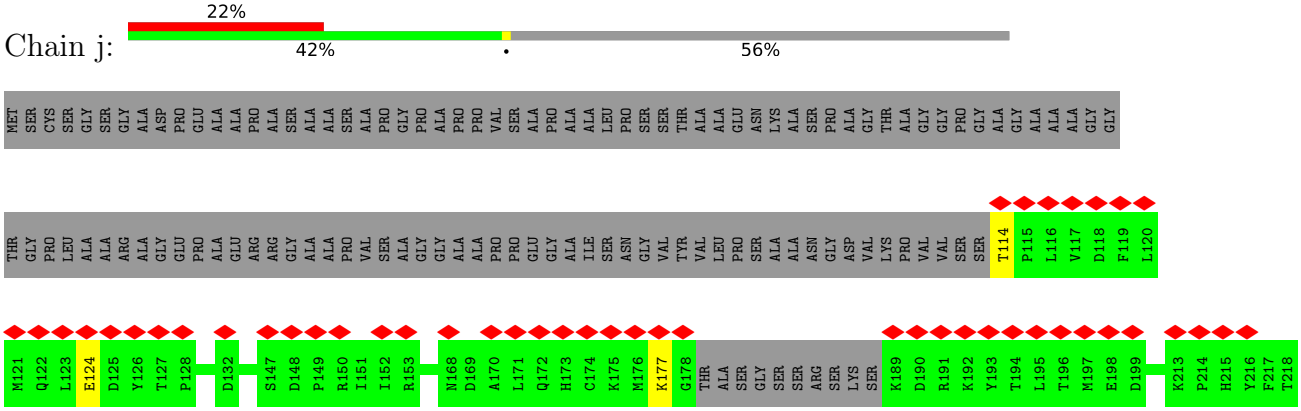


• Molecule 19: Transcription initiation factor TFIID subunit 10

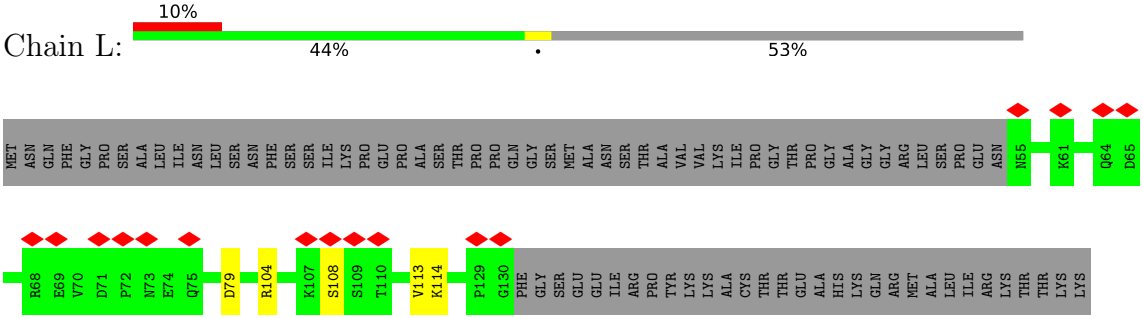
Chain J:



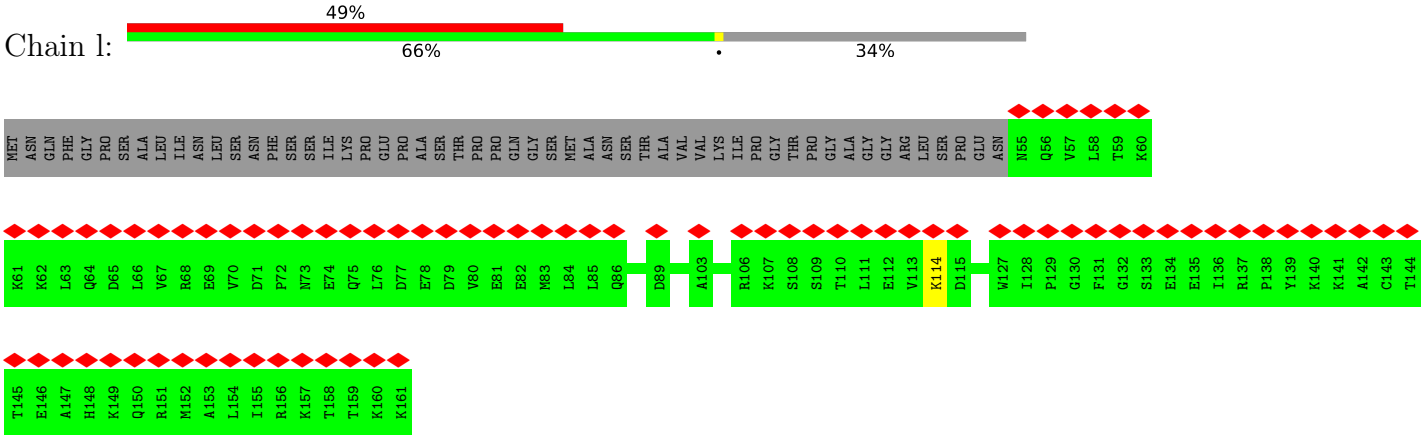
• Molecule 19: Transcription initiation factor TFIID subunit 10



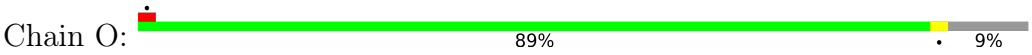
• Molecule 20: Transcription initiation factor TFIID subunit 12

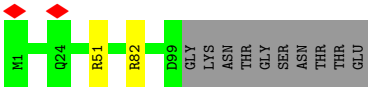


• Molecule 20: Transcription initiation factor TFIID subunit 12



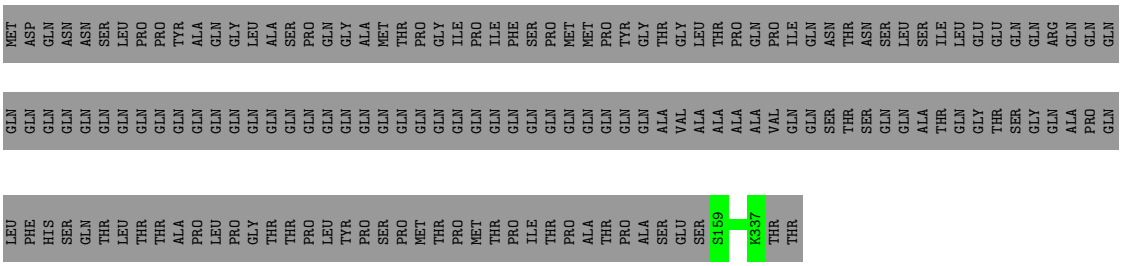
• Molecule 21: Transcription initiation factor IIA subunit 2





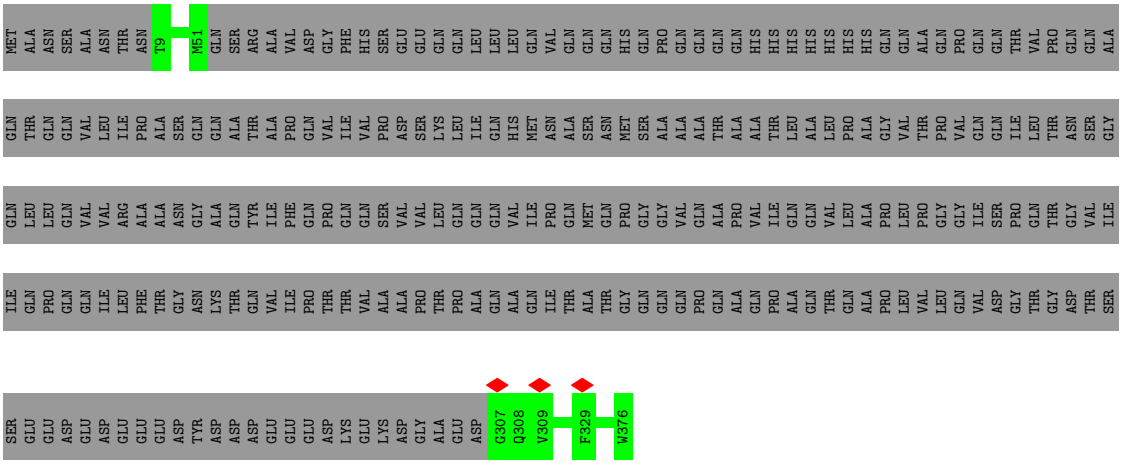
• Molecule 22: TATA-box-binding protein

Chain P:



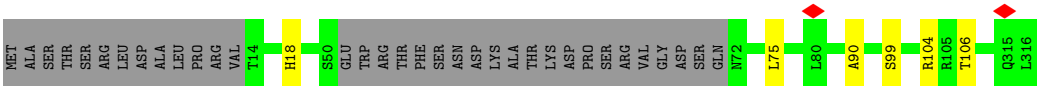
• Molecule 23: Transcription initiation factor IIA beta chain

Chain Q:



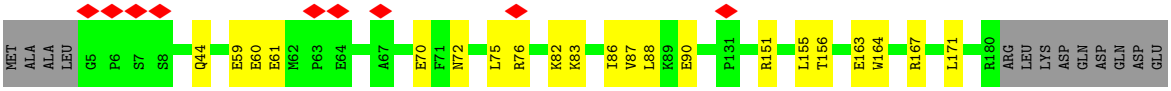
• Molecule 24: Transcription initiation factor IIB

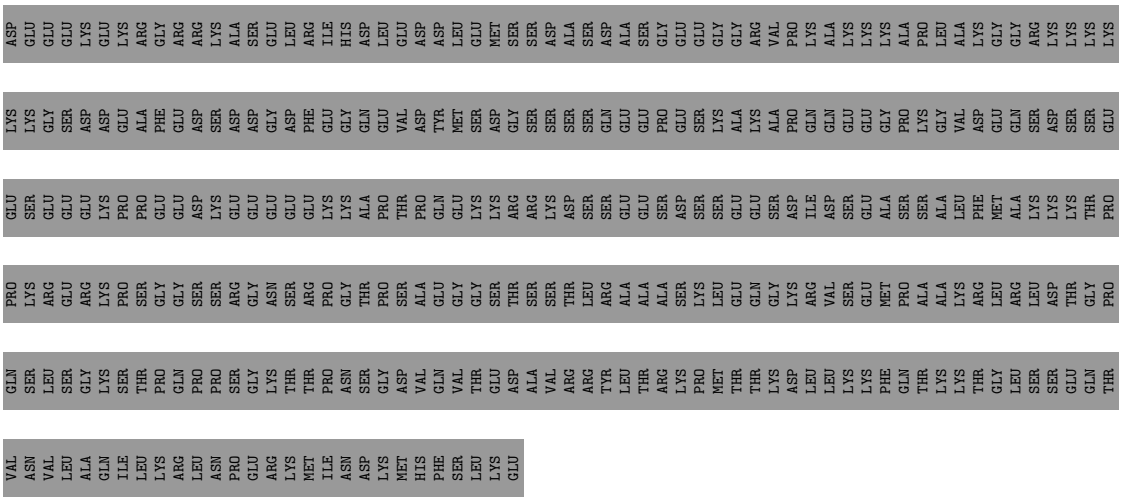
Chain R:



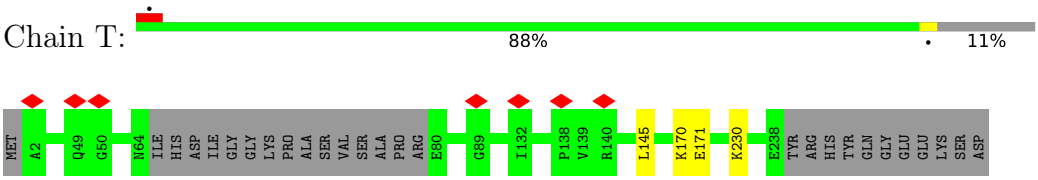
• Molecule 25: General transcription factor IIF subunit 1

Chain S:

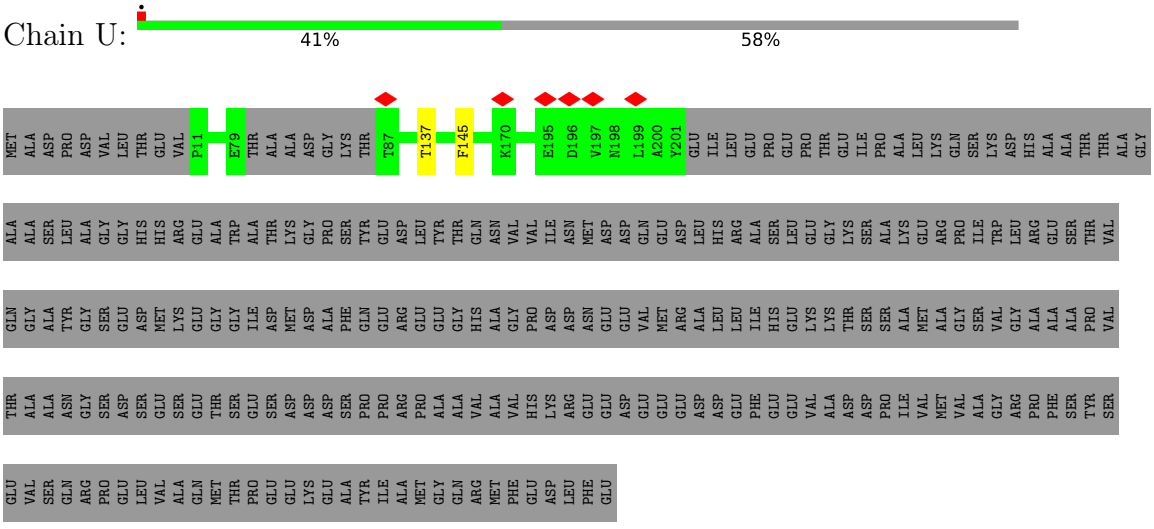




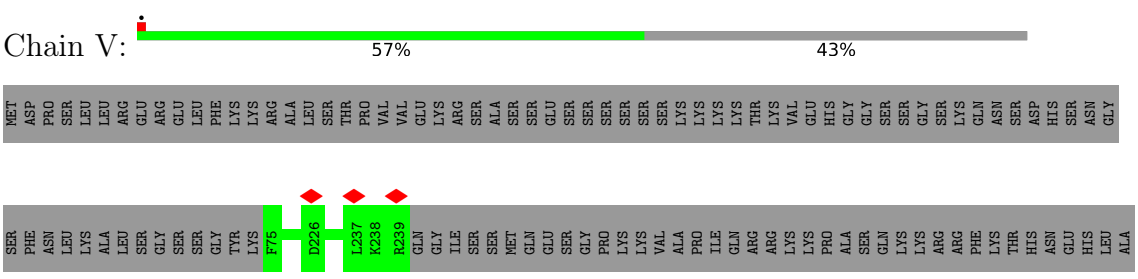
• Molecule 26: General transcription factor IIF subunit 2



• Molecule 27: General transcription factor IIE subunit 1

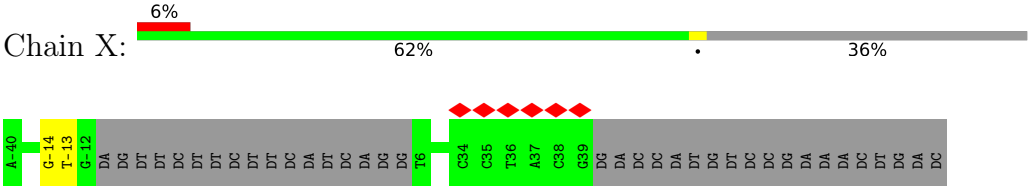


• Molecule 28: Transcription initiation factor IIE subunit beta



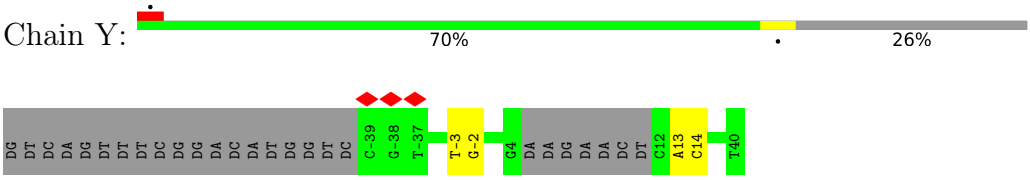
• Molecule 29: non-template DNA

Chain X:



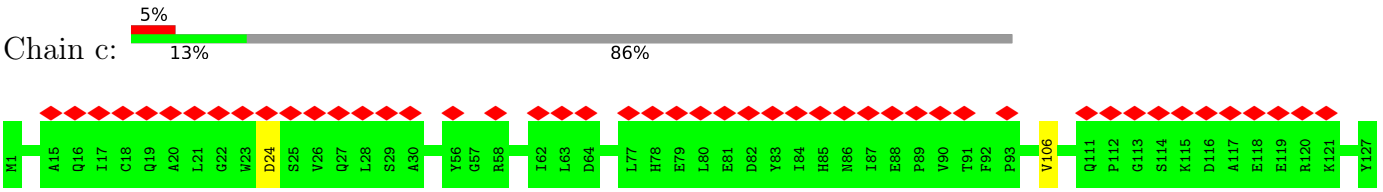
• Molecule 30: template DNA

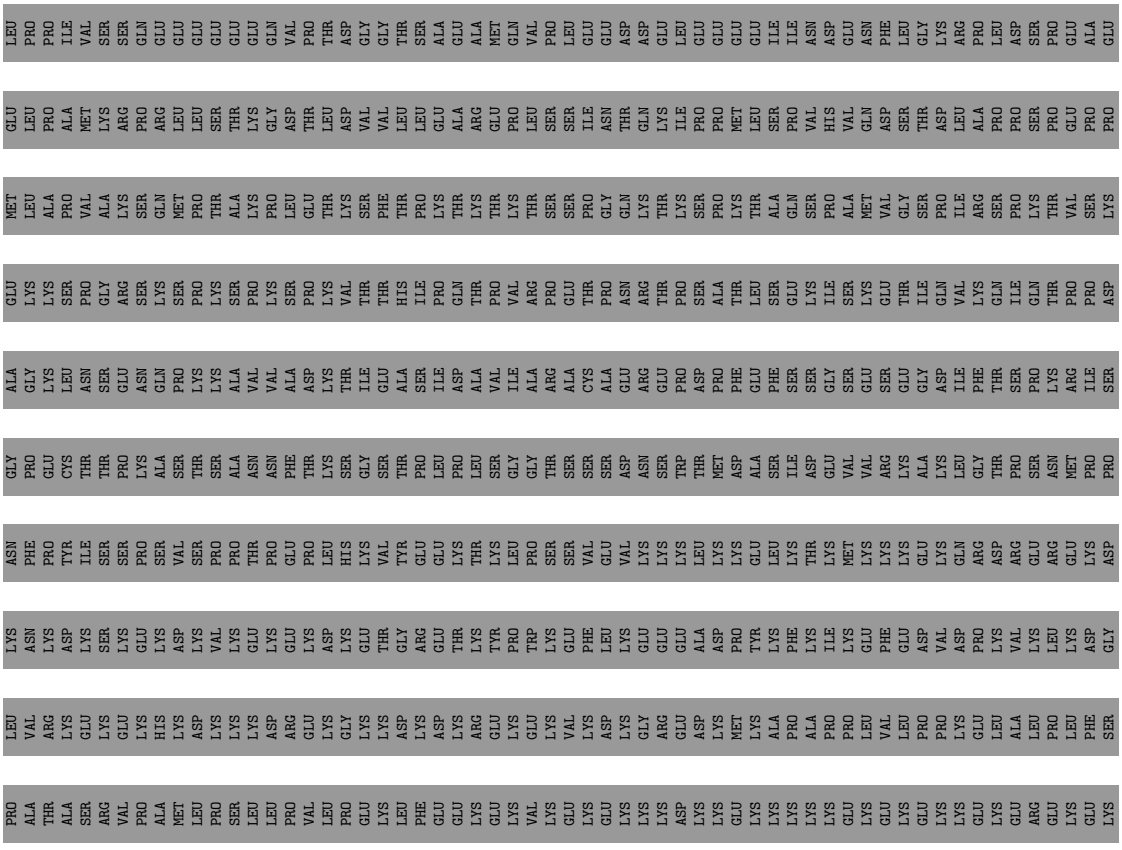
Chain Y:

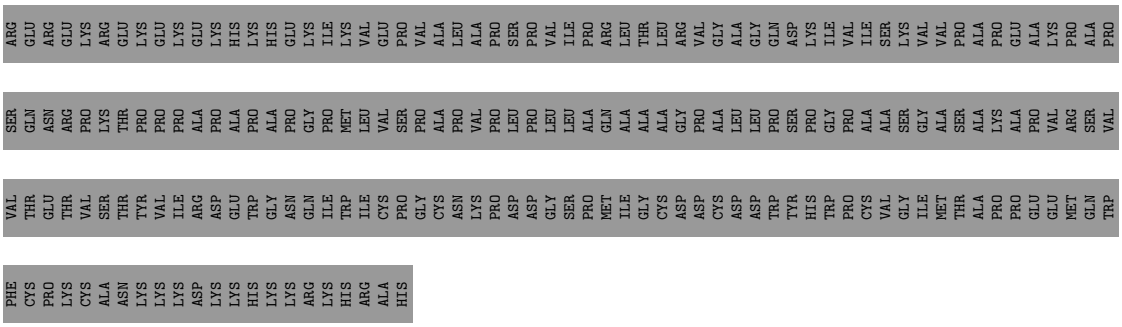


• Molecule 31: Transcription initiation factor TFIID subunit 3

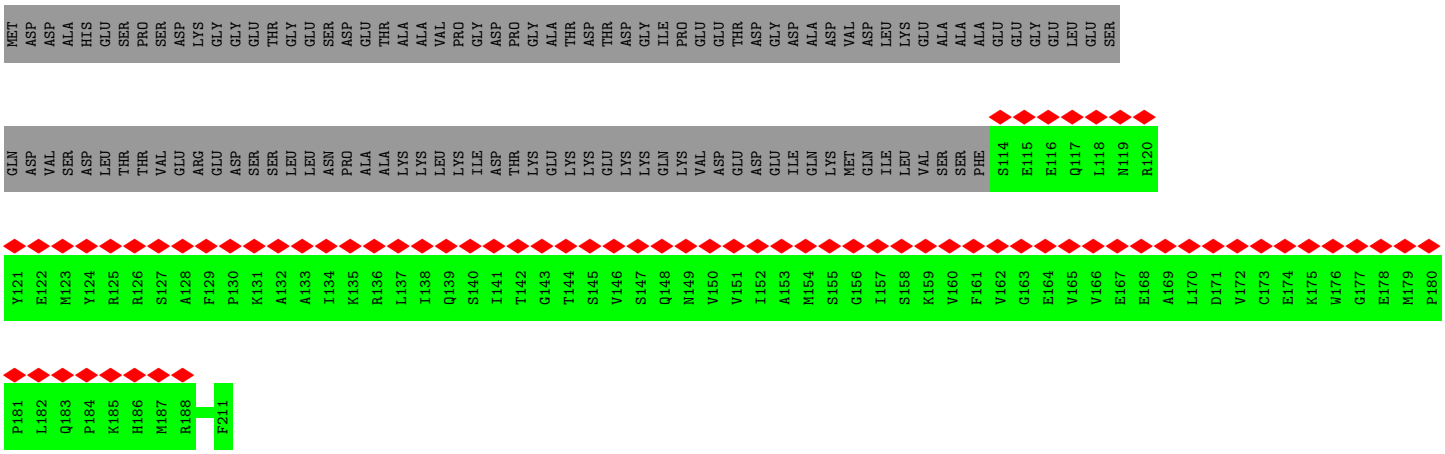
Chain c:



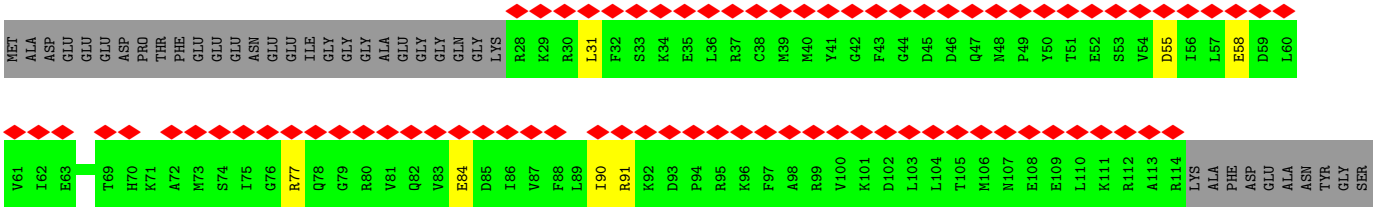




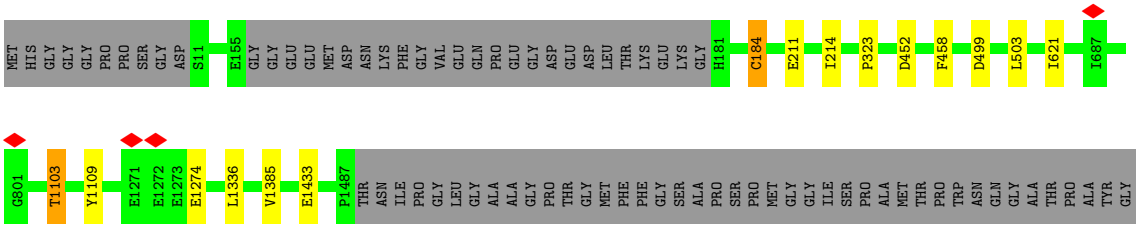
• Molecule 32: Transcription initiation factor TFIID subunit 11

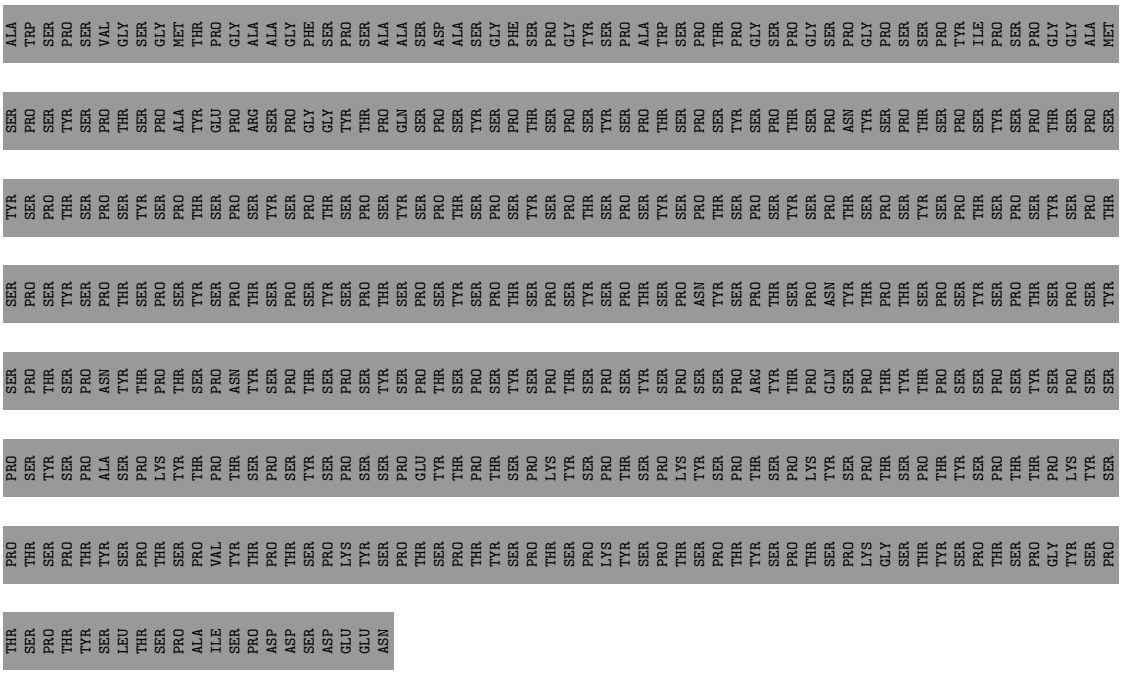


• Molecule 33: Transcription initiation factor TFIID subunit 13



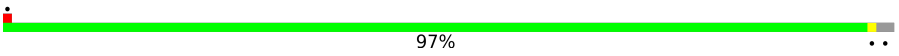
• Molecule 34: DNA-directed RNA polymerase subunit

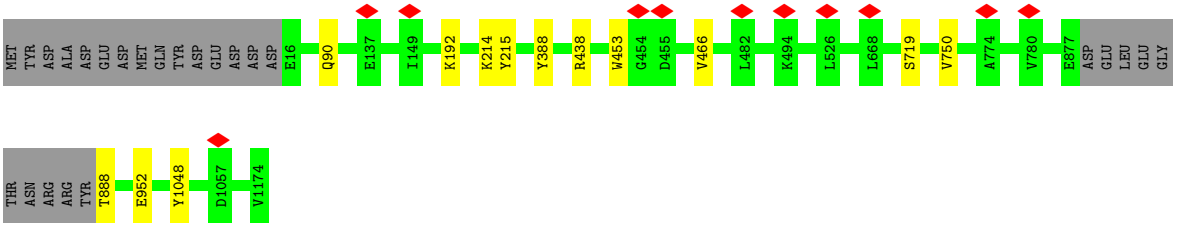




• Molecule 35: DNA-directed RNA polymerase subunit beta

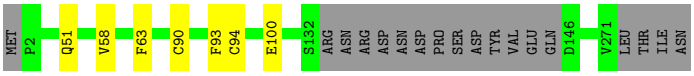
Chain p:





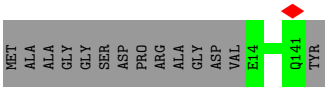
• Molecule 36: DNA-directed RNA polymerase II subunit RPB3

Chain q:



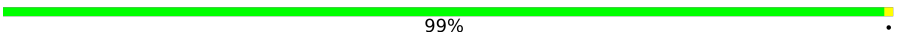
• Molecule 37: DNA-directed RNA polymerase II subunit RPB4

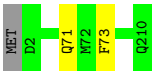
Chain r:



• Molecule 38: DNA-directed RNA polymerase II subunit E

Chain s:



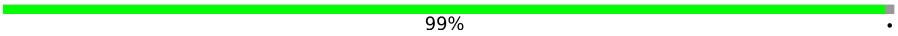


• Molecule 39: DNA-directed RNA polymerase II subunit F

Chain t:

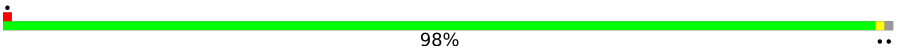
• Molecule 40: DNA-directed RNA polymerase II subunit RPB7

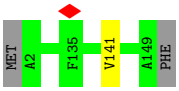
Chain u:



• Molecule 41: DNA-directed RNA polymerases I, II, and III subunit RPABC3

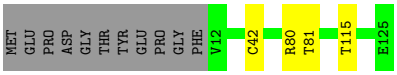
Chain v:





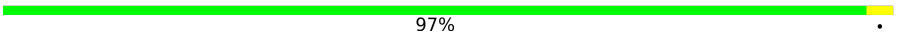
• Molecule 42: DNA-directed RNA polymerase II subunit RPB9

Chain w:



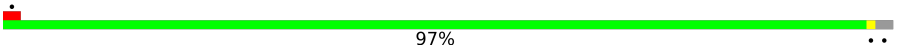
• Molecule 43: DNA-directed RNA polymerases I, II, and III subunit RPABC5

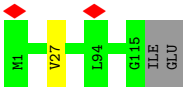
Chain x:



• Molecule 44: DNA-directed RNA polymerase II subunit RPB11-a

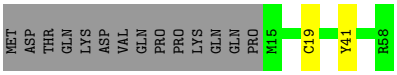
Chain y:





• Molecule 45: RPB12

Chain z:


MET
ASP
THR
GLN
LYS
ASP
VAL
GLN
PRO
PRO
LYS
GLN
GLN
PRO
M15
C19
Y41
R58

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5869	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.558	Depositor
Minimum map value	-1.961	Depositor
Average map value	0.047	Depositor
Map value standard deviation	0.200	Depositor
Recommended contour level	0.54	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.668, 2.668, 2.668	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: W0F, ZN, SF4, TRX, ILX, ATP, HYP, G2L, MG, CSX

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	0.36	0/1437	0.59	3/1926 (0.2%)
2	1	0.26	0/2210	0.41	0/2975
3	2	0.27	0/2624	0.43	0/3555
4	3	0.30	0/2103	0.46	0/2846
5	4	0.31	0/3262	0.46	1/4418 (0.0%)
6	5	0.35	0/433	0.57	0/585
7	6	0.26	0/4994	0.41	0/6745
8	7	0.26	0/5875	0.41	0/7955
9	N	0.46	0/22	1.00	0/26
10	Z	0.59	0/68	1.17	0/103
11	A	0.50	0/4698	0.66	0/6345
12	B	0.46	0/7993	0.61	0/10836
13	D	0.42	0/1379	0.63	1/1843 (0.1%)
13	d	0.39	0/1321	0.53	0/1772
14	E	0.39	0/4482	0.59	0/6069
14	e	0.44	0/4433	0.60	0/6004
15	F	0.48	0/3201	0.69	0/4347
15	f	0.41	0/3140	0.63	0/4268
16	G	0.51	0/1190	0.62	0/1601
17	H	0.46	0/1673	0.64	0/2285
18	I	0.28	0/981	0.47	0/1332
18	i	0.29	0/989	0.46	0/1343
19	J	0.57	0/736	0.69	0/998
19	j	0.54	0/775	0.63	0/1049
20	L	0.49	0/630	0.71	0/852
20	l	0.44	0/888	0.55	0/1194
21	O	0.28	0/816	0.44	0/1105
22	P	0.29	0/1448	0.51	0/1948
23	Q	0.26	0/945	0.43	0/1274
24	R	0.36	0/2199	0.55	1/2967 (0.0%)
25	S	0.27	0/1496	0.52	0/2013
26	T	0.28	0/1817	0.47	0/2445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
27	U	0.32	0/1545	0.55	0/2075
28	V	0.28	0/1380	0.53	0/1854
29	X	0.76	0/1461	1.14	5/2253 (0.2%)
30	Y	0.78	0/1666	1.06	5/2564 (0.2%)
31	c	0.39	0/1035	0.54	0/1406
32	k	0.31	0/799	0.47	0/1070
33	m	0.59	0/733	0.64	0/977
34	o	0.47	0/11723	0.57	1/15830 (0.0%)
35	p	0.53	0/9358	0.57	0/12633
36	q	0.57	0/2102	0.59	0/2857
37	r	0.25	0/1064	0.42	0/1428
38	s	0.44	0/1751	0.54	0/2366
39	t	0.52	0/667	0.57	0/901
40	u	0.37	0/1382	0.50	0/1874
41	v	0.53	0/1207	0.58	0/1628
42	w	0.40	0/948	0.53	0/1284
43	x	0.56	0/542	0.58	0/730
44	y	0.51	0/939	0.56	0/1271
45	z	0.49	0/377	0.64	0/500
All	All	0.43	0/110937	0.58	17/150525 (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
6	5	0	1
24	R	0	1
All	All	0	2

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	-14	DG	O4'-C1'-N9	9.00	114.30	108.00
1	0	55	LYS	CB-CA-C	-7.70	94.99	110.40
30	Y	-2	DG	O4'-C4'-C3'	-7.00	101.70	104.50
29	X	-14	DG	C1'-O4'-C4'	-6.96	103.14	110.10
1	0	8	ARG	N-CA-CB	-6.40	99.08	110.60
5	4	439	ARG	CB-CA-C	6.16	122.73	110.40
29	X	-14	DG	C3'-C2'-C1'	-5.96	95.34	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Y	13	DA	O4'-C1'-N9	5.89	112.12	108.00
13	D	1002	ARG	CB-CA-C	5.83	122.05	110.40
24	R	75	LEU	CA-CB-CG	5.76	128.56	115.30
30	Y	14	DC	O4'-C1'-C2'	-5.69	101.35	105.90
29	X	-13	DT	N3-C4-O4	5.64	123.29	119.90
29	X	-13	DT	C5-C4-O4	-5.47	121.07	124.90
30	Y	14	DC	O4'-C1'-N1	5.34	111.74	108.00
34	o	503	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	0	8	ARG	CB-CG-CD	-5.17	98.15	111.60
30	Y	-3	DT	O4'-C4'-C3'	-5.14	102.44	104.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	5	36	GLN	Mainchain
24	R	106	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	169/309 (55%)	157 (93%)	12 (7%)	0	100	100
2	1	253/548 (46%)	243 (96%)	10 (4%)	0	100	100
3	2	325/395 (82%)	312 (96%)	13 (4%)	0	100	100
4	3	259/308 (84%)	253 (98%)	6 (2%)	0	100	100
5	4	384/462 (83%)	365 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	5	52/71 (73%)	48 (92%)	2 (4%)	2 (4%)	3 24
7	6	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	47 81
8	7	710/760 (93%)	684 (96%)	26 (4%)	0	100 100
9	N	4/8 (50%)	3 (75%)	1 (25%)	0	100 100
11	A	543/1872 (29%)	519 (96%)	23 (4%)	1 (0%)	47 81
12	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100 100
13	D	158/1085 (15%)	153 (97%)	5 (3%)	0	100 100
13	d	154/1085 (14%)	150 (97%)	4 (3%)	0	100 100
14	E	541/800 (68%)	518 (96%)	22 (4%)	1 (0%)	47 81
14	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	47 81
15	F	408/677 (60%)	392 (96%)	15 (4%)	1 (0%)	47 81
15	f	399/677 (59%)	380 (95%)	19 (5%)	0	100 100
16	G	138/349 (40%)	135 (98%)	3 (2%)	0	100 100
17	H	207/310 (67%)	189 (91%)	13 (6%)	5 (2%)	6 33
18	I	118/264 (45%)	115 (98%)	3 (2%)	0	100 100
18	i	119/264 (45%)	115 (97%)	4 (3%)	0	100 100
19	J	86/218 (39%)	82 (95%)	4 (5%)	0	100 100
19	j	91/218 (42%)	85 (93%)	4 (4%)	2 (2%)	6 35
20	L	74/161 (46%)	72 (97%)	2 (3%)	0	100 100
20	l	105/161 (65%)	100 (95%)	5 (5%)	0	100 100
21	O	97/109 (89%)	95 (98%)	2 (2%)	0	100 100
22	P	177/339 (52%)	175 (99%)	2 (1%)	0	100 100
23	Q	109/376 (29%)	102 (94%)	7 (6%)	0	100 100
24	R	278/316 (88%)	261 (94%)	15 (5%)	2 (1%)	22 63
25	S	174/517 (34%)	161 (92%)	12 (7%)	1 (1%)	25 66
26	T	218/249 (88%)	210 (96%)	8 (4%)	0	100 100
27	U	180/439 (41%)	153 (85%)	26 (14%)	1 (1%)	25 66
28	V	163/291 (56%)	139 (85%)	24 (15%)	0	100 100
31	c	125/929 (14%)	116 (93%)	9 (7%)	0	100 100
32	k	96/211 (46%)	91 (95%)	5 (5%)	0	100 100
33	m	85/124 (68%)	82 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
34	o	1448/1970 (74%)	1395 (96%)	49 (3%)	4 (0%)	41 76
35	p	1145/1174 (98%)	1112 (97%)	33 (3%)	0	100 100
36	q	253/275 (92%)	246 (97%)	7 (3%)	0	100 100
37	r	126/142 (89%)	126 (100%)	0	0	100 100
38	s	207/210 (99%)	203 (98%)	4 (2%)	0	100 100
39	t	80/127 (63%)	79 (99%)	1 (1%)	0	100 100
40	u	169/172 (98%)	166 (98%)	3 (2%)	0	100 100
41	v	146/150 (97%)	142 (97%)	4 (3%)	0	100 100
42	w	112/125 (90%)	108 (96%)	4 (4%)	0	100 100
43	x	65/67 (97%)	63 (97%)	2 (3%)	0	100 100
44	y	113/117 (97%)	111 (98%)	2 (2%)	0	100 100
45	z	42/58 (72%)	40 (95%)	2 (5%)	0	100 100
All	All	12996/22270 (58%)	12412 (96%)	562 (4%)	22 (0%)	50 81

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	5	48	GLU
14	E	523	VAL
17	H	156	PRO
25	S	87	VAL
34	o	1103	THR
34	o	1274	GLU
14	e	522	ASP
19	j	124	GLU
11	A	502	LEU
15	F	411	VAL
17	H	154	PRO
24	R	90	ALA
19	j	177	LYS
6	5	39	ASP
17	H	136	ALA
17	H	139	ASN
24	R	99	SER
7	6	416	THR
34	o	1433	GLU
17	H	158	THR
27	U	137	THR

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Mol	Chain	Res	Type
34	o	184	CYS

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	164/283 (58%)	157 (96%)	7 (4%)	29 53
2	1	241/484 (50%)	241 (100%)	0	100 100
3	2	295/352 (84%)	293 (99%)	2 (1%)	84 90
4	3	234/272 (86%)	232 (99%)	2 (1%)	78 87
5	4	346/399 (87%)	339 (98%)	7 (2%)	55 74
6	5	48/64 (75%)	47 (98%)	1 (2%)	53 72
7	6	536/688 (78%)	533 (99%)	3 (1%)	86 92
8	7	624/664 (94%)	623 (100%)	1 (0%)	93 96
9	N	2/2 (100%)	2 (100%)	0	100 100
11	A	496/1665 (30%)	456 (92%)	40 (8%)	11 35
12	B	876/1083 (81%)	859 (98%)	17 (2%)	57 75
13	D	147/815 (18%)	137 (93%)	10 (7%)	16 41
13	d	146/815 (18%)	145 (99%)	1 (1%)	84 90
14	E	480/657 (73%)	466 (97%)	14 (3%)	42 64
14	e	475/657 (72%)	463 (98%)	12 (2%)	47 68
15	F	328/574 (57%)	310 (94%)	18 (6%)	21 47
15	f	322/574 (56%)	314 (98%)	8 (2%)	47 68
16	G	132/322 (41%)	124 (94%)	8 (6%)	18 44
17	H	181/270 (67%)	174 (96%)	7 (4%)	32 56
18	I	106/235 (45%)	106 (100%)	0	100 100
18	i	107/235 (46%)	107 (100%)	0	100 100
19	J	79/154 (51%)	72 (91%)	7 (9%)	9 30
19	j	83/154 (54%)	82 (99%)	1 (1%)	71 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	L	71/141 (50%)	66 (93%)	5 (7%)	15 40
20	l	98/141 (70%)	97 (99%)	1 (1%)	76 86
21	O	90/98 (92%)	88 (98%)	2 (2%)	52 71
22	P	154/293 (53%)	154 (100%)	0	100 100
23	Q	105/324 (32%)	105 (100%)	0	100 100
24	R	238/268 (89%)	236 (99%)	2 (1%)	81 89
25	S	154/448 (34%)	134 (87%)	20 (13%)	4 18
26	T	196/218 (90%)	192 (98%)	4 (2%)	55 74
27	U	167/373 (45%)	166 (99%)	1 (1%)	86 92
28	V	150/261 (58%)	150 (100%)	0	100 100
31	c	113/833 (14%)	111 (98%)	2 (2%)	59 77
32	k	87/182 (48%)	87 (100%)	0	100 100
33	m	80/106 (76%)	73 (91%)	7 (9%)	10 31
34	o	1280/1748 (73%)	1268 (99%)	12 (1%)	78 87
35	p	1004/1027 (98%)	991 (99%)	13 (1%)	69 82
36	q	234/252 (93%)	227 (97%)	7 (3%)	41 63
37	r	118/126 (94%)	118 (100%)	0	100 100
38	s	191/192 (100%)	189 (99%)	2 (1%)	76 86
39	t	71/111 (64%)	70 (99%)	1 (1%)	67 80
40	u	152/153 (99%)	152 (100%)	0	100 100
41	v	129/131 (98%)	128 (99%)	1 (1%)	81 89
42	w	103/112 (92%)	99 (96%)	4 (4%)	32 56
43	x	56/56 (100%)	54 (96%)	2 (4%)	35 59
44	y	104/106 (98%)	103 (99%)	1 (1%)	76 86
45	z	41/55 (74%)	39 (95%)	2 (5%)	25 50
All	All	11634/19173 (61%)	11379 (98%)	255 (2%)	54 71

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	8	ARG
1	0	10	LYS
1	0	11	THR

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Mol	Chain	Res	Type
1	0	28	HIS
1	0	41	ARG
1	0	127	LYS
1	0	128	GLU
3	2	69	ARG
3	2	343	ARG
4	3	257	CYS
4	3	258	HIS
5	4	33	ARG
5	4	400	ARG
5	4	401	LEU
5	4	404	THR
5	4	407	VAL
5	4	413	LEU
5	4	456	LYS
6	5	38	ILE
7	6	198	ARG
7	6	266	GLN
7	6	692	LYS
8	7	114	ASN
11	A	337	ARG
11	A	338	VAL
11	A	353	LEU
11	A	395	ASP
11	A	397	LEU
11	A	400	GLU
11	A	404	MET
11	A	408	LEU
11	A	415	ILE
11	A	416	TRP
11	A	417	ASP
11	A	419	GLU
11	A	468	PHE
11	A	470	ILE
11	A	475	LEU
11	A	481	GLU
11	A	491	MET
11	A	499	VAL
11	A	500	LEU
11	A	501	THR
11	A	502	LEU
11	A	505	ASN

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Mol	Chain	Res	Type
11	A	511	LEU
11	A	639	LEU
11	A	661	GLU
11	A	667	THR
11	A	711	ASP
11	A	727	THR
11	A	730	PHE
11	A	821	ARG
11	A	828	GLU
11	A	943	LYS
11	A	970	ASN
11	A	1052	ARG
11	A	1058	HIS
11	A	1059	GLN
11	A	1062	TYR
11	A	1073	GLN
11	A	1165	LEU
11	A	1203	GLU
12	B	21	GLU
12	B	24	ARG
12	B	71	ARG
12	B	140	GLU
12	B	184	ASN
12	B	225	TYR
12	B	262	MET
12	B	266	THR
12	B	293	GLU
12	B	431	LEU
12	B	488	PHE
12	B	559	LYS
12	B	603	LYS
12	B	638	ARG
12	B	640	VAL
12	B	771	VAL
12	B	818	THR
13	D	948	GLU
13	D	952	GLN
13	D	957	ARG
13	D	958	LYS
13	D	960	GLU
13	D	964	GLU
13	D	965	ILE

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Mol	Chain	Res	Type
13	D	966	LEU
13	D	1006	LEU
13	D	1009	LEU
14	E	258	ASN
14	E	268	HIS
14	E	270	ASP
14	E	274	TYR
14	E	278	ASP
14	E	280	ARG
14	E	326	ASN
14	E	327	ASN
14	E	519	GLU
14	E	522	ASP
14	E	593	PHE
14	E	761	LEU
14	E	774	MET
14	E	775	THR
15	F	86	PHE
15	F	91	PHE
15	F	94	PHE
15	F	219	GLU
15	F	258	ARG
15	F	261	THR
15	F	271	VAL
15	F	280	ILE
15	F	301	VAL
15	F	317	LEU
15	F	326	HIS
15	F	332	PHE
15	F	340	ILE
15	F	348	THR
15	F	354	ARG
15	F	368	THR
15	F	397	GLN
15	F	427	LEU
16	G	41	ASP
16	G	81	ASP
16	G	143	VAL
16	G	147	ARG
16	G	153	LYS
16	G	181	TRP
16	G	182	GLU

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Mol	Chain	Res	Type
16	G	183	ILE
17	H	27	ASP
17	H	33	ARG
17	H	36	THR
17	H	135	THR
17	H	157	HIS
17	H	161	LYS
17	H	162	THR
19	J	116	LEU
19	J	123	LEU
19	J	156	SER
19	J	164	SER
19	J	174	CYS
19	J	177	LYS
19	J	192	LYS
20	L	79	ASP
20	L	104	ARG
20	L	108	SER
20	L	113	VAL
20	L	114	LYS
21	O	51	ARG
21	O	82	ARG
24	R	18	HIS
24	R	104	ARG
25	S	44	GLN
25	S	59	GLU
25	S	60	GLU
25	S	61	GLU
25	S	70	GLU
25	S	72	ASN
25	S	75	LEU
25	S	76	ARG
25	S	82	LYS
25	S	83	LYS
25	S	86	ILE
25	S	88	LEU
25	S	90	GLU
25	S	151	ARG
25	S	155	LEU
25	S	156	THR
25	S	163	GLU
25	S	164	TRP

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Mol	Chain	Res	Type
25	S	167	ARG
25	S	171	LEU
26	T	145	LEU
26	T	170	LYS
26	T	171	GLU
26	T	230	LYS
27	U	145	PHE
31	c	24	ASP
31	c	106	VAL
33	m	31	LEU
33	m	55	ASP
33	m	58	GLU
33	m	77	ARG
33	m	84	GLU
33	m	90	ILE
33	m	91	ARG
34	o	184	CYS
34	o	211	GLU
34	o	214	ILE
34	o	323	PRO
34	o	452	ASP
34	o	458	PHE
34	o	499	ASP
34	o	621	ILE
34	o	1103	THR
34	o	1109	TYR
34	o	1336	LEU
34	o	1385	VAL
35	p	90	GLN
35	p	192	LYS
35	p	214	LYS
35	p	215	TYR
35	p	388	TYR
35	p	438	ARG
35	p	453	TRP
35	p	466	VAL
35	p	719	SER
35	p	750	VAL
35	p	888	THR
35	p	952	GLU
35	p	1048	TYR
36	q	51	GLN

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Mol	Chain	Res	Type
36	q	58	VAL
36	q	63	PHE
36	q	90	CYS
36	q	93	PHE
36	q	94	CYS
36	q	100	GLU
38	s	71	GLN
38	s	73	PHE
39	t	121	ASP
41	v	141	VAL
42	w	42	CYS
42	w	80	ARG
42	w	81	THR
42	w	115	THR
43	x	7	CYS
43	x	14	VAL
44	y	27	VAL
45	z	19	CYS
45	z	41	TYR
13	d	951	ASP
14	e	243	LEU
14	e	258	ASN
14	e	268	HIS
14	e	270	ASP
14	e	277	ASP
14	e	282	LEU
14	e	365	ARG
14	e	436	ASP
14	e	438	LEU
14	e	512	ASP
14	e	516	ILE
14	e	663	ARG
15	f	253	TYR
15	f	261	THR
15	f	272	VAL
15	f	322	ASP
15	f	323	VAL
15	f	326	HIS
15	f	356	THR
15	f	421	ASP
19	j	114	THR
20	l	114	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	24	ASN
1	0	136	ASN
4	3	240	GLN
5	4	352	GLN
5	4	411	GLN
5	4	458	GLN
5	4	460	HIS
7	6	415	HIS
11	A	401	ASN
11	A	472	ASN
11	A	489	GLN
11	A	590	GLN
11	A	860	ASN
11	A	896	GLN
12	B	30	HIS
12	B	137	HIS
12	B	176	HIS
12	B	183	GLN
12	B	184	ASN
12	B	235	HIS
12	B	348	GLN
12	B	432	HIS
12	B	439	HIS
12	B	450	GLN
12	B	509	ASN
12	B	750	GLN
12	B	813	ASN
12	B	882	HIS
12	B	908	GLN
12	B	916	ASN
13	D	875	GLN
13	D	936	GLN
13	D	956	GLN
13	D	998	GLN
13	D	1053	GLN
14	E	254	ASN
14	E	256	HIS
14	E	258	ASN
14	E	268	HIS
14	E	327	ASN
14	E	351	GLN

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Mol	Chain	Res	Type
14	E	616	HIS
14	E	640	ASN
14	E	758	HIS
14	E	800	GLN
15	F	59	HIS
15	F	79	ASN
15	F	89	GLN
15	F	119	ASN
15	F	221	GLN
15	F	270	ASN
15	F	273	GLN
15	F	275	ASN
16	G	48	HIS
17	H	145	HIS
18	I	21	GLN
18	I	38	GLN
18	I	98	GLN
19	J	210	ASN
20	L	117	GLN
24	R	98	ASN
25	S	44	GLN
25	S	72	ASN
25	S	96	GLN
25	S	152	HIS
25	S	178	GLN
26	T	182	HIS
27	U	142	ASN
27	U	183	GLN
28	V	83	ASN
28	V	90	GLN
28	V	117	GLN
28	V	157	GLN
28	V	160	GLN
33	m	70	HIS
33	m	107	ASN
34	o	181	HIS
34	o	412	GLN
34	o	439	HIS
34	o	449	HIS
34	o	493	ASN
34	o	531	ASN
34	o	671	ASN

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Mol	Chain	Res	Type
34	o	703	GLN
34	o	721	HIS
34	o	780	ASN
34	o	783	GLN
34	o	791	GLN
34	o	1105	ASN
34	o	1263	ASN
35	p	72	GLN
35	p	145	GLN
35	p	188	ASN
35	p	245	GLN
35	p	461	GLN
35	p	639	HIS
35	p	699	HIS
35	p	755	GLN
35	p	1021	HIS
35	p	1097	HIS
36	q	217	GLN
36	q	260	GLN
36	q	265	HIS
37	r	129	GLN
38	s	64	HIS
38	s	71	GLN
42	w	41	ASN
42	w	50	ASN
45	z	26	ASN
13	d	912	ASN
13	d	943	GLN
13	d	1069	ASN
14	e	246	HIS
14	e	294	ASN
14	e	336	HIS
14	e	616	HIS
15	f	325	ASN
18	i	81	GLN
19	j	160	GLN
19	j	173	HIS
20	l	73	ASN
20	l	105	HIS
20	l	119	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	Z	2/5 (40%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	Z	3	C

There are no RNA pucker outliers to report.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
10	G2L	Z	5	10,30	19,26,30	1.00	1 (5%)	18,38,44	1.33	3 (16%)
9	HYP	N	8	9	6,8,9	0.74	0	5,10,12	2.17	2 (40%)
9	TRX	N	2	9	14,16,17	0.98	0	15,22,24	2.00	4 (26%)
9	CSX	N	6	9	3,6,7	1.04	0	1,6,8	2.23	1 (100%)
9	ILX	N	1	9	8,9,10	0.60	0	9,11,13	1.32	2 (22%)

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
10	G2L	Z	5	10,30	-	2/5/27/31	0/3/3/3
9	HYP	N	8	9	-	0/0/11/13	0/1/1/1
9	TRX	N	2	9	-	0/4/6/8	0/2/2/2
9	CSX	N	6	9	-	1/1/5/7	-
9	ILX	N	1	9	-	7/11/12/14	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	5	G2L	C6-N1	-2.32	1.34	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	2	TRX	CG-CB-CA	5.78	123.47	114.53
9	N	8	HYP	O-C-CA	-3.27	116.21	124.78
9	N	8	HYP	CB-CG-CD	3.06	107.02	103.27
9	N	2	TRX	CB-CG-CD1	-2.94	124.33	127.97
9	N	1	ILX	OD1-CD1-CG1	-2.87	104.83	111.07
10	Z	5	G2L	C3'-C2'-C1'	2.72	105.92	99.89
9	N	2	TRX	CH2-CZ2-CE2	-2.49	116.66	119.29
10	Z	5	G2L	C8-N7-C5	2.38	107.52	102.99
10	Z	5	G2L	C5-C6-N1	2.32	118.04	113.95
9	N	2	TRX	CB-CG-CD2	2.25	129.75	126.25
9	N	6	CSX	CA-CB-SG	2.23	118.22	113.36
9	N	1	ILX	CB-CA-C	-2.06	110.16	112.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	N	1	ILX	C-CA-CB-CG2
9	N	1	ILX	OD1-CD1-CG1-CB
9	N	1	ILX	OD1-CD1-CG1-OG1
9	N	6	CSX	N-CA-CB-SG
10	Z	5	G2L	C3'-C4'-C5'-O5'
10	Z	5	G2L	O4'-C4'-C5'-O5'
9	N	1	ILX	C-CA-CB-CG1
9	N	1	ILX	CG2-CB-CG1-CD1
9	N	1	ILX	O-C-CA-CB
9	N	1	ILX	N-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 18 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	$\#\|Z\| > 2$
49	W0F	p	1201	-	25,35,35	3.21	7 (28%)	31,55,55	2.54	12 (38%)
47	SF4	7	1000	8	0,12,12	-	-	-		

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
49	W0F	p	1201	-	-	3/20/40/40	0/3/3/3
47	SF4	7	1000	8	-	-	0/6/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	p	1201	W0F	C03-C04	-9.45	1.27	1.52
49	p	1201	W0F	O05-C06	-9.22	1.28	1.41
49	p	1201	W0F	O05-C04	6.84	1.60	1.45
49	p	1201	W0F	C07-C03	-2.92	1.46	1.52
49	p	1201	W0F	C20-C04	2.46	1.59	1.51
49	p	1201	W0F	C17-N16	-2.16	1.34	1.39
49	p	1201	W0F	P22-O21	2.10	1.67	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	p	1201	W0F	O05-C06-C07	-6.30	97.72	106.93
49	p	1201	W0F	O05-C04-C03	-5.67	92.73	104.87
49	p	1201	W0F	O05-C04-C20	4.79	125.15	109.37
49	p	1201	W0F	O21-C20-C04	3.94	122.56	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	p	1201	W0F	O32-P30-O29	3.89	117.67	104.64
49	p	1201	W0F	O33-P30-O31	-3.29	97.80	110.68
49	p	1201	W0F	P26-O25-P22	-3.10	122.20	132.83
49	p	1201	W0F	P26-O29-P30	2.73	142.18	132.83
49	p	1201	W0F	O33-P30-O29	2.65	113.51	104.64
49	p	1201	W0F	O08-C07-C06	2.43	119.82	110.85
49	p	1201	W0F	C10-N11-C12	2.38	107.52	102.99
49	p	1201	W0F	O21-P22-O24	-2.36	99.86	109.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

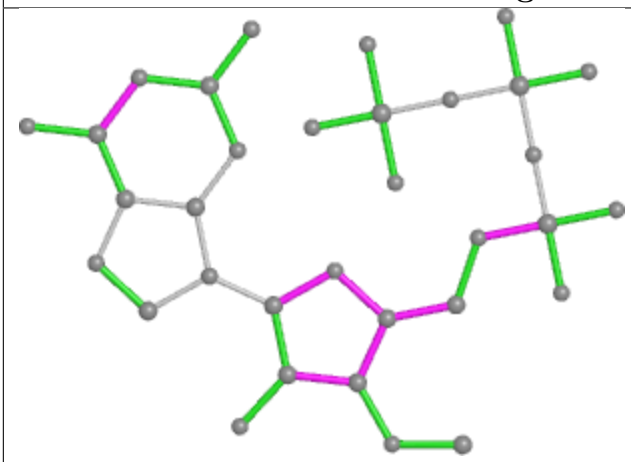
Mol	Chain	Res	Type	Atoms
49	p	1201	W0F	C20-O21-P22-O24
49	p	1201	W0F	C20-O21-P22-O25
49	p	1201	W0F	C03-C04-C20-O21

There are no ring outliers.

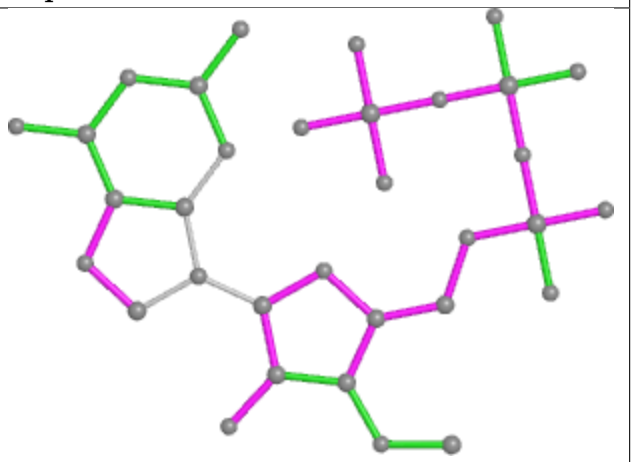
No monomer is involved in short contacts.

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.

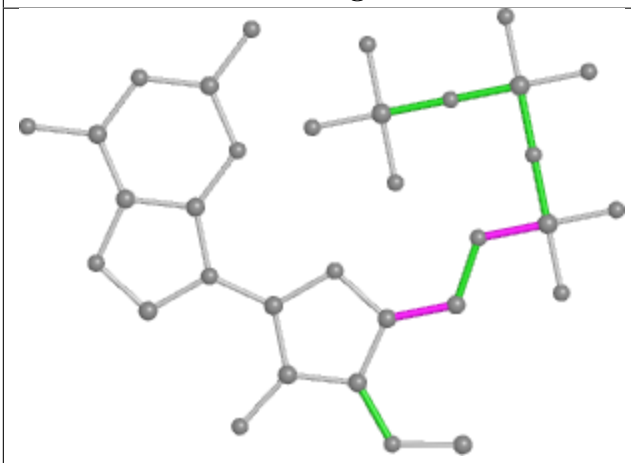
Ligand W0F p 1201



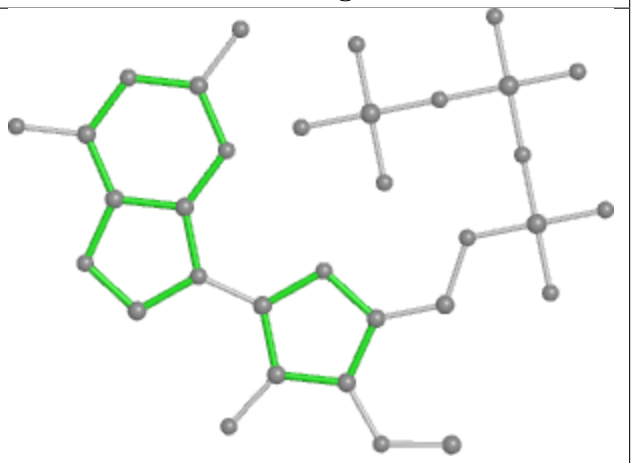
Bond lengths



Bond angles

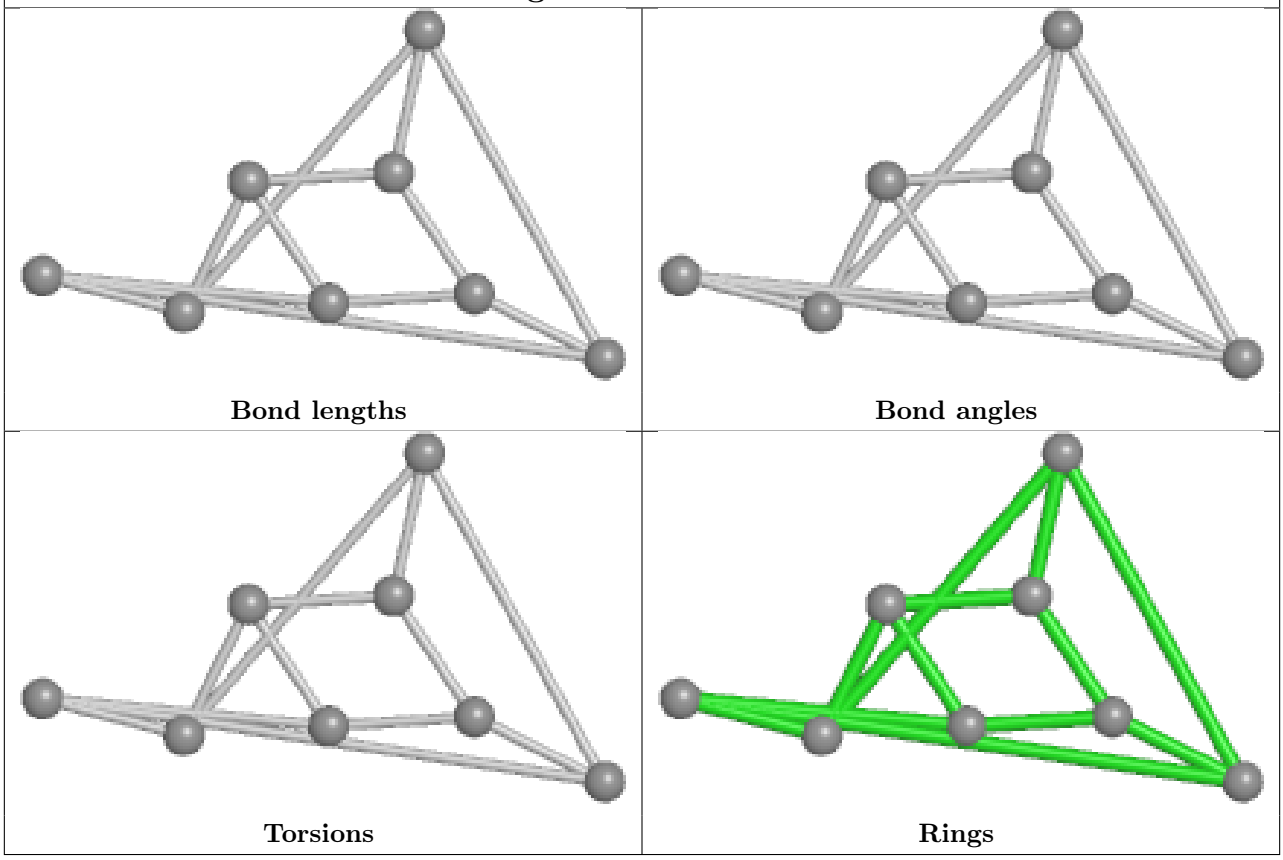


Torsions



Rings

Ligand SF4 7 1000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

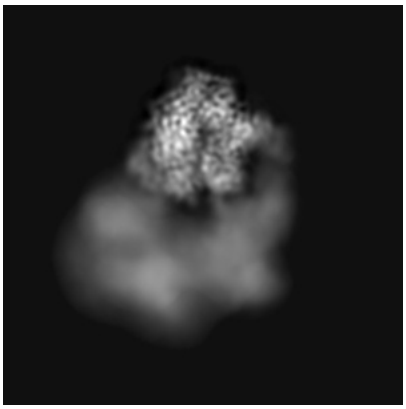
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37399. These allow visual inspection of the internal detail of the map and identification of artifacts.

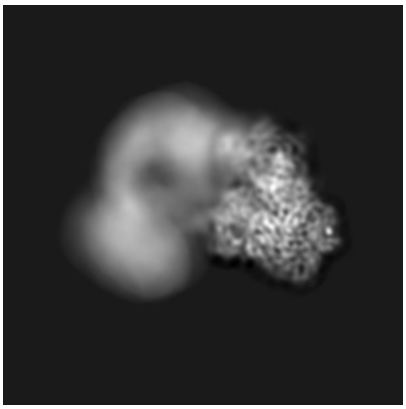
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

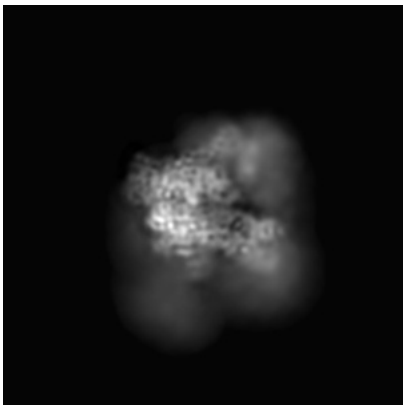
6.1.1 Primary map



X

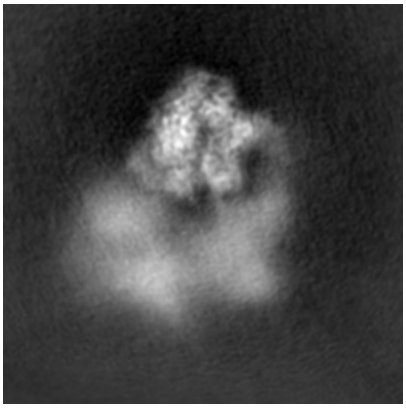


Y

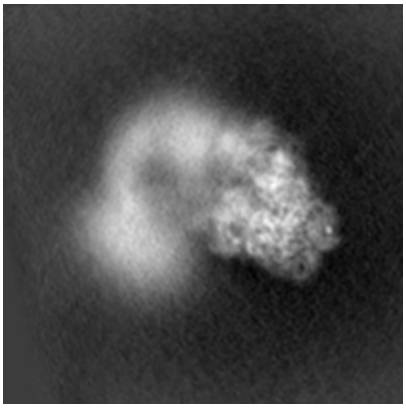


Z

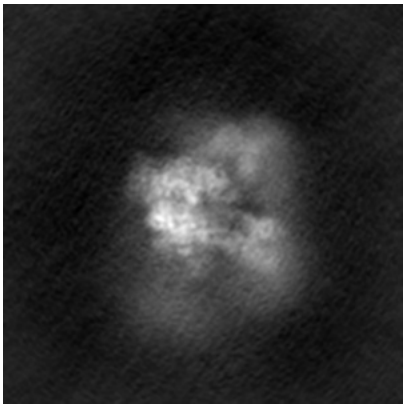
6.1.2 Raw map



X



Y

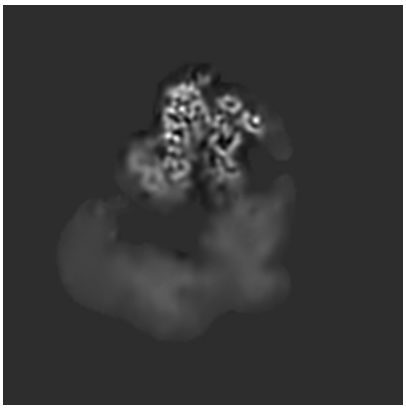


Z

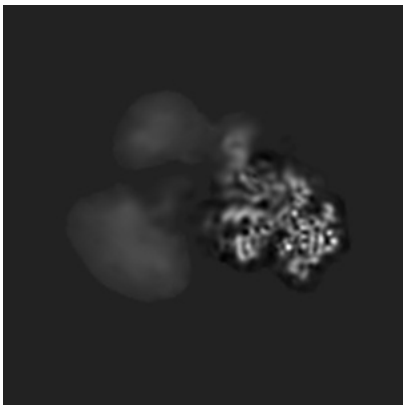
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

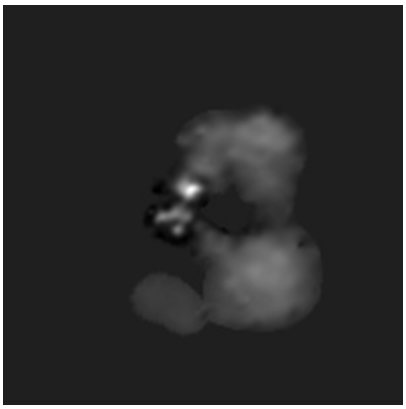
6.2.1 Primary map



X Index: 80

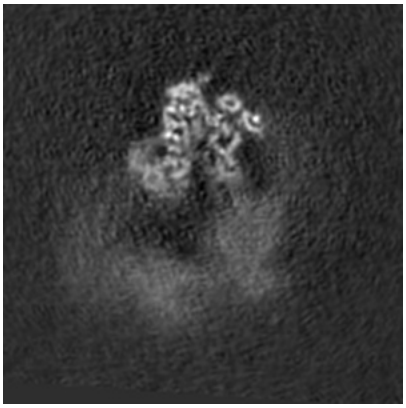


Y Index: 80

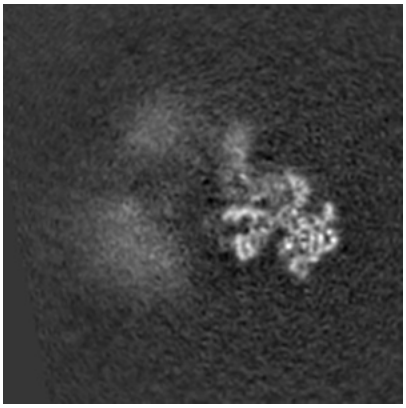


Z Index: 80

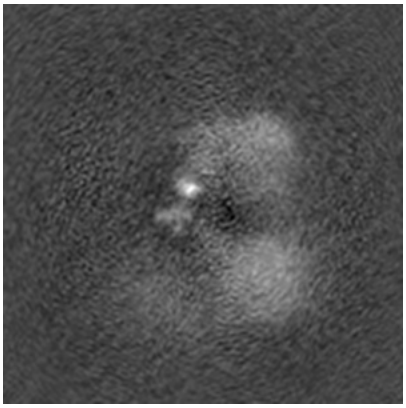
6.2.2 Raw map



X Index: 80



Y Index: 80

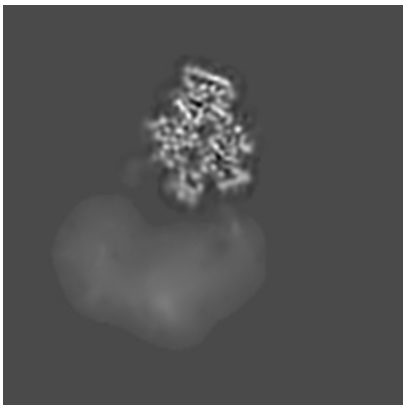


Z Index: 80

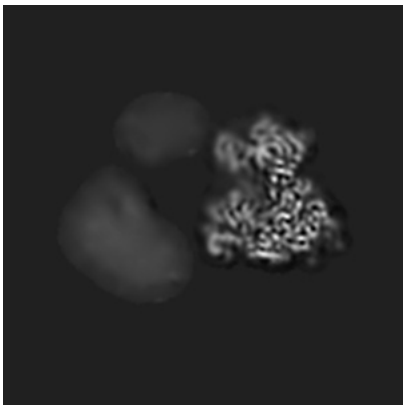
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



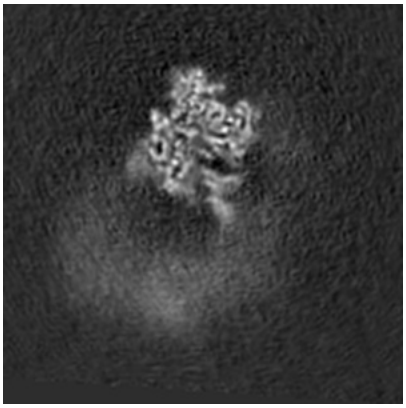
X Index: 66



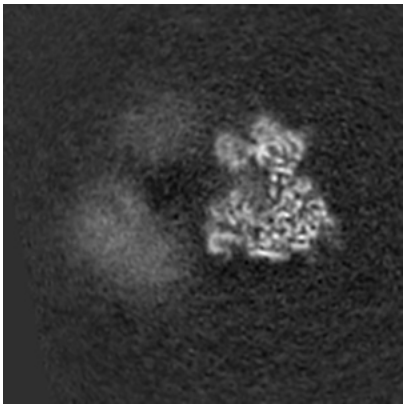
Y Index: 71

Z Index: 111

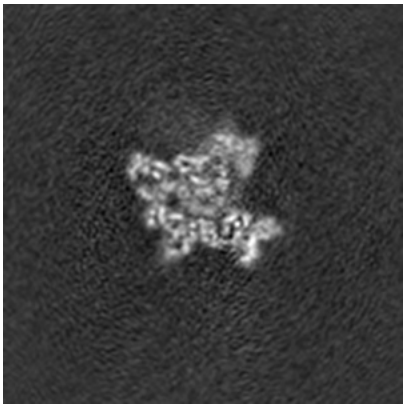
6.3.2 Raw map



X Index: 73



Y Index: 71

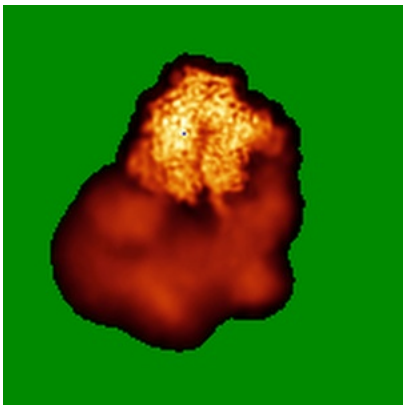


Z Index: 111

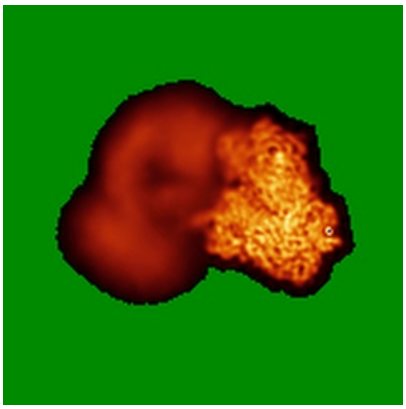
The images above show the largest variance slices of the map in three orthogonal directions.

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

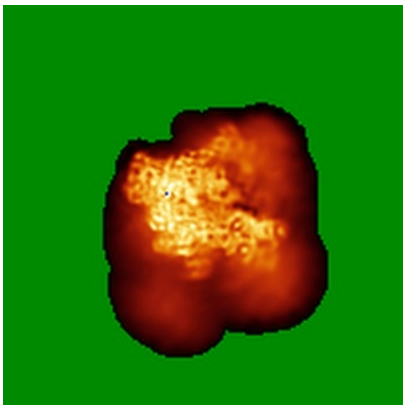
6.4.1 Primary map



X

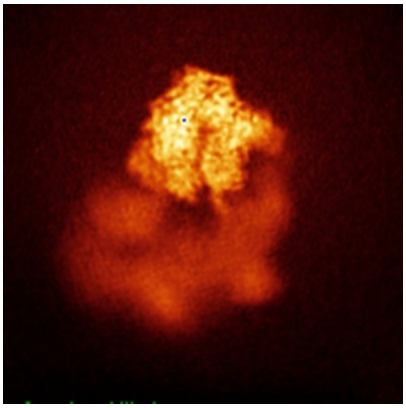


Y

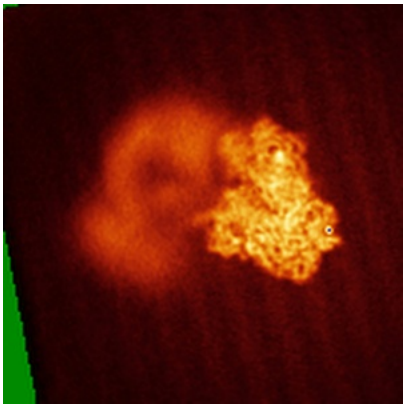


Z

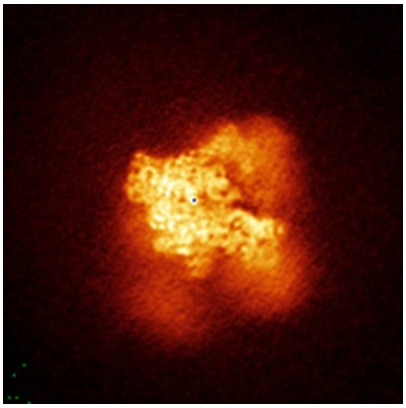
6.4.2 Raw map



X



Y

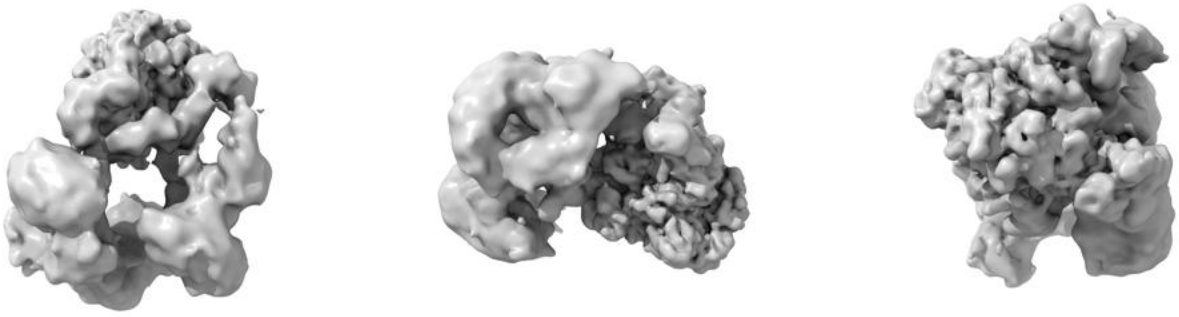


Z

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)

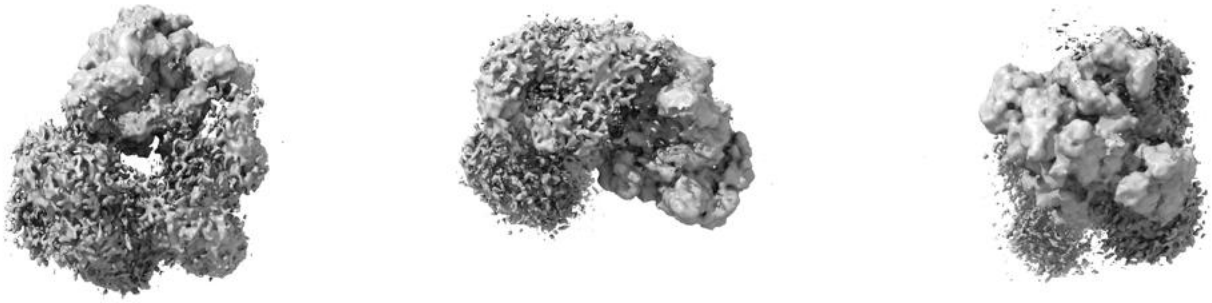
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.54. 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.

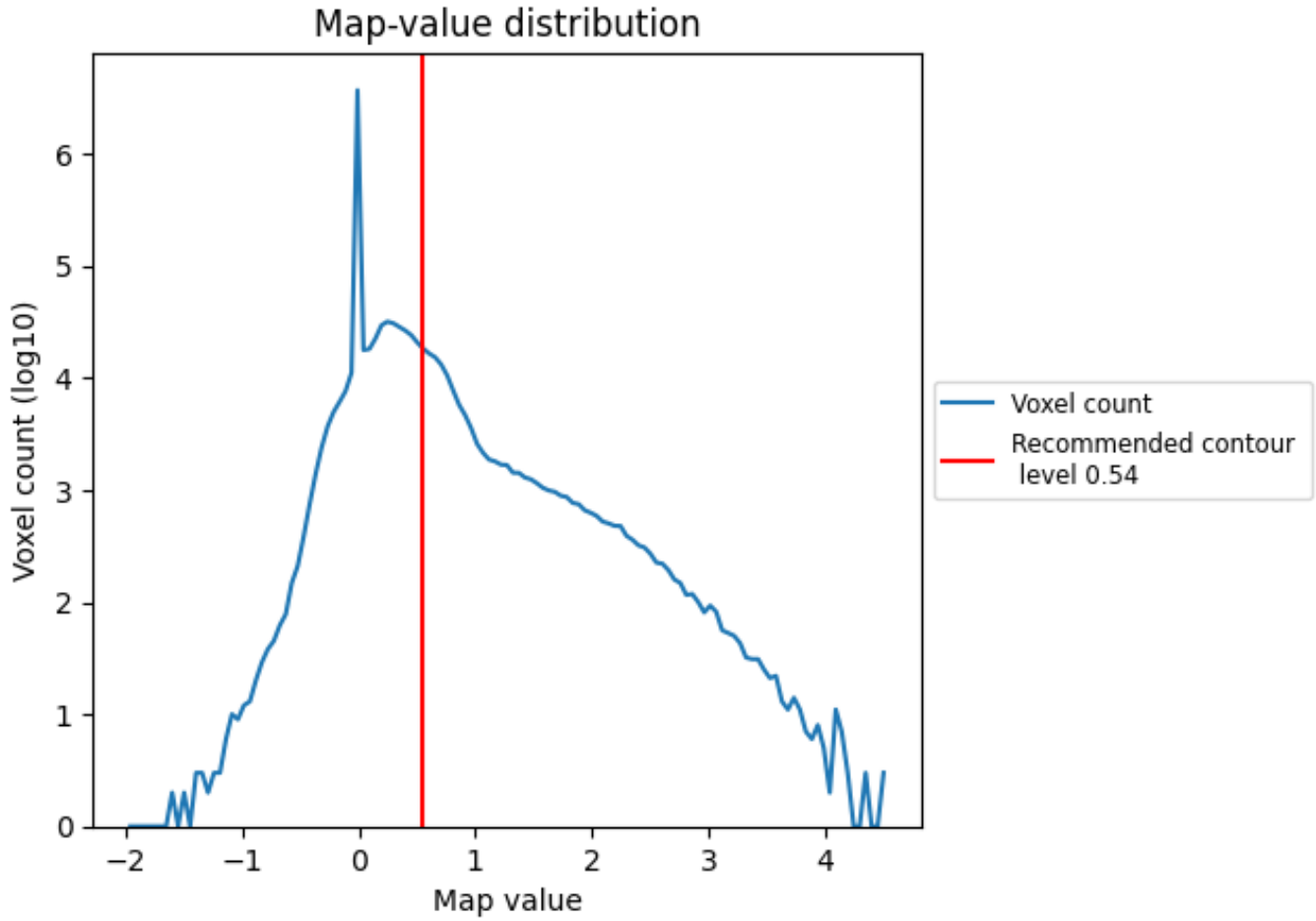
6.6 Mask visualisation (i)

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

7 Map analysis

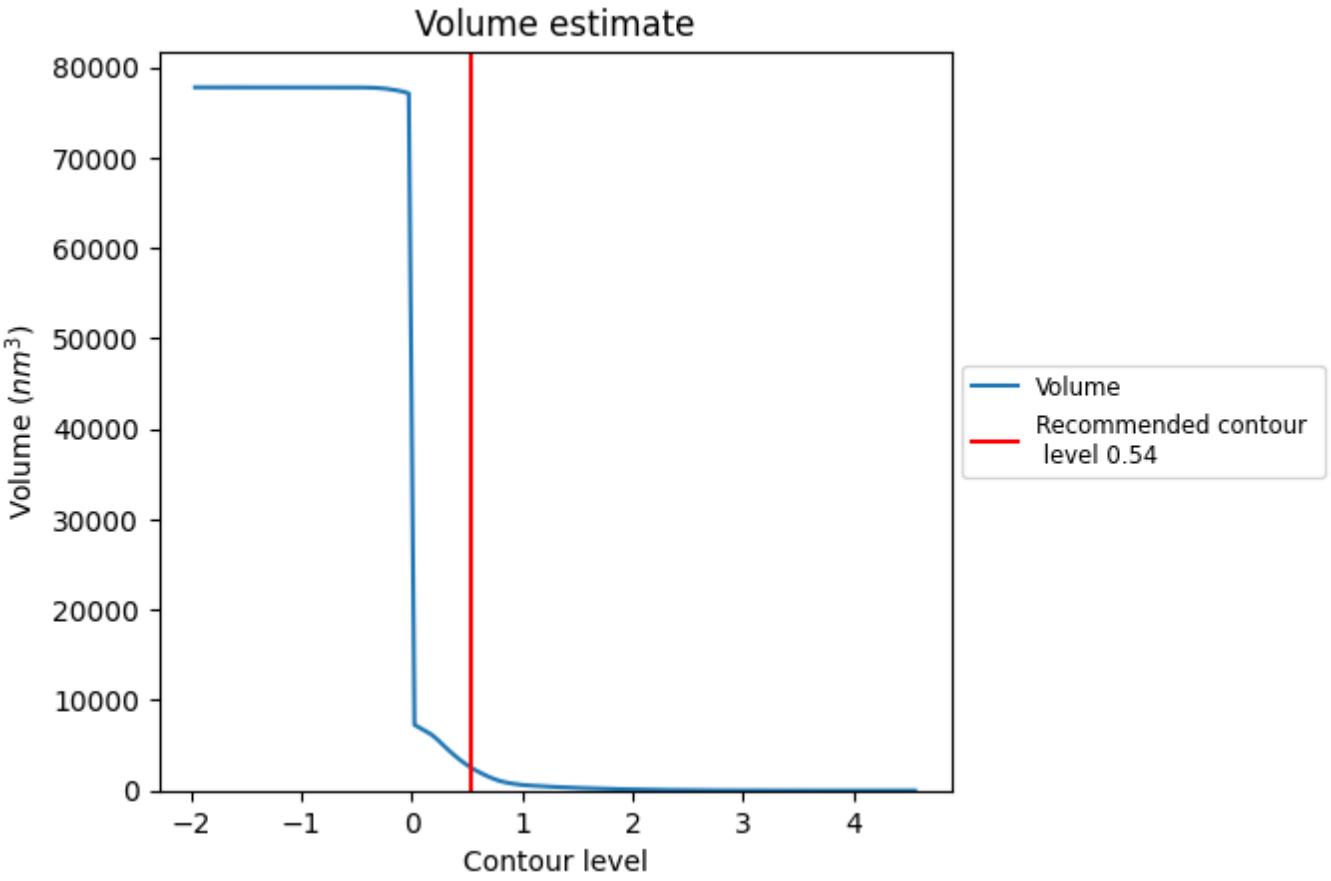
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

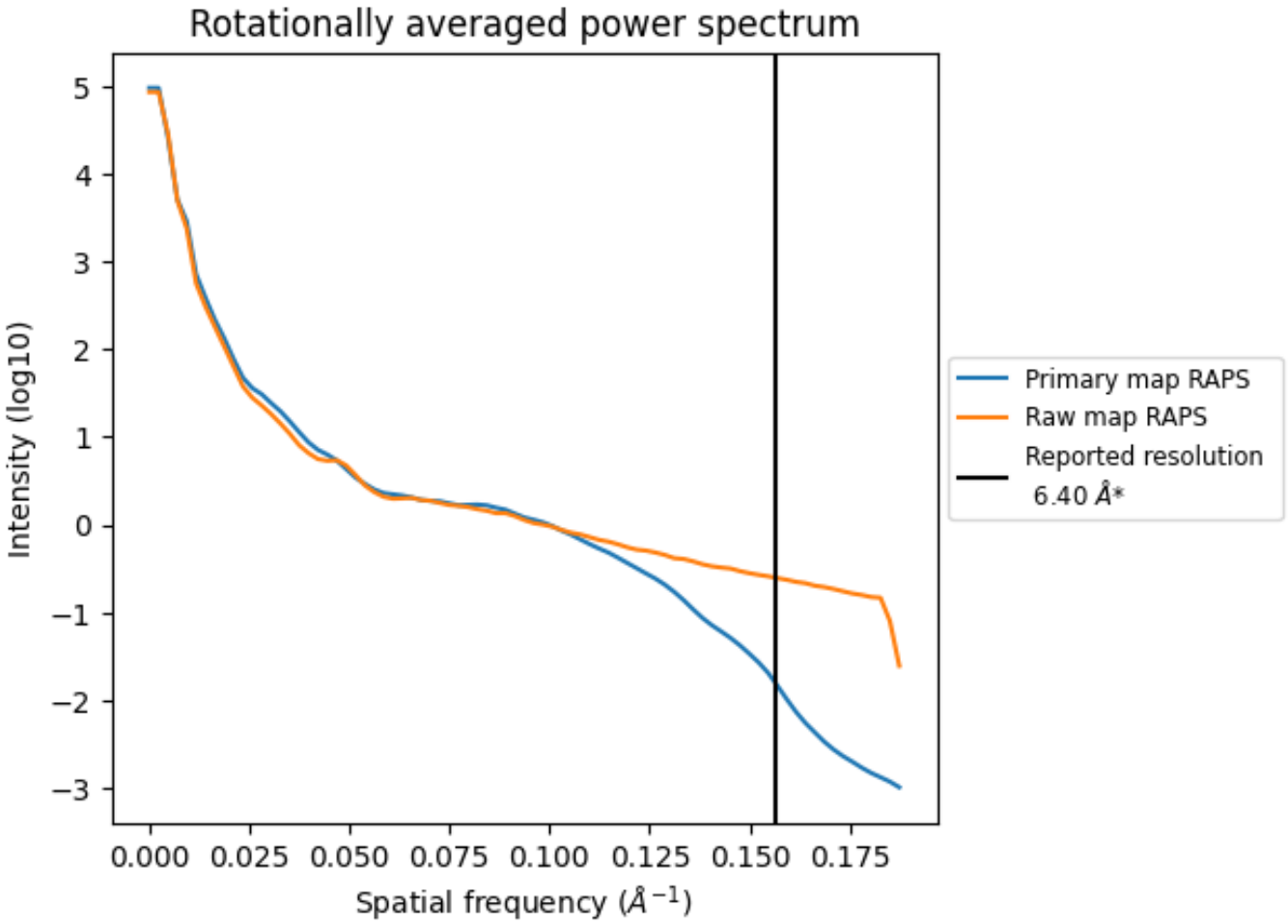
7.2 Volume estimate



The volume at the recommended contour level is 2520 nm^3; this corresponds to an approximate mass of 2276 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)

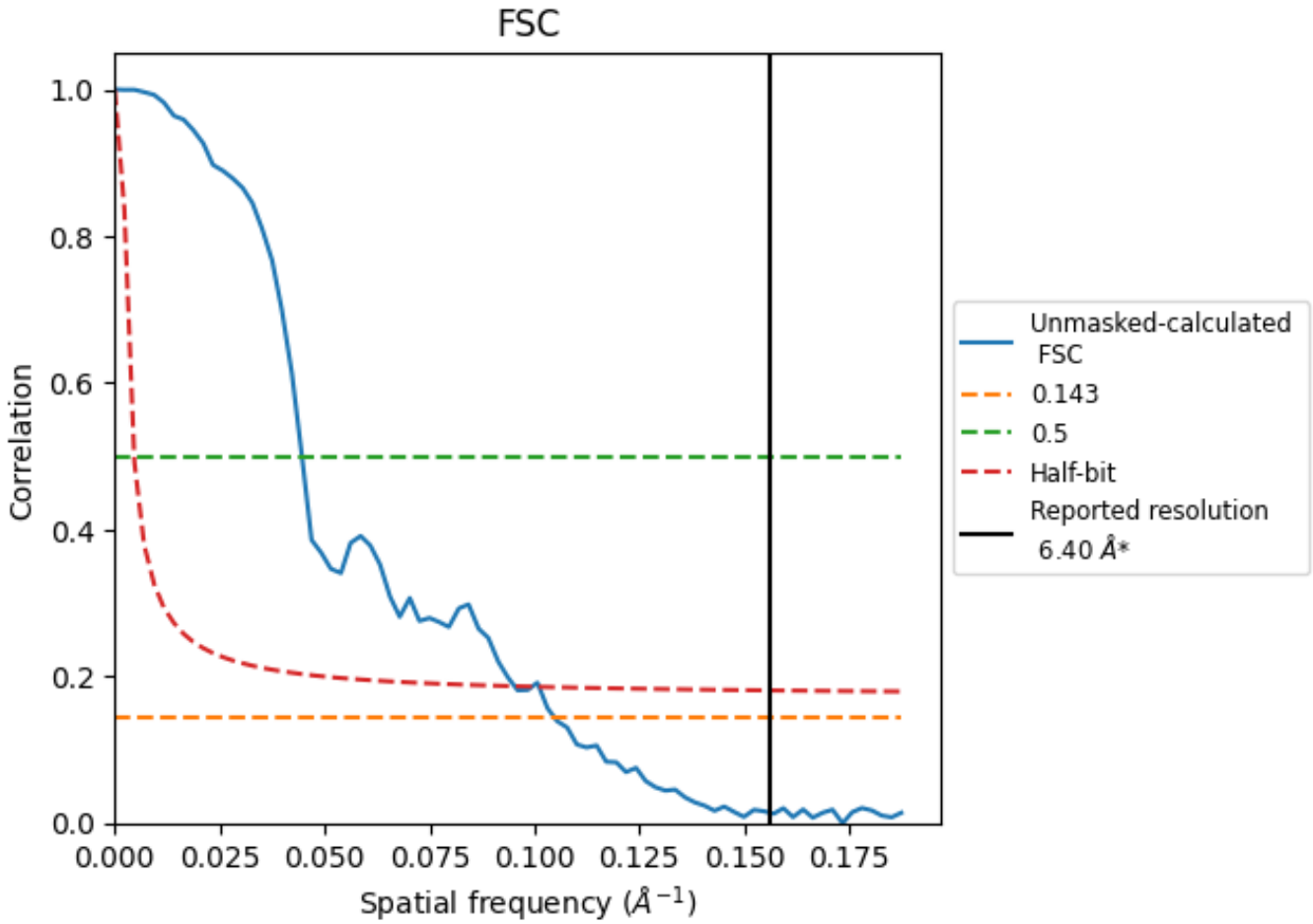


*Reported resolution corresponds to spatial frequency of 0.156 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.156 Å^{-1}

8.2 Resolution estimates (i)

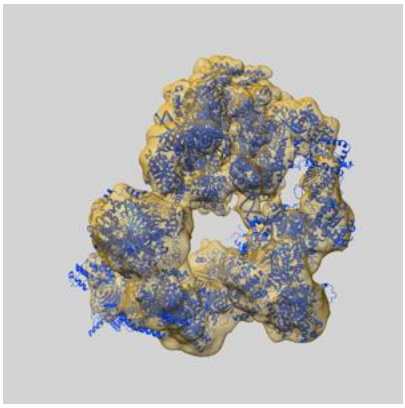
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.54	22.42	10.49

*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 9.54 differs from the reported value 6.4 by more than 10 %

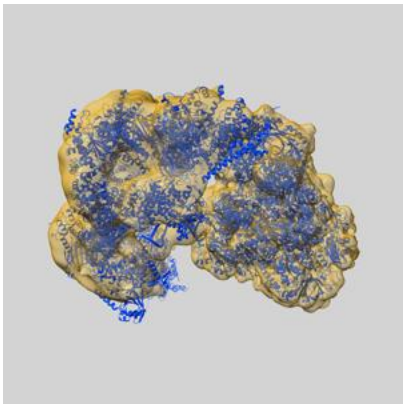
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37399 and PDB model 8WAO. Per-residue inclusion information can be found in section 3 on page 14.

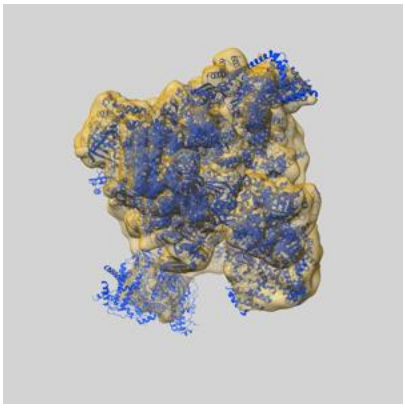
9.1 Map-model overlay



X



Y



Z

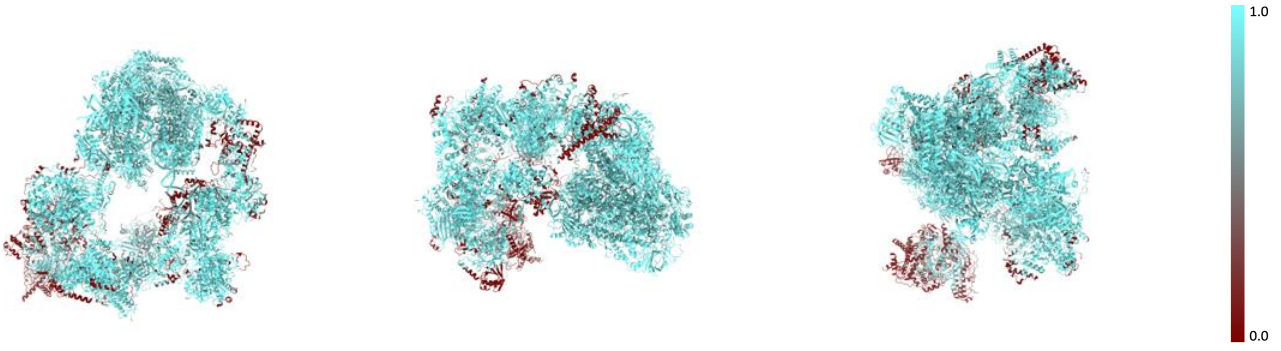
The images above show the 3D surface view of the map at the recommended contour level 0.54 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

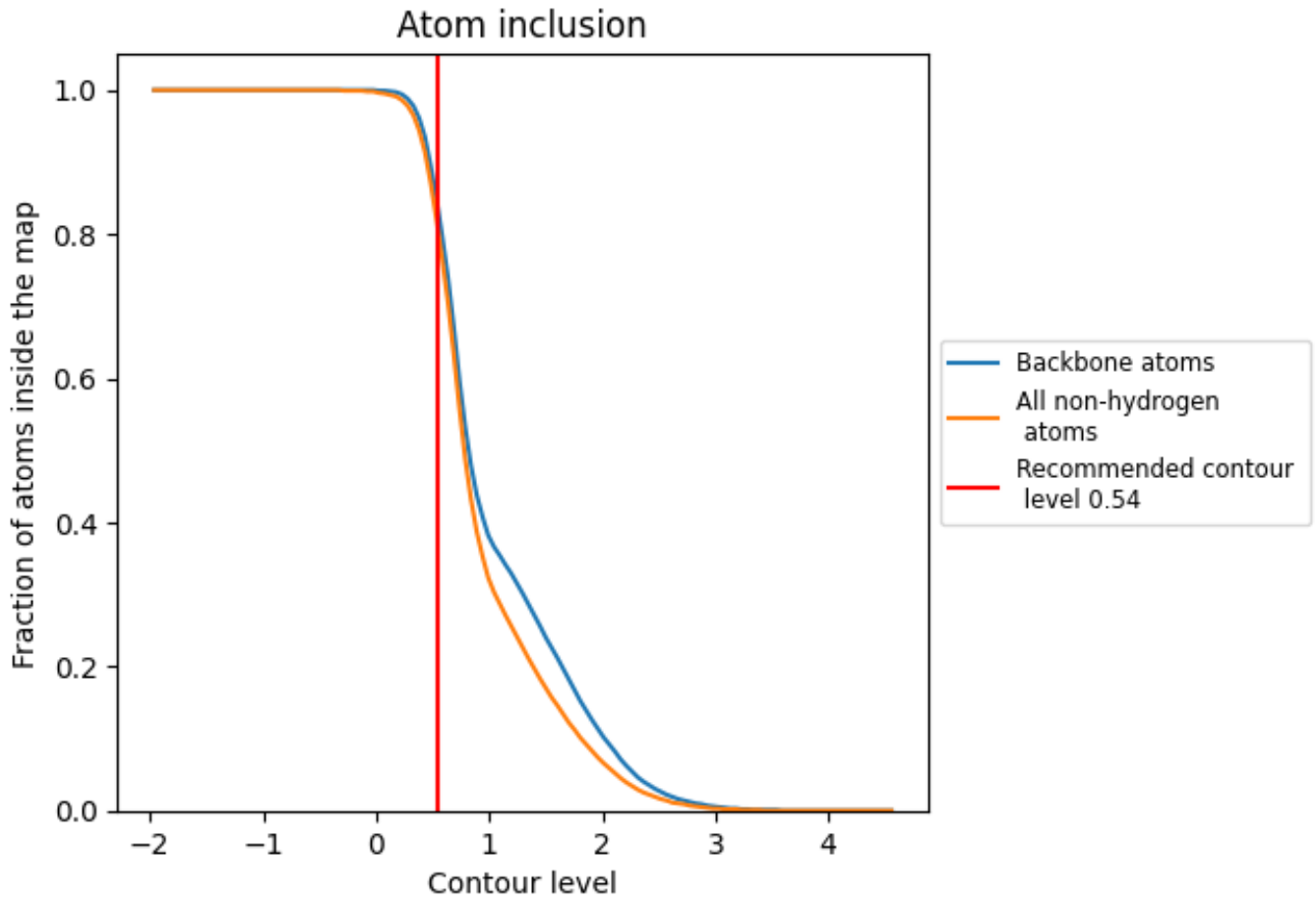
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.54).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.54) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.0750
0	0.1910	0.0660
1	0.6880	0.0450
2	0.9130	0.0510
3	0.9380	0.0460
4	0.9050	0.0580
5	0.8710	0.0720
6	0.6850	0.0460
7	0.8120	0.0550
A	0.7170	0.0320
B	0.9270	0.0420
D	0.8050	0.0540
E	0.8400	0.0450
F	0.8770	0.0510
G	0.3080	0.0190
H	0.8830	0.0370
I	0.9340	0.0400
J	0.9680	0.0460
L	0.7840	0.0330
N	0.9520	0.1450
O	0.9700	0.0830
P	0.9860	0.1160
Q	0.9510	0.0900
R	0.9360	0.1120
S	0.9340	0.1100
T	0.9470	0.1150
U	0.9510	0.0990
V	0.9750	0.1260
X	0.9140	0.1630
Y	0.9380	0.1580
Z	0.9570	0.1830
c	0.5940	0.0350
d	0.2120	0.0230
e	0.4770	0.0220
f	0.6890	0.0380

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.4630	0.0170
j	0.4540	0.0300
k	0.2280	0.0350
l	0.2490	0.0140
m	0.0900	0.0550
o	0.9240	0.1290
p	0.9130	0.1040
q	0.9430	0.1040
r	0.9640	0.1390
s	0.9380	0.1550
t	0.9150	0.1300
u	0.9780	0.1190
v	0.9280	0.1190
w	0.9410	0.1060
x	0.9120	0.0960
y	0.9220	0.1130
z	0.9580	0.1100