



wwPDB EM Validation Summary Report ⓘ

Aug 24, 2026 – 06:22 am BST

PDB ID : 8CEO / pdb_00008ceo
EMDB ID : EMD-16611
Title : Yeast RNA polymerase II transcription pre-initiation complex with core Mediator and the +1 nucleosome
Authors : Wang, H.; Cramer, P.
Deposited on : 2023-02-02
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

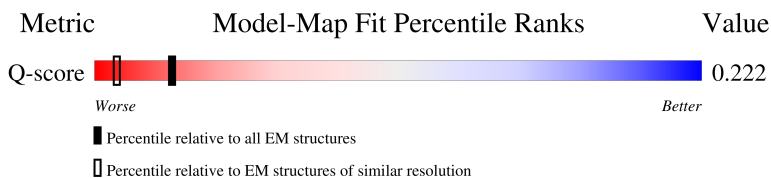
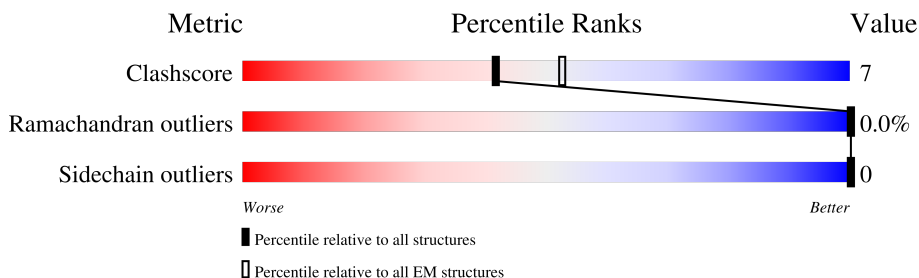
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal 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 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	778	80% 17% .
2	1	642	70% 11% 19%
3	2	513	76% 12% 12%
4	3	321	33% 7% 59%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	4	338	
6	5	72	
7	6	461	
8	7	843	
9	A	1733	
10	B	1224	
11	C	347	
12	D	221	
13	E	215	
14	F	155	
15	G	177	
16	H	146	
17	I	122	
18	J	70	
19	K	120	
20	L	70	
21	M	352	
22	N	209	
23	O	240	
24	Q	735	
25	R	400	
26	T	209	
27	U	286	
28	V	122	
29	W	492	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	X	328	
31	a	295	
32	b	223	
33	c	115	
34	d	687	
35	e	307	
36	f	210	
37	g	121	
38	h	284	
39	i	222	
40	j	149	
41	k	157	
42	l	1082	
43	m	220	
44	n	140	
45	o	127	
46	p	566	
47	r	135	
47	v	135	
48	s	102	
48	w	102	
49	t	129	
49	x	129	
50	u	125	
50	y	125	

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 113584 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 General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	752	Total	C	N	O	S	0	0
			6091	3882	1029	1142	38		

- Molecule 2 is a protein called TFB1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	522	Total	C	N	O	S	0	0
			4214	2660	734	798	22		

- Molecule 3 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	452	Total	C	N	O	S	0	0
			3647	2354	600	677	16		

- Molecule 4 is a protein called RNA polymerase II transcription factor B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	131	Total	C	N	O	S	0	0
			1089	692	180	209	8		

- Molecule 5 is a protein called General transcription and DNA repair factor IIIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	302	Total	C	N	O	S	0	0
			2338	1492	390	442	14		

- Molecule 6 is a protein called General transcription and DNA repair factor IIIH subunit TFB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	65	Total	C	N	O	S	0	0
			514	326	90	95	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	383	Total	C	N	O	S	0	0
			3019	1915	523	552	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	615	Total	C	N	O	S	0	0
			4954	3153	860	914	27		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1508	Total	C	N	O	S	0	0
			11815	7442	2042	2269	62		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	1180	Total	C	N	O	S	0	0
			9404	5946	1643	1760	55		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	266	Total	C	N	O	S	0	0
			2092	1315	348	416	13		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	initiating methionine	UNP P16370
C	-27	GLY	-	expression tag	UNP P16370
C	-26	SER	-	expression tag	UNP P16370
C	-25	HIS	-	expression tag	UNP P16370
C	-24	HIS	-	expression tag	UNP P16370
C	-23	HIS	-	expression tag	UNP P16370
C	-22	HIS	-	expression tag	UNP P16370
C	-21	HIS	-	expression tag	UNP P16370
C	-20	HIS	-	expression tag	UNP P16370
C	-19	SER	-	expression tag	UNP P16370

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	ASN	-	expression tag	UNP P16370
C	-17	SER	-	expression tag	UNP P16370
C	-16	GLY	-	expression tag	UNP P16370
C	-15	LEU	-	expression tag	UNP P16370
C	-14	ASN	-	expression tag	UNP P16370
C	-13	ASP	-	expression tag	UNP P16370
C	-12	ILE	-	expression tag	UNP P16370
C	-11	PHE	-	expression tag	UNP P16370
C	-10	GLU	-	expression tag	UNP P16370
C	-9	ALA	-	expression tag	UNP P16370
C	-8	GLN	-	expression tag	UNP P16370
C	-7	LYS	-	expression tag	UNP P16370
C	-6	ILE	-	expression tag	UNP P16370
C	-5	GLU	-	expression tag	UNP P16370
C	-4	TRP	-	expression tag	UNP P16370
C	-3	HIS	-	expression tag	UNP P16370
C	-2	GLU	-	expression tag	UNP P16370
C	-1	ASP	-	expression tag	UNP P16370
C	0	THR	-	expression tag	UNP P16370
C	1	GLY	-	expression tag	UNP P16370
C	2	SER	-	expression tag	UNP P16370
C	3	SER	-	expression tag	UNP P16370

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	167	Total	C	N	O	S	0	0
			1343	829	242	270	2		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	118	Total	C	N	O	S	0	0
			983	623	164	193	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	171	Total	C	N	O	S	0	0
			1339	861	222	248	8		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	HIS	-	expression tag	UNP P34087
G	173	HIS	-	expression tag	UNP P34087
G	174	HIS	-	expression tag	UNP P34087
G	175	HIS	-	expression tag	UNP P34087
G	176	HIS	-	expression tag	UNP P34087
G	177	HIS	-	expression tag	UNP P34087

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	140	Total	C	N	O	S	0	0
			1120	704	188	224	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 19 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	115	Total	C	N	O	S	0	0
			924	593	157	172	2		

- Molecule 20 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	45	Total	C	N	O	S	0	0
			359	221	71	63	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	310	Total	C	N	O	S	0	0
			2379	1504	408	449	18		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	346	LYS	-	expression tag	UNP P29055
M	347	HIS	-	expression tag	UNP P29055
M	348	HIS	-	expression tag	UNP P29055
M	349	HIS	-	expression tag	UNP P29055
M	350	HIS	-	expression tag	UNP P29055
M	351	HIS	-	expression tag	UNP P29055
M	352	HIS	-	expression tag	UNP P29055

- Molecule 22 is a DNA chain called Nontemplate DNA (209-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	209	Total	C	N	O	P	0	0
			4263	2035	761	1259	208		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	181	Total	C	N	O	S	0	0
			1422	925	243	248	6		

- Molecule 24 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	221	Total	C	N	O	S	0	0
			1871	1179	346	339	7		

- Molecule 25 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	268	Total	C	N	O	S	0	0
			2230	1409	392	419	10		

- Molecule 26 is a DNA chain called Template DNA (209-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	209	Total	C	N	O	P	0	0
			4300	2045	802	1245	208		

- Molecule 27 is a protein called TOA1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	107	Total	C	N	O	S	0	0
			885	559	147	176	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	104	Total	C	N	O	S	0	0
			815	511	136	164	4		

- Molecule 29 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	304	Total	C	N	O	S	0	0
			2473	1558	431	477	7		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	483	ALA	-	expression tag	UNP P36100
W	484	ALA	-	expression tag	UNP P36100
W	485	ALA	-	expression tag	UNP P36100
W	486	LEU	-	expression tag	UNP P36100
W	487	GLU	-	expression tag	UNP P36100
W	488	HIS	-	expression tag	UNP P36100
W	489	HIS	-	expression tag	UNP P36100
W	490	HIS	-	expression tag	UNP P36100
W	491	HIS	-	expression tag	UNP P36100
W	492	HIS	-	expression tag	UNP P36100

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	211	Total	C	N	O	S	0	0
			1708	1089	293	320	6		

- Molecule 31 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	178	Total	C	N	O	S	0	0
			1495	970	240	278	7		

- Molecule 32 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	172	Total	C	N	O	S	0	0
			1407	895	240	269	3		

- Molecule 33 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	111	Total	C	N	O	S	0	0
			902	566	154	178	4		

- Molecule 34 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	501	Total	C	N	O	S	0	0
			4063	2613	684	752	14		

- Molecule 35 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	256	Total	C	N	O	S	0	0
			2017	1280	336	390	11		

- Molecule 36 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	206	Total	C	N	O	S	0	0
			1578	998	266	309	5		

- Molecule 37 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	102	Total	C	N	O	S	0	0
			815	512	134	164	5		

- Molecule 38 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	171	Total	C	N	O	S	0	0
			1394	884	234	271	5		

- Molecule 39 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	181	Total	C	N	O	S	0	0
			1512	973	253	280	6		

- Molecule 40 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	102	Total	C	N	O	S	0	0
			852	533	156	162	1		

- Molecule 41 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	157	Total	C	N	O	S	0	0
			1259	777	222	257	3		

- Molecule 42 is a protein called Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	535	Total	C	N	O	S	0	0
			4385	2846	759	763	17		

- Molecule 43 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	130	Total	C	N	O	S	0	0
			1068	672	185	209	2		

- Molecule 44 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	136	Total	C	N	O	S	0	0
			1095	685	185	220	5		

- Molecule 45 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	110	Total	C	N	O	S	0	0
			922	607	143	166	6		

- Molecule 46 is a protein called Mediator of RNA polymerase II transcription subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	225	Total	C	N	O	S	0	0
			1863	1193	298	366	6		

- Molecule 47 is a protein called Histone H3.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	97	Total	C	N	O	S	0	0
			801	506	155	138	2		
47	v	98	Total	C	N	O	S	0	0
			810	512	157	139	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
r	102	ALA	GLY	conflict	UNP P84233
r	110	ALA	CYS	engineered mutation	UNP P84233
v	102	ALA	GLY	conflict	UNP P84233
v	110	ALA	CYS	engineered mutation	UNP P84233

- Molecule 48 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	82	Total	C	N	O	S	0	0
			653	412	127	113	1		
48	w	80	Total	C	N	O	S	0	0
			638	401	125	111	1		

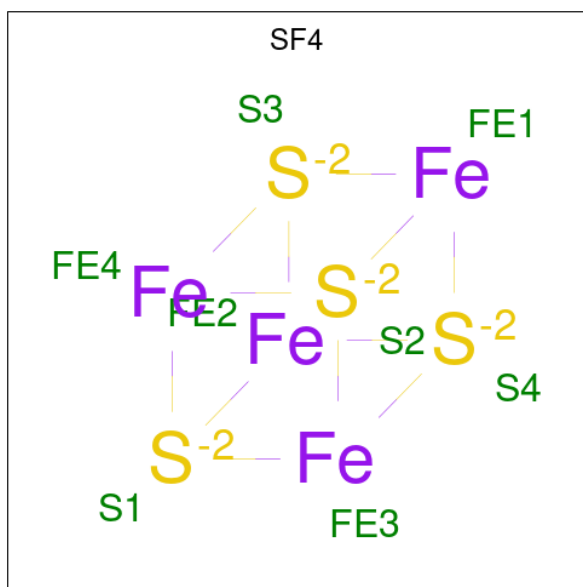
- Molecule 49 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	t	109	Total	C	N	O	0	0
			843	531	167	145		
49	x	106	Total	C	N	O	0	0
			818	516	160	142		

- Molecule 50 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	97	Total	C	N	O	S	0	0
			767	481	142	142	2		
50	y	95	Total	C	N	O	S	0	0
			745	469	134	140	2		

- Molecule 51 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
51	0	1	Total	Fe	S	0
			8	4	4	

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	2	Total	Zn	0
			2	2	
52	4	1	Total	Zn	0
			1	1	
52	6	4	Total	Zn	0
			4	4	
52	A	2	Total	Zn	0
			2	2	
52	B	1	Total	Zn	0
			1	1	
52	C	1	Total	Zn	0
			1	1	
52	I	2	Total	Zn	0
			2	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	J	1	Total 1	Zn 1	0
52	L	1	Total 1	Zn 1	0
52	M	1	Total 1	Zn 1	0
52	W	1	Total 1	Zn 1	0

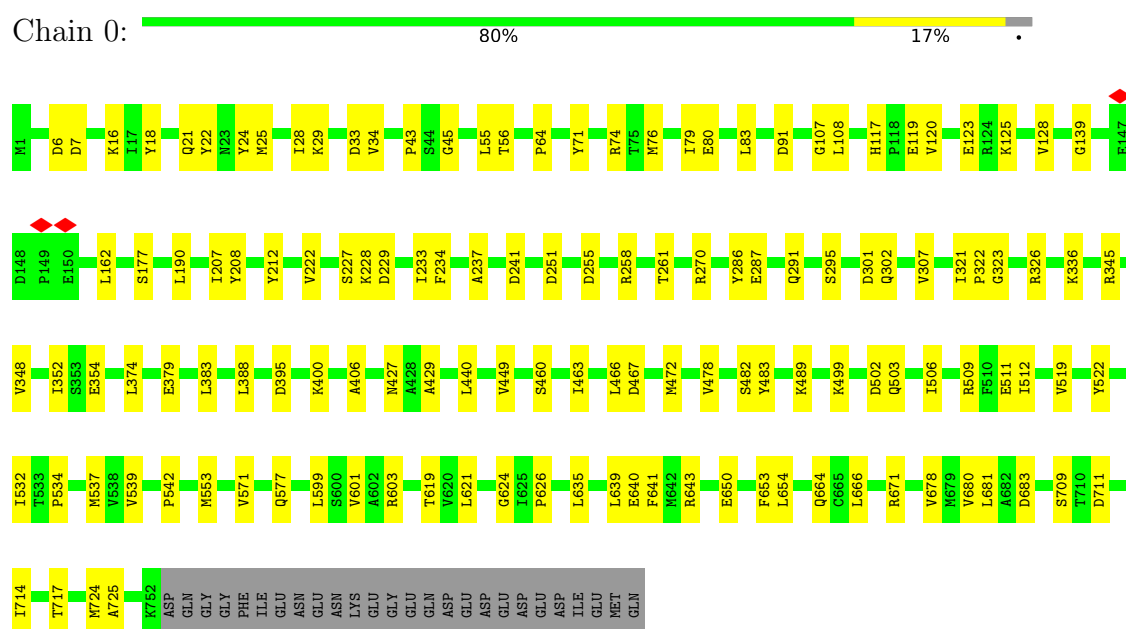
- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	A	1	Total 1	Mg 1	0

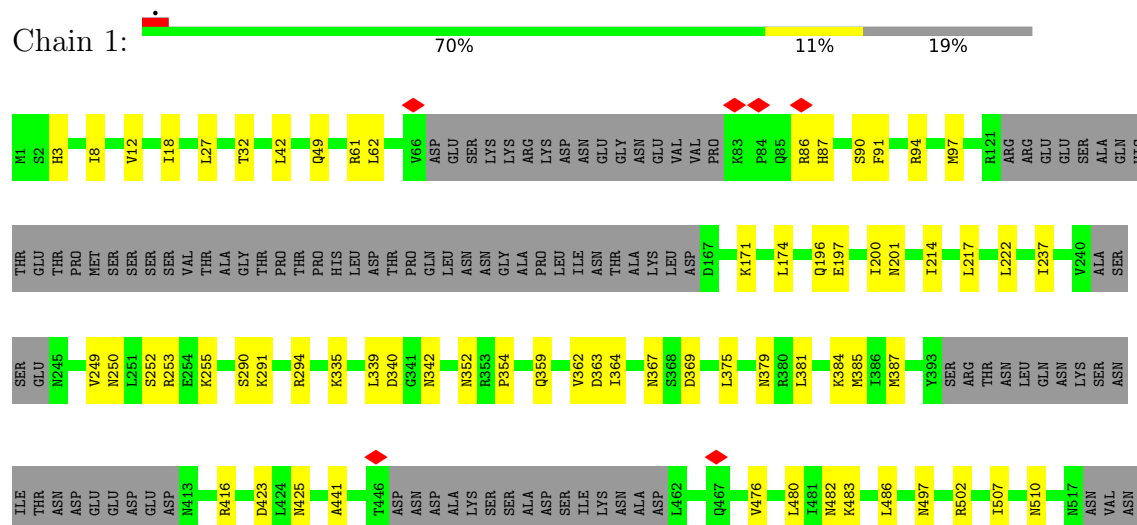
3 Residue-property plots

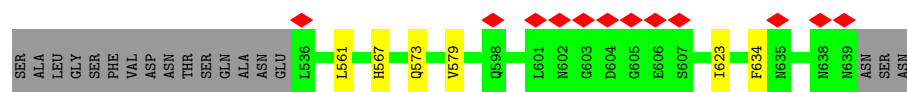
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: General transcription and DNA repair factor IIH helicase subunit XPD



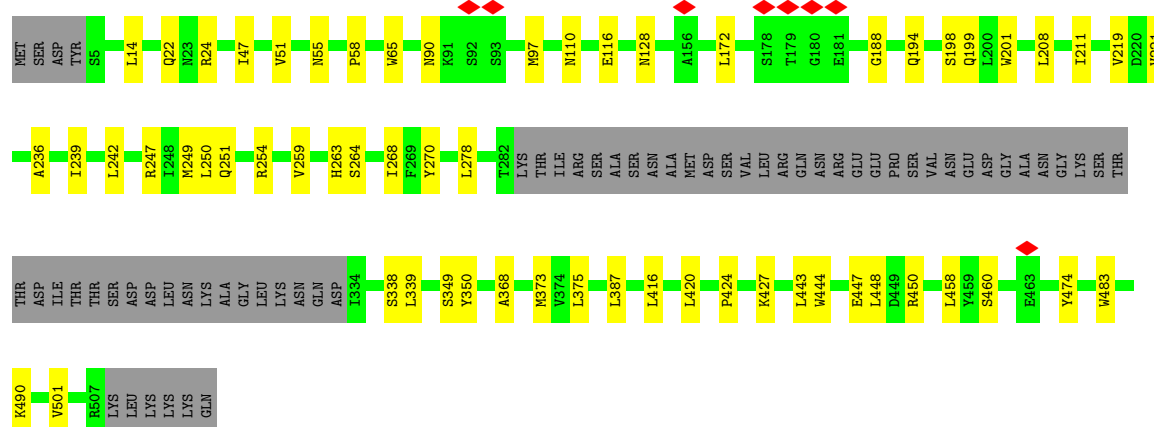
- Molecule 2: TFB1 isoform 1





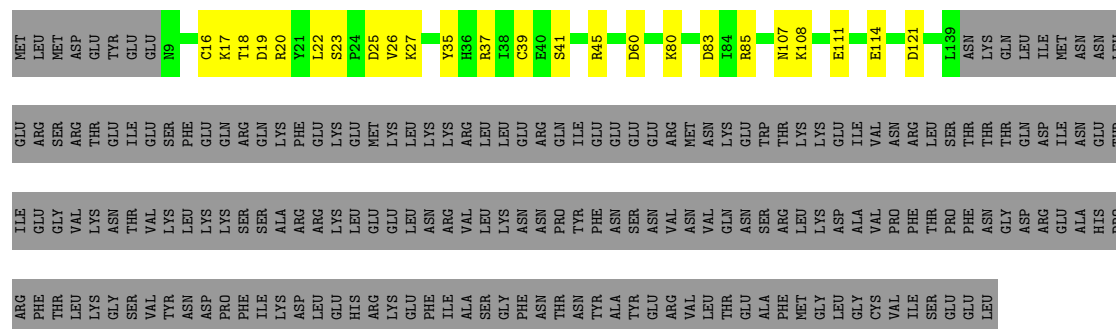
• Molecule 3: RNA polymerase II transcription factor B subunit 2

Chain 2: 76% 12% 12%



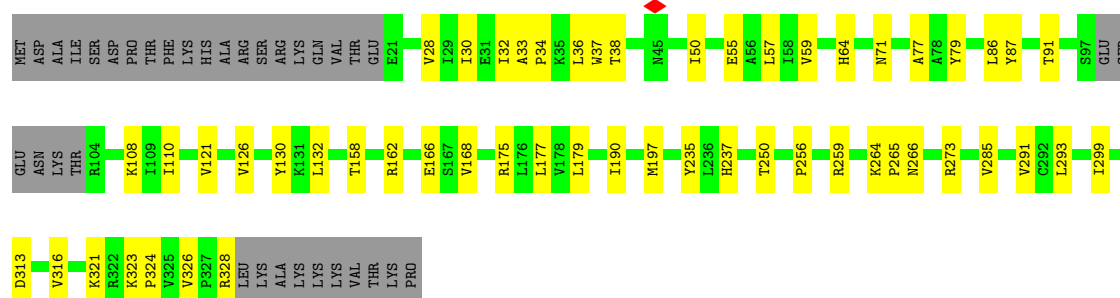
• Molecule 4: RNA polymerase II transcription factor B subunit 3

Chain 3: 33% 7% 59%



• Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

Chain 4: 73% 16% 11%



• Molecule 6: General transcription and DNA repair factor IIH subunit TFB5

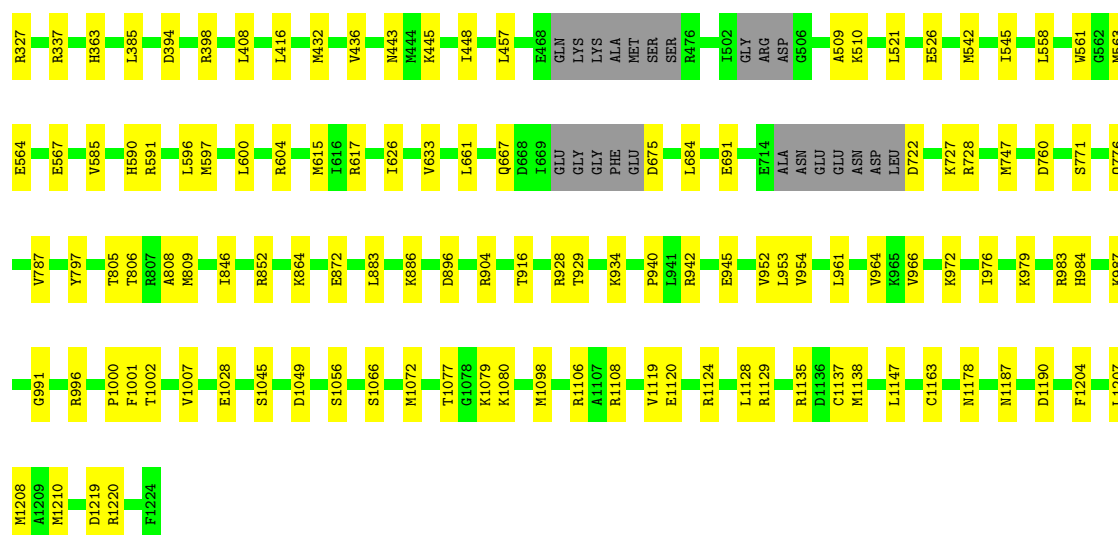
Amino Acid	Relative Abundance (%)
MET	100
A2	85
R5	75
D13	65
K17	55
D29	45
I30	35
V31	25
L32	15
L35	10
D36	5
D37	5
L40	5
L41	5
M66	5
ASP	5
GLU	5
GIU	5
GLU	5
ASN	5
GLN	5

Chain 6: 69% 14% 17%

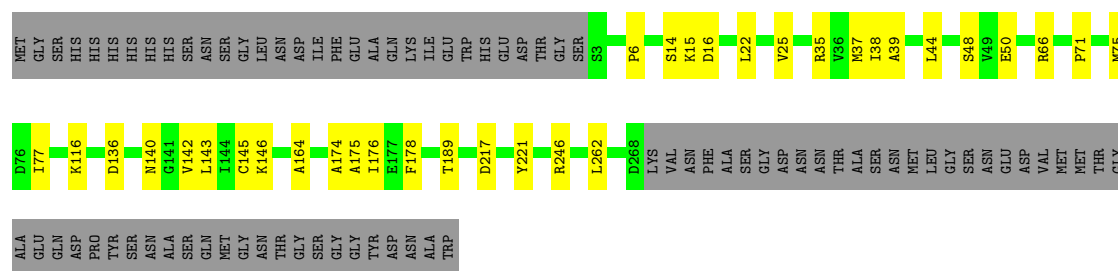
K397	F398	R399	D402	S405	C406	R409	F410	P411	L412	L413	H416	K417	M418	G419	K420	L421	L422	Y427	K433	V459	ILE	THR																												
R200	K205	G206	Q211	M216	L220	L221	R230	T234	G237	S238	L239	D246	V263	L266	T290	L291	L297	P325	T326	E330	D331	T332	P333	C338	H339	L342	Y347	N351	K365	L376	A377	Y380	F389	T394																
ARG	LEU	PRO	ASN	VAL	ASN	LEU	GLN	GLY	SER	GLU	ASP	GLY	GLY	ASP	GLN	LYS	GLN	VAL	HIS	PHE	ASP	GLY	GLY	GLY	ASP	ASP	ARG	VAL	ASP	GLN	GLN	GLN	HIS	SER	SER	SER	HIS	ARG	ASP	ARG	ASP	LYS	HIS	VAL	GLN	ARG	LYS	LYS	LYS	LYS

Chain 7: 58% 15% 27%

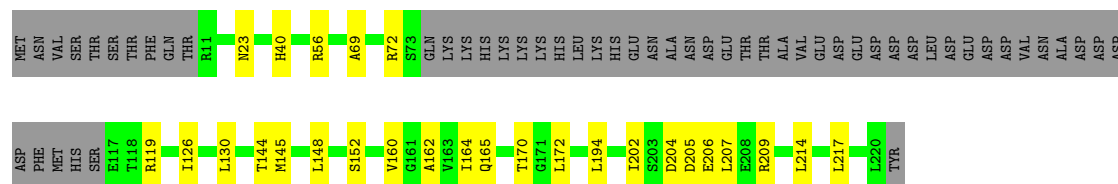
ARG	PHE	S679	R519	I382	GLN	THR	THR	MET
LYS	Q682	L527	L527	E367	GLN	GLY	GLY	THR
SER	N528	F529	N528	K372	LEU	ASP	LEU	ASP
ALA	Q685	L530	L530	R380	GLN	GLU	LYS	VAL
VAL	L687	L535	L535	S331	THR	PRO	PRO	GLY
ARG	G688	G689	G688	I383	ALA	GLN	ARG	TYR
GLY	R689	A538	A538	L386	LYS	LYS	LYS	PRO
GLY	R692	E542	E542	G389	PRO	ALA	SER	LYS
SER	A703	K546	K546	T393	THR	ASP	SER	GLY
LEU	L708	V552	V552	I397	ASN	ALA	GLY	LYS
GLY	K711	F665	F665	T398	VAL	THR	ARG	LYS
ALA	D712	V666	V666	K405	VAL	HIS	ILE	LYS
GLY	M716	Q667	Q667	V409	ASN	ALA	ALA	PHE
GLY	Q668	E568	E568	Q423	ASP	ASP	ASP	SER
ASP	K721	R722	R722	F438	VAL	ASP	ASP	PRO
MET	R722	A574	A574	T439	GLU	ASP	ASP	ASP
ALA	R722	M583	M583	S440	GLY	GLY	ASP	MET
TYR	V735	C591	C591	K443	GLY	GLY	ASP	ASP
MET	H738	Q592	Q592	Q447	GLY	GLY	ASP	ASP
GLU	N747	L748	L748	V454	GLY	GLY	ASP	ASP
SER	L748	A751	A751	T456	GLY	GLY	ASP	ASP
THR	A751	R601	R601	V460	GLY	GLY	ASP	ASP
ASN	L760	G602	G602	I486	GLY	GLY	ASP	ASN
LYS	N767	D603	D603	V490	GLY	GLY	ASP	ASN
GLY	H830	L832	L832	A495	GLY	GLY	ASP	ASN
THR	P831	L832	L832	A496	GLY	GLY	ASP	ASN
ASN	L832	P831	P831	A497	GLY	GLY	ASP	ASN
LYS	L832	F626	F626	F498	GLY	GLY	ASP	ASN
GLY	L832	R636	R636	R499	GLY	GLY	ASP	ASN
GLY	L832	L654	L654	R500	GLY	GLY	ASP	ASN
GLY	L832	T660	T660	I505	GLY	GLY	ASP	ASN
GLY	L832	A615	A615	T514	GLY	GLY	ASP	ASN
GLY	L832	L673	L673	T516	GLY	GLY	ASP	ASN
GLY	L832	H151	H151	L517	GLY	GLY	ASP	ASN
GLY	L832	V578	V578	L518	GLY	GLY	ASP	ASN
GLY	L832	L518	L518	L519	GLY	GLY	ASP	ASN
GLY	L832	L519	L519	L520	GLY	GLY	ASP	ASN
GLY	L832	L520	L520	L521	GLY	GLY	ASP	ASN
GLY	L832	L521	L521	L522	GLY	GLY	ASP	ASN
GLY	L832	L522	L522	L523	GLY	GLY	ASP	ASN
GLY	L832	L523	L523	L524	GLY	GLY	ASP	ASN
GLY	L832	L524	L524	L525	GLY	GLY	ASP	ASN
GLY	L832	L525	L525	L526	GLY	GLY	ASP	ASN
GLY	L832	L526	L526	L527	GLY	GLY	ASP	ASN
GLY	L832	L527	L527	L528	GLY	GLY	ASP	ASN
GLY	L832	L528	L528	L529	GLY	GLY	ASP	ASN
GLY	L832	L529	L529	L530	GLY	GLY	ASP	ASN
GLY	L832	L530	L530	L531	GLY	GLY	ASP	ASN
GLY	L832	L531	L531	L532	GLY	GLY	ASP	ASN
GLY	L832	L532	L532	L533	GLY	GLY	ASP	ASN
GLY	L832	L533	L533	L534	GLY	GLY	ASP	ASN
GLY	L832	L534	L534	L535	GLY	GLY	ASP	ASN
GLY	L832	L535	L535	L536	GLY	GLY	ASP	ASN
GLY	L832	L536	L536	L537	GLY	GLY	ASP	ASN
GLY	L832	L537	L537	L538	GLY	GLY	ASP	ASN
GLY	L832	L538	L538	L539	GLY	GLY	ASP	ASN
GLY	L832	L539	L539	L540	GLY	GLY	ASP	ASN
GLY	L832	L540	L540	L541	GLY	GLY	ASP	ASN
GLY	L832	L541	L541	L542	GLY	GLY	ASP	ASN
GLY	L832	L542	L542	L543				



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



- Molecule 12: DNA-directed RNA polymerase II subunit RPB4

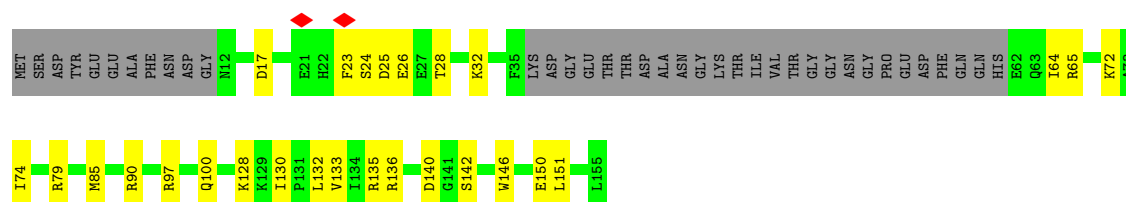


- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC1



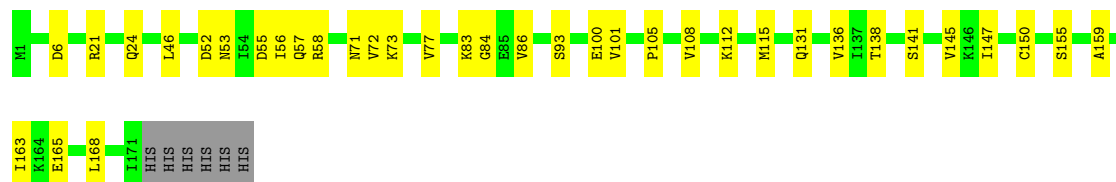
- Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC2





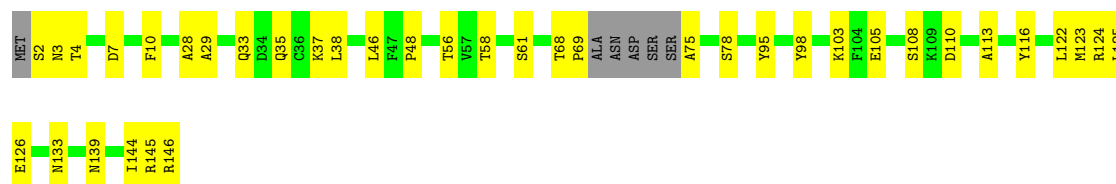
- Molecule 15: DNA-directed RNA polymerase II subunit RPB7

Chain G: 76% 20% .



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

Chain H: 70% 26% .



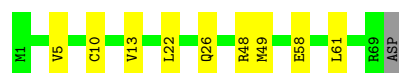
- Molecule 17: DNA-directed RNA polymerase II subunit RPB9

Chain I: 75% 20% 5% .



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

Chain J: 86% 13% .



- Molecule 19: DNA-directed RNA polymerase II subunit RPB11

Chain K: 88% 8% .



- Molecule 20: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  51% 13% 36%

MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN ALA LEU ASP ALA ALA ALA GLY THR SER GLN ARG ALA THR ALA T26 Y29 I30 C31 C34 V46 L56 L64 F65 Q66 F67 F68 A69 R70

• Molecule 21: Transcription initiation factor IIB

Chain M:  74% 14% 12%

MET MET THR ARG GLU SER ILE ASP LYS THR ALA ALA GLY ARG R14 I20 V21 L22 E26 R37 E40 V43 V44 I213 I212 L214 R215 D58 ARG SER GLU TRP ARG THR PHE SER ASN ASP ASP HIS ASN ASP GLY ASP PRO SER R78 L92 A113 N117 K121 I133 A140 E160 M172 C180 R181 V185 A186 R187 T188 E191 L195 K199 E202 K205 N212 I213 L214 R215 S231 G232 A233 Q234 S244 T259 I269 P274 V280 S281 N285 Q303 G312 Y313 L316 L323 V324 P326 Q327 P340 G341 V342 GLU LYS LYS LYS HIS HIS HIS HIS HIS HIS

• Molecule 22: Nontemplate DNA (209-MER)

Chain N:  33% 84% 16%

A-73 G-65 A-59 T-58 T-42 G-39 A-38 T-26 G-25 C-15 A-14 T-13 A-12 A1 T2 A3 T8 T9 C10 T11 G12 C13 G14 G17 T18 G19 T20 T21 G22 G23 T24 C25 G26 T27 A30 C31 A32 G33 C34 T35 C36 T37 C40 A41 C42 C43 G44 C45 T46 T47 A48 A49 A50 C51 G52 C53 A54 C55 G56 T57 A58 C59 C68 C69 C70 G89 G90 C100 T104 C105 T106 C107 A109 G110 G111 C112 A113 C114 G115 G116 T117 T118 C119 T123 A124 T125 A126 T127 A128 C129 A130 T131 C132 G133 A134 T135

• Molecule 23: TATA-binding protein

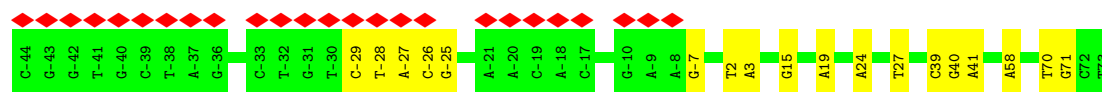
Chain O:  62% 14% 25%

MET ALA ASP GLU ARG GLU LEU LYS GLU PHE THR LYS GLU ALA ASN LYS ILE VAL PHE ASP PRO ASN THR ARG GLN VAL TRP GLU ASN GLN ASN SER ARG ASP GLY THR LYS PRO ALA THR THR PHE GLN SER GLY LEU ASP ILE LYS ARG ALA PRO GLU SER LYS ASP THR ALA T60 V74 T75 L76 L82 V85 H88 K97 R105 I106 R107 E108 P109 M121 Y139 I143 I146 G147 F148 A149 A150 I157 Q158 N159 I160 L172 G180 S183 S184 Y185 L193 M197 L204 L205 V208 V213 L214 I230 L234 M240

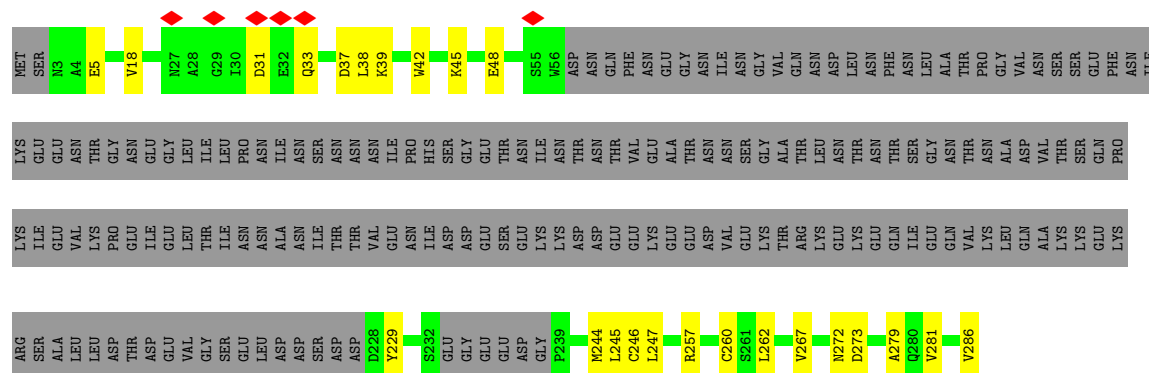
• Molecule 24: Transcription initiation factor IIF subunit alpha

Chain Q:  24% 6% 70%

MET SER ARG ASN PRO PRO GLY SER ASN ASN GLY GLY THR M17 D25 R35 MET GLY GLN ASN GLY SER ASN F148 SER SER SER PRO GLY VAL THR PRO ASN GLY ASP ASN SER ARG GLY SER LEU VAL LYS LYS ASP ASP PRO GLU THR ALA GLU ARG GLU ARG LYS MET LEU



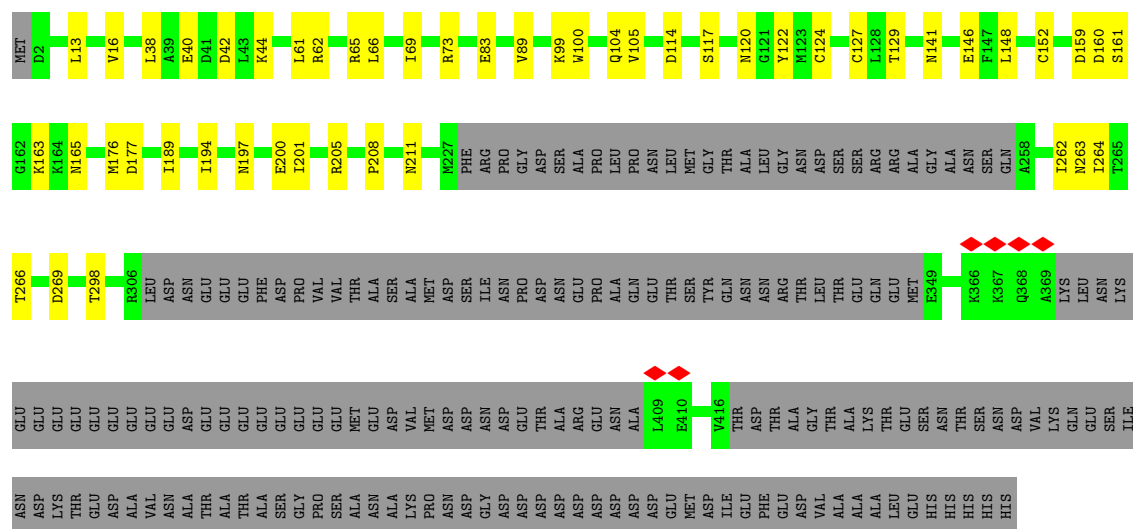
• Molecule 27: TOA1 isoform 1



• Molecule 28: Transcription initiation factor IIA subunit 2

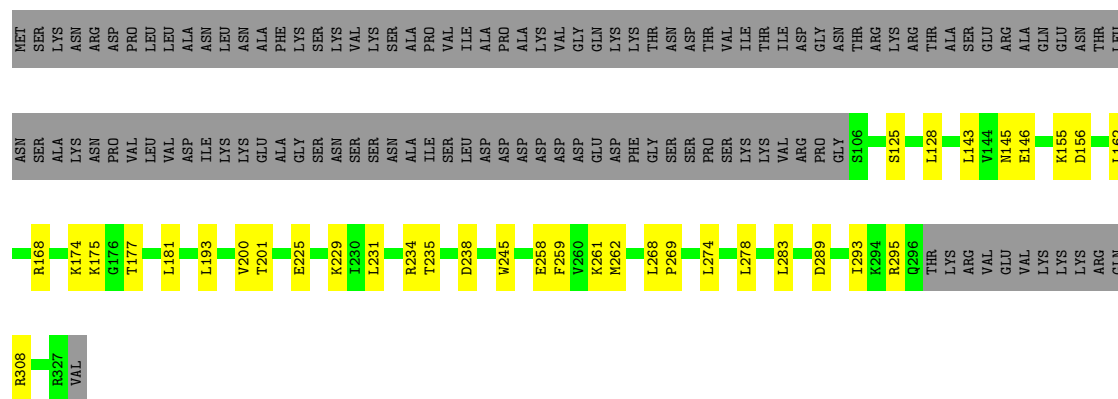


• Molecule 29: Transcription initiation factor IIE subunit alpha

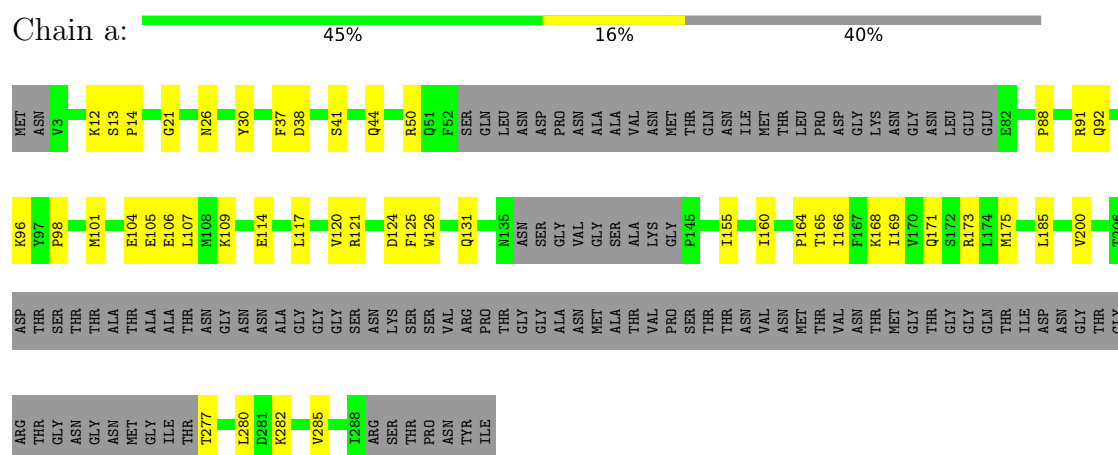


• Molecule 30: Transcription initiation factor IIE subunit beta

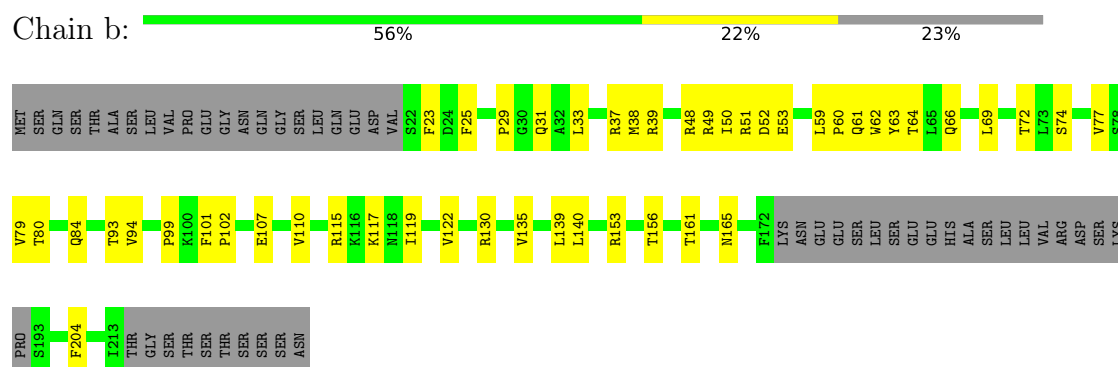




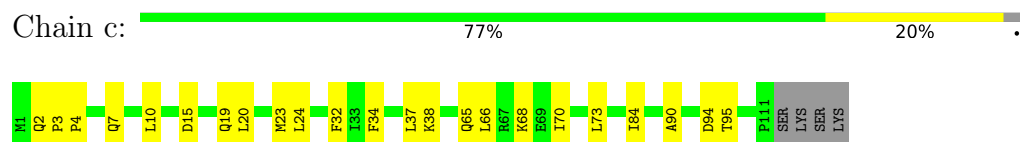
- Molecule 31: Mediator of RNA polymerase II transcription subunit 6



- Molecule 32: Mediator of RNA polymerase II transcription subunit 8

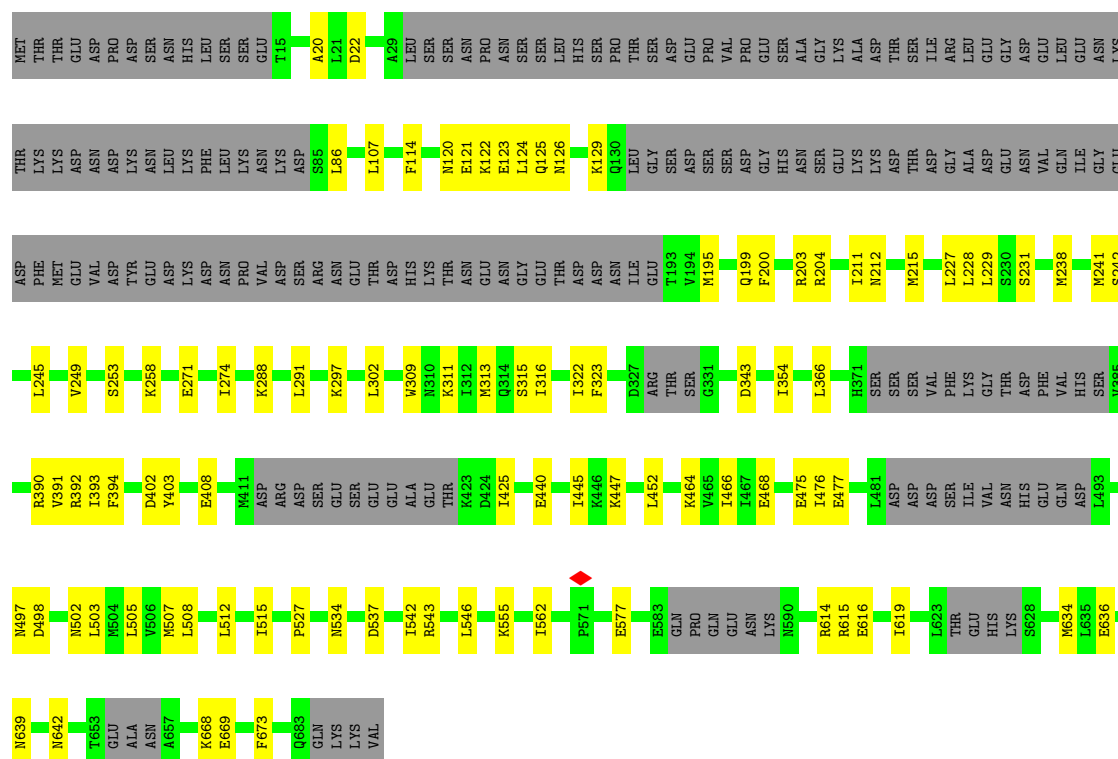


- Molecule 33: Mediator of RNA polymerase II transcription subunit 11



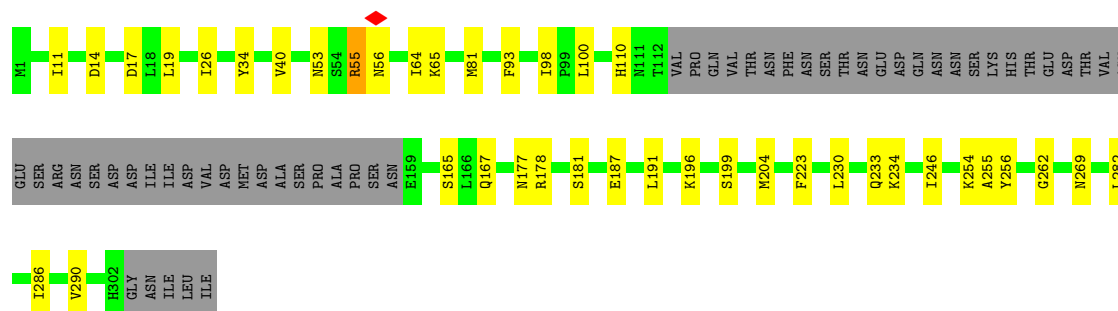
- Molecule 34: Mediator of RNA polymerase II transcription subunit 17

Chain d:  59% 14% 27%



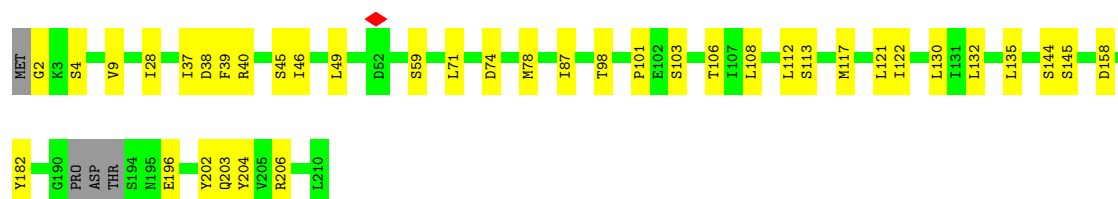
• Molecule 35: Mediator of RNA polymerase II transcription subunit 18

Chain e:  70% 13% 17%



• Molecule 36: Mediator of RNA polymerase II transcription subunit 20

Chain f:  80% 18%



• Molecule 37: Mediator of RNA polymerase II transcription subunit 22

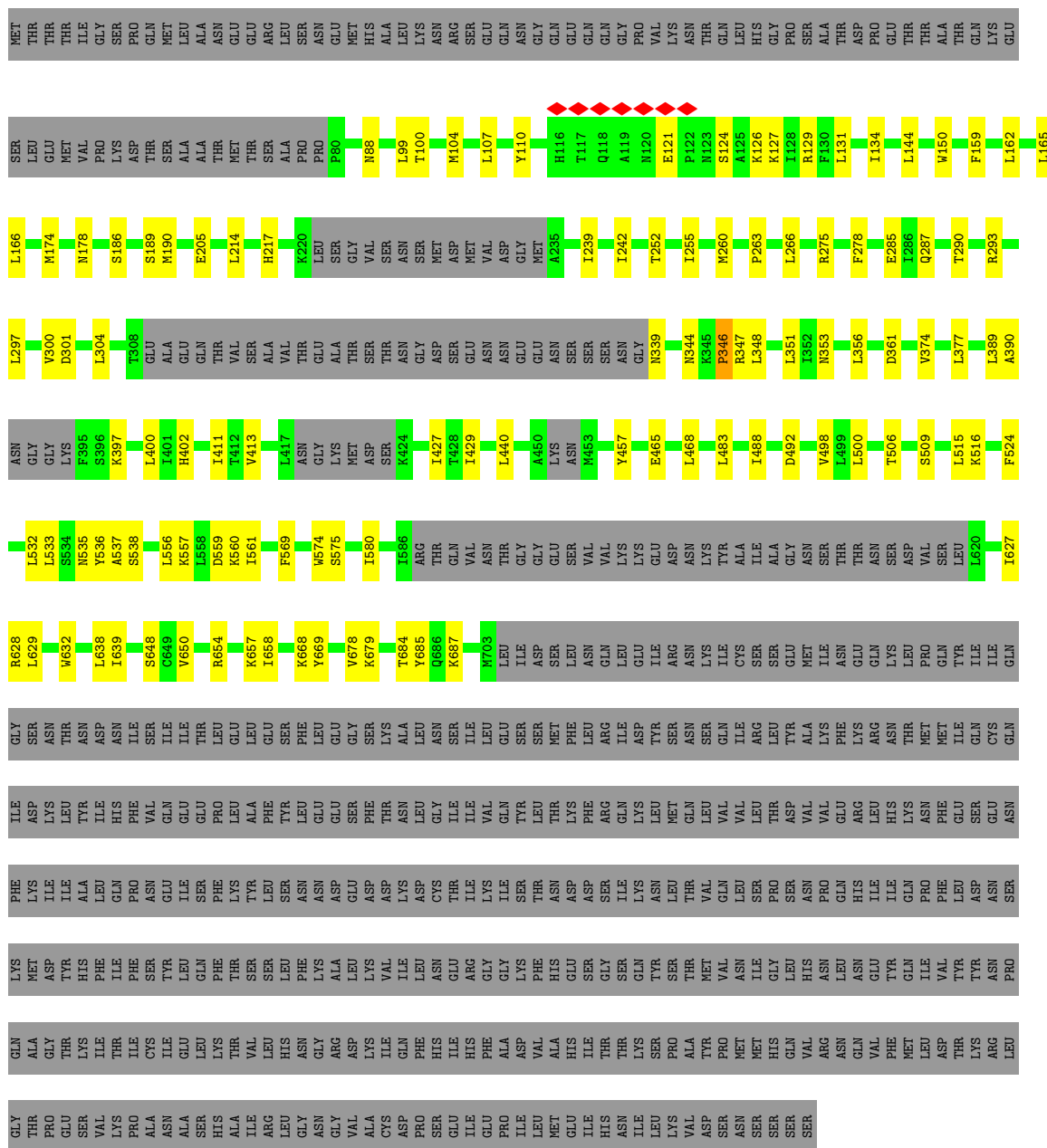
T97	E118	LYS	THR	THR	MET	S2	N3	Q4	L10	E11	Q12	T15	K20	E23	M27	D52	ARG	ASN	ASP	ASP	ASP	GLU	GLY	SER	PHE	A42	N45	T52	T53	S54	V55	H56	N60	Q61	T62	M63	Q64	L65	L66	K67	L73	T74	L75	M83	L84	V90	THR	GLU	HIS	SER	LYS	VAL
-----	------	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- | Amino Acid | Position |
|------------|----------|
| PHE | L107 |
| ASP | K110 |
| GLY | T111 |
| THR | R112 |
| ALA | K113 |
| LYS | C121 |
| GLU | L125 |
| VAL | L131 |
| ASP | R145 |
| ASN | Y156 |
| THR | L160 |
| LYS | L193 |
| GLU | P207 |
| ASN | GLY |
| ASN | GLU |
| ASP | GLU |
| ASP | ALA |
| ASP | ALA |
| LEU | GLU |
| ASP | GLU |
| LEU | THR |
| ASP | GLU |
| ASP | VAL |
| ASP | PRO |
| PHE | VAL |
| ASP | PRO |
| PRO | PRO |
| ASP | SER |
| ASP | GLN |
| PHE | SER |
| | GLU |
| | GLN |
| | GLY |
| | GLN |
| | MET |
| | ALA |
| | LYS |
| | LYS |
| | GLU |
| | GLY |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | ASP |
| | GLU |
| | GLY |
| | THR |
| | PRO |
| | LYS |
| | ASP |
| | SER |
| | GLU |
| | ASP |
| | THR |
| | ASN |
| | SER |
| | THR |
| | ASN |
| | SER |
| | THR |
| | ALA |
| | GLU |
| | GLU |
| | ASP |
| | LYS |
| | L37 |
| | S38 |
| | Q41 |
| | C47 |
| | L56 |
| | V57 |
| | V60 |
| | D61 |
| | R62 |
| | L73 |
| | N83 |
| | Y90 |
| | D91 |
| | N92 |
| | I93 |
| | Y94 |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |
| | LYS |
| | THR |
| | PRO |
| | LYS |
| | THR |
| | ASP |
| | SER |
| | PHE |
| | THR |

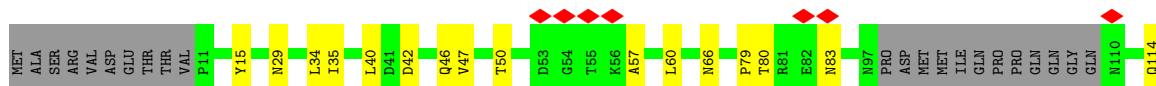
- [illegible]

- [illegible]

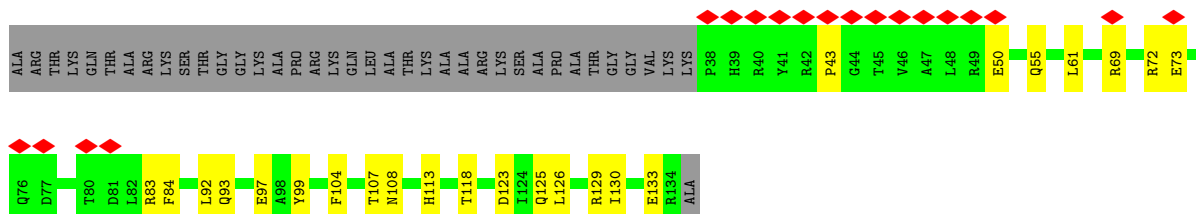
-



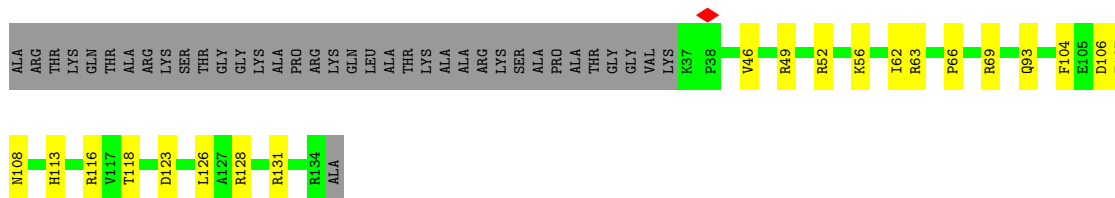
- Molecule 43: Mediator of RNA polymerase II transcription subunit 19



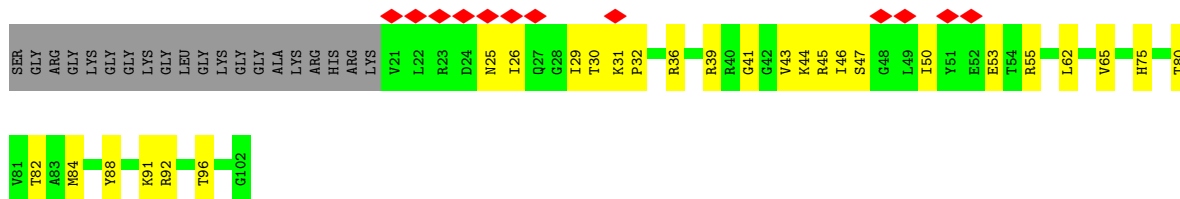
- Molecule 47: Histone H3.2



- Molecule 47: Histone H3.2



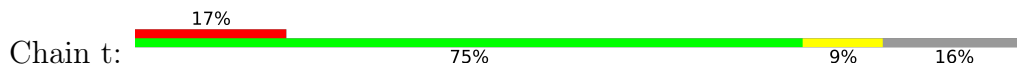
- Molecule 48: Histone H4



- Molecule 48: Histone H4

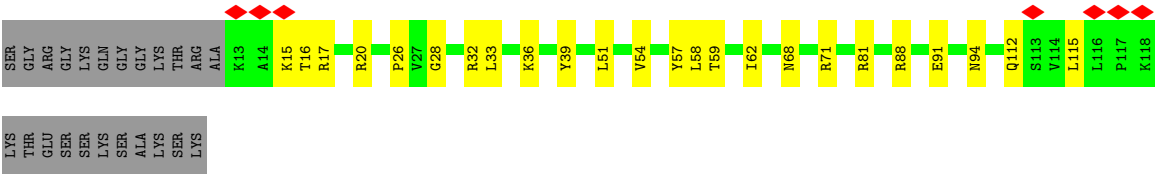


- Molecule 49: Histone H2A

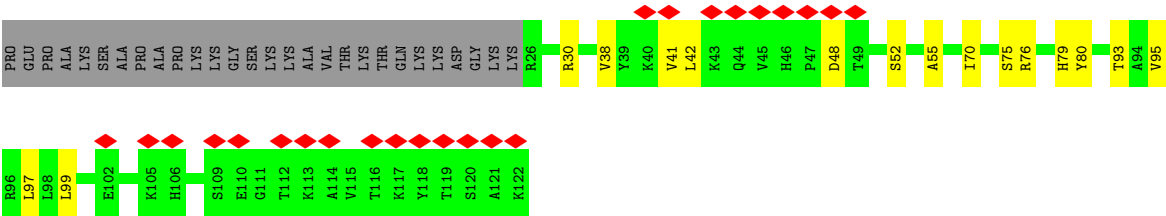


SER
LYS
SER
SER
LYS
LYS
SER
SER
ALA
LYS
SER
LYS

● Molecule 49: Histone H2A



● Molecule 50: Histone H2B



● Molecule 50: Histone H2B



K122

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.234	Depositor
Minimum map value	-0.121	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.16	0/6209	0.34	0/8384
2	1	0.14	0/4277	0.33	0/5755
3	2	0.17	0/3717	0.42	0/5028
4	3	0.13	0/1109	0.36	0/1492
5	4	0.16	0/2377	0.35	0/3216
6	5	0.20	0/520	0.51	0/701
7	6	0.16	0/3082	0.39	0/4165
8	7	0.16	0/5059	0.35	0/6841
9	A	0.20	0/12048	0.37	0/16321
10	B	0.22	0/9589	0.36	0/12934
11	C	0.23	0/2130	0.36	0/2887
12	D	0.14	0/1351	0.37	0/1811
13	E	0.19	0/1788	0.45	2/2406 (0.1%)
14	F	0.22	0/1001	0.44	0/1347
15	G	0.18	0/1367	0.44	0/1844
16	H	0.20	0/1139	0.40	0/1544
17	I	0.19	0/962	0.43	0/1295
18	J	0.25	0/578	0.43	0/775
19	K	0.23	0/942	0.44	0/1272
20	L	0.23	0/361	0.49	0/478
21	M	0.17	0/2408	0.42	0/3241
22	N	0.23	0/4776	0.41	0/7366
23	O	0.21	0/1449	0.45	0/1952
24	Q	0.17	0/1907	0.37	0/2556
25	R	0.15	0/2270	0.37	0/3052
26	T	0.22	0/4830	0.37	0/7457
27	U	0.17	0/898	0.47	0/1212
28	V	0.17	0/822	0.45	0/1109
29	W	0.13	0/2513	0.34	0/3388
30	X	0.13	0/1739	0.37	0/2339
31	a	0.16	0/1531	0.45	0/2072
32	b	0.18	0/1436	0.50	0/1947

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.20	0/913	0.46	0/1228
34	d	0.17	0/4118	0.42	0/5532
35	e	0.17	0/2054	0.41	1/2782 (0.0%)
36	f	0.18	0/1602	0.36	0/2169
37	g	0.20	0/818	0.48	0/1104
38	h	0.23	0/1415	0.62	0/1907
39	i	0.17	0/1543	0.45	1/2084 (0.0%)
40	j	0.24	0/865	0.71	0/1166
41	k	0.19	0/1277	0.48	0/1727
42	l	0.18	0/4468	0.49	3/6048 (0.0%)
43	m	0.15	0/1093	0.40	0/1481
44	n	0.21	0/1106	0.61	0/1488
45	o	0.19	0/949	0.48	0/1294
46	p	0.15	0/1898	0.40	0/2559
47	r	0.20	0/813	0.51	0/1091
47	v	0.18	0/822	0.44	0/1103
48	s	0.23	0/660	0.59	0/883
48	w	0.21	0/645	0.53	0/862
49	t	0.22	0/853	0.53	0/1149
49	x	0.18	0/828	0.45	0/1117
50	u	0.20	0/778	0.50	0/1043
50	y	0.20	0/756	0.54	0/1015
All	All	0.19	0/116459	0.41	7/159019 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	l	346	PRO	CA-N-CD	-11.55	95.84	112.00
42	l	346	PRO	N-CA-C	6.33	122.98	114.18
35	e	55	ARG	CA-CB-CG	6.29	126.69	114.10
42	l	346	PRO	N-CD-CG	-5.39	95.11	103.20
39	i	190	ARG	CB-CG-CD	5.21	123.28	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	6091	0	6155	90	0
2	1	4214	0	4288	52	0
3	2	3647	0	3732	38	0
4	3	1089	0	1069	19	0
5	4	2338	0	2404	40	0
6	5	514	0	541	10	0
7	6	3019	0	3040	47	0
8	7	4954	0	4946	81	0
9	A	11815	0	11816	156	0
10	B	9404	0	9398	112	0
11	C	2092	0	2050	28	0
12	D	1343	0	1366	18	0
13	E	1752	0	1776	12	0
14	F	983	0	968	22	0
15	G	1339	0	1357	23	0
16	H	1120	0	1086	27	0
17	I	944	0	899	15	0
18	J	569	0	585	6	0
19	K	924	0	934	7	0
20	L	359	0	381	7	0
21	M	2379	0	2488	38	0
22	N	4263	0	2359	37	0
23	O	1422	0	1500	25	0
24	Q	1871	0	1883	36	0
25	R	2230	0	2254	35	0
26	T	4300	0	2352	29	0
27	U	885	0	866	23	0
28	V	815	0	822	18	0
29	W	2473	0	2476	35	0
30	X	1708	0	1761	25	0
31	a	1495	0	1476	29	0
32	b	1407	0	1404	42	0
33	c	902	0	918	18	0
34	d	4063	0	4247	71	0
35	e	2017	0	2024	31	0
36	f	1578	0	1595	23	0
37	g	815	0	839	21	0
38	h	1394	0	1420	18	0
39	i	1512	0	1544	34	0
40	j	852	0	857	23	0
41	k	1259	0	1241	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	l	4385	0	4612	76	0
43	m	1068	0	1021	25	0
44	n	1095	0	1116	31	0
45	o	922	0	907	18	0
46	p	1863	0	1819	17	0
47	r	801	0	841	23	0
47	v	810	0	853	16	0
48	s	653	0	696	27	0
48	w	638	0	676	13	0
49	t	843	0	908	12	0
49	x	818	0	877	16	0
50	u	767	0	799	15	0
50	y	745	0	773	15	0
51	0	8	0	0	0	0
52	3	2	0	0	0	0
52	4	1	0	0	0	0
52	6	4	0	0	0	0
52	A	2	0	0	0	0
52	B	1	0	0	0	0
52	C	1	0	0	0	0
52	I	2	0	0	0	0
52	J	1	0	0	0	0
52	L	1	0	0	0	0
52	M	1	0	0	0	0
52	W	1	0	0	0	0
53	A	1	0	0	0	0
All	All	113584	0	111015	1429	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1429 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)
20:L:31:CYS:HB3	20:L:34:CYS:SG	2.08	0.93
16:H:75:ALA:N	16:H:98:TYR:HH	1.70	0.89
29:W:127:CYS:HB3	29:W:152:CYS:SG	2.13	0.88
41:k:82:GLU:O	41:k:86:TYR:HB2	1.84	0.78
32:b:80:THR:HG21	37:g:52:THR:HG21	1.67	0.76

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	750/778 (96%)	735 (98%)	15 (2%)	0	100	100
2	1	508/642 (79%)	504 (99%)	4 (1%)	0	100	100
3	2	448/513 (87%)	434 (97%)	14 (3%)	0	100	100
4	3	129/321 (40%)	127 (98%)	2 (2%)	0	100	100
5	4	298/338 (88%)	288 (97%)	10 (3%)	0	100	100
6	5	63/72 (88%)	61 (97%)	2 (3%)	0	100	100
7	6	379/461 (82%)	367 (97%)	12 (3%)	0	100	100
8	7	609/843 (72%)	584 (96%)	25 (4%)	0	100	100
9	A	1494/1733 (86%)	1449 (97%)	45 (3%)	0	100	100
10	B	1168/1224 (95%)	1131 (97%)	37 (3%)	0	100	100
11	C	264/347 (76%)	258 (98%)	6 (2%)	0	100	100
12	D	163/221 (74%)	160 (98%)	3 (2%)	0	100	100
13	E	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
14	F	114/155 (74%)	111 (97%)	3 (3%)	0	100	100
15	G	169/177 (96%)	161 (95%)	8 (5%)	0	100	100
16	H	136/146 (93%)	134 (98%)	2 (2%)	0	100	100
17	I	114/122 (93%)	109 (96%)	5 (4%)	0	100	100
18	J	67/70 (96%)	67 (100%)	0	0	100	100
19	K	113/120 (94%)	110 (97%)	3 (3%)	0	100	100
20	L	43/70 (61%)	42 (98%)	1 (2%)	0	100	100
21	M	306/352 (87%)	295 (96%)	11 (4%)	0	100	100
23	O	179/240 (75%)	170 (95%)	9 (5%)	0	100	100
24	Q	215/735 (29%)	205 (95%)	10 (5%)	0	100	100
25	R	264/400 (66%)	255 (97%)	9 (3%)	0	100	100
27	U	101/286 (35%)	96 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	V	100/122 (82%)	99 (99%)	1 (1%)	0	100	100
29	W	296/492 (60%)	290 (98%)	6 (2%)	0	100	100
30	X	207/328 (63%)	200 (97%)	7 (3%)	0	100	100
31	a	170/295 (58%)	161 (95%)	9 (5%)	0	100	100
32	b	168/223 (75%)	162 (96%)	6 (4%)	0	100	100
33	c	109/115 (95%)	108 (99%)	1 (1%)	0	100	100
34	d	481/687 (70%)	468 (97%)	13 (3%)	0	100	100
35	e	252/307 (82%)	244 (97%)	8 (3%)	0	100	100
36	f	202/210 (96%)	194 (96%)	8 (4%)	0	100	100
37	g	96/121 (79%)	93 (97%)	3 (3%)	0	100	100
38	h	169/284 (60%)	166 (98%)	3 (2%)	0	100	100
39	i	175/222 (79%)	173 (99%)	2 (1%)	0	100	100
40	j	98/149 (66%)	93 (95%)	5 (5%)	0	100	100
41	k	155/157 (99%)	154 (99%)	1 (1%)	0	100	100
42	l	521/1082 (48%)	503 (96%)	17 (3%)	1 (0%)	43	72
43	m	126/220 (57%)	120 (95%)	6 (5%)	0	100	100
44	n	134/140 (96%)	132 (98%)	2 (2%)	0	100	100
45	o	108/127 (85%)	108 (100%)	0	0	100	100
46	p	221/566 (39%)	207 (94%)	14 (6%)	0	100	100
47	r	95/135 (70%)	94 (99%)	1 (1%)	0	100	100
47	v	96/135 (71%)	95 (99%)	1 (1%)	0	100	100
48	s	80/102 (78%)	78 (98%)	2 (2%)	0	100	100
48	w	78/102 (76%)	76 (97%)	2 (3%)	0	100	100
49	t	107/129 (83%)	103 (96%)	4 (4%)	0	100	100
49	x	104/129 (81%)	104 (100%)	0	0	100	100
50	u	95/125 (76%)	91 (96%)	4 (4%)	0	100	100
50	y	93/125 (74%)	90 (97%)	3 (3%)	0	100	100
All	All	12842/17410 (74%)	12464 (97%)	377 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	l	648	SER

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	684/707 (97%)	684 (100%)	0	100	100
2	1	483/589 (82%)	483 (100%)	0	100	100
3	2	414/468 (88%)	414 (100%)	0	100	100
4	3	125/303 (41%)	125 (100%)	0	100	100
5	4	267/300 (89%)	267 (100%)	0	100	100
6	5	59/66 (89%)	59 (100%)	0	100	100
7	6	346/418 (83%)	346 (100%)	0	100	100
8	7	547/737 (74%)	547 (100%)	0	100	100
9	A	1330/1520 (88%)	1330 (100%)	0	100	100
10	B	1024/1061 (96%)	1024 (100%)	0	100	100
11	C	234/299 (78%)	234 (100%)	0	100	100
12	D	149/200 (74%)	149 (100%)	0	100	100
13	E	196/197 (100%)	196 (100%)	0	100	100
14	F	108/137 (79%)	108 (100%)	0	100	100
15	G	152/158 (96%)	152 (100%)	0	100	100
16	H	123/128 (96%)	123 (100%)	0	100	100
17	I	110/116 (95%)	110 (100%)	0	100	100
18	J	64/65 (98%)	64 (100%)	0	100	100
19	K	99/102 (97%)	99 (100%)	0	100	100
20	L	40/57 (70%)	40 (100%)	0	100	100
21	M	267/306 (87%)	267 (100%)	0	100	100
23	O	153/205 (75%)	153 (100%)	0	100	100
24	Q	204/641 (32%)	204 (100%)	0	100	100
25	R	252/363 (69%)	252 (100%)	0	100	100
27	U	99/260 (38%)	99 (100%)	0	100	100
28	V	94/108 (87%)	94 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	W	275/436 (63%)	275 (100%)	0	100	100
30	X	193/295 (65%)	193 (100%)	0	100	100
31	a	170/259 (66%)	170 (100%)	0	100	100
32	b	161/207 (78%)	161 (100%)	0	100	100
33	c	104/108 (96%)	104 (100%)	0	100	100
34	d	469/642 (73%)	469 (100%)	0	100	100
35	e	232/280 (83%)	232 (100%)	0	100	100
36	f	174/178 (98%)	174 (100%)	0	100	100
37	g	95/113 (84%)	95 (100%)	0	100	100
38	h	158/258 (61%)	158 (100%)	0	100	100
39	i	174/208 (84%)	174 (100%)	0	100	100
40	j	100/144 (69%)	100 (100%)	0	100	100
41	k	145/145 (100%)	145 (100%)	0	100	100
42	l	505/1001 (50%)	505 (100%)	0	100	100
43	m	119/195 (61%)	119 (100%)	0	100	100
44	n	128/132 (97%)	128 (100%)	0	100	100
45	o	103/117 (88%)	103 (100%)	0	100	100
46	p	212/528 (40%)	212 (100%)	0	100	100
47	r	84/109 (77%)	84 (100%)	0	100	100
47	v	85/109 (78%)	85 (100%)	0	100	100
48	s	67/78 (86%)	67 (100%)	0	100	100
48	w	65/78 (83%)	65 (100%)	0	100	100
49	t	86/101 (85%)	86 (100%)	0	100	100
49	x	84/101 (83%)	84 (100%)	0	100	100
50	u	83/105 (79%)	83 (100%)	0	100	100
50	y	81/105 (77%)	81 (100%)	0	100	100
All	All	11775/15543 (76%)	11775 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such sidechains are listed below:

Mol	Chain	Res	Type
27	U	40	ASN
46	p	203	GLN
32	b	165	ASN
46	p	177	GLN
42	l	403	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
51	SF4	0	801	1	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
51	SF4	0	801	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1614:PRO	C	1629:THR	N	22.84

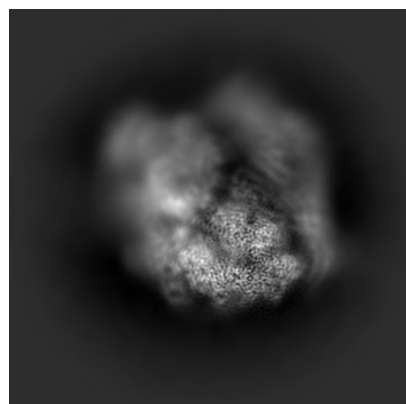
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16611. These allow visual inspection of the internal detail of the map and identification of artifacts.

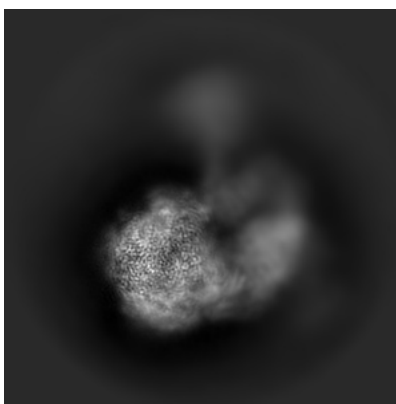
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

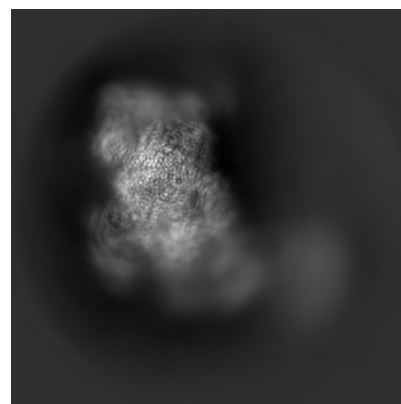
6.1.1 Primary map



X

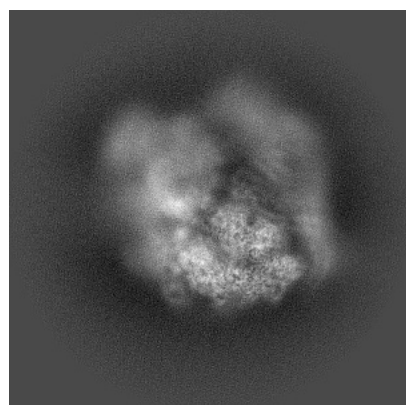


Y

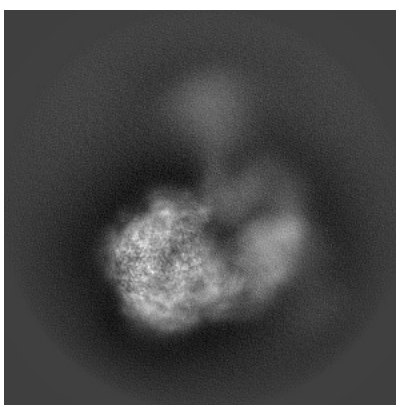


Z

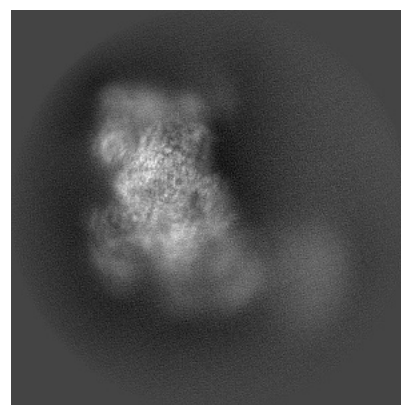
6.1.2 Raw map



X



Y

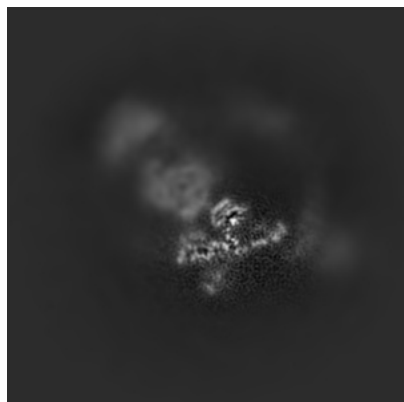


Z

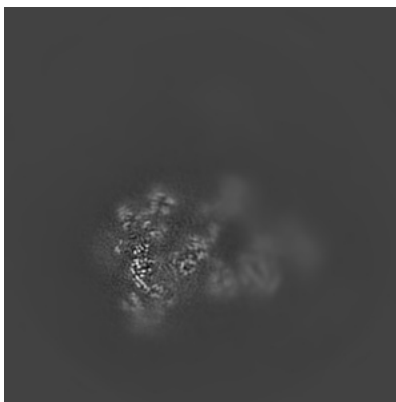
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

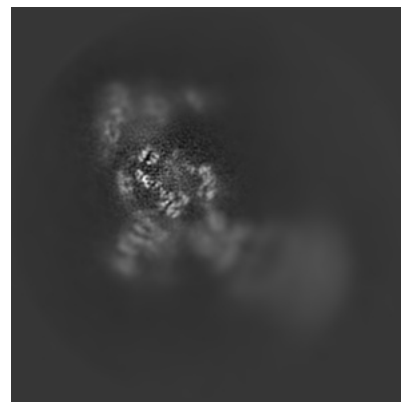
6.2.1 Primary map



X Index: 200

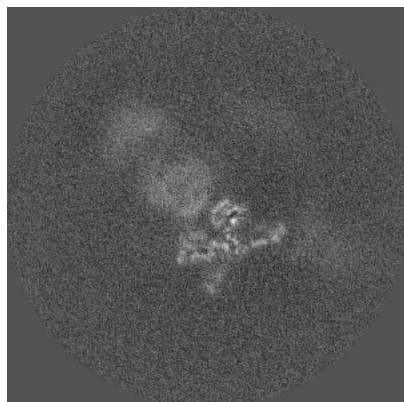


Y Index: 200

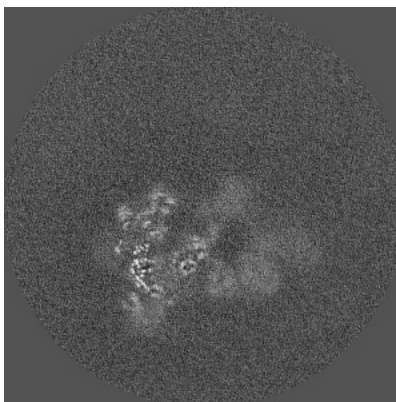


Z Index: 200

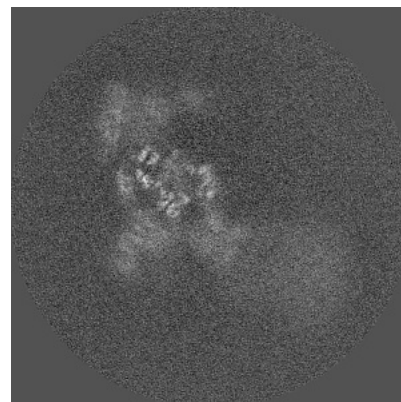
6.2.2 Raw map



X Index: 200



Y Index: 200

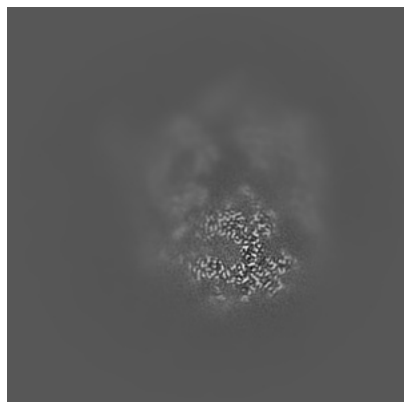


Z Index: 200

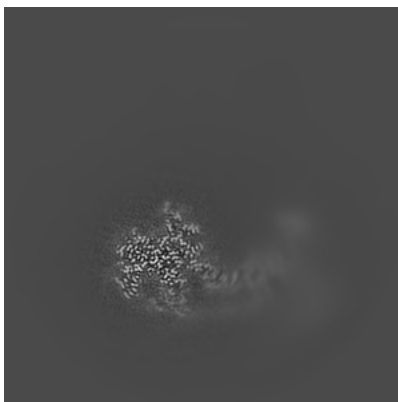
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

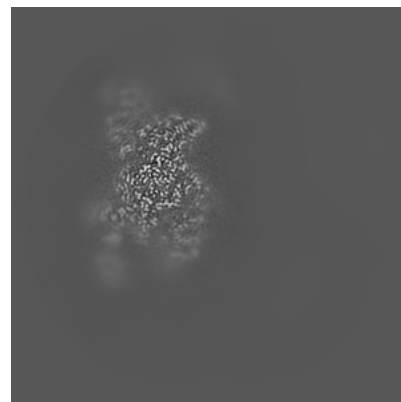
6.3.1 Primary map



X Index: 145

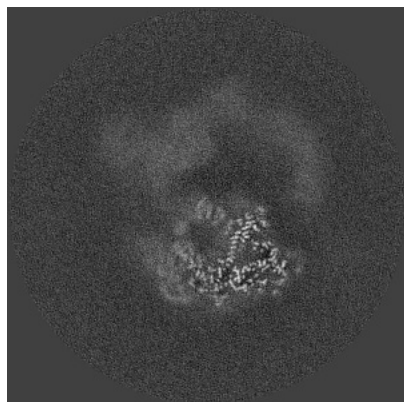


Y Index: 248

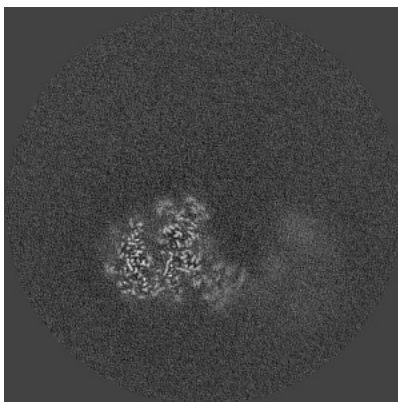


Z Index: 138

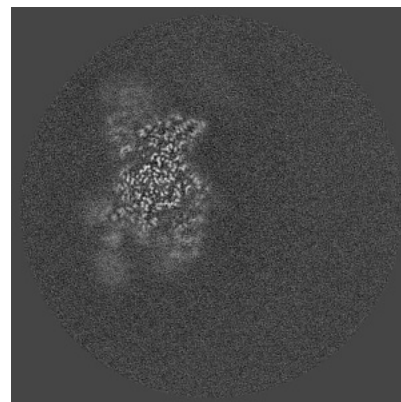
6.3.2 Raw map



X Index: 163



Y Index: 232

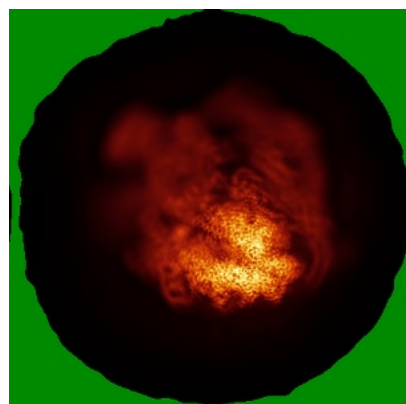


Z Index: 138

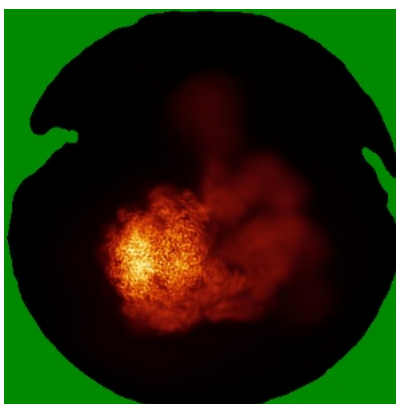
The images above show the largest variance slices of the map in three orthogonal directions.

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

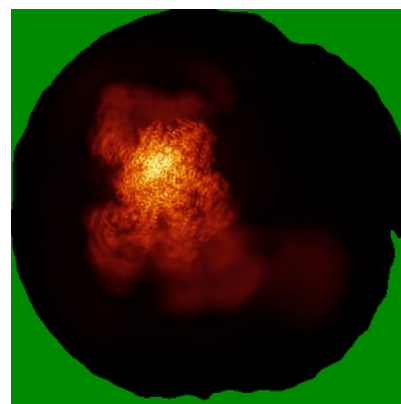
6.4.1 Primary map



X

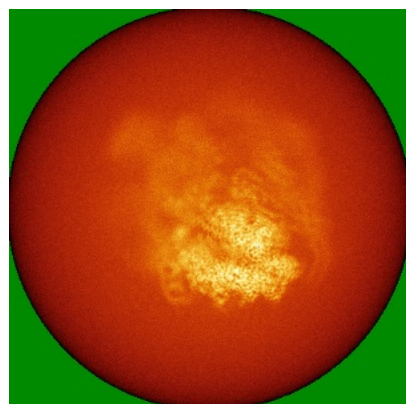


Y

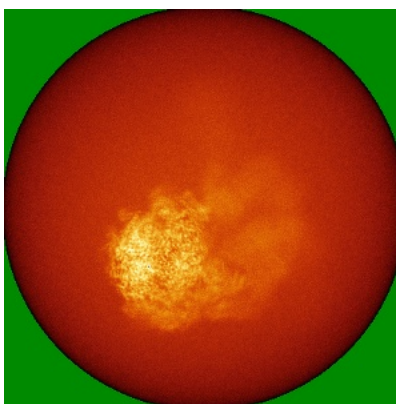


Z

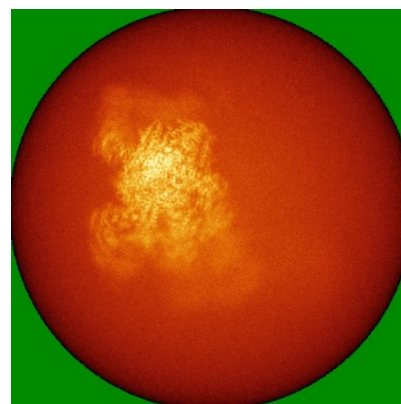
6.4.2 Raw map



X



Y

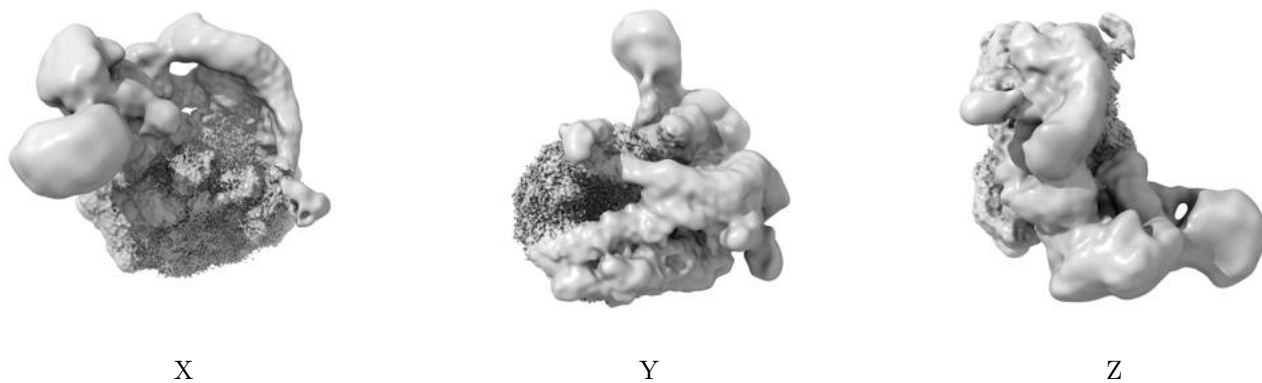


Z

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.

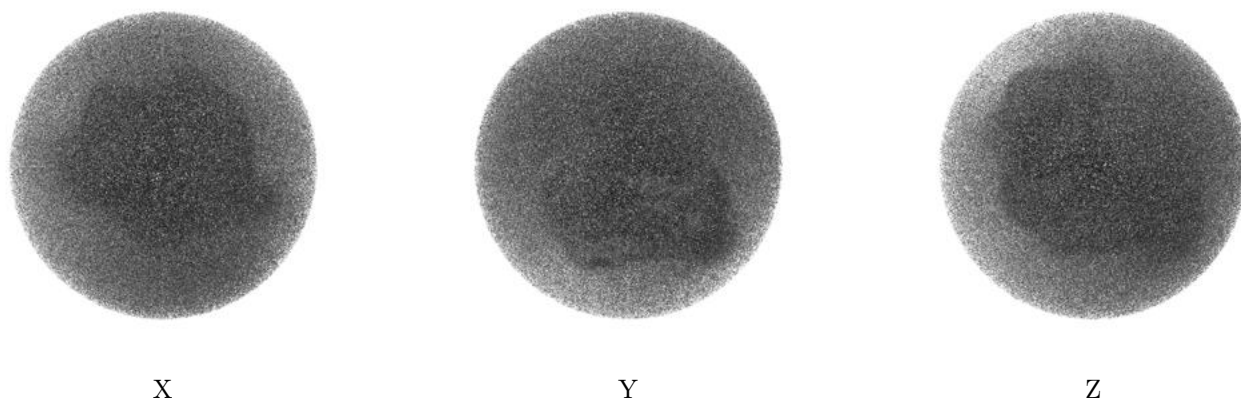
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

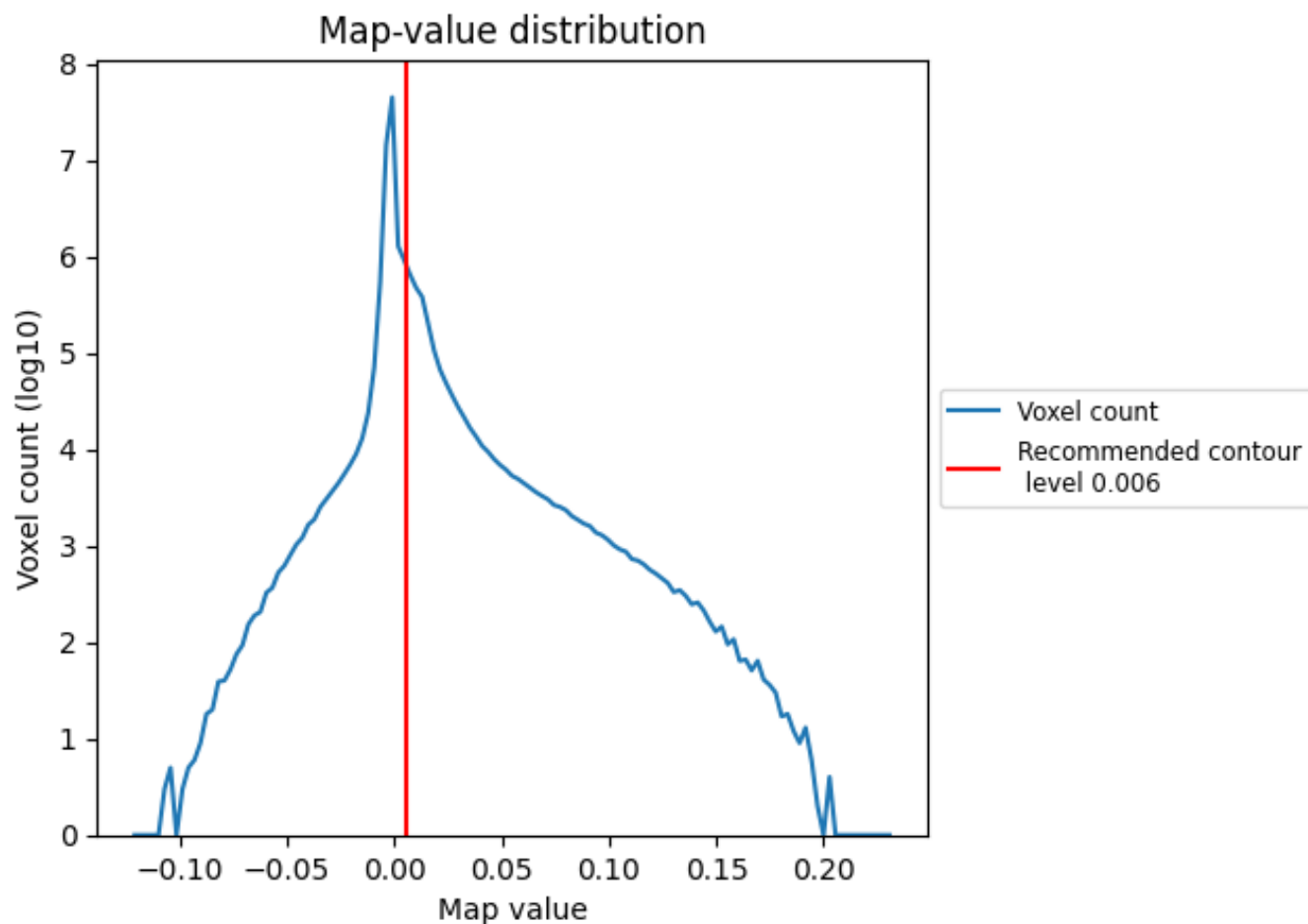
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

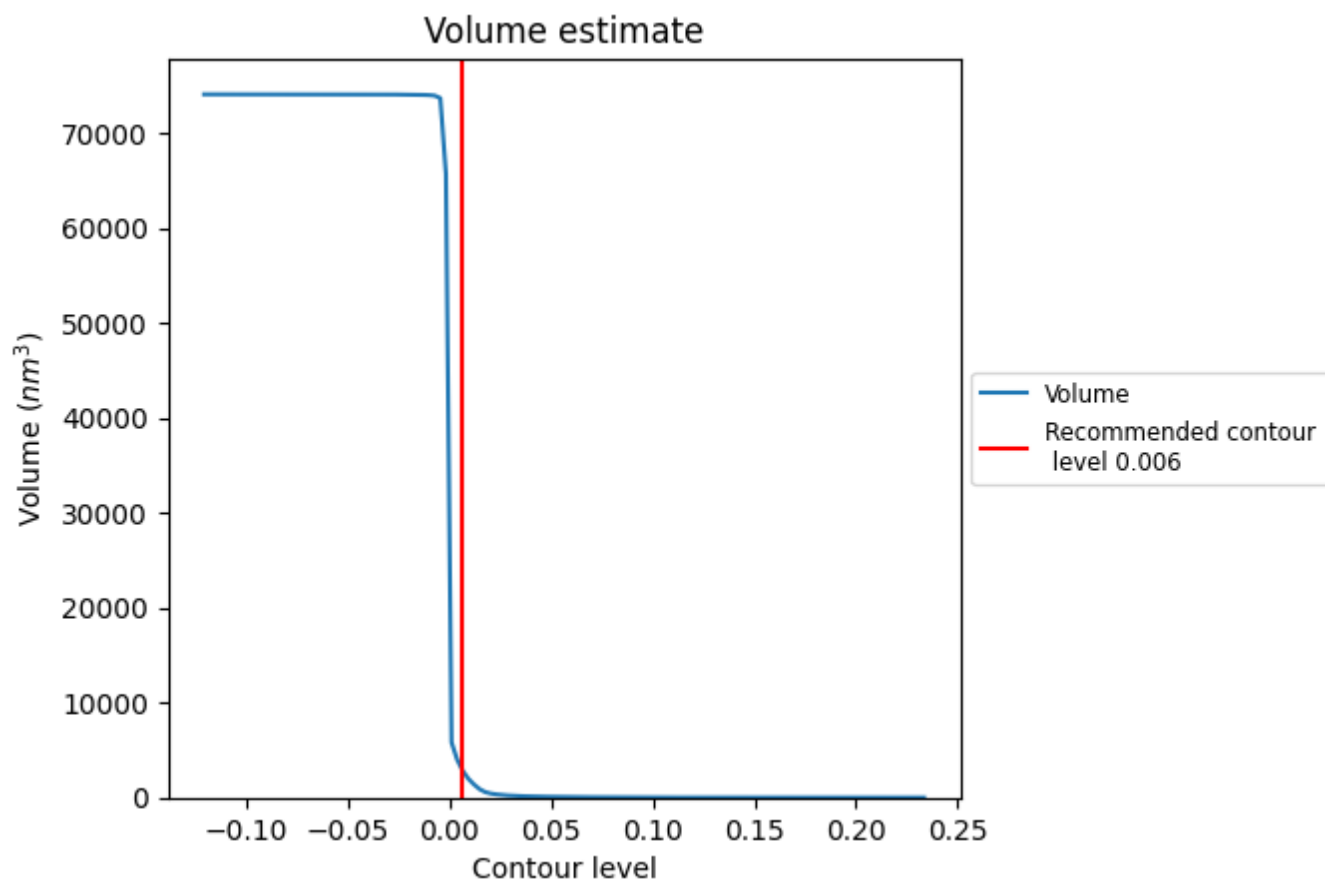
This section contains the results of statistical analysis of the map.

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.

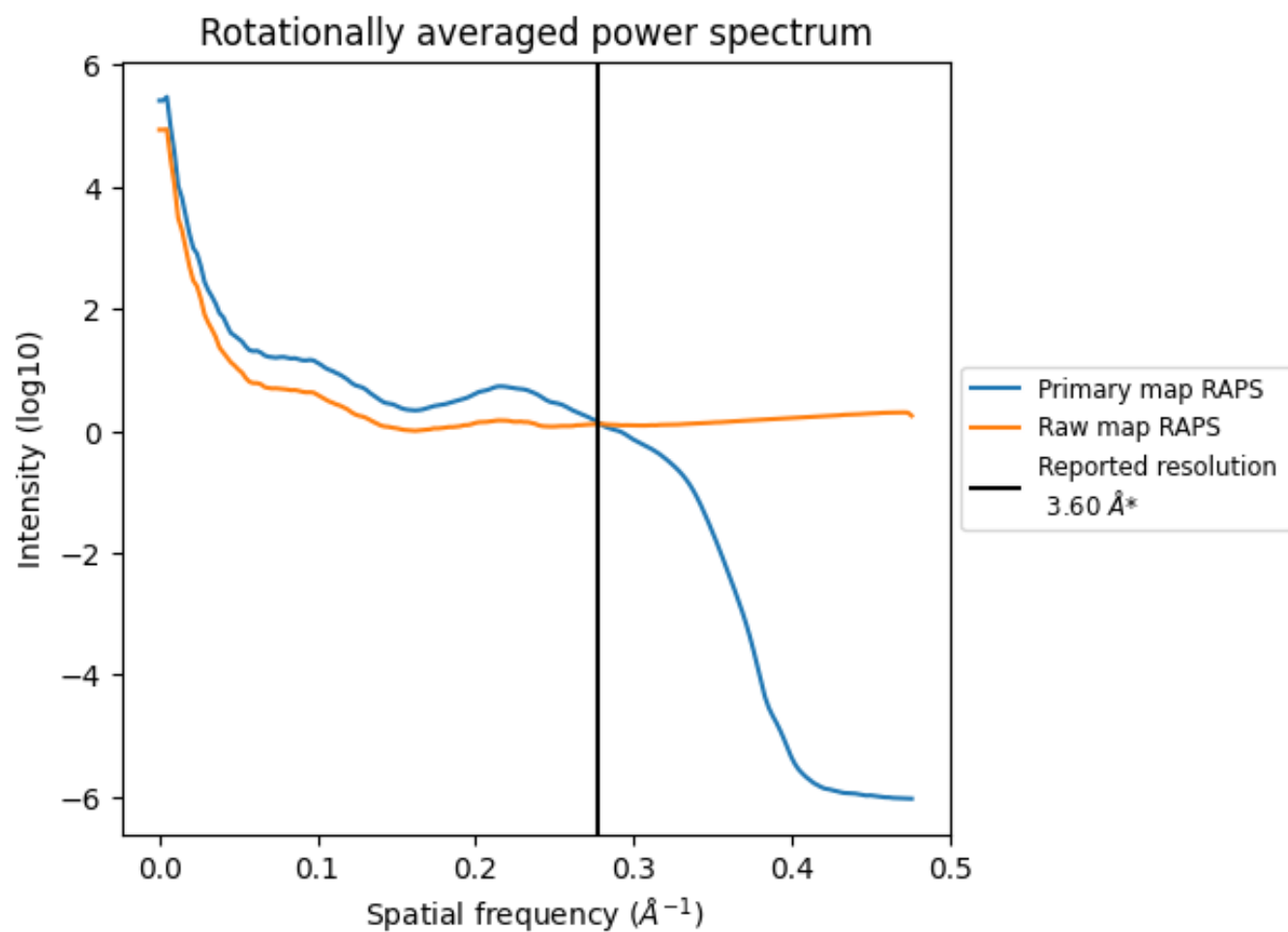
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2978 nm^3 ; this corresponds to an approximate mass of 2690 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 ⓘ

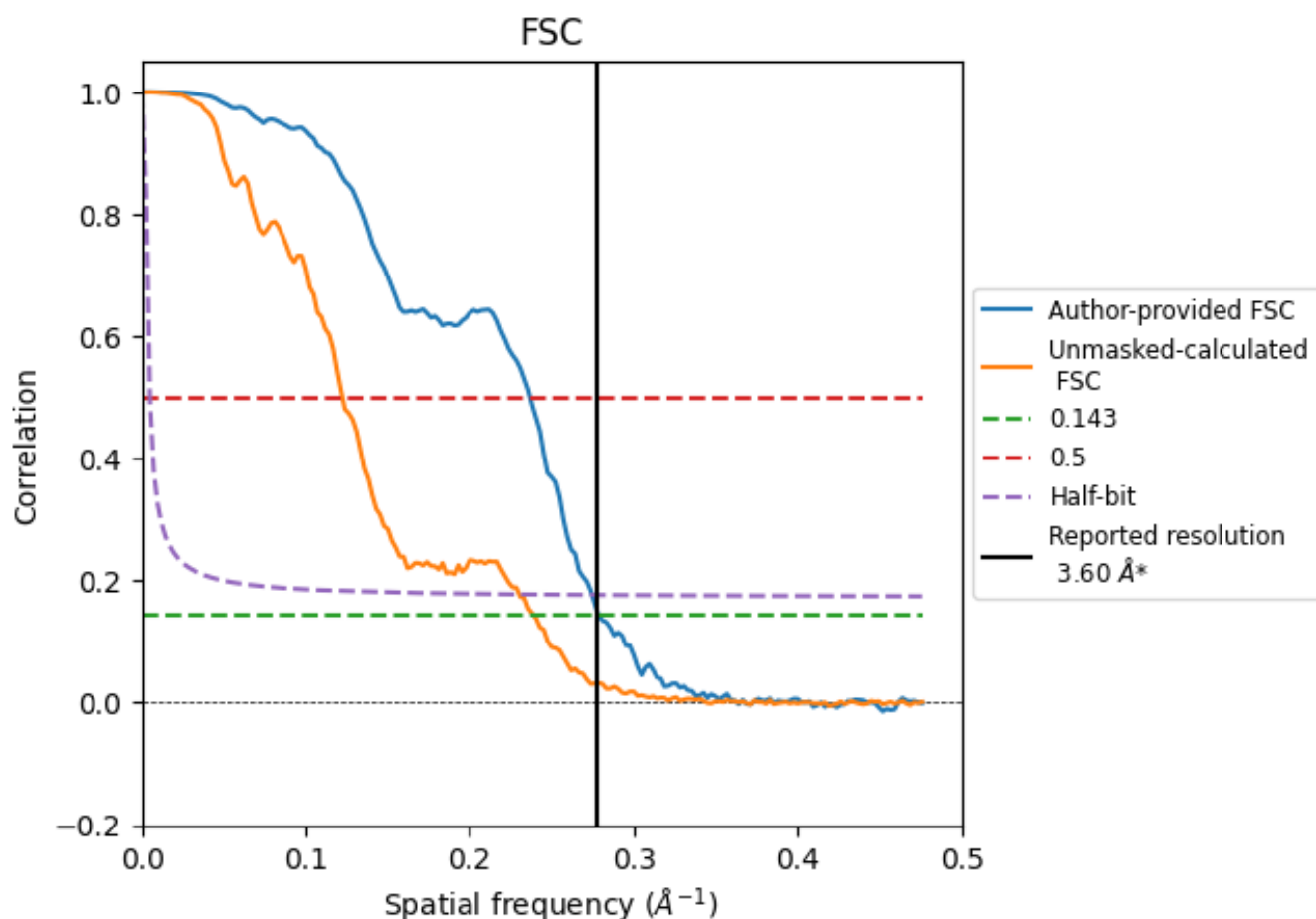


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

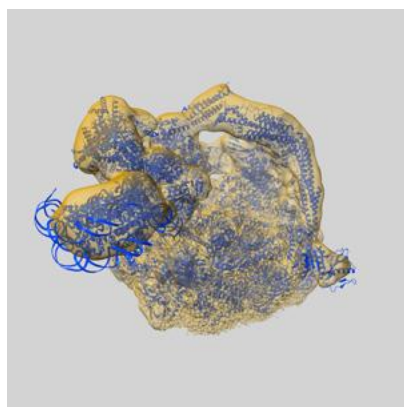
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.59	4.22	3.64
Unmasked-calculated*	4.18	8.18	4.34

*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 4.18 differs from the reported value 3.6 by more than 10 %

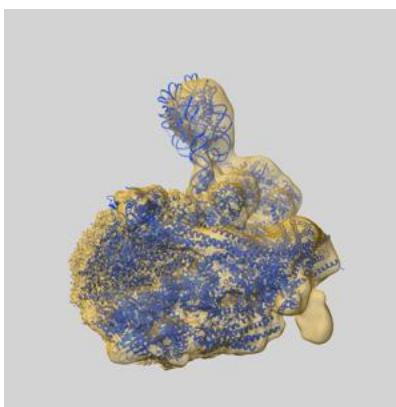
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16611 and PDB model 8CEO. Per-residue inclusion information can be found in section 3 on page 16.

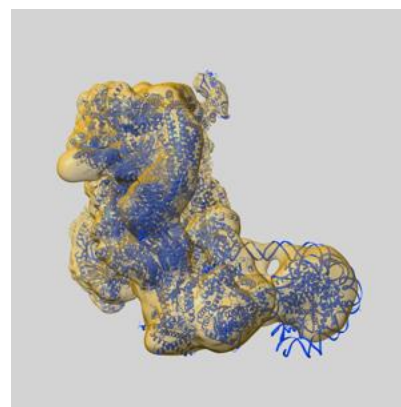
9.1 Map-model overlay [i](#)



X



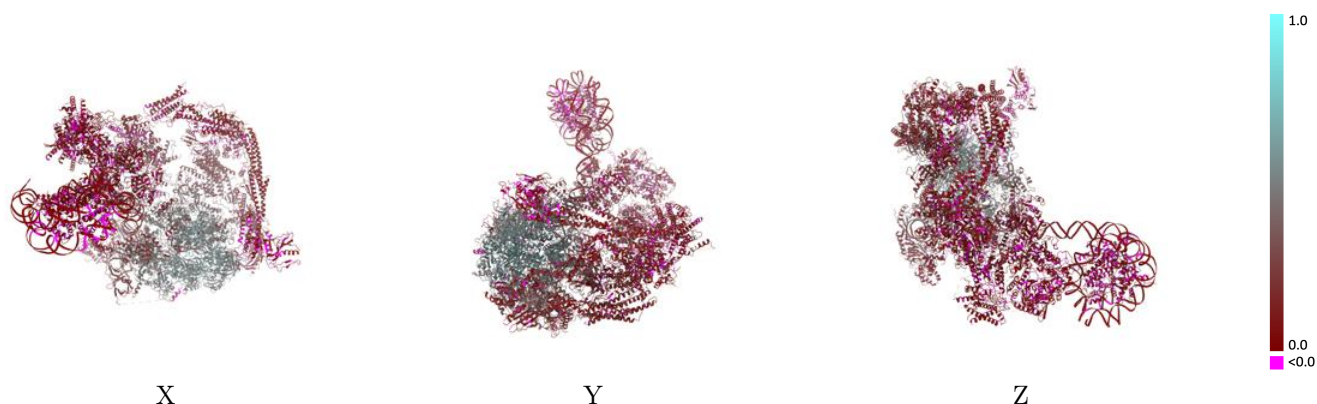
Y



Z

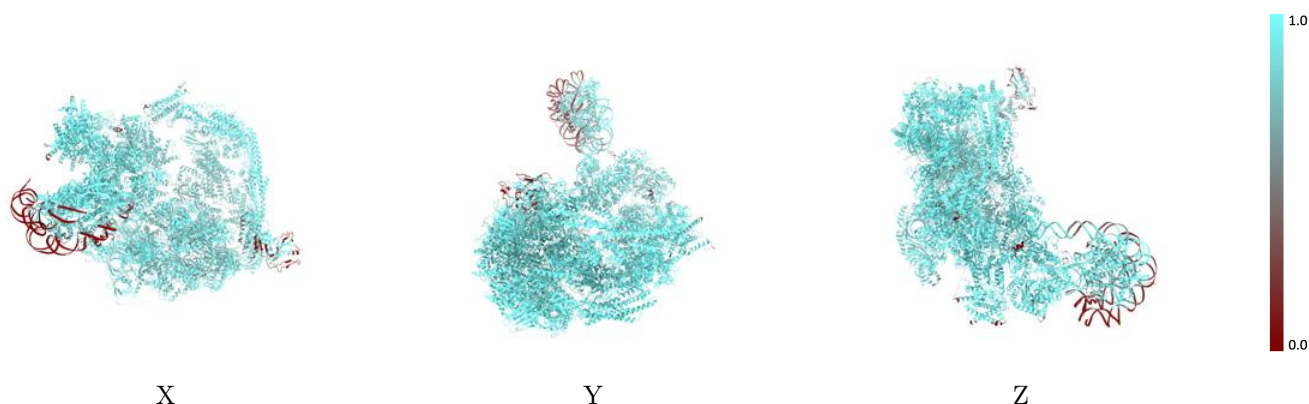
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



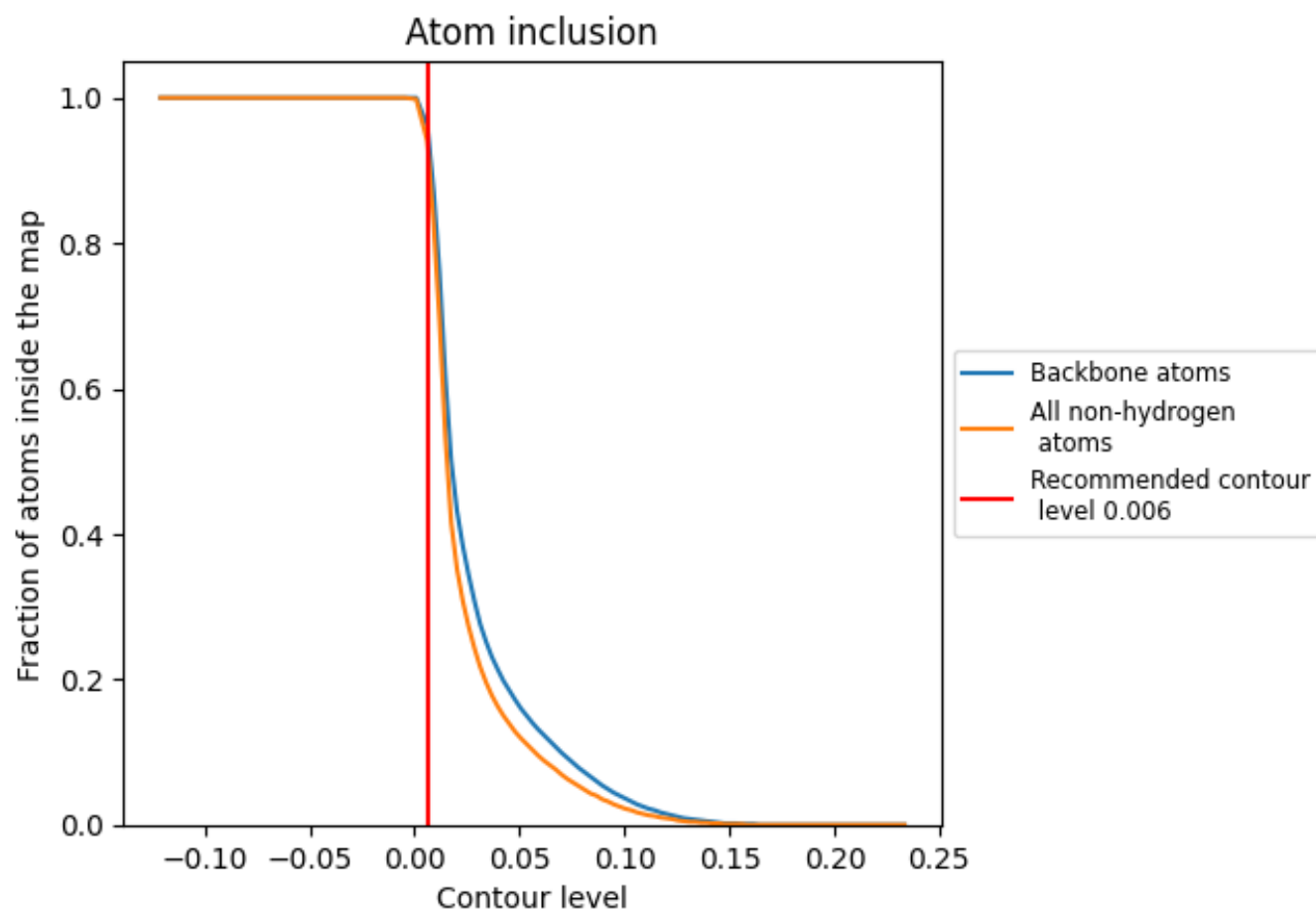
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 94% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.2220
0	 0.9880	 0.1100
1	 0.9590	 0.0830
2	 0.9790	 0.0750
3	 0.9880	 0.1710
4	 0.9970	 0.0610
5	 1.0000	 0.0720
6	 0.9640	 0.0820
7	 0.9890	 0.1030
A	 0.9860	 0.4510
B	 0.9850	 0.5000
C	 0.9890	 0.5120
D	 0.9670	 0.1990
E	 0.9900	 0.3850
F	 0.9220	 0.3790
G	 0.9840	 0.3480
H	 0.9780	 0.4460
I	 0.9910	 0.3480
J	 0.9910	 0.5340
K	 0.9770	 0.5050
L	 0.9860	 0.4710
M	 0.9770	 0.3570
N	 0.6520	 0.0940
O	 0.9940	 0.2260
Q	 0.9790	 0.2350
R	 0.9950	 0.2040
T	 0.6500	 0.0970
U	 0.9270	 0.1280
V	 0.9930	 0.1340
W	 0.9690	 0.1600
X	 0.9910	 0.1520
a	 0.9970	 0.1340
b	 0.9870	 0.1620
c	 0.9970	 0.1800
d	 0.9940	 0.1620



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.9620	 0.3730
f	 0.9630	 0.3520
g	 0.9960	 0.1630
h	 0.9550	 0.1030
i	 0.9980	 0.1290
j	 0.8210	 0.1120
k	 0.9450	 0.0840
l	 0.9750	 0.1270
m	 0.9210	 0.0650
n	 0.9680	 0.0960
o	 0.9790	 0.1190
p	 0.5320	 0.0620
r	 0.7950	 0.0260
s	 0.7970	 0.0360
t	 0.7720	 0.0170
u	 0.7470	 0.0230
v	 0.9740	 0.0510
w	 1.0000	 0.0850
x	 0.9280	 0.0490
y	 0.9930	 0.0530