



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 12:11 AM JST

PDB ID : 8WAS / pdb_00008was
EMDB ID : EMD-37403
Title : Structure of transcribing complex 9 (TC9), the initially transcribing complex with Pol II positioned 9nt downstream of TSS.
Authors : Chen, X.; Liu, W.; Wang, Q.; Wang, X.; Ren, Y.; Qu, X.; Li, W.; Xu, Y.
Deposited on : 2023-09-08
Resolution : 6.13 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

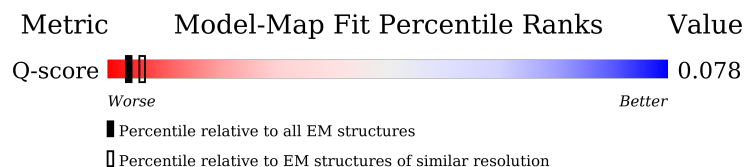
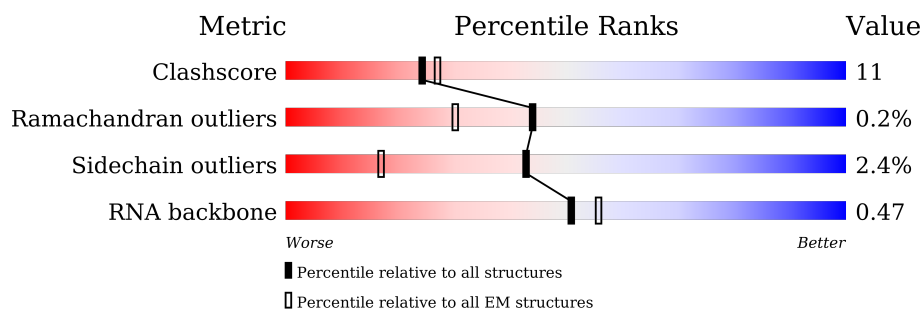
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

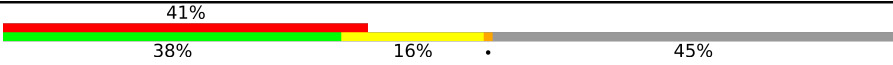
The reported resolution of this entry is 6.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	501 (5.63 - 6.63)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	309	
2	1	548	
3	2	395	

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Mol	Chain	Length	Quality of chain
4	3	308	
5	4	462	
6	5	71	
7	6	782	
8	7	760	
9	N	8	
10	Z	9	
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	

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Mol	Chain	Length	Quality of chain
23	Q	376	
24	R	316	
25	S	517	
26	T	249	
27	U	439	
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 [i](#)

There are 49 unique types of molecules in this entry. The entry contains 108702 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
1	0	171	Total	C	N	O	S	0	0
			1420	882	249	279	10		

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

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

- Molecule 3 is a protein called General transcription factor IIH subunit 2.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	394	Total	C	N	O	S	0	0
			3189	2068	552	557	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	54	Total	C	N	O	S	0	0
			428	277	67	82	2		

- Molecule 7 is a protein called General transcription and DNA repair factor IIIH 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 IIIH 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	9	Total	C	N	O	P	0	0
			199	86	32	70	11		

- 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
			1303	615	249	376	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
			1485	706	266	440	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		

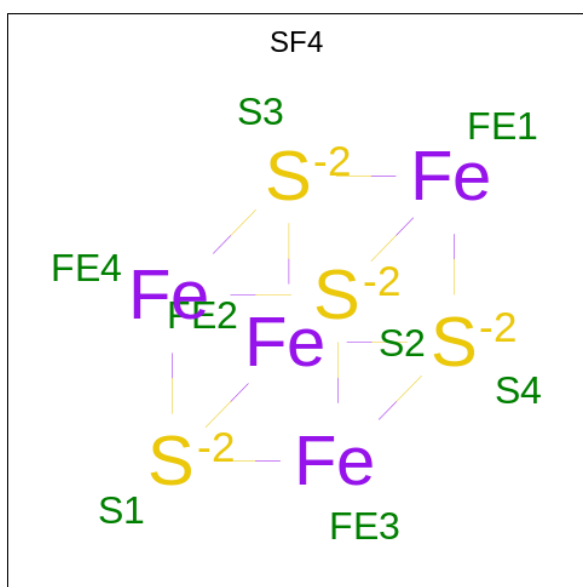
- Molecule 45 is a protein called RPB12.

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 (CCD ID: ZN) (formula: Zn).

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

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

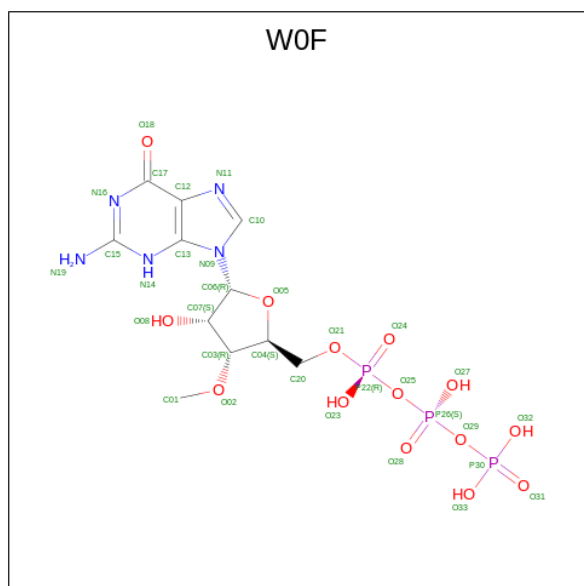


Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total	Fe	S	0
			8	4	4	

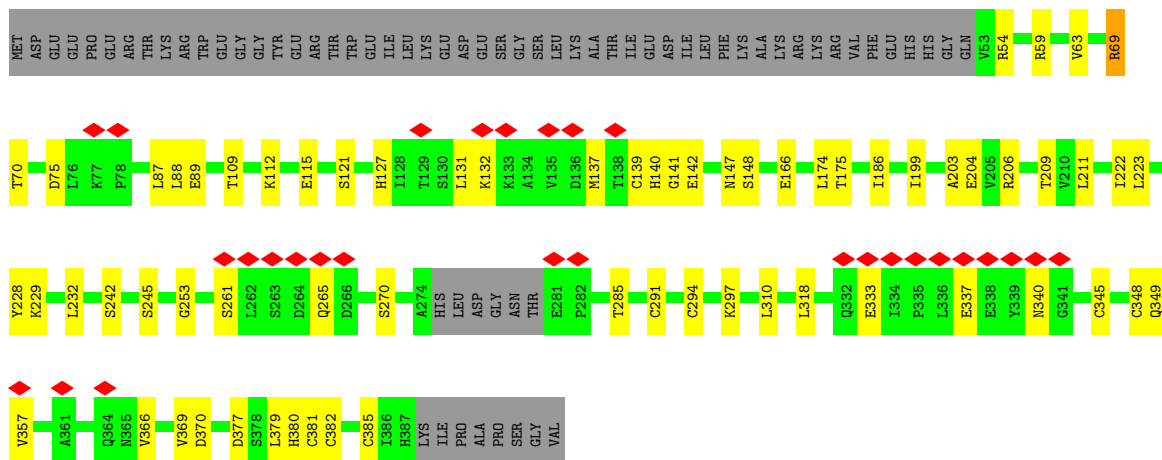
- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- 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 (CCD ID: W0F) (formula: C₁₁H₁₈N₅O₁₄P₃).



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

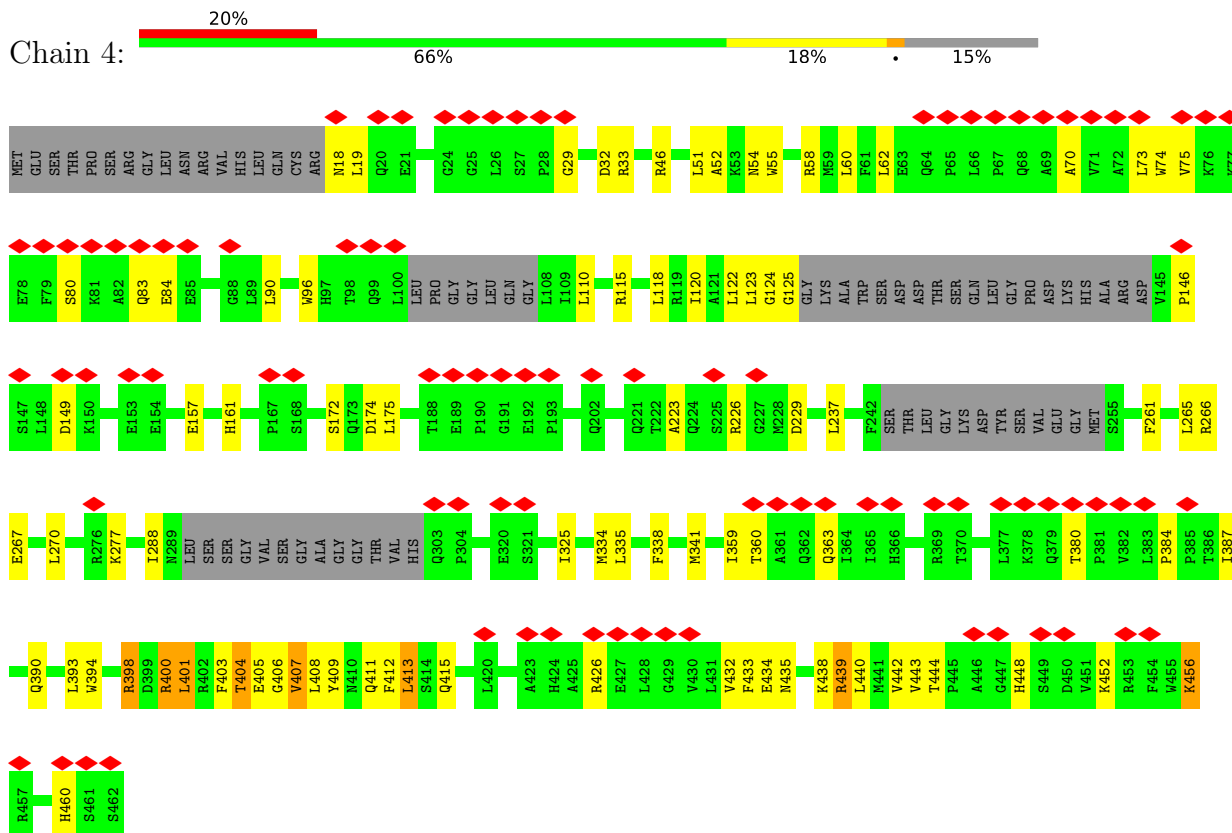


Chain 3: 9% 65% 19% 15%

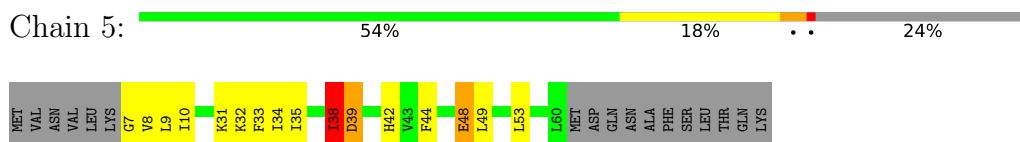


VAL
SER
ALA

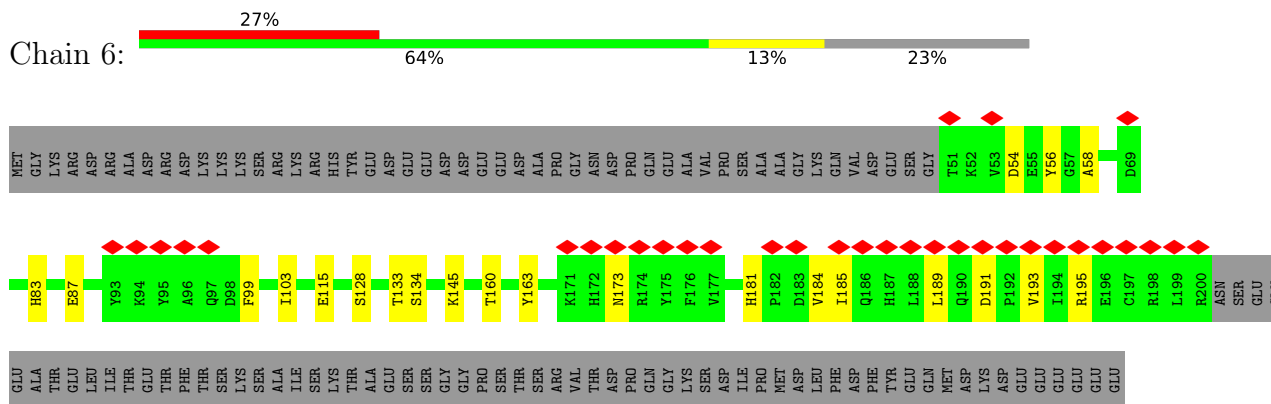
• Molecule 5: General transcription factor IIH subunit 4

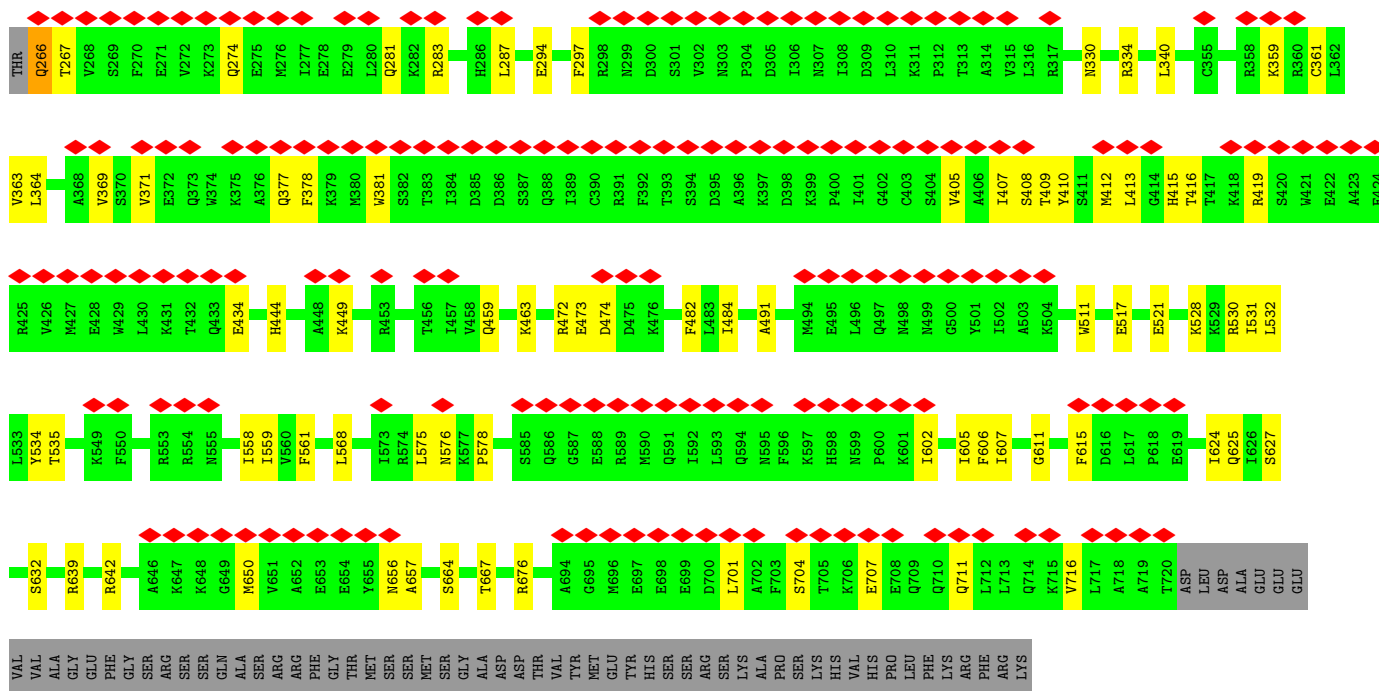


• Molecule 6: General transcription factor IIH subunit 5

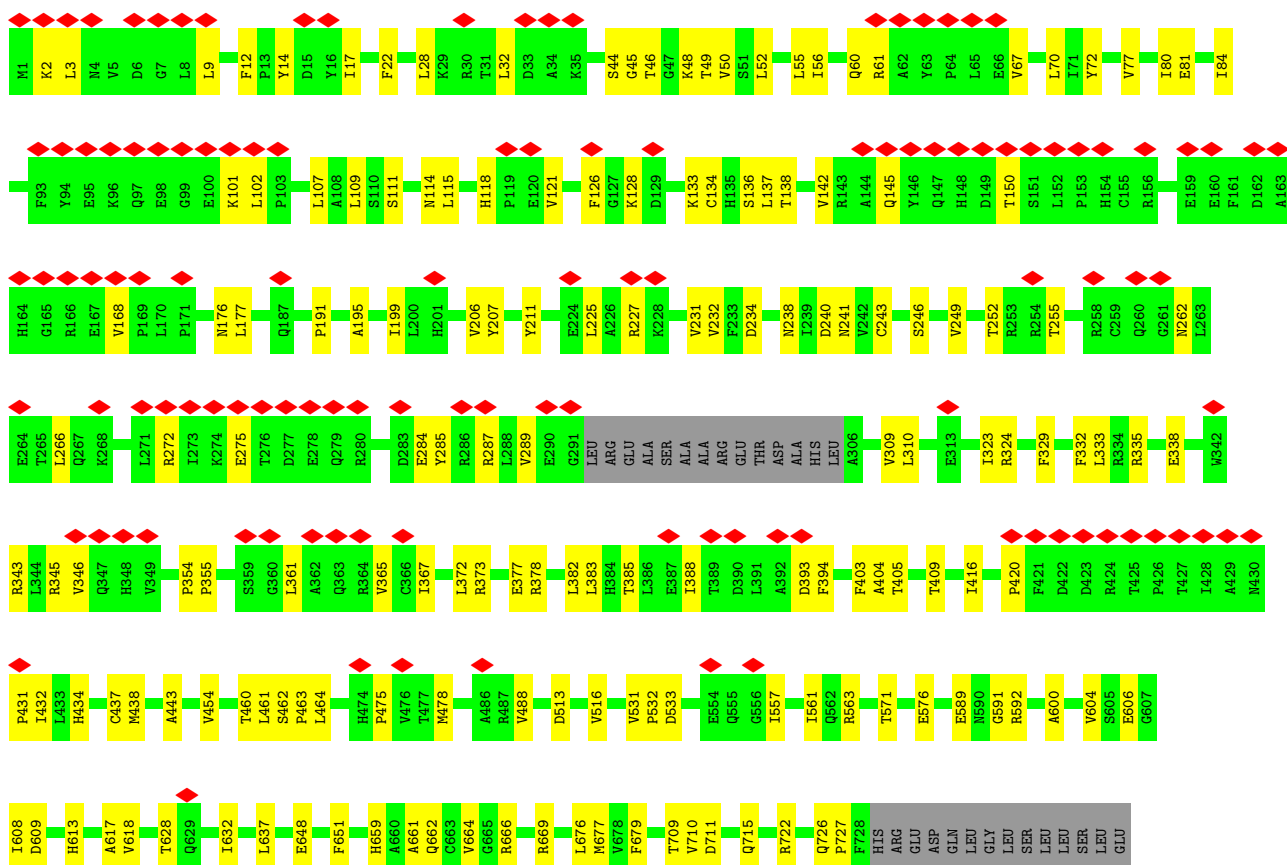


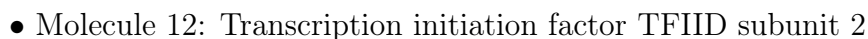
• Molecule 7: General transcription and DNA repair factor IIH helicase subunit XPB

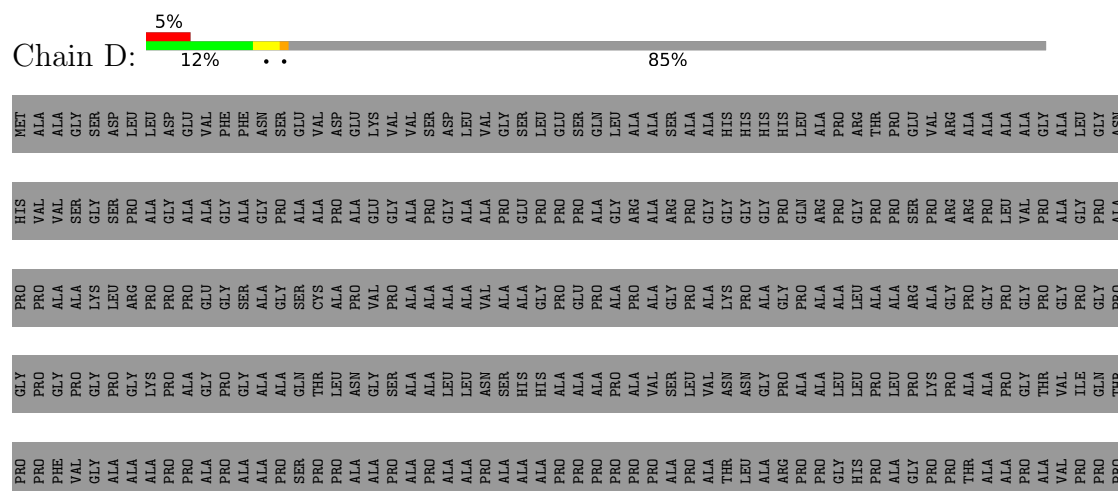
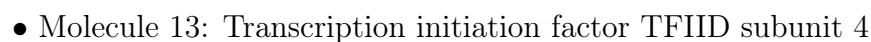




• Molecule 8: General transcription and DNA repair factor IHH helicase subunit XPD

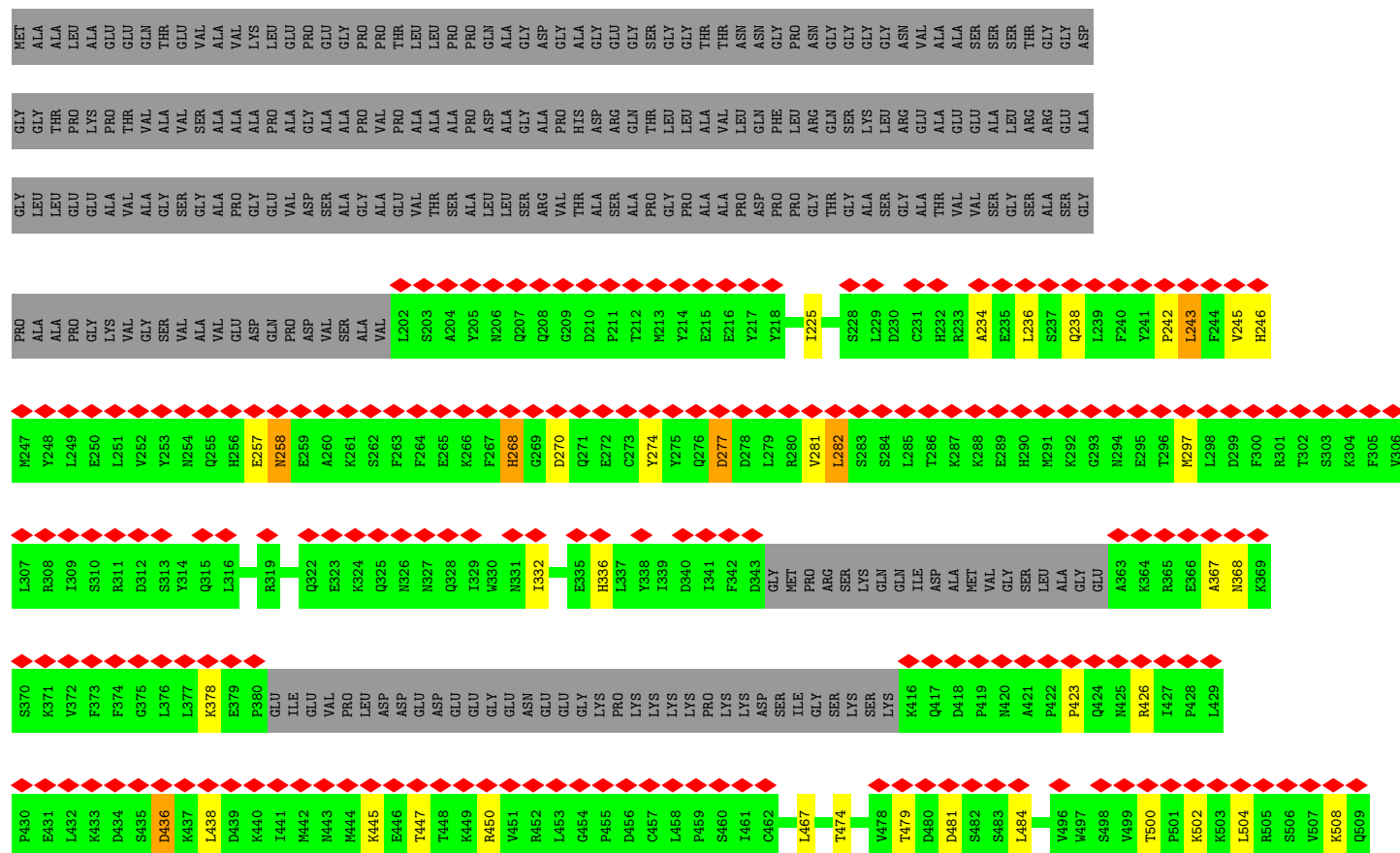




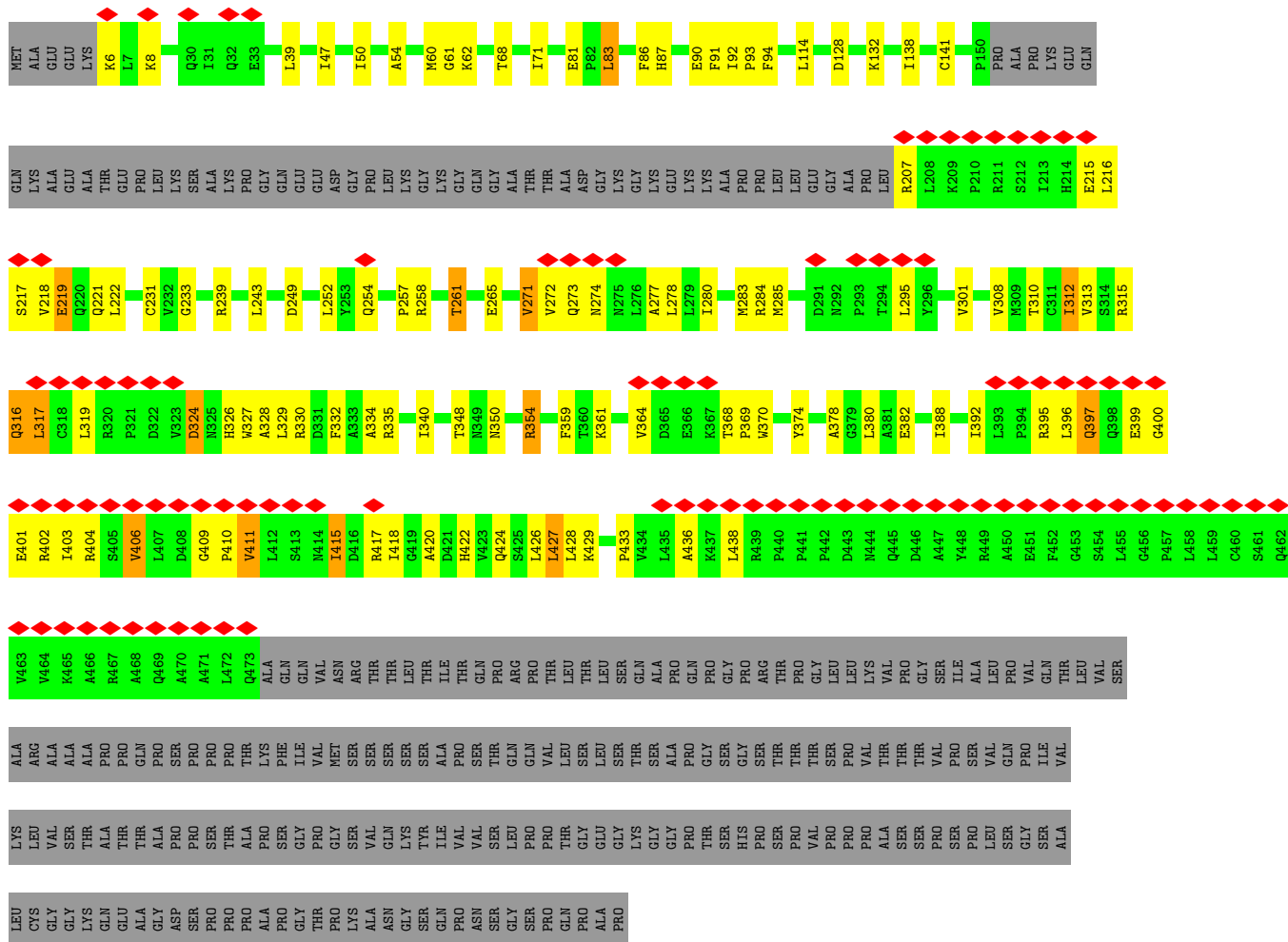
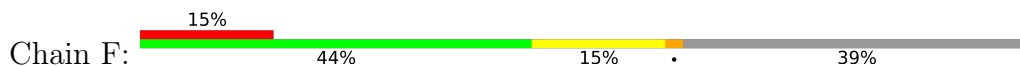


- Molecule 13: Transcription initiation factor TFIID subunit 4

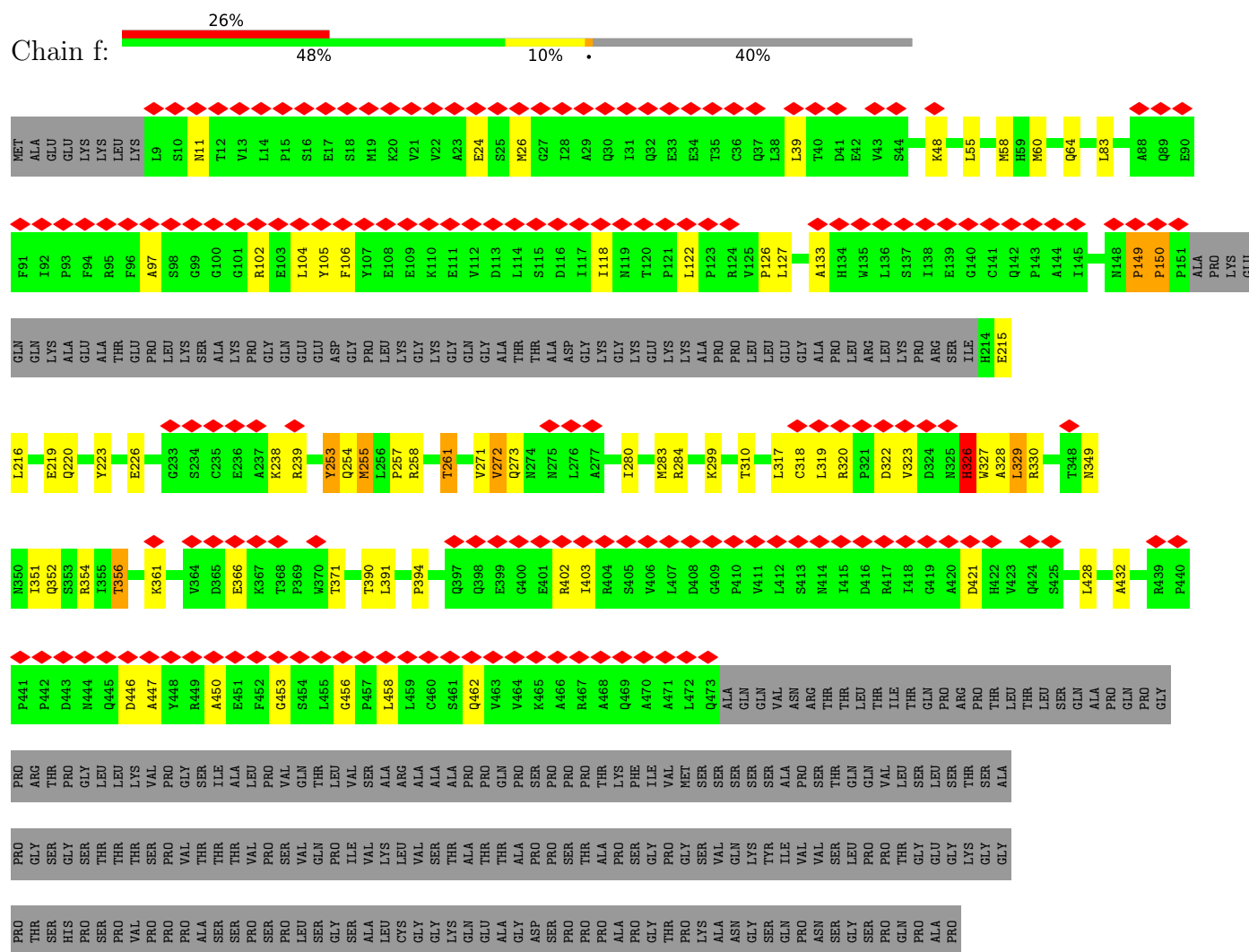
[illegible]



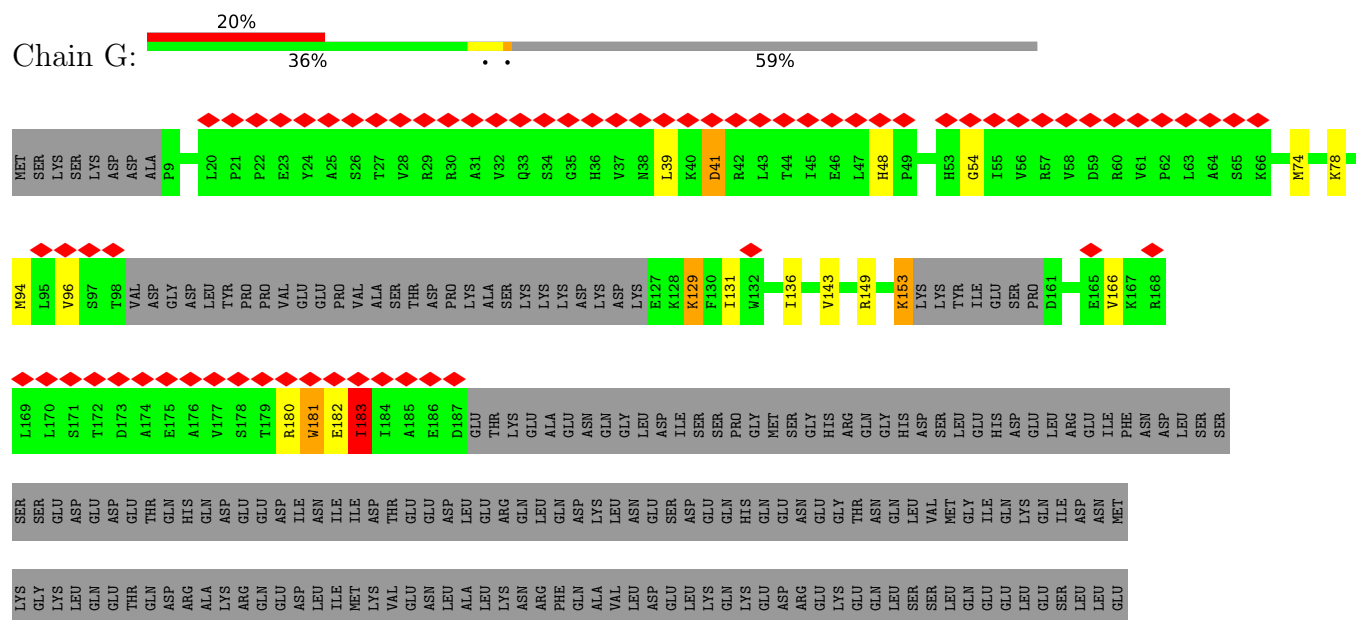
- Molecule 15: Transcription initiation factor TFIID subunit 6

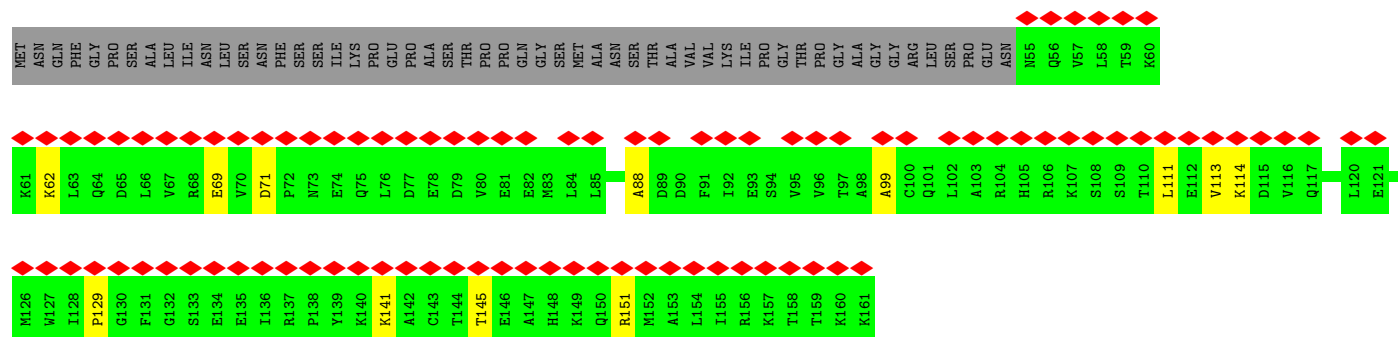


- Molecule 15: Transcription initiation factor TFIID subunit 6

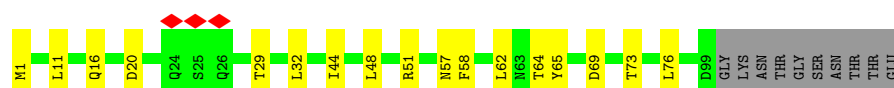
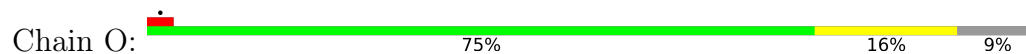


- Molecule 16: Transcription initiation factor TFIID subunit 7

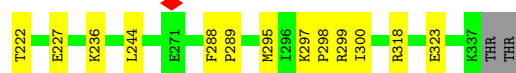
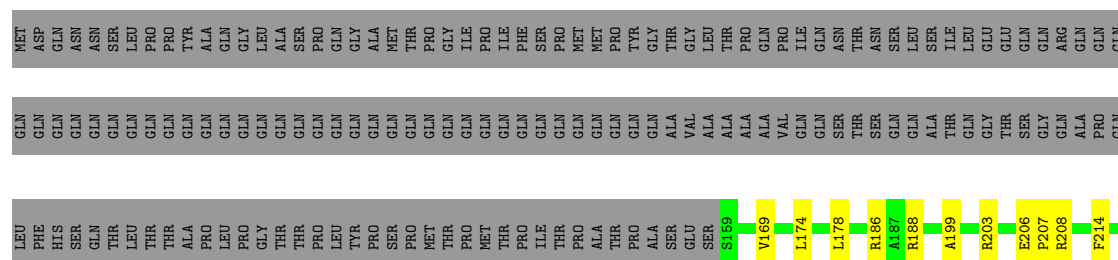




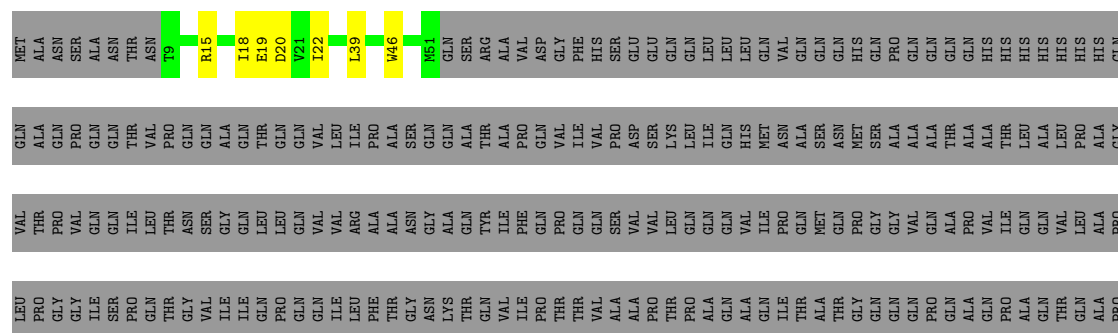
• Molecule 21: Transcription initiation factor IIA subunit 2



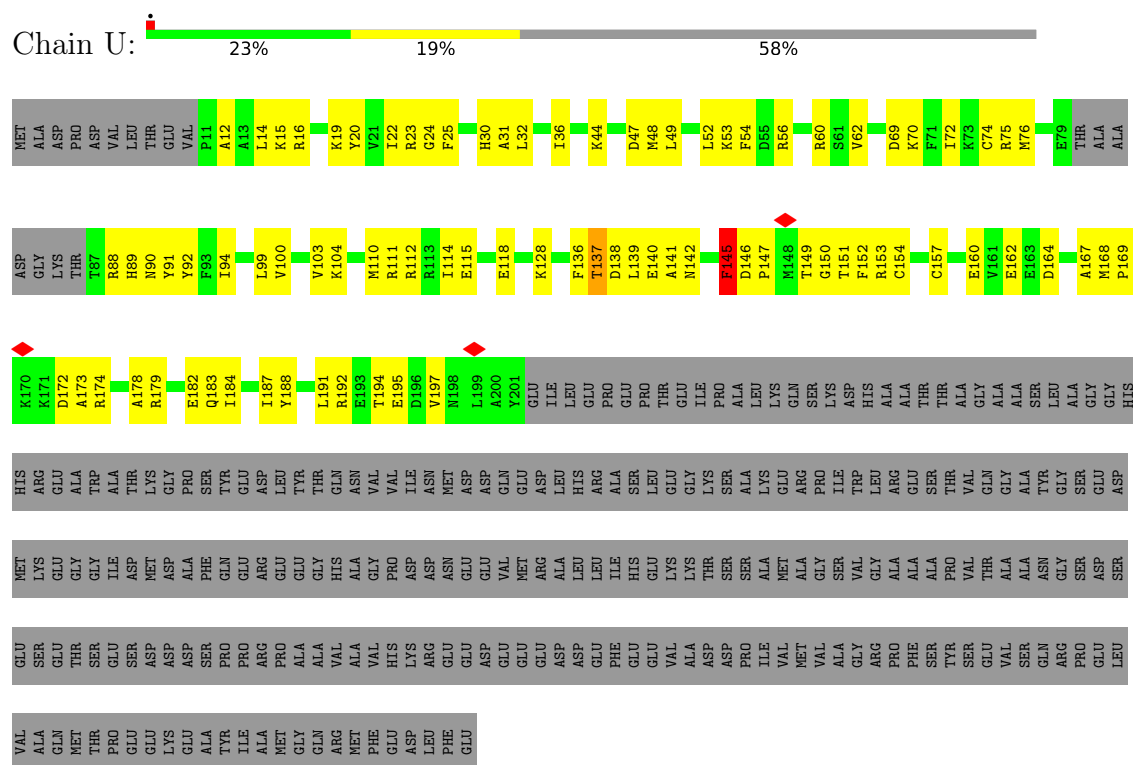
• Molecule 22: TATA-box-binding protein



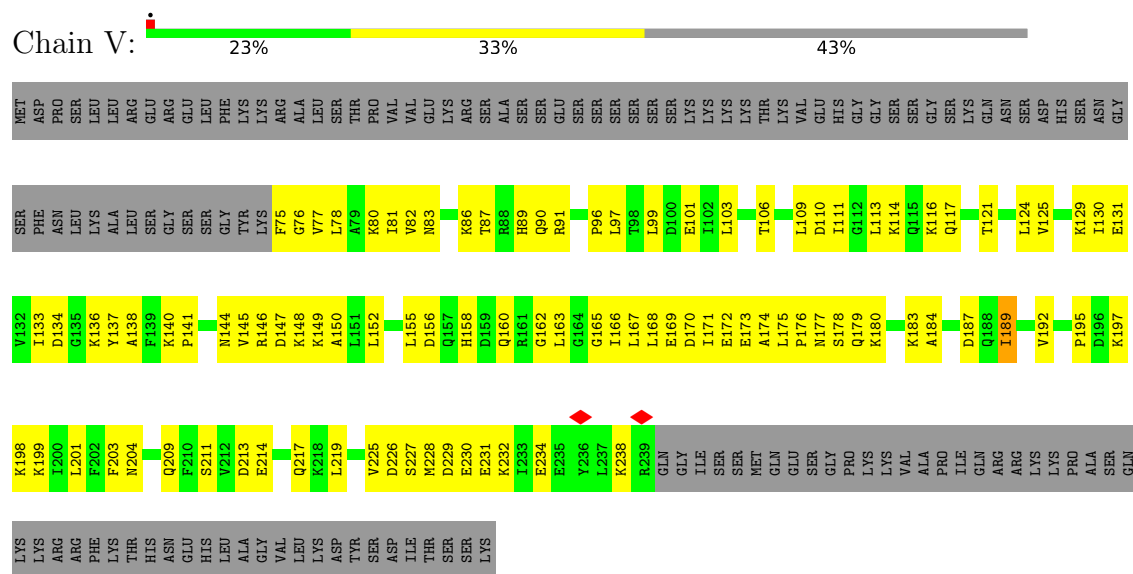
• Molecule 23: Transcription initiation factor IIA beta chain



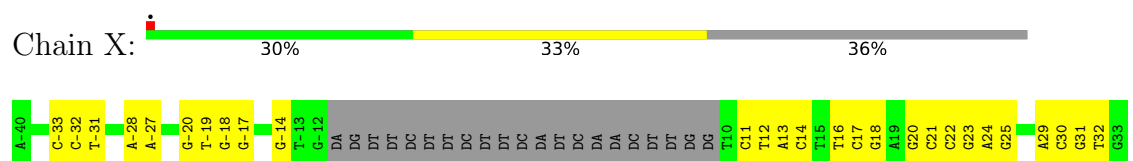
• Molecule 27: General transcription factor IIE subunit 1

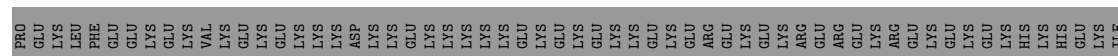
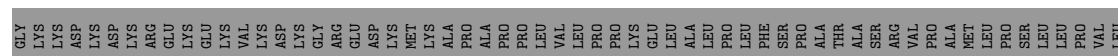
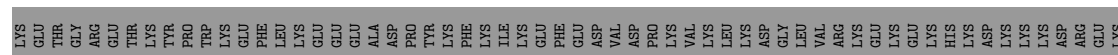
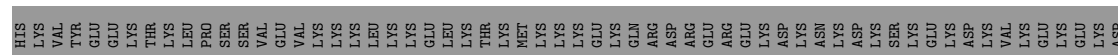
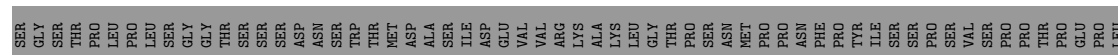
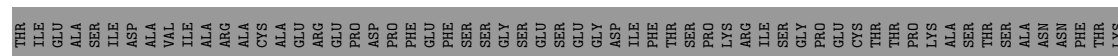
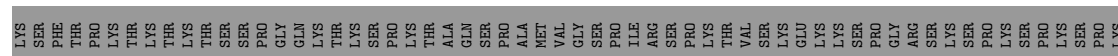
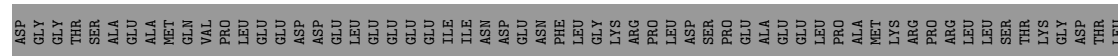
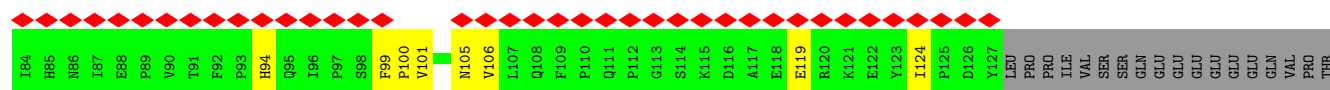
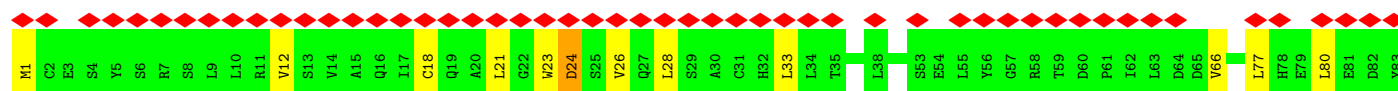
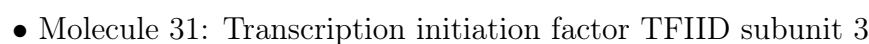
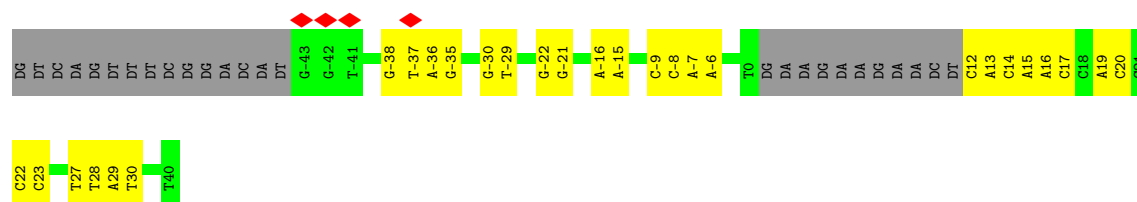
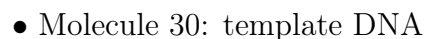


• Molecule 28: Transcription initiation factor IIE subunit beta



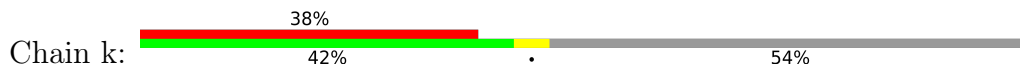
• Molecule 29: non-template DNA





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

- Molecule 32: Transcription initiation factor TFIID subunit 11



NET	ASP	ASP	ASP	HIS	GLU	SER	PRO	SER	ASP	LYS	GLY	GLY	GLU	THR	ALA	ALA	VAL	PRO	PRO	ASP	ASP	PRO	GLY	GLY	ALA	THR	THR	THR	ILE	PRO	GLU	GLU	GLU	THR	THR	ASP	GLY	ASP	ALA	ALA	ASP	VAL	ASP	LEU	LYS	GLU	ALA	ALA	ALA	GLU	GLU	GLY	GLY	LEU	GLU	GLF
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GLN	ASP	VAL	VAL	SER	ASP	LEU	THR	THR	GLU	GLU	ARG	GLU	ASP	SER	SER	LEU	LEU	ASN	PRO	ALA	ALA	LYS	LYS	LEU	LYS	ILE	THR	THR	LYS	GLU	LYS	LYS	GLU	LYS	LYS	GLN	LYS	VAL	ASP	GLU	ASP	GLU	GLU	ILE	GLN	LYS	MET	GLN	ILE	LEU	VAL	SER	SER	PHE	S114	E115	E116	Q117	L118	N119	S120	S121	S122	S123	S124	S125	S126	S127	S128	S129	S130	S131	S132	S133	S134	S135	S136	S137	S138	S139	S140	S141	S142	S143	S144	S145	S146	S147	S148	S149	S150	S151	S152	S153	S154	S155	S156	S157	S158	S159	S160	S161	S162	S163	S164	S165	S166	S167	S168	S169	S170	S171	S172	S173	S174	S175	S176	S177	S178	S179	S180	S181	S182	S183	S184	S185	S186	S187	S188	S189	S190	S191	S192	S193	S194	S195	S196	S197	S198	S199	S200	S201	S202	S203	S204	S205	S206	S207	S208	S209	S210	S211	S212	S213	S214	S215	S216	S217	S218	S219	S220	S221	S222	S223	S224	S225	S226	S227	S228	S229	S230	S231	S232	S233	S234	S235	S236	S237	S238	S239	S240	S241	S242	S243	S244	S245	S246	S247	S248	S249	S250	S251	S252	S253	S254	S255	S256	S257	S258	S259	S260	S261	S262	S263	S264	S265	S266	S267	S268	S269	S270	S271	S272	S273	S274	S275	S276	S277	S278	S279	S280	S281	S282	S283	S284	S285	S286	S287	S288	S289	S290	S291	S292	S293	S294	S295	S296	S297	S298	S299	S300	S301	S302	S303	S304	S305	S306	S307	S308	S309	S310	S311	S312	S313	S314	S315	S316	S317	S318	S319	S320	S321	S322	S323	S324	S325	S326	S327	S328	S329	S330	S331	S332	S333	S334	S335	S336	S337	S338	S339	S340	S341	S342	S343	S344	S345	S346	S347	S348	S349	S350	S351	S352	S353	S354	S355	S356	S357	S358	S359	S360	S361	S362	S363	S364	S365	S366	S367	S368	S369	S370	S371	S372	S373	S374	S375	S376	S377	S378	S379	S380	S381	S382	S383	S384	S385	S386	S387	S388	S389	S390	S391	S392	S393	S394	S395	S396	S397	S398	S399	S400	S401	S402	S403	S404	S405	S406	S407	S408	S409	S410	S411	S412	S413	S414	S415	S416	S417	S418	S419	S420	S421	S422	S423	S424	S425	S426	S427	S428	S429	S430	S431	S432	S433	S434	S435	S436	S437	S438	S439	S440	S441	S442	S443	S444	S445	S446	S447	S448	S449	S450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554	S555	S556	S557	S558	S559	S560	S561	S562	S563	S564	S565	S566	S567	S568	S569	S570	S571	S572	S573	S574	S575	S576	S577	S578	S579	S580	S581	S582	S583	S584	S585	S586	S587	S588	S589	S590	S591	S592	S593	S594	S595	S596	S597	S598	S599	S600	S601	S602	S603	S604	S605	S606	S607	S608	S609	S610	S611	S612	S613	S614	S615	S616	S617	S618	S619	S620	S621	S622	S623	S624	S625	S626	S627	S628	S629	S630	S631	S632	S633	S634	S635	S636	S637	S638	S639	S640	S641	S642	S643	S644	S645	S646	S647	S648	S649	S650	S651	S652	S653	S654	S655	S656	S657	S658	S659	S660	S661	S662	S663	S664	S665	S666	S667	S668	S669	S670	S671	S672	S673	S674	S675	S676	S677	S678	S679	S680	S681	S682	S683	S684	S685	S686	S687	S688	S689	S690	S691	S692	S693	S694	S695	S696	S697	S698	S699	S700	S701	S702	S703	S704	S705	S706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935	S936	S937	S938	S939	S940	S941	S942	S943	S944	S945	S946	S947	S948	S949	S950	S951	S952	S953	S954	S955	S956	S957	S958	S959	S960	S961	S962	S963	S964	S965	S966	S967	S968	S969	S970	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000
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- Molecule 33: Transcription initiation factor TFIID subunit 13



Met	ALA	ASP	GLU	GLU	GLU	ASP	GLU	GLU	GLU	GLU	GLU	ASN	GLN	GLU	ILE	GLY	GLY	GLY	GLY	GLY	GLN	GLY	LYS	R28	R29	R30	L31	F32	F33	S33	S34	E35	L36	R37	R38	M39	M40	Y41	G42	F43	G44	G44	D44	D46	Q47	M48	P49	Y50	T51	E52	S53	Y54	D55	L56	L57	E58	D59	L60
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ASN
TYR
GLY
SER

- Molecule 34: DNA-directed RNA polymerase subunit

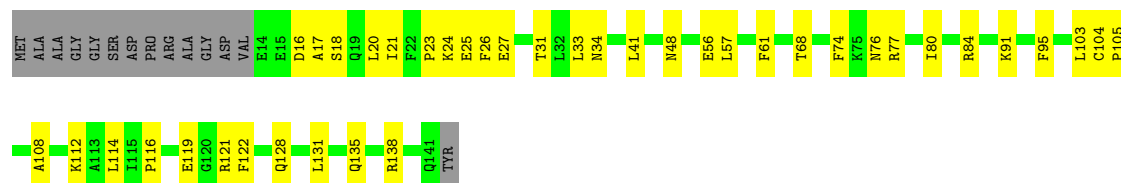
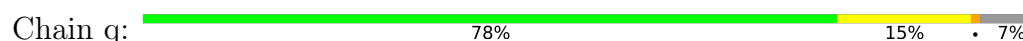


MET	HIS	GLY	GLY	GLY	P80	P80	SER	GLY	ASP	S11	A12	C13	I18	L26	L31	M34	S35	V36	G40	Y43	T46	T47	E48	G49	G50	R51	P52	K53	L57	Q62	T73	G76	E80	H84	H87	P93	F95	H96	V97	G98	V110	A111
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	G14	S115	V119	D120	I126	I129	L130	A131	K134	I153	E154	E155	GLY	GLY	GLU	GLU	MET	ASP	ASN	LVS	PHE	GLY	VAL	GLN	PRO	I181	I187	P189	E201	Z202	K203	E204	V205	E211	K212	K213
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Chain p: 77% 20% .



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

Chain x:  84% 15% .



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

Chain y:  79% 18% ..



- Molecule 45: RPB12

Chain z:  53% 22% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3757	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 ($e^-/\text{\AA}^2$)	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	4.605	Depositor
Minimum map value	-1.871	Depositor
Average map value	0.049	Depositor
Map value standard deviation	0.204	Depositor
Recommended contour level	0.6	Depositor
Map size ($\text{\AA}$)	426.88, 426.88, 426.88	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.668, 2.668, 2.668	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, SF4, CSX, MG, G2L, W0F, HYP, TRX, ZN, ILX

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	0.41	0/1437	0.71	3/1926 (0.2%)
2	1	0.20	0/2210	0.34	0/2975
3	2	0.18	0/2624	0.33	1/3555 (0.0%)
4	3	0.24	0/2103	0.36	0/2846
5	4	0.31	0/3262	0.45	1/4418 (0.0%)
6	5	0.41	0/433	0.79	1/585 (0.2%)
7	6	0.19	0/4994	0.33	0/6745
8	7	0.17	0/5875	0.30	0/7955
9	N	0.41	0/22	0.98	0/26
10	Z	0.26	0/159	0.37	0/244
11	A	0.63	0/4698	0.95	5/6345 (0.1%)
12	B	0.46	1/7993 (0.0%)	0.69	6/10836 (0.1%)
13	D	0.56	0/1379	0.88	3/1843 (0.2%)
13	d	0.47	0/1321	0.71	0/1772
14	E	0.45	1/4482 (0.0%)	0.72	3/6069 (0.0%)
14	e	0.55	1/4433 (0.0%)	0.77	0/6004
15	F	0.63	1/3201 (0.0%)	1.00	7/4347 (0.2%)
15	f	0.47	0/3140	0.80	6/4268 (0.1%)
16	G	0.68	0/1190	0.94	1/1601 (0.1%)
17	H	0.63	3/1673 (0.2%)	0.86	5/2285 (0.2%)
18	I	0.20	0/981	0.41	0/1332
18	i	0.22	0/989	0.40	0/1343
19	J	0.83	0/736	1.15	2/998 (0.2%)
19	j	0.74	0/775	0.96	0/1049
20	L	0.69	0/630	1.14	1/852 (0.1%)
20	l	0.59	0/888	0.88	0/1194
21	O	0.27	0/816	0.36	0/1105
22	P	0.11	0/1448	0.24	0/1948
23	Q	0.19	0/945	0.35	0/1274
24	R	0.19	0/2199	0.37	0/2967
25	S	0.16	0/1496	0.37	0/2013
26	T	0.13	0/1817	0.29	0/2445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	U	0.35	0/1545	0.69	1/2075 (0.0%)
28	V	0.24	0/1380	0.58	0/1854
29	X	0.29	0/1463	0.59	0/2256
30	Y	0.31	0/1661	0.53	0/2556
31	c	0.48	0/1035	0.67	0/1406
32	k	0.28	0/799	0.53	1/1070 (0.1%)
33	m	0.85	0/733	1.18	1/977 (0.1%)
34	o	0.28	0/11723	0.39	0/15830
35	p	0.30	0/9358	0.37	0/12633
36	q	0.32	0/2102	0.38	0/2857
37	r	0.10	0/1064	0.22	0/1428
38	s	0.24	0/1751	0.32	0/2366
39	t	0.28	0/667	0.33	0/901
40	u	0.16	0/1382	0.30	0/1874
41	v	0.26	0/1207	0.32	0/1628
42	w	0.19	0/948	0.31	0/1284
43	x	0.33	0/542	0.38	0/730
44	y	0.32	0/939	0.37	0/1271
45	z	0.23	0/377	0.32	0/500
All	All	0.39	7/111025 (0.0%)	0.59	48/150661 (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
24	R	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	28	ASN	C-O	-7.47	1.15	1.24
17	H	27	ASP	C-O	-7.11	1.15	1.24
17	H	31	LEU	C-O	-6.20	1.16	1.24
12	B	61	ASN	C-O	-6.14	1.18	1.24
14	E	524	LEU	C-O	5.74	1.30	1.24

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	55	LYS	CB-CA-C	-11.48	94.97	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	491	HIS	N-CA-C	-9.42	101.01	111.28
15	f	149	PRO	O-C-N	8.98	125.44	121.31
14	E	756	THR	N-CA-C	-8.39	103.18	113.50
17	H	32	ALA	N-CA-C	-8.26	102.23	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	R	106	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1420	0	1420	125	0
2	1	2167	0	2175	39	0
3	2	2567	0	2539	93	0
4	3	2066	0	2097	102	0
5	4	3189	0	3243	141	0
6	5	428	0	434	43	0
7	6	4890	0	4949	96	0
8	7	5751	0	5794	145	0
9	N	64	0	51	8	0
10	Z	199	0	95	8	0
11	A	4580	0	4502	98	0
12	B	7796	0	7751	116	0
13	D	1366	0	1390	75	0
13	d	1307	0	1318	15	0
14	E	4376	0	4256	74	0
14	e	4327	0	4197	60	0
15	F	3143	0	3093	100	0
15	f	3081	0	3012	69	0
16	G	1171	0	1222	16	0
17	H	1633	0	1621	35	0
18	I	959	0	969	13	0
18	i	967	0	977	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	J	720	0	719	13	0
19	j	759	0	759	14	0
20	L	622	0	620	19	0
20	l	876	0	893	10	0
21	O	806	0	818	18	0
22	P	1422	0	1514	19	0
23	Q	930	0	888	12	0
24	R	2167	0	2193	38	0
25	S	1461	0	1429	42	0
26	T	1788	0	1819	54	0
27	U	1520	0	1520	212	0
28	V	1357	0	1381	90	0
29	X	1303	0	707	44	0
30	Y	1485	0	822	33	0
31	c	1011	0	975	19	0
32	k	785	0	818	8	0
33	m	724	0	744	23	0
34	o	11510	0	11615	259	0
35	p	9175	0	9196	176	0
36	q	2059	0	2007	31	0
37	r	1050	0	1033	24	0
38	s	1720	0	1737	25	0
39	t	657	0	684	9	0
40	u	1351	0	1358	131	0
41	v	1186	0	1147	16	0
42	w	927	0	860	29	0
43	x	533	0	553	10	0
44	y	920	0	942	18	0
45	z	372	0	378	11	0
46	0	2	0	0	0	0
46	2	3	0	0	0	0
46	3	2	0	0	0	0
46	R	1	0	0	0	0
46	U	1	0	0	0	0
46	o	2	0	0	0	0
46	p	1	0	0	0	0
46	q	1	0	0	0	0
46	w	2	0	0	0	0
46	x	1	0	0	0	0
46	z	1	0	0	0	0
47	7	8	0	0	0	0
48	o	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	p	33	0	0	8	0
All	All	108702	0	107234	2308	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 11.

The worst 5 of 2308 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)
27:U:152:PHE:CE1	40:u:95:VAL:HB	1.25	1.66
27:U:139:LEU:HB2	40:u:160:ILE:CG1	1.22	1.59
1:0:41:ARG:CG	27:U:169:PRO:HG2	1.34	1.54
27:U:139:LEU:CB	40:u:160:ILE:HG12	1.41	1.49
6:5:33:PHE:CE1	6:5:49:LEU:HD12	1.44	1.49

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	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%)	313 (96%)	12 (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
6	5	52/71 (73%)	48 (92%)	2 (4%)	2 (4%)	2	19
7	6	601/782 (77%)	573 (95%)	27 (4%)	1 (0%)	43	77
8	7	710/760 (93%)	682 (96%)	28 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	N	4/8 (50%)	3 (75%)	1 (25%)	0	100	100
11	A	543/1872 (29%)	519 (96%)	23 (4%)	1 (0%)	43	77
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%)	517 (96%)	23 (4%)	1 (0%)	43	77
14	e	531/800 (66%)	482 (91%)	48 (9%)	1 (0%)	43	77
15	F	408/677 (60%)	392 (96%)	15 (4%)	1 (0%)	43	77
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%)	4	27
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%)	5	29
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%)	18	56
25	S	174/517 (34%)	161 (92%)	12 (7%)	1 (1%)	21	59
26	T	218/249 (88%)	211 (97%)	7 (3%)	0	100	100
27	U	180/439 (41%)	153 (85%)	26 (14%)	1 (1%)	21	59
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
34	o	1448/1970 (74%)	1397 (96%)	47 (3%)	4 (0%)	36	72
35	p	1145/1174 (98%)	1106 (97%)	39 (3%)	0	100	100
36	q	253/275 (92%)	246 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	62 (95%)	3 (5%)	0	100	100
44	y	113/117 (97%)	110 (97%)	3 (3%)	0	100	100
45	z	42/58 (72%)	40 (95%)	2 (5%)	0	100	100
All	All	12996/22270 (58%)	12405 (96%)	569 (4%)	22 (0%)	44	77

5 of 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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	164/283 (58%)	158 (96%)	6 (4%)	30	51
2	1	241/484 (50%)	241 (100%)	0	100	100
3	2	295/352 (84%)	294 (100%)	1 (0%)	86	85
4	3	234/272 (86%)	232 (99%)	2 (1%)	70	79
5	4	346/399 (87%)	339 (98%)	7 (2%)	48	66
6	5	48/64 (75%)	47 (98%)	1 (2%)	47	65
7	6	536/688 (78%)	535 (100%)	1 (0%)	87	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	7	624/664 (94%)	624 (100%)	0	100	100
9	N	2/2 (100%)	2 (100%)	0	100	100
11	A	496/1665 (30%)	452 (91%)	44 (9%)	9	28
12	B	876/1083 (81%)	862 (98%)	14 (2%)	55	70
13	D	147/815 (18%)	136 (92%)	11 (8%)	12	33
13	d	146/815 (18%)	144 (99%)	2 (1%)	59	72
14	E	480/657 (73%)	467 (97%)	13 (3%)	39	60
14	e	475/657 (72%)	462 (97%)	13 (3%)	39	60
15	F	328/574 (57%)	308 (94%)	20 (6%)	17	38
15	f	322/574 (56%)	312 (97%)	10 (3%)	35	56
16	G	132/322 (41%)	124 (94%)	8 (6%)	17	38
17	H	181/270 (67%)	175 (97%)	6 (3%)	33	55
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	28
19	j	83/154 (54%)	82 (99%)	1 (1%)	63	75
20	L	71/141 (50%)	66 (93%)	5 (7%)	14	35
20	l	98/141 (70%)	97 (99%)	1 (1%)	68	78
21	O	90/98 (92%)	90 (100%)	0	100	100
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%)	235 (99%)	3 (1%)	61	74
25	S	154/448 (34%)	134 (87%)	20 (13%)	4	15
26	T	196/218 (90%)	193 (98%)	3 (2%)	57	72
27	U	167/373 (45%)	166 (99%)	1 (1%)	78	83
28	V	150/261 (58%)	149 (99%)	1 (1%)	76	81
31	c	113/833 (14%)	111 (98%)	2 (2%)	51	67
32	k	87/182 (48%)	87 (100%)	0	100	100
33	m	80/106 (76%)	71 (89%)	9 (11%)	5	19
34	o	1280/1748 (73%)	1261 (98%)	19 (2%)	57	72
35	p	1004/1027 (98%)	984 (98%)	20 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	q	234/252 (93%)	227 (97%)	7 (3%)	36	57
37	r	118/126 (94%)	118 (100%)	0	100	100
38	s	191/192 (100%)	187 (98%)	4 (2%)	47	65
39	t	71/111 (64%)	71 (100%)	0	100	100
40	u	152/153 (99%)	150 (99%)	2 (1%)	61	74
41	v	129/131 (98%)	127 (98%)	2 (2%)	55	70
42	w	103/112 (92%)	99 (96%)	4 (4%)	28	49
43	x	56/56 (100%)	54 (96%)	2 (4%)	31	52
44	y	104/106 (98%)	101 (97%)	3 (3%)	37	58
45	z	41/55 (74%)	40 (98%)	1 (2%)	43	63
All	All	11634/19173 (61%)	11358 (98%)	276 (2%)	43	63

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	s	7	THR
41	v	141	VAL
14	e	515	LEU
14	E	761	LEU
14	E	521	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 202 such sidechains are listed below:

Mol	Chain	Res	Type
27	U	183	GLN
34	o	791	GLN
20	l	86	GLN
28	V	157	GLN
34	o	412	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	Z	8/9 (88%)	2 (25%)	1 (12%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	Z	7	U
10	Z	9	G2L

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	Z	1	ATP

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

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	9	30,48,10	23,26,30	1.21	3 (13%)	32,38,44	2.07	7 (21%)
9	TRX	N	2	9	15,16,17	0.99	1 (6%)	19,22,24	1.53	2 (10%)
9	CSX	N	6	9	3,6,7	1.03	0	1,6,8	2.23	1 (100%)
9	ILX	N	1	9	8,9,10	0.62	0	9,11,13	1.32	2 (22%)
9	HYP	N	8	9	6,8,9	0.76	0	5,10,12	2.19	2 (40%)

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	9	30,48,10	-	2/9/27/31	0/3/3/3
9	TRX	N	2	9	-	2/5/6/8	0/2/2/2
9	CSX	N	6	9	-	1/1/5/7	-
9	ILX	N	1	9	-	7/11/12/14	-
9	HYP	N	8	9	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Z	9	G2L	C5-C4	3.15	1.47	1.38
10	Z	9	G2L	C6-N1	-2.36	1.34	1.38
10	Z	9	G2L	C5-N7	-2.11	1.35	1.39
9	N	2	TRX	CD2-CE2	2.02	1.44	1.41

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Z	9	G2L	C5-C4-N3	-6.15	118.48	128.46
9	N	2	TRX	CA-CB-CG	5.21	123.46	113.51
10	Z	9	G2L	C2-N3-C4	4.92	121.06	112.30
10	Z	9	G2L	N9-C4-N3	4.60	135.17	125.94
9	N	8	HYP	O-C-CA	-3.28	116.17	124.78

There are no chirality outliers.

5 of 12 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	9	G2L	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	Z	9	G2L	3	0
9	N	2	TRX	1	0
9	N	6	CSX	1	0
9	N	1	ILX	3	0
9	N	8	HYP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	31,35,35	2.89	10 (32%)	38,55,55	3.53	16 (42%)
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	-	-	3/24/40/40	0/3/3/3
47	SF4	7	1000	8	-	-	0/6/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	p	1201	W0F	C03-C04	-9.42	1.27	1.52
49	p	1201	W0F	O05-C04	6.85	1.60	1.45
49	p	1201	W0F	O05-C06	-5.82	1.28	1.42
49	p	1201	W0F	C12-C13	5.73	1.47	1.38
49	p	1201	W0F	C13-N09	-3.08	1.34	1.37

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	p	1201	W0F	O05-C06-N09	-14.46	75.32	108.36
49	p	1201	W0F	C07-C06-N09	8.15	136.32	113.22
49	p	1201	W0F	O05-C04-C03	-5.65	92.76	104.87
49	p	1201	W0F	O05-C04-C20	4.78	125.11	109.37
49	p	1201	W0F	O05-C06-C07	-4.09	97.74	106.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

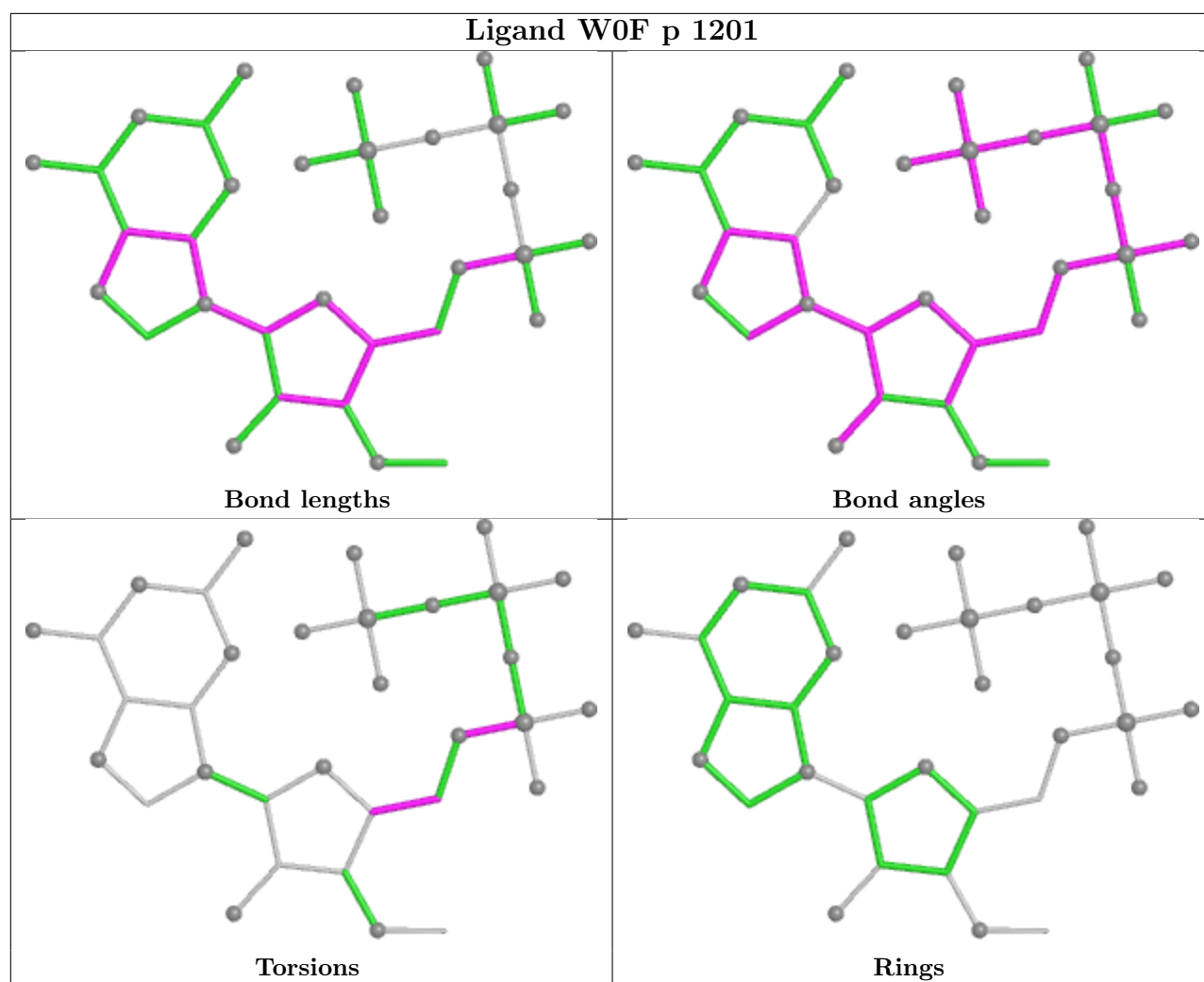
Mol	Chain	Res	Type	Atoms
49	p	1201	W0F	C20-O21-P22-O24
49	p	1201	W0F	C20-O21-P22-O25
49	p	1201	W0F	C03-C04-C20-O21

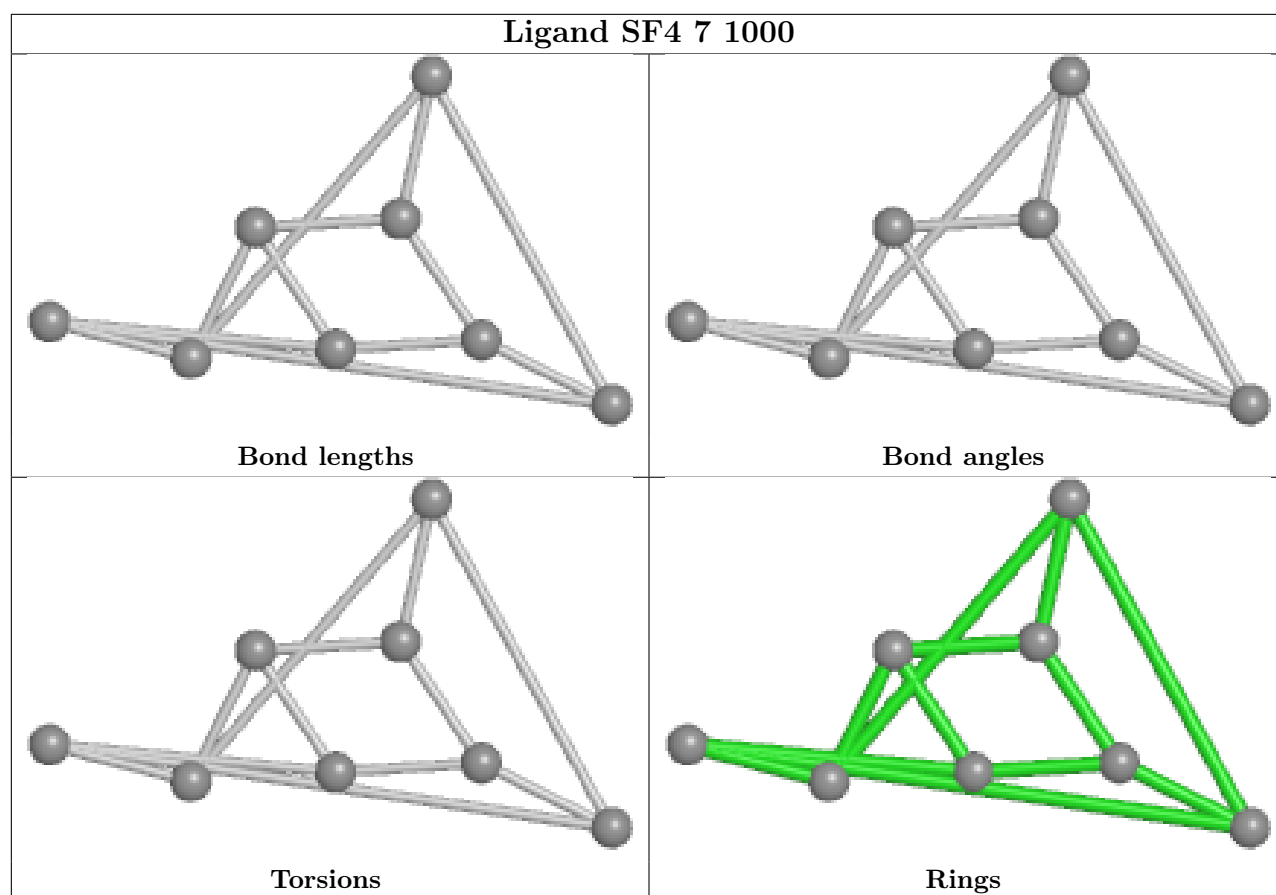
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	p	1201	W0F	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

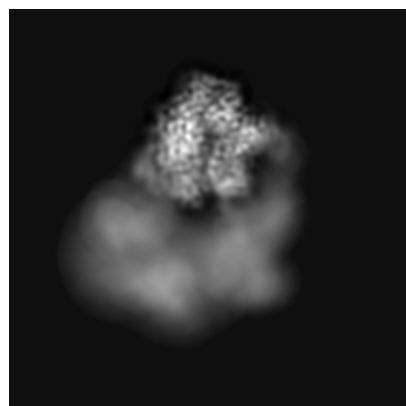
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37403. These allow visual inspection of the internal detail of the map and identification of artifacts.

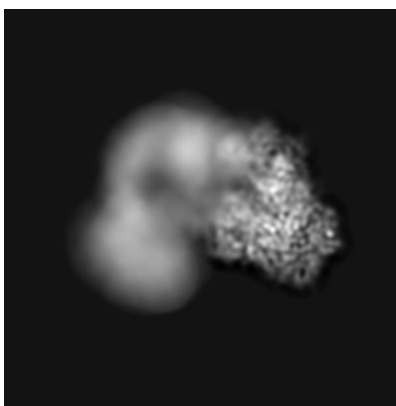
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

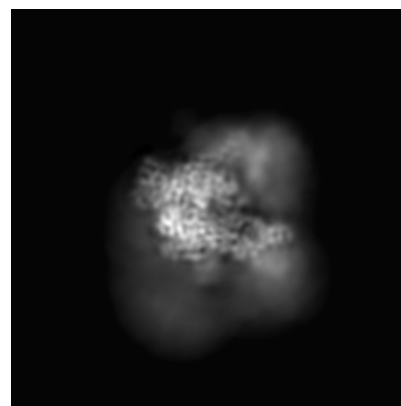
6.1.1 Primary map



X

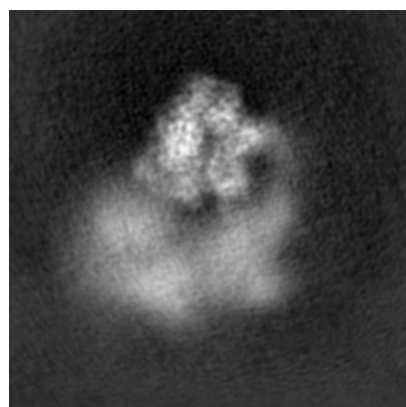


Y

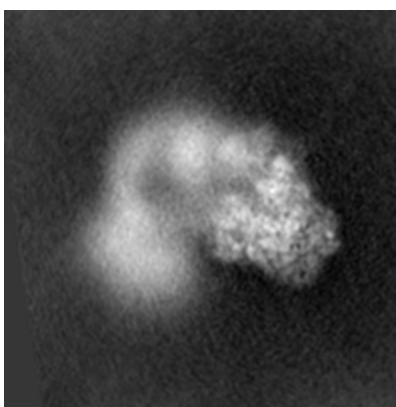


Z

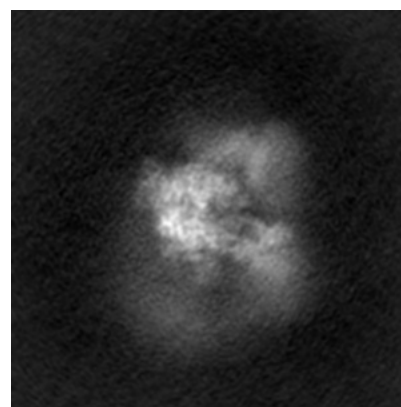
6.1.2 Raw map



X



Y

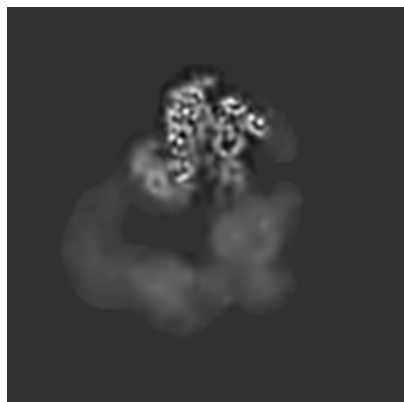


Z

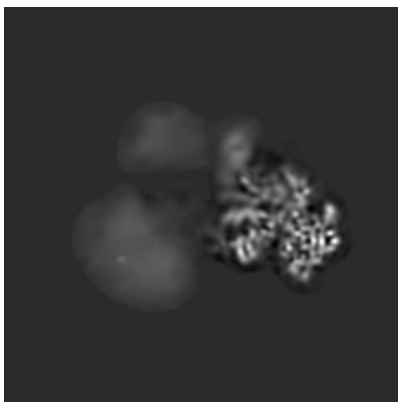
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

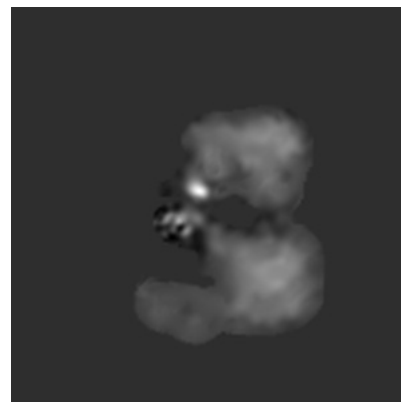
6.2.1 Primary map



X Index: 80

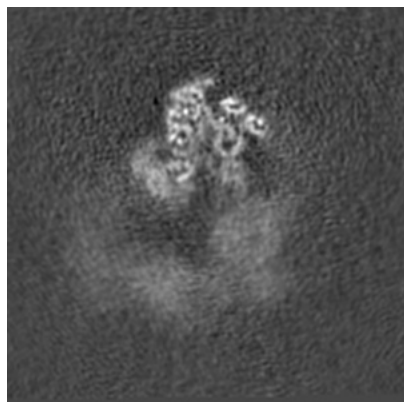


Y Index: 80

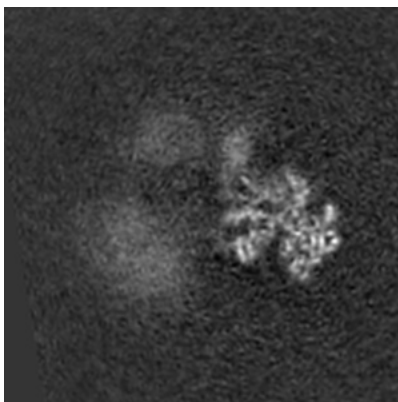


Z Index: 80

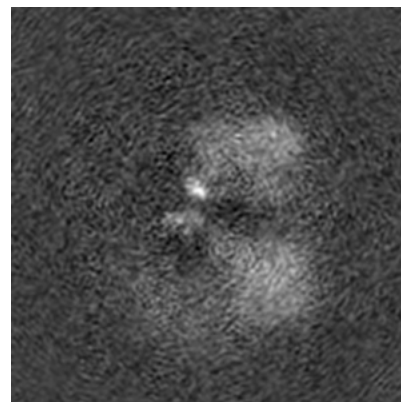
6.2.2 Raw map



X Index: 80



Y Index: 80

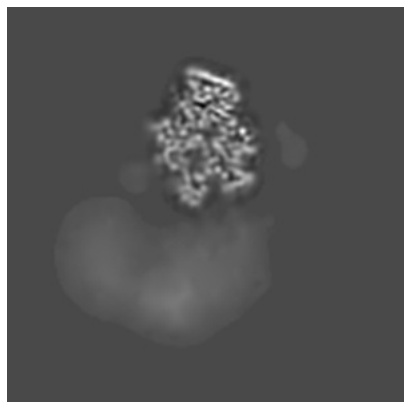


Z Index: 80

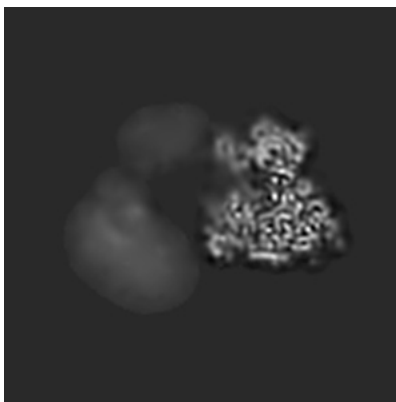
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

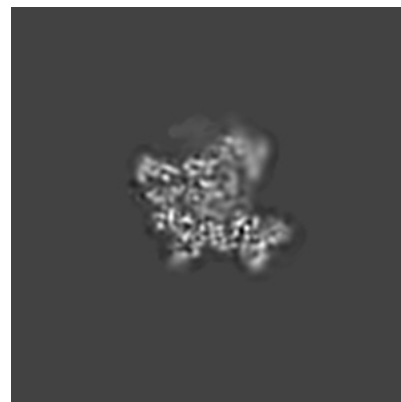
6.3.1 Primary map



X Index: 66

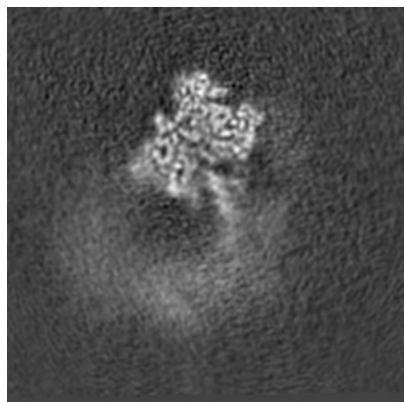


Y Index: 71

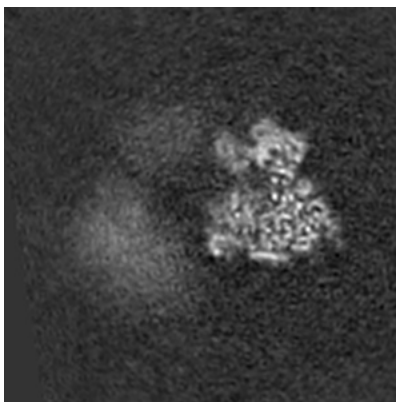


Z Index: 111

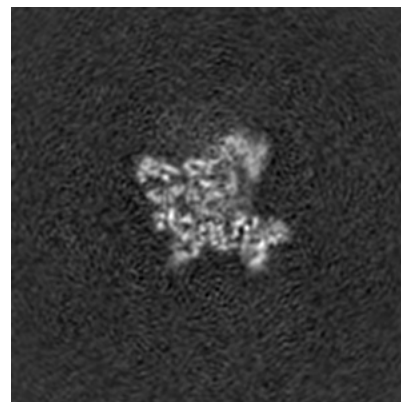
6.3.2 Raw map



X Index: 74



Y Index: 71

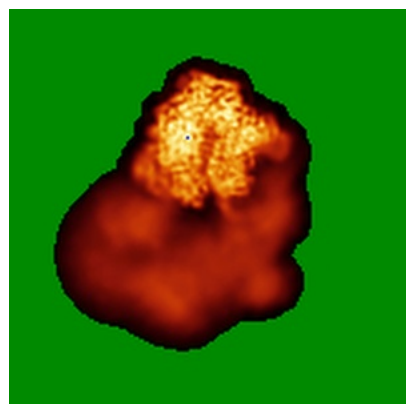


Z Index: 111

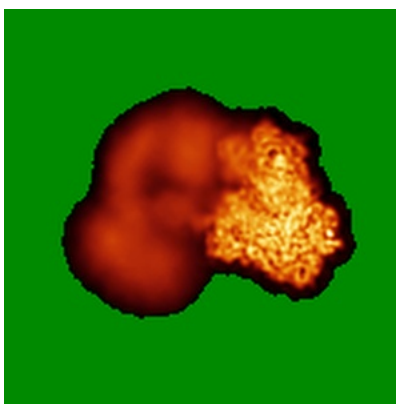
The images above show the largest variance slices of the map in three orthogonal directions.

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

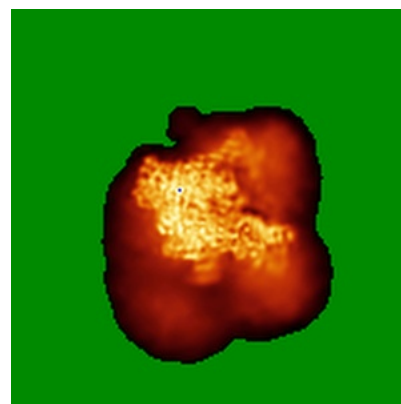
6.4.1 Primary map



X

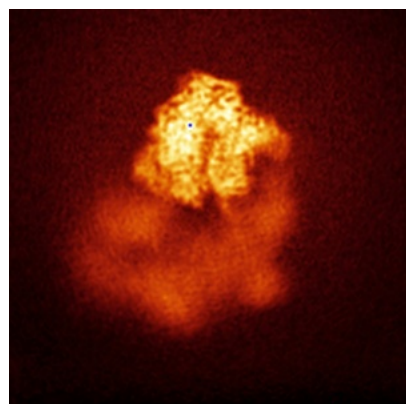


Y

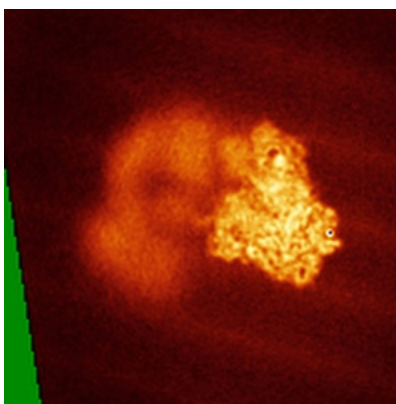


Z

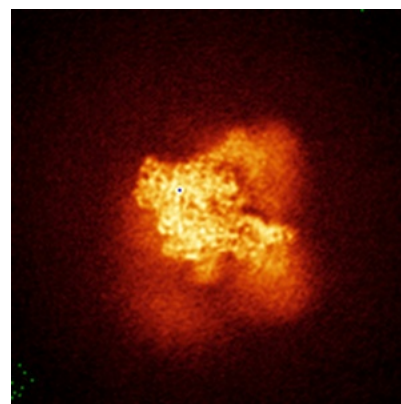
6.4.2 Raw map



X



Y

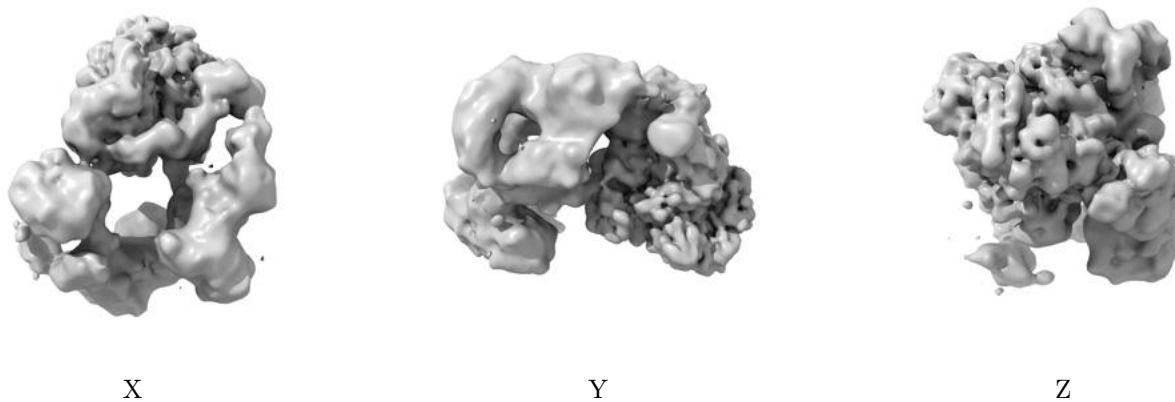


Z

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.

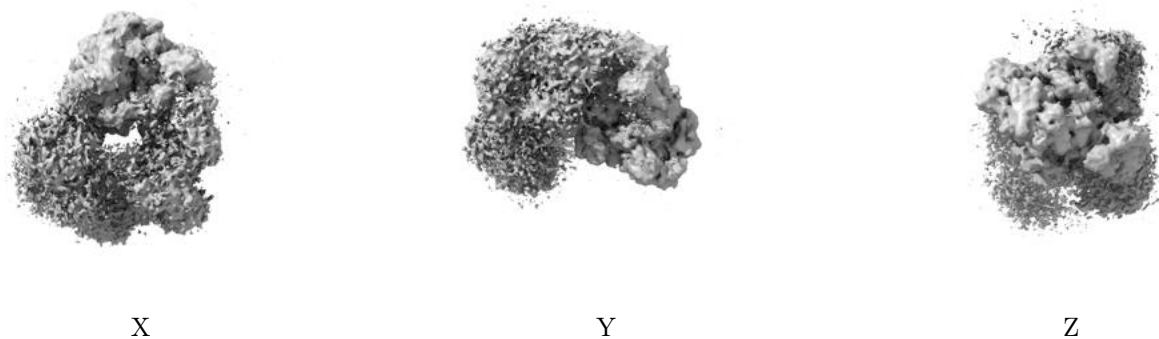
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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



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.

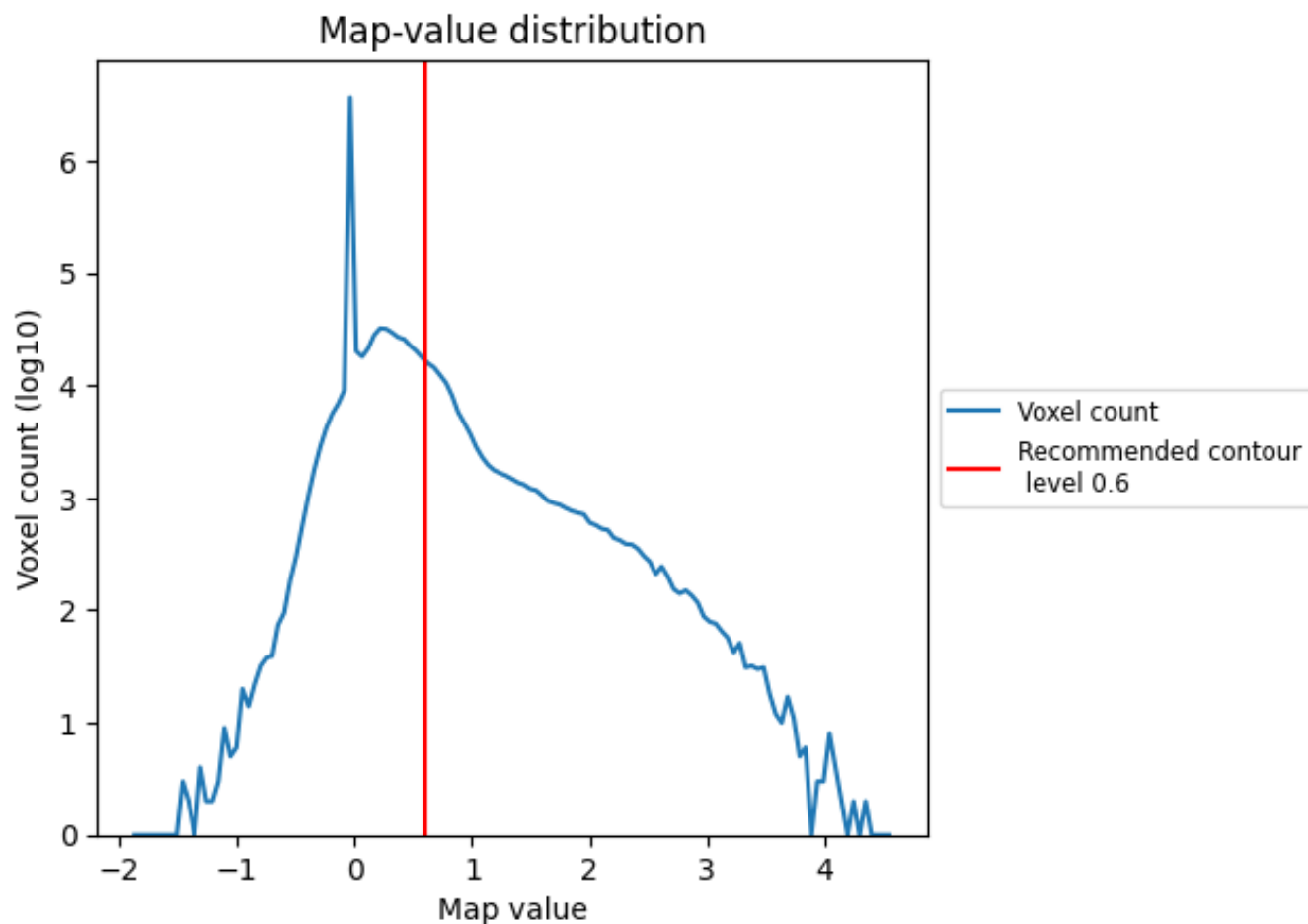
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

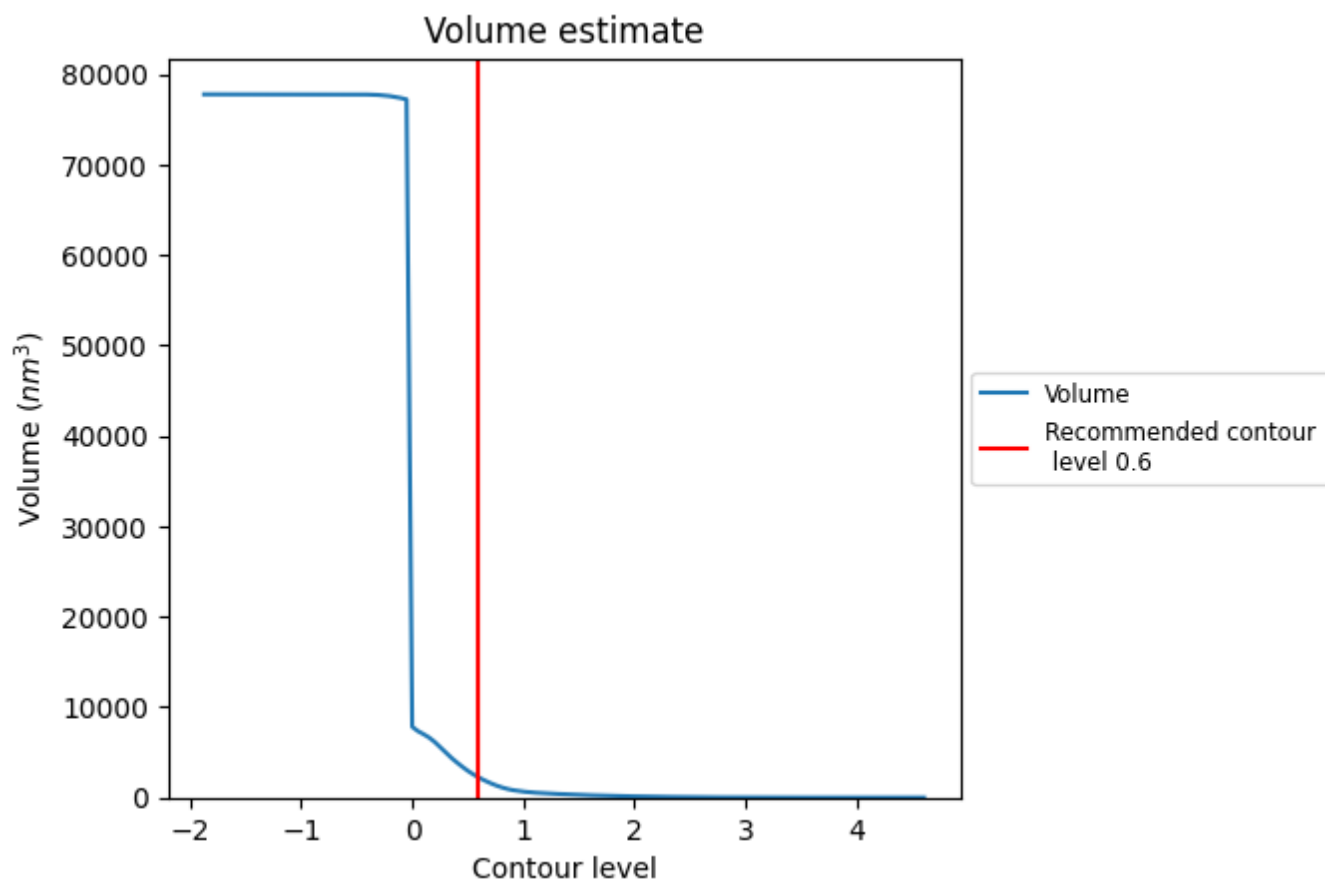
This section contains the results of statistical analysis of the map.

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.

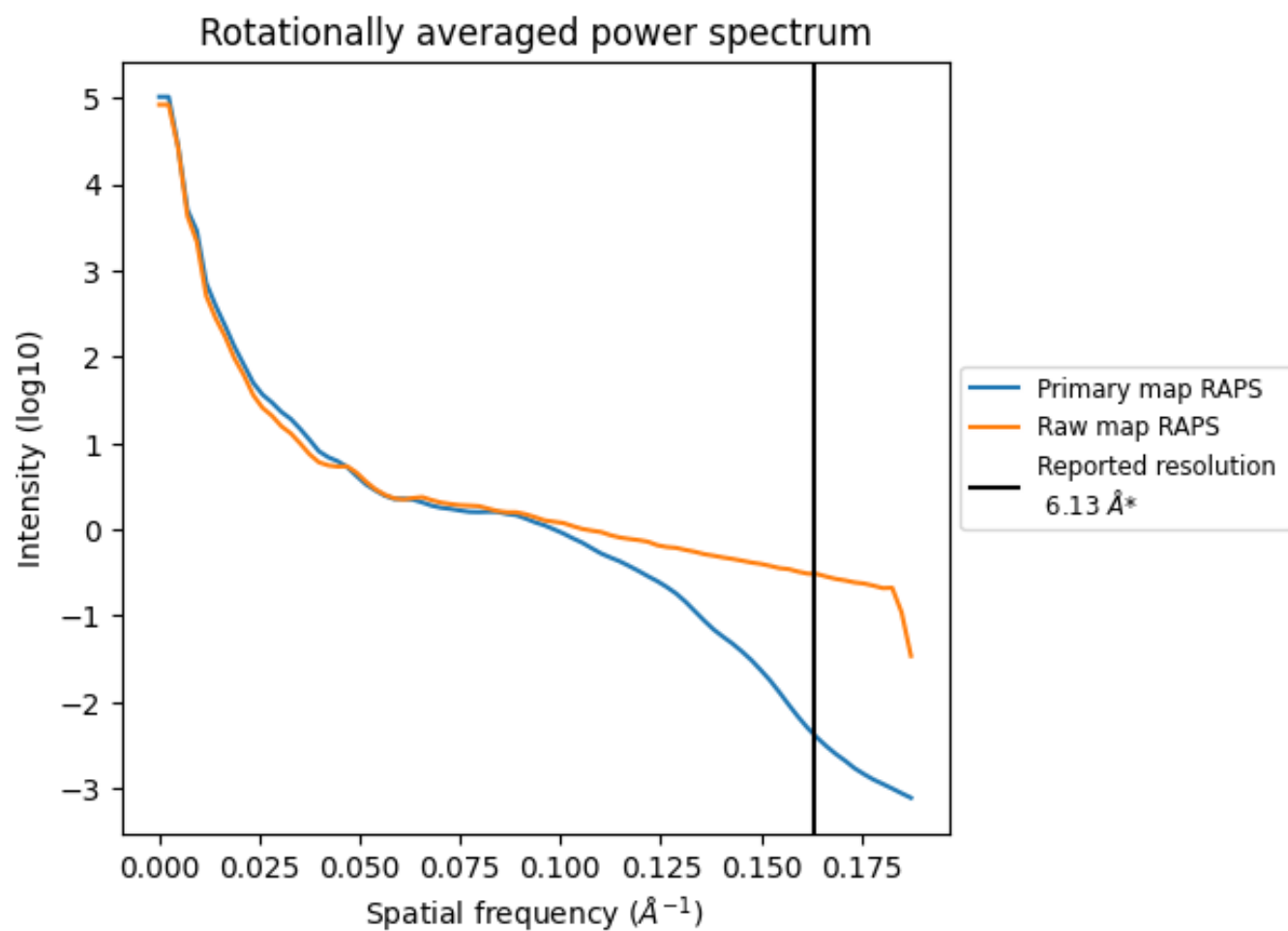
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2224 nm³; this corresponds to an approximate mass of 2009 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

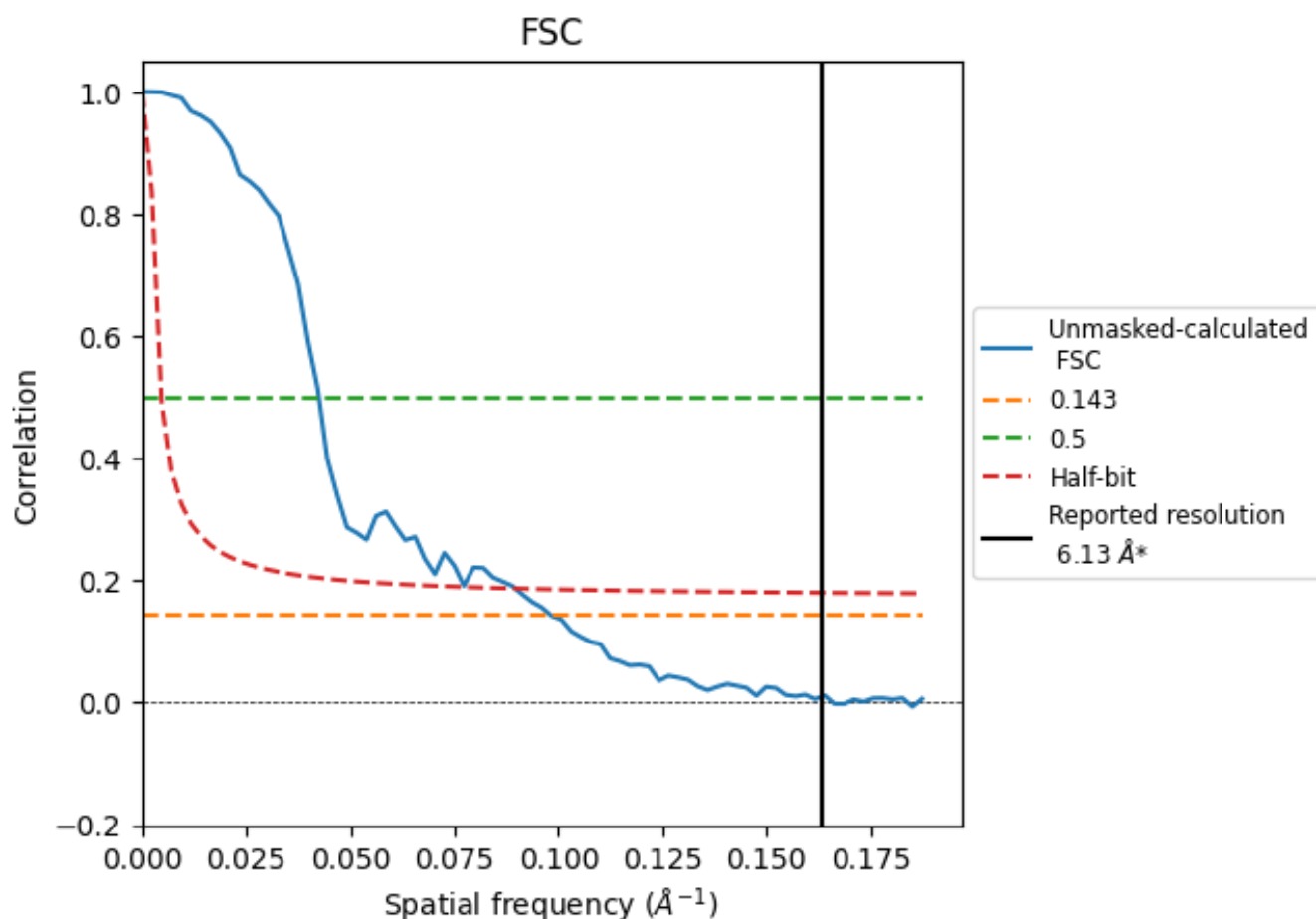


*Reported resolution corresponds to spatial frequency of 0.163 Å⁻¹

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 0.163 Å⁻¹

8.2 Resolution estimates [i](#)

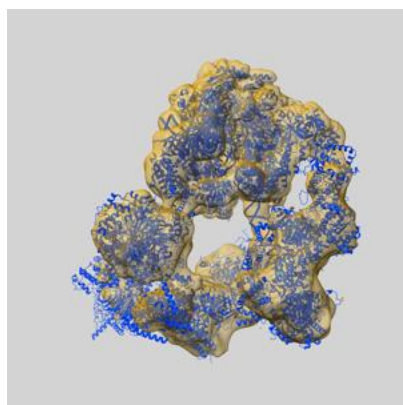
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.18	23.58	11.15

*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 10.18 differs from the reported value 6.13 by more than 10 %

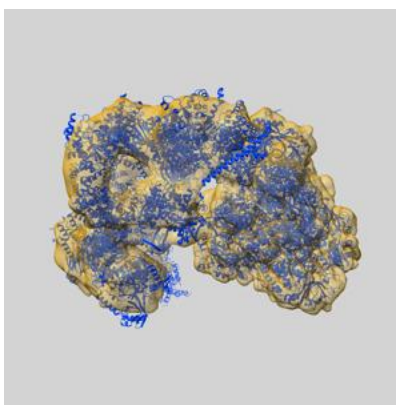
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37403 and PDB model 8WAS. Per-residue inclusion information can be found in section [3](#) on page [14](#).

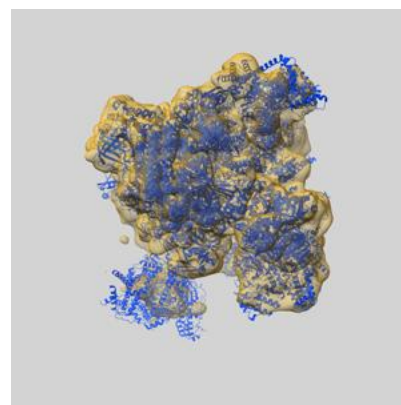
9.1 Map-model overlay [i](#)



X



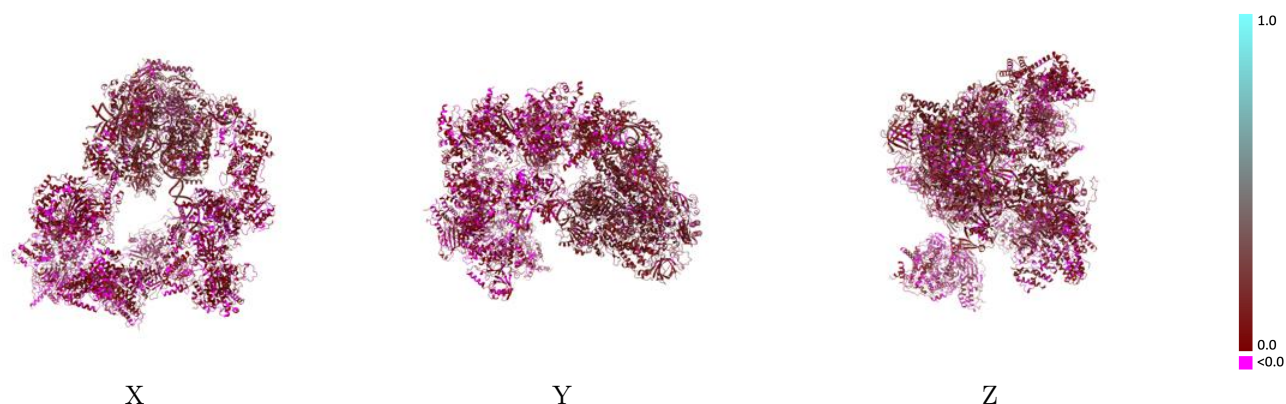
Y



Z

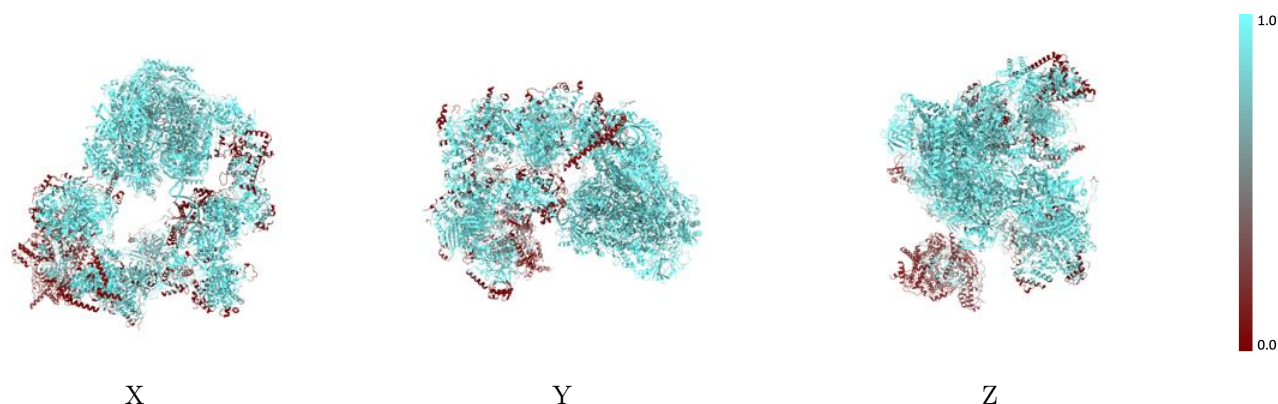
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



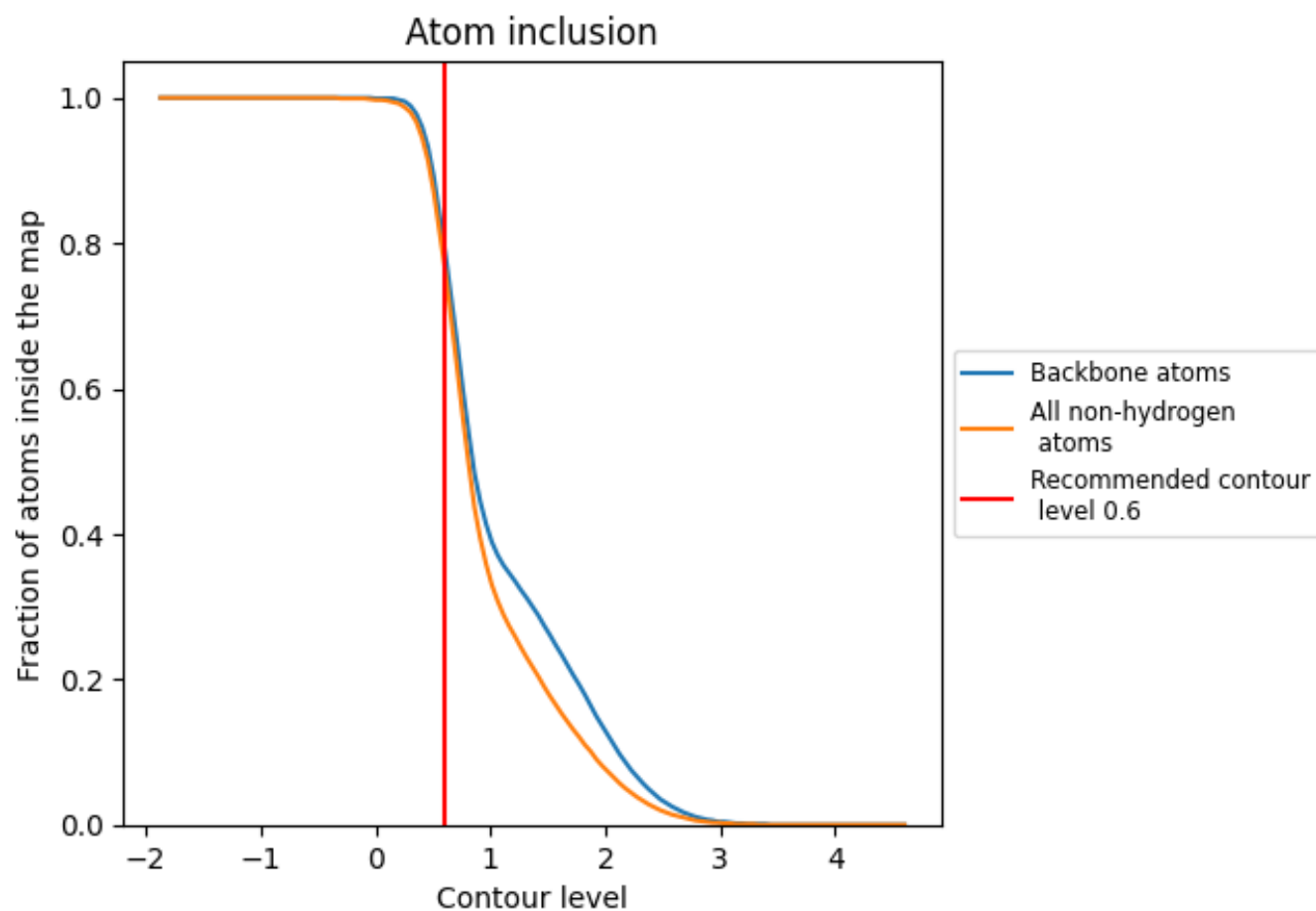
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.0780
0	 0.2180	 0.0490
1	 0.4880	 0.0340
2	 0.8890	 0.0600
3	 0.8670	 0.0390
4	 0.7470	 0.0500
5	 0.9220	 0.0350
6	 0.6130	 0.0360
7	 0.8020	 0.0560
A	 0.7020	 0.0360
B	 0.8850	 0.0410
D	 0.6520	 0.0410
E	 0.8140	 0.0450
F	 0.7730	 0.0350
G	 0.5140	 0.0270
H	 0.8490	 0.0370
I	 0.8800	 0.0340
J	 0.9580	 0.0360
L	 0.7500	 0.0550
N	 0.9840	 0.1640
O	 0.9510	 0.0860
P	 0.9710	 0.1170
Q	 0.9400	 0.0760
R	 0.9160	 0.1270
S	 0.9390	 0.0990
T	 0.9590	 0.1310
U	 0.9570	 0.0840
V	 0.9680	 0.1270
X	 0.9560	 0.1760
Y	 0.9060	 0.1510
Z	 0.9700	 0.1740
c	 0.2570	 0.0110
d	 0.1510	 0.0100
e	 0.2560	 0.0170
f	 0.5620	 0.0270



Continued on next page...

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Chain	Atom inclusion	Q-score
i	 0.2770	 0.0210
j	 0.1640	 0.0140
k	 0.1840	 0.0370
l	 0.1230	 0.0240
m	 0.1380	 0.0410
o	 0.9210	 0.1380
p	 0.9120	 0.1310
q	 0.9380	 0.1440
r	 0.9670	 0.1250
s	 0.9400	 0.1500
t	 0.9390	 0.1430
u	 0.9670	 0.1160
v	 0.9400	 0.1490
w	 0.9460	 0.1410
x	 0.9140	 0.1220
y	 0.9460	 0.1480
z	 0.9640	 0.1510